CrysFML

Welcome

***Crys**tallographic **F**ortran **M**odules **L**ibrary*

Version: 5.0

The Crystallographic Fortran Modules Library (***CrysFML***) is a set of Fortran 90/95 modules containing procedures of interest in Crystallographic applications.

This set of modules has been, and is still being, developed by us in order to facilitate the design and the development of crystallographic computing programs.
Many of the algorithms and procedures of the library come from adaptations and modifications of existing codes of different sources. We make the source code
available publicly without any licence (we have to time to think in legal stuff). We hope that academic groups interested in cooperative scientific software
development will take some benefit of the library and we expect that additional individuals will contribute to the development of the library. If somebody is interested
in working in the library at the level of developer we can add his(her) name in the list of developer by contacting us by e-mail.

The ***CrysFML*** library is distributed in the hope that it will be useful, but **without any warranty** of being free of internal errors. in no event will the authors be liable
to you for damages, including any general, special, incidental or consequential damages arising out of the use or inability to use the library (including but not limited
to loss of data or data being rendered inaccurate or losses sustained by you or third parties or a failure of the library to operate with any other programs).

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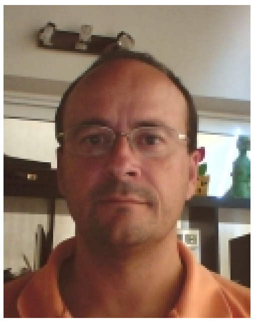

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Structure of CrysFML

The present distribution of ***CrysFML*** have the following directory structure:

Src	**CFGL**	
	CFML	
	Scripts	**Linux**
		MacOS
		Windows
<Compiler>	**LibC**	
Absoft		
G95	**LibGL**	
GFortran		
Intel	**LibR (*)**	
Lahey		
	LibW	
Help (**)		
Html (**)	**files**	
Program_Examples	**CFML4C**	
	Cryscal_TR	
	Cryst_Calculator_Console	
	Magnetism	
	Metrics	
	HKL_Gen	
	PowderPattern	
	Simbo-Enermag	
	SpaceGroups	
	StructureFactors	
	Structures_GlobalOptimization	
	Twins	

(*) Using Lahey compiler and RealWin library (obsolete)
(**) Windows Help format (chm)
(***) Html format for use in Linux,MacOS,Windows

Installing and Compiling CrysFML

The installation of ***CrysFML*** depends of your operating system. Presently we have tested it in the following operating systems:

- Linux
  MacOS
  Windows

Linux

Please, follow the following steps to install the ***CrysFML*** library in your Linux System.

1. Create a new directory to install ***CrysFML*** (<*CRYSFMLDIR*>)
   For example: *$HOME/CrysFML*

2. Download the last version of ***CrysFML*** from the ILL forge site.
   You can do it directly from the site or using a ***svn*** program as RapidSVN or KDESvn that is integrated in the KDE file system.

3. After downloading the Library you should have at <*CRYSFMLDIR*>, ***Src***, ***Help*** and ***Program_Examples*** subdirectories.
   Then, go to ***Src*** directory.

4. Check that you have a file called ***makecrys*** with execute permission.

5. Run the script file with the name of the command invoking your compiler. More info if you run the script file without arguments. At present ***CrysFML*** exist in two versions:
   - **Console**
     Run: **makecrys** <*compiler-command*>

   - **Graphical**
     in this case, ***CrysFML*** will be linked together with the Winteracter Library
     Run: **makecrys** <*compiler-command*> *all*

6. If the script runs properly you'll have ***CrysFML*** compiled in the form of a library and the list of module files (*.mod) in <CRYSFMLDIR>*/Compiler/LibC*
   Where *Compiler* can be: *Absoft, intel, Lahey, G95, GFortran*

   If you have compiled and linked with the Winteracter library, you will get two additional subdirectories: *LibW* and *LibGL*

MacOS

Please, follow the following steps to install the ***CrysFML*** library in your MacOS X System.

4. Create a new directory to install the ***CrysFML*** library (<*CRYSFMLDIR*>)
   For example: *$HOME/CrysFML*

5. Download the last version of ***CrysFML*** from the ILL forge site.
   You can do it directly from the site or using a ***svn*** program as ZigZig, RapidSVN or SvnX .

6. After downloading the Library you should have at <*CRYSFMLDIR*>, ***Src***, ***Help*** and ***Program_Examples*** subdirectories.
   Then, go to ***Src*** directory.

4. Check that you have a file called ***makecrys*** with execute permission.

5. Run the script file with the name of the command invoking your compiler. More info if you run the script file without

arguments. At present ***CrysFML*** exist in two versions:

- **Console**
  Run: **makecrys** <*compiler-command*>

- **Graphical**
  in this case, ***CrysFML*** will be linked together with the Winteracter Library
  Run: **makecrys** <*compiler-command*> *all*

6. If the script runs properly you'll have ***CrysFML*** compiled in the form of a library and the list of module files (*.mod) in <CRYSFMLDIR>*/Compiler/LibC*
   Where *Compiler* can be: *Absoft, intel, G95, GFortran*

   If you have compiled and linked with the Winteracter library, you will get two additional subdirectories: *LibW* and *LibGL*

Windows

Please, follow the following steps to install the ***CrysFML*** library in your Windows System.

7. Create a new directory to install the ***CrysFML*** library (<*CRYSFMLDIR*>)
   For example: *C:\CrysFML*

8. Download the last version of ***CrysFML*** from the ILL forge site.
   You can do it directly from the site or using a ***svn*** program as Tortoise.

9. After downloading the Library you should have at <*CRYSFMLDIR*>, ***Src***, ***Help*** and ***Program_Examples*** subdirectories.
   Then, go to ***Src*** directory.

4. Check that you have a file called ***makecrys.bat***

5. Run the batch file with the name of the command invoking your compiler. More info if you run the batch file without arguments. At present ***CrysFML*** exist in two versions:
   - **Console**
     Run: **makecrys** <*compiler-command*>

   - **Graphical**
     in this case, ***CrysFML*** will be linked together with the Winteracter Library
     Run: **makecrys** <*compiler-command*> *all*

6. If the batch file runs properly you'll have ***CrysFML*** compiled in the form of a library and the list of module files (*.mod) in <CRYSFMLDIR>*\Compiler\LibC*
   Where *Compiler* can be: *Absoft, G95, GFortran, Intel, Lahey*

   If you have compiled and linked with the Winteracter library, you will get two additional subdirectories: *LibW* and *LibGL*

Compiling and Running the Examples

Some examples programs are distributed together with the ***CrysFML*** library in order to facilitate the understanding of how you can make programs. At the moment, the examples are:

- CFML4C
- Cryscal_TR
- Cryst_Calculator_Console
- Magnetism
- Metrics
- Hkl_Gen
- PowderPattern
- Simbo-Enermag
- SpaceGroups
- StructureFactors
- Structures_GlobalOptimization
- Twins

CFML4C

This is a sample to use ***CFML*** in C language.

Building the executable file

Run the script (for Linux or MacOS). The user must have installed the GFortran and GCC compilers.

make_xtl

Running the program

./xtl *test*

Cryscal_TR

Console program for crystallographic calculations from Thierry Roisnel.

Building the executable file

Run the batch file (for Windows) located in scripts directory

make_cryscal lf95| g95 |all

Running the program

The program is invoked at the prompt using the name of the executable file.

Cryst_Calculator_Console

Initial example about the use of CrysFML to do some crystallograhic calculations.

Building the executable file

Run the batch file (for Windows) or the script (for Linux or MacOS)

make_cryscal <*compiler-command*>

Running the program

The program is invoked at the prompt using the name of the executable file.

Magnetism

Examples about the use of ***CrysFML*** for calculations of Magnetic structure factors and interaction

MagPolar program calculates magnetic structure factors, and magnetic interaction, vectors from magnetic structures by reading a *.CFL file and
Magnetic S-domains and chirality domains are considered.

MagRef calculates magnetic structure factors, and magnetic interaction, vectors from magnetic structures by reading a *.CFL file

Building the executable file

Run the batch file (for Windows)

make_magref *g95* **|** *gfortran* **|** *ifort* **|** *lf95*
make_magpolar3d *g95* **|** *gfortran* **|** *ifort* **|** *lf95*

Running the program

The program is invoked at the prompt using the name of the executable file.

Metrics

Get_Conven_Cell is a program to calculate the conventional unit cell parameters from an input unit cell using ***CFML***.

Building the executable file

Run the batch file (for Windows) or the script (for Linux or MacOS)

make_convcell <*compiler-command*>

Running the program

The program is invoked at the prompt using the name of the executable file.

Hkl_Gen

Hkl_Gen is a program that generates HKL reflections using a minimal information

Building the executable file

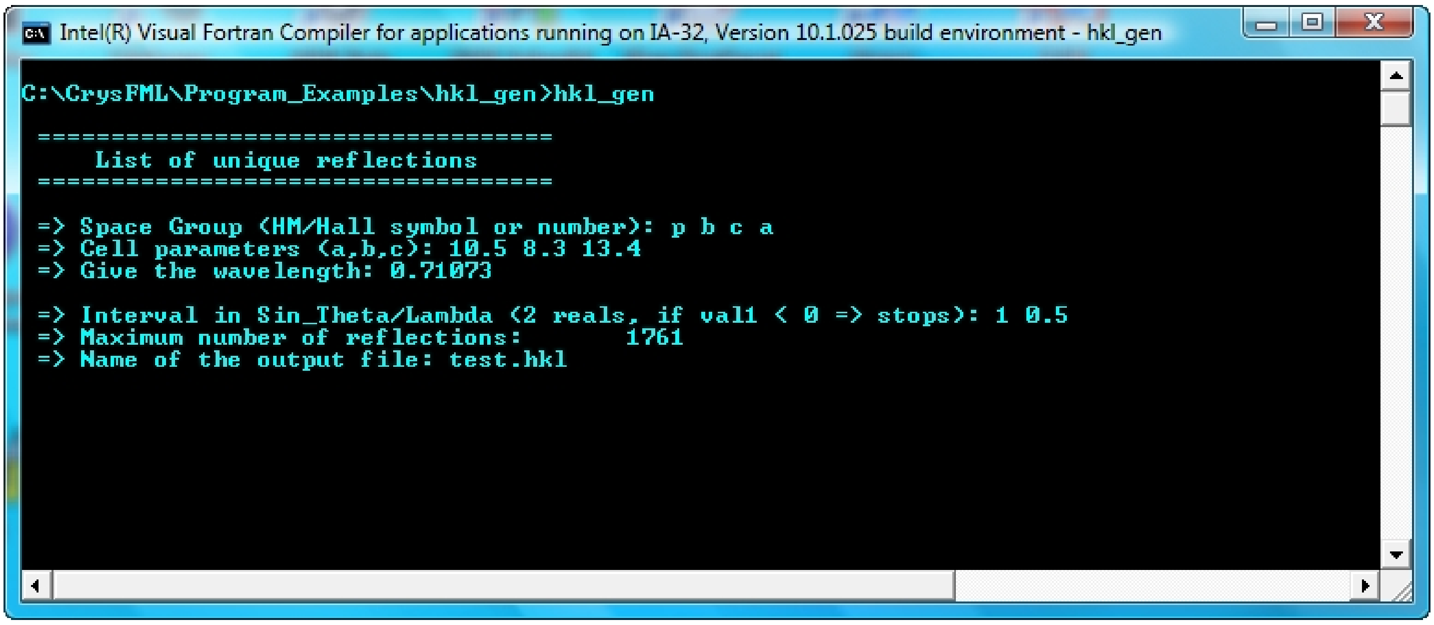
Run the batch file (for Windows) or the script (for Linux or MacOS)

make_hkl_gen <*compiler-command*>

Running the program

The program is invoked at the prompt using the name of the executable file generated in the previous step.

The program calculate a list of unique reflections and for it the user will have to introduce the space group, cell parameters, wavelength and the range on sin / . All reflections calculated will be written in output file.



```
C:\CrysFML\Program_Examples\hkl_gen>hkl_gen

 ===================================
     List of unique reflections
 ===================================

 => Space Group (HM/Hall symbol or number): p b c a
 => Cell parameters (a,b,c): 10.5 8.3 13.4
 => Give the wavelength: 0.71073

 => Interval in Sin_Theta/Lambda (2 reals, if val1 < 0 => stops): 1 0.5
 => Maximum number of reflections:        1761
 => Name of the output file: test.hkl
```

PowderPattern

There are two examples about the calculation of powder pattern reading CIF or CFL file.

Simple_Calc_Powder is a very simple program for calculating powder patterns by reading a CIF or a CFL file while ***Calc_Powder*** is an extended version
of the previous program. In this case the user can use it for generating a super-cell and perturb the atom positions to see the effect on the powder
diffraction pattern.

Building the executable file

Run the batch file (for Windows) or the script (for Linux or MacOS)

> **make_simple_calc_powder** <*compiler-command*>
> **make_calc_powder** <*compiler-command*>

Running the program

The program is invoked at the prompt using the name of the executable file.

Simbo-Enermag

Simbo program generate files with neighbouring information around magnetic atoms for simulation purposes.

Enermag program calculate the classical magnetic energy for a set of k-vectors and exchange parameters. The input file is created by the program ***Simbo***.

Phase_Diagram is a console program helps to visualise a magnetic phase diagram as a function of exchange interactions using ***GFourier*** from the **FullProf Suite**.
The program reads a file (with extension *.res) coming from ***Enermag*** (when used for generating a phase diagram). A maximum of three variable exchange interactions
are taken into account. And generates some information in the screen as well as a binary file that can be read from ***GFourier***

Building the executable file

Run the batch file (for Windows) to compile the programs

make_Simbo	<*compiler-command*>
make_EnerMag	<*compiler-command*>
make_Phas_Diag	<*compiler-command*>

Running the program

The program is invoked at the prompt using the name of the executable file.

SpaceGroups

Program that give all information related with the Space group.

Building the executable file

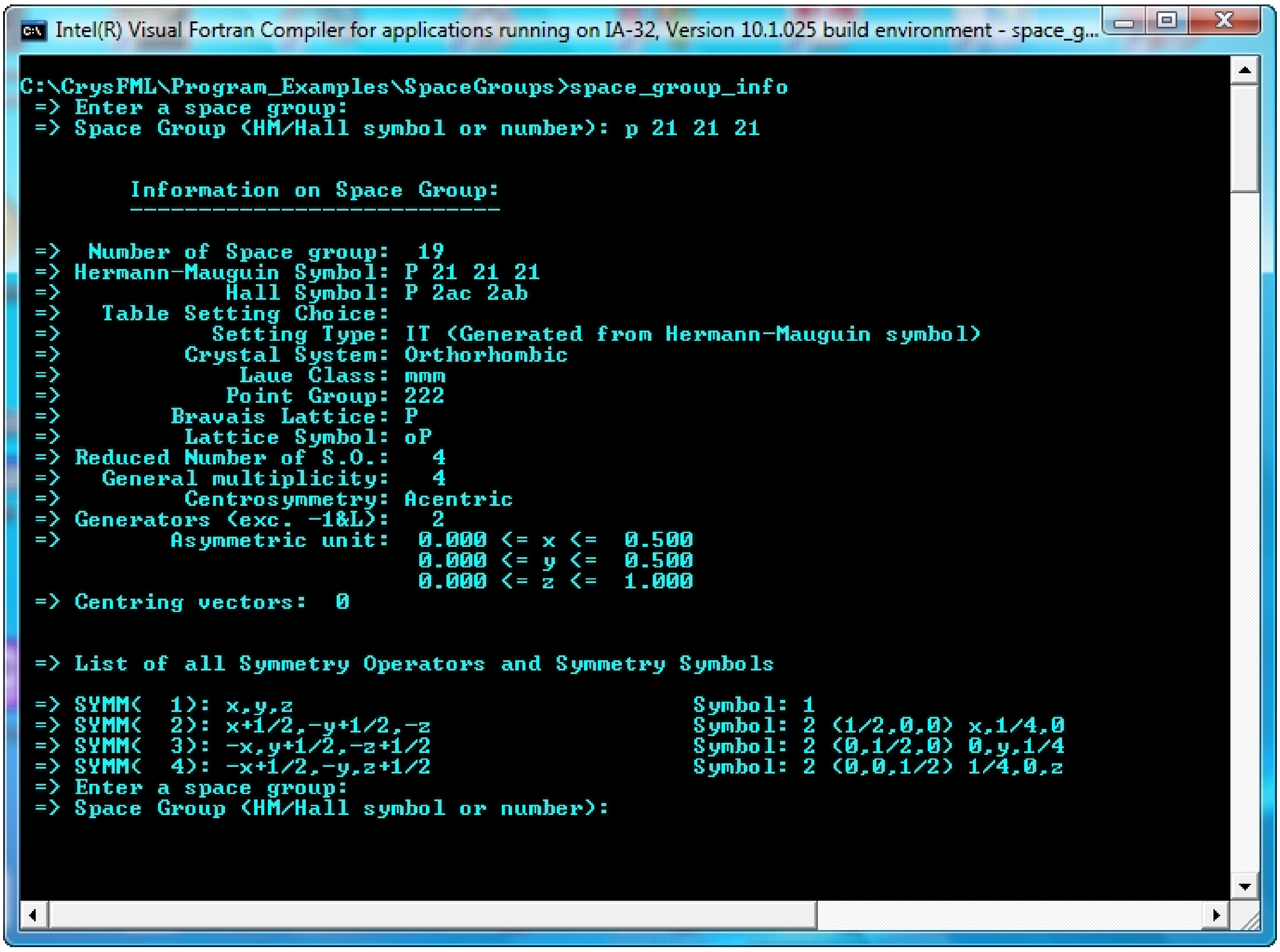
Run the batch file (for Windows) or the script (for Linux or MacOS)

make_space_group_info <*compiler-command*>

Running the program

The program is invoked at the prompt using the name of the executable file generated in the previous step: space_group_info.

To the question about the space group the user can answer with the number of the space group, the Hermann-Mauguin symbol or the Hall symbol.
After striking the <enter> key the program shows all information about the space group.


Intel(R) Visual Fortran Compiler for applications running on IA-32, Version 10.1.025 build environment - space_g...

```
C:\CrysFML\Program_Examples\SpaceGroups>space_group_info
 => Enter a space group:
 => Space Group (HM/Hall symbol or number): p 21 21 21


        Information on Space Group:
        ---------------------------

 =>  Number of Space group:  19
 => Hermann-Mauguin Symbol: P 21 21 21
 =>            Hall Symbol: P 2ac 2ab
 =>   Table Setting Choice:
 =>           Setting Type: IT (Generated from Hermann-Mauguin symbol)
 =>         Crystal System: Orthorhombic
 =>             Laue Class: mmm
 =>            Point Group: 222
 =>        Bravais Lattice: P
 =>         Lattice Symbol: oP
 => Reduced Number of S.O.:   4
 =>   General multiplicity:   4
 =>         Centrosymmetry: Acentric
 => Generators (exc. -1&L):   2
 =>        Asymmetric unit:  0.000 <= x <=  0.500
                             0.000 <= y <=  0.500
                             0.000 <= z <=  1.000
 => Centring vectors:  0


 => List of all Symmetry Operators and Symmetry Symbols

 => SYMM(  1): x,y,z                                 Symbol: 1
 => SYMM(  2): x+1/2,-y+1/2,-z                       Symbol: 2 (1/2,0,0) x,1/4,0
 => SYMM(  3): -x,y+1/2,-z+1/2                       Symbol: 2 (0,1/2,0) 0,y,1/4
 => SYMM(  4): -x+1/2,-y,z+1/2                       Symbol: 2 (0,0,1/2) 1/4,0,z
 => Enter a space group:
 => Space Group (HM/Hall symbol or number):
```

Example showing the screen where Space_Group_info is ran

StructureFactors

Simple program to do Structure factors calculations using ***CrysFML***.

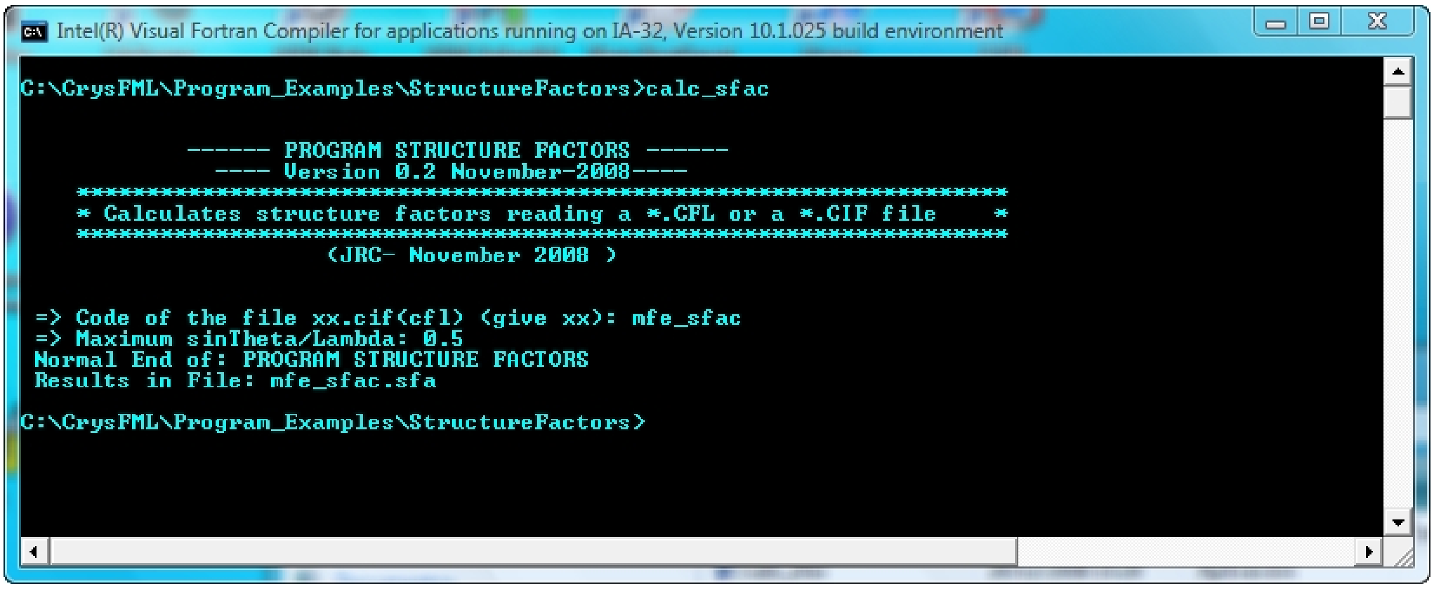
Building the executable file

Run the batch file (for Windows) or the script (for Linux or MacOS)

> **make_calc_sfac** <*compiler-command*>

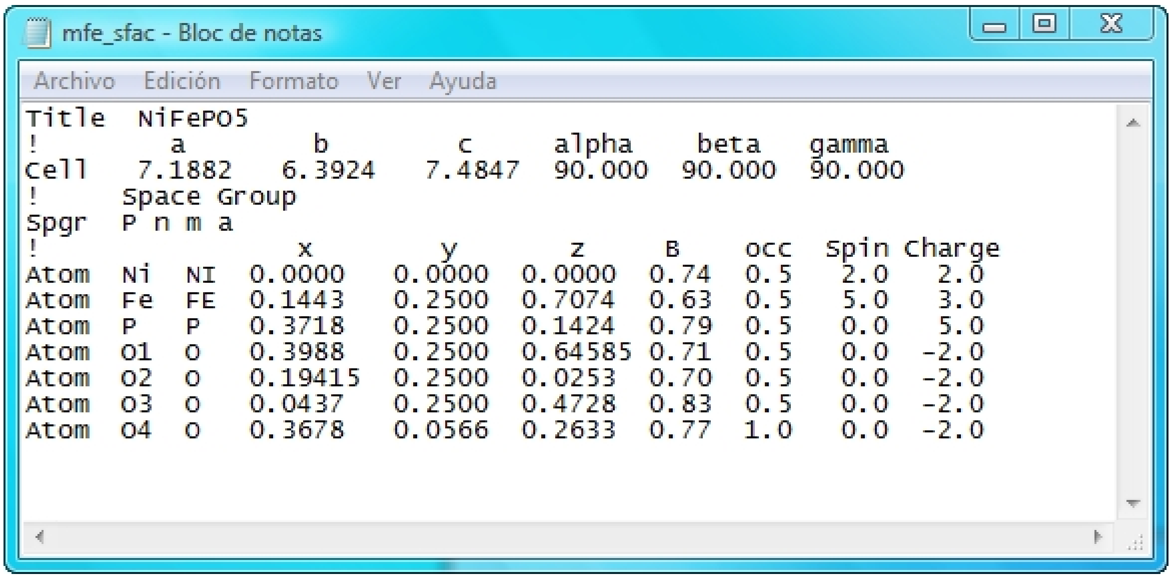
Running the program

The program is invoked at the prompt using the name of the executable file: **calc_sfac**


Intel(R) Visual Fortran Compiler for applications running on IA-32, Version 10.1.025 build environment

```
C:\CrysFML\Program_Examples\StructureFactors>calc_sfac

            ------ PROGRAM STRUCTURE FACTORS ------
              ---- Version 0.2 November-2008----
    *******************************************************************
    * Calculates structure factors reading a *.CFL or a *.CIF file    *
    *******************************************************************
                      (JRC- November 2008 )

 => Code of the file xx.cif(cfl) (give xx): mfe_sfac
 => Maximum sinTheta/Lambda: 0.5
 Normal End of: PROGRAM STRUCTURE FACTORS
 Results in File: mfe_sfac.sfa

C:\CrysFML\Program_Examples\StructureFactors>
```

The input file requires a minimal information to do the calculations. Here an example for use with this program.



```
Title  NiFePO5
!        a         b          c      alpha    beta   gamma
Cell    7.1882    6.3924     7.4847  90.000   90.000  90.000
!      Space Group
Spgr   P n m a
!                x         y        z       B     occ   Spin Charge
Atom   Ni   NI  0.0000    0.0000   0.0000   0.74   0.5    2.0    2.0
Atom   Fe   FE  0.1443    0.2500   0.7074   0.63   0.5    5.0    3.0
Atom   P    P   0.3718    0.2500   0.1424   0.79   0.5    0.0    5.0
Atom   O1   O   0.3988    0.2500   0.64585  0.71   0.5    0.0   -2.0
Atom   O2   O   0.19415   0.2500   0.0253   0.70   0.5    0.0   -2.0
Atom   O3   O   0.0437    0.2500   0.4728   0.83   0.5    0.0   -2.0
Atom   O4   O   0.3678    0.0566   0.2633   0.77   1.0    0.0   -2.0
```

Structures_GlobalOptimization

More elaborate example using CrysFML about simulated annealing procedure.

Building the executable file

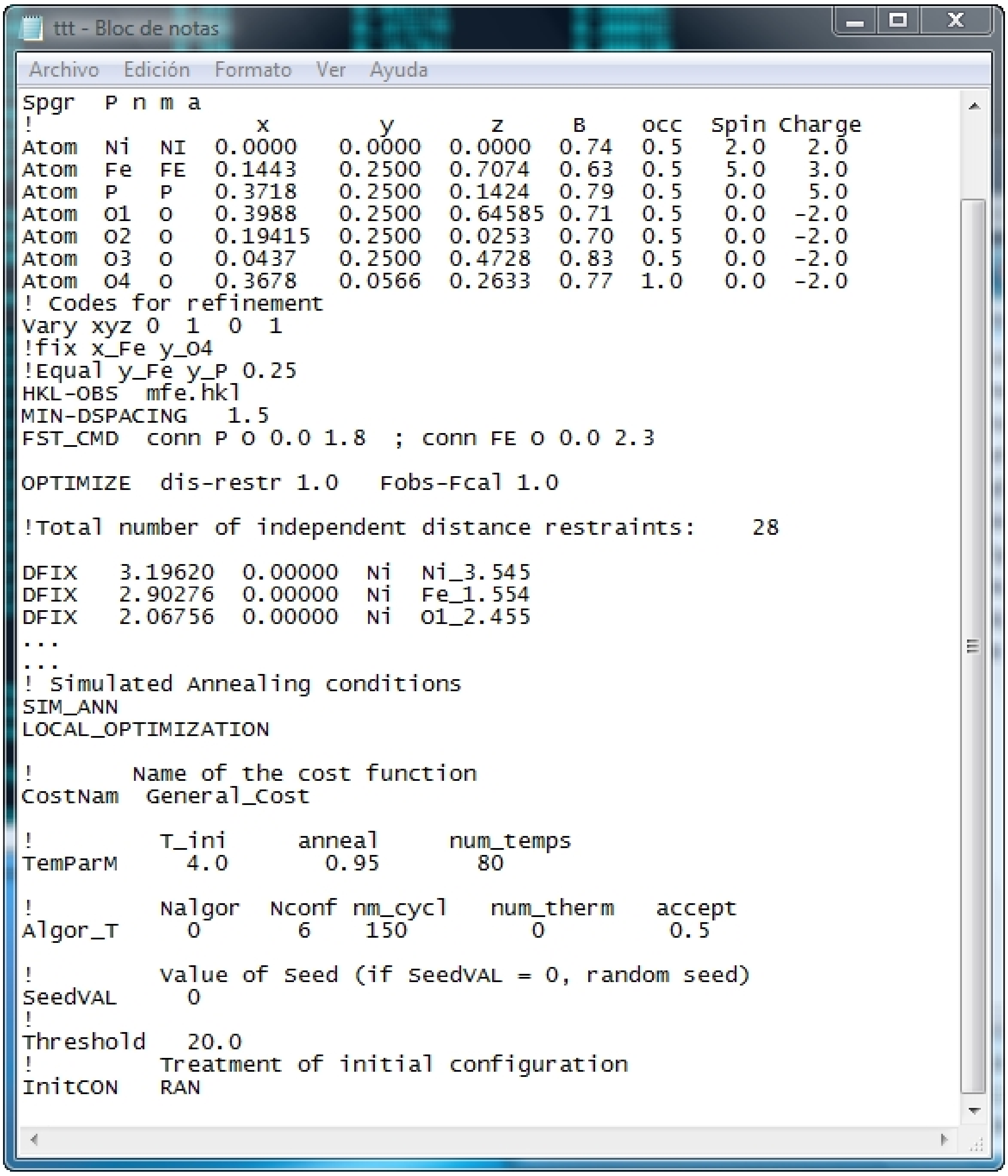
Run the batch file (for Windows) or the script (for Linux or MacOS)

make_optim_gen <*compiler-command*>

Running the program

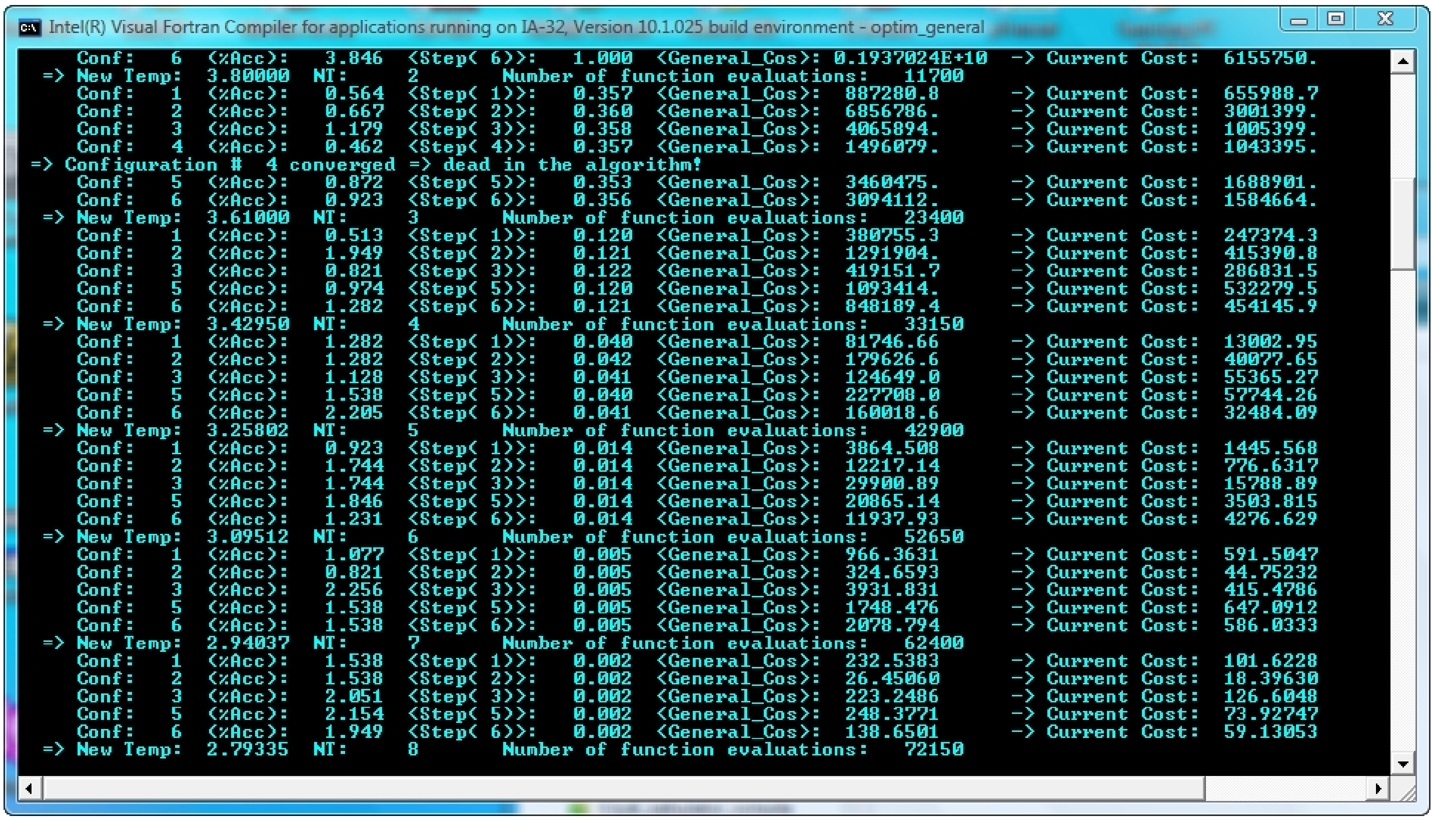
The program is invoked at the prompt using the name of the executable file generated in the previous step.
The user need a file containing the reflections and an input file to introduce the information for calculations.

This is a piece of general example to do Simulated annealing refinement



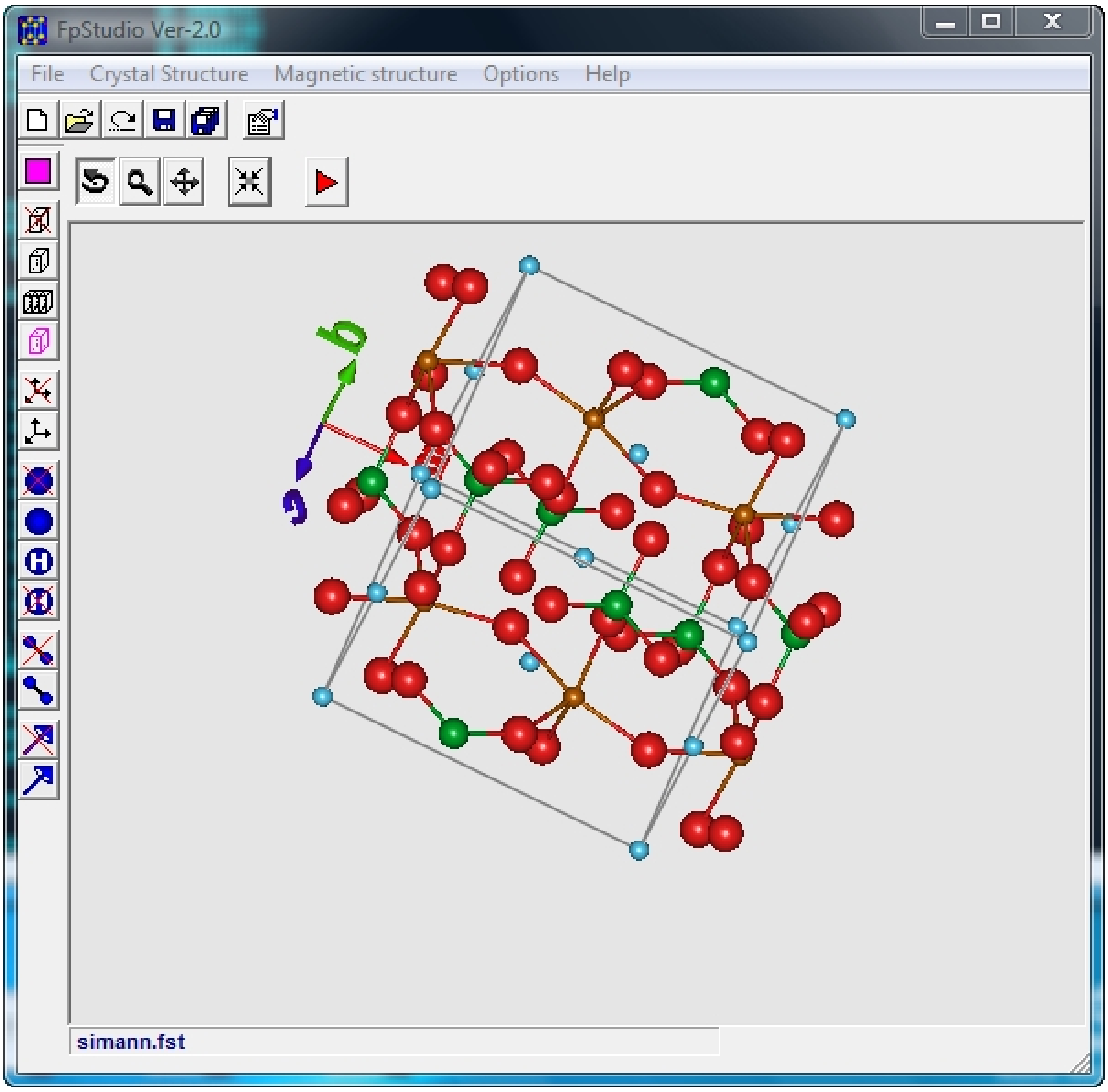
```
Spgr  P n m a
!                   x         y         z       B     occ   Spin Charge
Atom  Ni   NI  0.0000   0.0000  0.0000  0.74  0.5   2.0   2.0
Atom  Fe   FE  0.1443   0.2500  0.7074  0.63  0.5   5.0   3.0
Atom  P    P   0.3718   0.2500  0.1424  0.79  0.5   0.0   5.0
Atom  O1   O   0.3988   0.2500  0.64585 0.71  0.5   0.0  -2.0
Atom  O2   O   0.19415  0.2500  0.0253  0.70  0.5   0.0  -2.0
Atom  O3   O   0.0437   0.2500  0.4728  0.83  0.5   0.0  -2.0
Atom  O4   O   0.3678   0.0566  0.2633  0.77  1.0   0.0  -2.0
! Codes for refinement
Vary xyz 0  1  0  1
!fix x_Fe y_O4
!Equal y_Fe y_P 0.25
HKL-OBS  mfe.hkl
MIN-DSPACING   1.5
FST_CMD  conn P O 0.0 1.8  ; conn FE O 0.0 2.3

OPTIMIZE  dis-restr 1.0   Fobs-Fcal 1.0

!Total number of independent distance restraints:    28

DFIX   3.19620  0.00000  Ni   Ni_3.545
DFIX   2.90276  0.00000  Ni   Fe_1.554
DFIX   2.06756  0.00000  Ni   O1_2.455
...
...
! Simulated Annealing conditions
SIM_ANN
LOCAL_OPTIMIZATION

!       Name of the cost function
CostNam  General_Cost

!         T_ini     anneal     num_temps
TemParM     4.0       0.95       80

!         Nalgor  Nconf nm_cycl   num_therm   accept
Algor_T     0       6    150         0          0.5

!         Value of Seed (if SeedVAL = 0, random seed)
SeedVAL     0
!
Threshold   20.0
!         Treatment of initial configuration
InitCON   RAN
```

output information is showed during execution about the Cost-Function parameter


Intel(R) Visual Fortran Compiler for applications running on IA-32, Version 10.1.025 build environment - optim_general

```
    Conf:   6  (%Acc):   3.846  <Step( 6)>:   1.000  <General_Cos>: 0.1937024E+10  -> Current Cost:  6155750.
 => New Temp:  3.80000  NT:      2        Number of function evaluations:   11700
    Conf:   1  (%Acc):   0.564  <Step( 1)>:   0.357  <General_Cos>:  887280.8      -> Current Cost:  655988.7
    Conf:   2  (%Acc):   0.667  <Step( 2)>:   0.360  <General_Cos>:  6856786.      -> Current Cost:  3001399.
    Conf:   3  (%Acc):   1.179  <Step( 3)>:   0.358  <General_Cos>:  4065894.      -> Current Cost:  1005399.
    Conf:   4  (%Acc):   0.462  <Step( 4)>:   0.357  <General_Cos>:  1496079.      -> Current Cost:  1043395.
=> Configuration #  4 converged => dead in the algorithm!
    Conf:   5  (%Acc):   0.872  <Step( 5)>:   0.353  <General_Cos>:  3460475.      -> Current Cost:  1688901.
    Conf:   6  (%Acc):   0.923  <Step( 6)>:   0.356  <General_Cos>:  3094112.      -> Current Cost:  1584664.
 => New Temp:  3.61000  NT:      3        Number of function evaluations:   23400
    Conf:   1  (%Acc):   0.513  <Step( 1)>:   0.120  <General_Cos>:  380755.3      -> Current Cost:  247374.3
    Conf:   2  (%Acc):   1.949  <Step( 2)>:   0.121  <General_Cos>:  1291904.      -> Current Cost:  415390.8
    Conf:   3  (%Acc):   0.821  <Step( 3)>:   0.122  <General_Cos>:  419151.7      -> Current Cost:  286831.5
    Conf:   5  (%Acc):   0.974  <Step( 5)>:   0.120  <General_Cos>:  1093414.      -> Current Cost:  532279.5
    Conf:   6  (%Acc):   1.282  <Step( 6)>:   0.121  <General_Cos>:  848189.4      -> Current Cost:  454145.9
 => New Temp:  3.42950  NT:      4        Number of function evaluations:   33150
    Conf:   1  (%Acc):   1.282  <Step( 1)>:   0.040  <General_Cos>:  81746.66      -> Current Cost:  13002.95
    Conf:   2  (%Acc):   1.282  <Step( 2)>:   0.042  <General_Cos>:  179626.6      -> Current Cost:  40077.65
    Conf:   3  (%Acc):   1.128  <Step( 3)>:   0.041  <General_Cos>:  124649.0      -> Current Cost:  55365.27
    Conf:   5  (%Acc):   1.538  <Step( 5)>:   0.040  <General_Cos>:  227708.0      -> Current Cost:  57744.26
    Conf:   6  (%Acc):   2.205  <Step( 6)>:   0.041  <General_Cos>:  160018.6      -> Current Cost:  32484.09
 => New Temp:  3.25802  NT:      5        Number of function evaluations:   42900
    Conf:   1  (%Acc):   0.923  <Step( 1)>:   0.014  <General_Cos>:  3864.508      -> Current Cost:  1445.568
    Conf:   2  (%Acc):   1.744  <Step( 2)>:   0.014  <General_Cos>:  12217.14      -> Current Cost:  776.6317
    Conf:   3  (%Acc):   1.744  <Step( 3)>:   0.014  <General_Cos>:  29900.89      -> Current Cost:  15788.89
    Conf:   5  (%Acc):   1.846  <Step( 5)>:   0.014  <General_Cos>:  20865.14      -> Current Cost:  3503.815
    Conf:   6  (%Acc):   1.231  <Step( 6)>:   0.014  <General_Cos>:  11937.93      -> Current Cost:  4276.629
 => New Temp:  3.09512  NT:      6        Number of function evaluations:   52650
    Conf:   1  (%Acc):   1.077  <Step( 1)>:   0.005  <General_Cos>:  966.3631      -> Current Cost:  591.5047
    Conf:   2  (%Acc):   0.821  <Step( 2)>:   0.005  <General_Cos>:  324.6593      -> Current Cost:  44.75232
    Conf:   3  (%Acc):   2.256  <Step( 3)>:   0.005  <General_Cos>:  3931.831      -> Current Cost:  415.4786
    Conf:   5  (%Acc):   1.538  <Step( 5)>:   0.005  <General_Cos>:  1748.476      -> Current Cost:  647.0912
    Conf:   6  (%Acc):   1.538  <Step( 6)>:   0.005  <General_Cos>:  2078.794      -> Current Cost:  586.0333
 => New Temp:  2.94037  NT:      7        Number of function evaluations:   62400
    Conf:   1  (%Acc):   1.538  <Step( 1)>:   0.002  <General_Cos>:  232.5383      -> Current Cost:  101.6228
    Conf:   2  (%Acc):   1.538  <Step( 2)>:   0.002  <General_Cos>:  26.45060      -> Current Cost:  18.39630
    Conf:   3  (%Acc):   2.051  <Step( 3)>:   0.002  <General_Cos>:  223.2486      -> Current Cost:  126.6048
    Conf:   5  (%Acc):   2.154  <Step( 5)>:   0.002  <General_Cos>:  248.3771      -> Current Cost:  73.92747
    Conf:   6  (%Acc):   1.949  <Step( 6)>:   0.002  <General_Cos>:  138.6501      -> Current Cost:  59.13053
 => New Temp:  2.79335  NT:      8        Number of function evaluations:   72150
```

And also the structure can be investigated at the same time if you have the **FP_Studio** program



Twins

Search_TwinLaws program calculate possible twin laws from special metrics using the method of A. Santoro (Acta Cryst A30, 224 (1974)).

The input data are simply the unit cell parameters and the symbol of the space group, and the keyword *TOL* (for tolerance) followed by its value.
If the value is greater than 1 it is supposed to be given in percentage and a division by 100 is performed. The input file should have the extension
CFL

Building the executable file

Run the batch file (for Windows) or the script (for Linux or MacOS)

make_twin <*compiler-command*>

Running the program

The program is invoked at the prompt using the name of the executable file.

Modules on CrysFML Library

CrysFML library presents different levels of complexity, but this is not important for the end user.

Level 0

Concept	*Module Name*	*Purpose*
Constants...	CFML_GlobalDeps	Global parameters on the ***CrysFML*** library

Level 1

Concept	*Module Name*	*Purpose*
Mathematics...	CFML_FFT	FFT calculations
	CFML_LSQ_TypeDef	Definitions of Types for LSQ routines
	CFML_Math_General	General mathematic utilities for use in Crystallography, Solid State Physics and Chemistry.
	CFML_Random_Generators	Random number generators for different kind of statistical distributions
	CFML_Spherical_Harmonics	Spherical Harmonics routines
Messages...	CFML_IO_Messages	Input/Output messages using ***CrysFML***
Profiles...	CFML_PowderProfiles_CW	Calculation of peak profile functions
	CFML_PowderProfiles_Finger	Routines for calculations of asymmetry due to axial divergence (Finger, Cox and Jephcoat)
	CFML_PowderProfiles_TOF	Contains variables and procedures used by programs aiming to handle T.O.F. powder diffraction patterns
Strings...	CFML_String_Utilities	Manipulation of strings with alphanumeric characters

Level 2

Concept	*Module Name*	*Purpose*
Chemical Tables...	CFML_Scattering_Chemical_Tables	Tabulated information about atomic chemical and scattering data
Mathematics...	CFML_Math_3D	Simple mathematics general utilities for 3D Systems
Optimization...	CFML_Optimization_General	Module implementing several algorithms for global and local optimization
	CFML_Optimization_LSQ	Module implementing Marquard algorithm for non-linear least-squares

Patterns...	CFML_Diffraction_Patterns	Diffraction Patterns data structures and procedures for reading different powder diffraction formats.
Symmetry Tables...	CFML_Symmetry_Tables	Tabulated information on Crystallographic Symmetry

Level 3

Concept	***Module Name***	***Purpose***
Bonds Tables...	CFML_Bond_Tables	Contain a simple subroutine providing the list of the usual bonds between atoms
Crystal Metrics...	CFML_Crystal_Metrics	Define crystallographic types and to provide automatic crystallographic metrics operations
instrumentation on ILL...	CFML_ILL_Instrm_Data	Procedures to access the (single crystals) instrument output data base at ILL
Symmetry information...	CFML_Crystallographic_Symmetry	Contain nearly everything needed for handling symmetry in Crystallography.

Level 4

Concept	***Module Name***	***Purpose***
Atoms...	CFML_Atom_TypeDef	Module defining different data structures concerned with atoms
Geometry...	CFML_Geometric_SXTAL	Module for geometrical calculations in single crystal instruments
Reflections...	CFML_Reflections_Utilities	Procedures handling operation with Bragg reflections

Level 5

Concept	***Module Name***	***Purpose***
Geometry...	CFML_Geometry_Calc	Geometry Calculations
Propagation vectors...	CFML_Propagation_Vectors	Procedures handling operations with propagation/modulation vectors
Structure Factors...	CFML_Structure_Factors	Structure Factors Calculations

Level 6

Concept	***Module Name***	***Purpose***
Configurations...	**CFML_BVS_Energy_Calc**	Procedures related to calculations of energy or configuration properties depending on the crystal structure: BVS, Energy,...
Maps...	**CFML_Maps_Calculations**	Procedures related to operations on arrays describing maps
Molecular...	**CFML_Molecular_Crystals**	Types and procedures related to molecules in crystals

Level 7

Concept	***Module Name***	***Purpose***
Formats...	**CFML_IO_Formats**	Procedures for handling different formats for input/output

Level 8

Concept	***Module Name***	***Purpose***
Refinement...	**CFML_Keywords_Code_Parser**	Refinable Codes parser
Magnetic Symmetry...	**CFML_Magnetic_Symmetry**	Procedures handling operations with Magnetic Symmetry and Magnetic Structures
Simulated Annealing...	**CFML_Simulated_Annealing**	Module for Global Optimization using Simulated Annealing

Level 9

Concept	***Module Name***	***Purpose***
Magnetic Structure Factors...	**CFML_Magnetic_Structure_Factors**	Magnetic Structure Factors Calculations
Polarimetry...	**CFML_Polarimetry**	Procedures to calculate the polarization tensor as measured using CRYOPAD

Level 0

Concept	***Module Name***	***Purpose***
Constants...	**CFML_GlobalDeps**	Global parameters on the ***CrysFML*** library

CFML_GlobalDeps

Precision parameters for ***CrysFML*** library and Operating System information.

Numeric parameters

- CP
- DEps
- DP
- Eps
- SP
- Pi
- To_Deg
- To_Rad
- TPi

Operative system parameters

- Ops
- Ops_Name
- Ops_Sep

Functions

- Directory_Exists

Fortran Filenames

Windows:

CFML_GlobalDeps_Windows.f90	(to be use for all Fortran compilers except intel)
CFML_GlobalDeps_Windows_Intel.f90	(to be use with intel Fortran Compiler)

Linux:

CFML_GlobalDeps_Linux.f90
CFML_GlobalDeps_Linux_Intel.f90

MacOS:

CFML_GlobalDeps_MacOS.f90
CFML_GlobalDeps_MacOS_Intel.f90

CFML_GlobalDeps: Numeric Parameters

- CP
- DEps
- DP
- Eps
- SP
- Pi
- To_Deg
- To_Rad
- TPi

CFML_GlobalDeps: Numeric Parameters

Integer, Parameter :: CP

Define the current precision

(***Default***: Simple precision)

CFML_GlobalDeps: Numeric Parameters

Real (Kind=DP), Parameter :: DEps

Epsilon value parameters in double precision

CFML_GlobalDeps: Numeric Parameters

Integer, Parameter :: DP

Define the double precision for real variables

CFML_GlobalDeps: Numeric Parameters

Real (Kind=CP), Parameter :: Eps

Epsilon value parameter in current precision

CFML_GlobalDeps: Numeric Parameters

Real (Kind=DP), Parameter :: Pi

Real parameter containing the value of in double precision

CFML_GlobalDeps: Numeric Parameters

Integer, Parameter :: SP

Define the simple precision for real variables

CFML_GlobalDeps: Numeric Parameters

Real (Kind=DP), Parameter :: To_Deg

Real parameter containing the conversion factor from Radians to Degrees

CFML_GlobalDeps: Numeric Parameters

Real (Kind=DP), Parameter :: To_Rad

Real parameter containing the conversion factor from Degrees to Radians

CFML_GlobalDeps: Numeric Parameters

Real (Kind=DP), Parameter :: TPi

Real parameter containing the value of 2

CFML_GlobalDeps: Operative System Parameters

CFML_GlobalDeps: Operative System Parameters

Integer, Parameter :: Ops

Integer parameter that define the operative system that you are using. The values are:

Value	***Operative System***
1	Windows
2	Linux
3	MacOS

CFML_GlobalDeps: Operative System Parameters

Character (Len=*), Parameter :: Ops_Name

String containing the name of the Operative System.

Value	***Operative System***
Windows	Windows
Linux	Linux
MacOS	MacOS

CFML_GlobalDeps: Operative System Parameters

Character (Len=*), Parameter :: Ops_Sep

String containing the character to define the directory separator.

Value	***Operative System***
\	Windows
/	Linux, MacOS

CFML_GlobalDeps: Functions

CFML_GlobalDeps: Functions

Logical Function Directory_Exists (DirName)

Character (Len=*)	**Intent(in)**	DirName	String containing the name of the directory

Return ***.TRUE.*** or ***.FALSE.*** depending if the directory name in the variable *DirName* exists or not.

Level 1

Concept	*Module Name*	*Purpose*
Mathematics...	**CFML_FFT**	FFT calculations
	CFML_LSQ_TypeDef	Type definitions for LSQ routines
	CFML_Math_General	General mathematic utilities for use in Crystallography, Solid State Physics and Chemistry.
	CFML_Random_Generators	Random number generators for different kind of statistical distributions
	CFML_Spherical_Harmonics	Spherical Harmonics routines
Messages...	**CFML_IO_Messages**	input / output general messages
Profiles...	**CFML_PowderProfiles_CW**	Calculation of peak profile functions
	CFML_PowderProfiles_Finger	Routines for calculations of asymmetry due to axial divergence (Finger, Cox and Jephcoat)
	CFML_PowderProfiles_TOF	Contains variables and procedures used by programs aiming to handle T.O.F. powder diffraction patterns
Strings...	**CFML_String_Utilities**	Manipulation of strings with alphanumeric characters

CFML_FFT

Module for multivariate Fast Fourier Transform calculations

Variables

Points_Interval_Type

Functions

Convol
Convol_Peaks
F_FFT
FFT

Subroutines

HFFT
SFFT

Fortran Filename

CFML_FFTs.f90

CFML_FFT: Variables

Points_Interval_Type

CFML_FFT: Variables

	Variable	*Definition*
Type :: Points_Interval_Type		
Integer	Np	Number of points
Real(Kind=CP)	Low	Lower range value
Real(Kind=CP)	High	Higher range value
End Type Points_Interval_Type		

CFML_FFT: Functions

Convol
Convol_Peaks
F_FFT
FFT

CFML_FFT: Functions

Real Function Convol (F, PF, G, PG, Interval)

Defined Function F		F	
Real(Kind=CP), Dimension (:)	**Intent(in)**	PF	Parameters of the function F
Defined Function G		G	
Real(Kind=CP), Dimension (:)	**Intent(in)**	PG	Parameters of the function G
Type (Points_Interval_Type)	**Intent(in)**	Interval	Give the number of points and the limits of the interval for calculation.

With

Function F (X, ParF)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension (:)	**Intent(in)**	ParF	

End Function F

and

Function G (X, ParG)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension (:)	**Intent(in)**	ParG	

End Function G

Return a real vector of dimension ***interval%NP*** with the convolution of the user-provided centered at x=0 of peak functions **F** and **G**. The convolution function is normalized to unit area.

Example:

h = **convol**(*Pseudo_Voigt*, *P_PV*, *Hat*, *P_Hat*, *My_interval*)

generates my_interval%np values h(i), i=1,my_interval%np corresponding to the convolution of a pseudo-Voigt function with a hat function

CFML_FFT: Functions

Real Function Convol_Peaks (F, PF, G, PG, WD, NP)

Defined Function F		F	
Real(Kind=CP), Dimension (:)	**Intent(in)**	PF	Parameters of the function F (starting with FWHM)
Defined Function G		G	
Real(Kind=CP), Dimension (:)	**Intent(in)**	PG	Parameters of the function G (starting with FWHM)
Real(Kind=CP)	**Intent(in)**	WD	Number of times a FWHM of the f-function to calculate range
Integer	**Intent(in)**	NP	Number of points (it is increased internally up to the closest power of 2)

With

Function F (X, ParF)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension (:)	**Intent(in)**	ParF	

End Function F

and

Function G (X, ParG)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension (:)	**Intent(in)**	ParG	

End Function G

Return a real vector of dimension ***NP*** with the convolution of the user-provided centered at x=0 of peak functions **F** and **G**. The convolution function is normalized to unit area.

The definition interval [a,b] of the peaks is calculated as:

a=-b
b=WD*FWHM=WD*PF(1)

Example:

h = **convol_peaks**(*Pseudo_Voigt*, *P_PV*, *Hat*, *P_Hat*, 15.0, 150)

generates 150 values h(i), i=1,150 corresponding to the convolution of a pseudo-Voigt function with a hat function

Complex Function F_FFT (Array, Mode)

Complex, Dimension (:)	**Intent(in)**	Array	Complex vector containing real parts of transform
Character (Len=*), Optional	**Intent(in)**	Mode	= ***inv*** backward transform. ***inv*** forward transform for the rest

This function is similar to subroutine SFFT and it is useful only when one want to retain the original array. It is a slight modification of a complex split radix FFT routine presented by C.S. Burrus.

NOTE: There is no control of the error consisting in giving a dimension that is not a power of two. It is the responsibility of the user to provide a complex array of dimension equal to a power of 2.

Example:

FX = F_FFT(X)

Y = F_FFT(FY,"inv")

Complex Function FFT (Array, Dim, Inv)

Complex, Dimension (:) **or** **Complex, Dimension (:,:)** **or** **Complex, Dimension (:,:,:)** **or** **...** **or** **Complex, Dimension (:,:,:,:,:,:,:)**	**Intent(in)**	Array	Complex array
Integer, Dimension (:), Optional	**Intent(in)**	Dim	array containing the dimensions to be transformed
Logical, Optional	**Intent(in)**	Inv	= ***.False.*** Forward transformation (Default) = ***.True.*** inverse transformation will be performed.

Multivariate Fast Fourier Transform (from 1 to up 7 dimensions). It is an implementation of Singleton's mixed-radix algorithm, RC Singleton, Stanford Research institute, Sept. 1968.

NOTE: Transformation results will always be scaled by the square root of the product of sizes of each dimension in Dim.

Example:

Let A be a L*M*N three dimensional complex array. Then result = fft(A) will produce a three dimensional transform, scaled by sqrt(L*M*N).

result = fft(A, dim=(/1,3/)) will transform with respect to the first and the third dimension, scaled by sqrt(L*N).
result = fft(fft(A), inv=.true.) should (approximately) reproduce A.

CFML_FFT: Subroutines

- HFFT
- SFFT

CFML_FFT: Subroutines

Subroutine HFFT (Array, IfSet, IfErr)

Complex, Dimension (:)	**Intent(in out)**	Array	Contains the complex 3D array to be transformed
Integer	**Intent(in)**	IfSet	= ***1*** or ***2*** inverse Fourier Transform =***-1*** or ***-2*** Fourier Transform
Integer	**Intent(out)**	IfErr	Flags to error. 0 for no error.

Performs Discrete Complex Fourier Transforms on a complex three dimensional array. This subroutine is to be used for complex, 3-dimensional arrays in which each dimension is a power of 2. The maximum m(i) must not be less than 3 or greater than 20,

For ***IfSet*** = -1, or -2, the Fourier transform of complex array a is obtained.

$$X(J1,J2,J3)=\sum_{K1=0}^{N1-1}\sum_{K2=0}^{N2-1}\sum_{K3=0}^{N3-1}A(K1,K2,K3)W1^{L1}W2^{L2}W3^{L3}$$

where Wi is the n(i) root of unit and L1=K1*J1,L2=K2*J2, L3=K3*J3.

For ***IfSet*** = +1, or +2, the inverse Fourier transform a of complex array x is obtained.

$$A(K1,K2,K3)=\frac{1}{N1N2N3}\sum_{J1=0}^{N1-1}\sum_{J2=0}^{N2-1}\sum_{J3=0}^{N3-1}X(J1,J2,J3)W1^{-L1}W2^{-L2}W3^{-L3}$$

CFML_FFT: Subroutines

Subroutine SFFT (Array, Mode, IfErr)

Complex, Dimension (:)	**Intent(in out)**	Array	Real array containing real parts of transform
Character (Len=*), Optional	**Intent(in)**	Mode	= ***inv*** backward transform. ***inv*** forward transform for the rest
Integer, Optional	**Intent(out)**	IfErr	Flags to error. 0 for no error

The forward transform computes:

$$X(k)=\sum_{j=0}^{N-1}x(j)\cdot e^{(-i2jk\pi/N)}$$

The backward transform computes

$$x(j)=\frac{1}{N}\sum_{k=0}^{N-1}X(k)\cdot e^{(2ijk\pi/N)}$$

CFML_IO_Messages

Input/Output general messages for ***CrysFML*** library

It is convenient to use these intermediate procedures instead of fortran ***write(*,*)*** or ***print****, because it is much more simple to modify a program for making a GUI. Usually GUI tools and libraries need special calls to dialog boxes for screen messages.

Variables

- Win_Console

Subroutines

- Close_Scroll_Window
- Error_Message
- info_Message
- Print_Message
- Question_Message
- Stop_Message
- Wait_Message
- Warning_Message
- Write_Scroll_Text

Fortran Filenames

Console:
CFML_IO_Mess.f90

Realwin:
CFML_IO_MessRW.f90

Winteracter:
CFML_IO_MessWin.f90

CFML_IO_Messages: Variables

- Win_Console

CFML_IO_Messages: Variables

Integer :: Win_Console

Integer value that identify a scroll window when ***Winteracter*** library is used.

NOTE: Only available using ***Winteracter*** library

CFML_IO_Messages: Subroutines

- Close_Scroll_Window
- Error_Message
- info_Message

CFML_IO_Messages: Subroutines

Subroutine Close_Scroll_Window( )

Close the scroll window if still open.

NOTE: Only available using ***Winteracter*** library

CFML_IO_Messages: Subroutines

Subroutine Error_Message(Mess, Iunit, Routine, Fatal)

Character (Len=*)	**Intent(in)**	Mess	String containing the error information
Integer, Optional	**Intent(in)**	Iunit	Write information on unit=Iunit
Character (Len=*), Optional	**Intent(in)**	Routine	Name of the subroutine where occurs the error
Logical, Optional	**Intent(in)**	Fatal	Flag to stop the program or not

Print an error message on the screen and/or in unit defined by ***Iunit*** variable if it is present

CFML_IO_Messages: Subroutines

Subroutine Info_Message(Mess, Iunit, Scroll_Window)

Character (Len=*)	**Intent(in)**	Mess	String Info message
Integer, Optional	**Intent(in)**	Iunit	Write information on unit=Iunit
Integer, Optional	**Intent(in)**	Scroll_Window	Write information on Scroll Window

Print an Information message on the screen and/or in the unit defined by ***Iunit*** if present.

NOTE: The last option is only available using ***RealWin*** library

CFML_IO_Messages: Subroutines

Subroutine Print_Message(Mess)

Character (Len=*)	**Intent(in)**	Mess	Print information

Print an message on the screen.

NOTE: Only available for ***Console*** version

CFML_IO_Messages: Subroutines

Subroutine Question_Message(Mess, Title)

Character (Len=*)	**Intent(in)**	Mess	string containing the message
Character (Len=*), Optional	**Intent(in)**	Title	Title on Dialog

Show a question dialog on the screen

NOTE: Only available using ***Winteracter*** library

CFML_IO_Messages: Subroutines

Subroutine Stop_Message(Mess, Title)

Character (Len=*)	**Intent(in)**	Mess	string containing the message
Character (Len=*), Optional	**Intent(in)**	Title	Title on Dialog

Show a stop dialog on the screen

NOTE: Only available using ***Winteracter*** library

CFML_IO_Messages: Subroutines

Subroutine Wait_Message(Mess)

Character (Len=*)	**Intent(in)**	Mess	String a message and the wait an answer or action by the user

Similar to Pause for Console version

NOTE: Only available for ***Console*** version

CFML_IO_Messages: Subroutines

Subroutine Warning_Message(Mess, Iunit)

Character (Len=*)	**Intent(in)**	Mess	String containing the message
Integer, Optional	**Intent(in)**	Iunit	Write information on unit=Iunit

Show a warning dialog on the screen

NOTE: Only available using ***Winteracter*** library

CFML_IO_Messages: Subroutines

Subroutine Write_Scroll_Text(Mess, ICmd)

Character (Len=*)	**Intent(in)**	Mess	String to print
Integer, Optional	**Intent(in)**	ICmd	Define the type of the Editor Window opened = 0 Editor with command line = 1 Editor without command line

Print the string in a actual scroll window /default terminal/Editor window. The procedure will open a scroll window or editor if it wasn't opened before.

NOTE: The last option is only available using ***Winteracter*** library

CFML_LSQ TypeDef

Definitions for LSQ routines into ***CrysFML*** library

Parameters

Max_Free_Par

Variables

LSQ_Conditions_Type
LSQ_Data_Type
LSQ_State_Vector_Type

Fortran Filename

CFML_LSQ_TypeDef.f90

CFML_LSQ TypeDef: Parameters

Max_Free_Par

CFML_LSQ TypeDef: Parameters

Integer, Parameter :: Max_Free_Par=809

Maximum number of free parameters for use on **CFML_Optimization_LSQ**

CFML_LSQ TypeDef: Variables

LSQ_Conditions_Type
LSQ_State_Vector_Type

LSQ_Data_Type

CFML_LSQ TypeDef: Variables

	Variable	***Definition***
Type :: LSQ_Conditions_Type		
Logical	Constr	if true box constraint of PERCENT are applied to parameters
Logical	Reached	if true convergence was reached in the algorithm
Integer	CorrMax	Value of correlation in % to output
Integer	NFEv	Number of function evaluations (output component, useful for assessing LM algorithm)

Integer	NJEv	Number of Jacobian evaluations
Integer	ICyc	Number of cycles of refinement
Integer	NPVar	Number of effective free parameters of the model
Integer	Iw	indicator for weighting scheme = 1 w=1/yc
Real(Kind=CP)	Tol	Tolerance value for applying stopping criterion in LM algorithm
Real(Kind=CP)	Percent	%value of maximum variation of a parameter w.r.t. the intial value before fixing it
End Type LSQ_Conditions_Type		

Definition of a derived type encapsulating all necessary to establish the conditions for running the LSQ algorithm

CFML_LSQ TypeDef: Variables

	Variable	***Definition***
Type :: LSQ_State_Vector_Type		
Integer	NP	Total number of model parameters <= Max_Free_Par
Real(Kind=CP), Dimension(Max_Free_Par)	PV	Vector of parameters
Real(Kind=CP), Dimension(Max_Free_Par)	SPV	Vector of standard deviations
Real(Kind=CP), Dimension(Max_Free_Par)	DPV	Vector of derivatives at a particular point
Integer, Dimension(Max_Free_Par)	Code	Pointer for selecting variable parameters
Character (Len=40), Dimension(Max_Free_Par)	NamPar	Names of parameters
End Type LSQ_State_Vector_Type		

Definition of derived type encapsulating the vector state defining a set of parameter for calculating the model function and running the LSQ algorithm.

CFML_LSQ TypeDef: Variables

	Variabl e	***Definition***
Type :: LSQ_Data_Type		
Integer	NObs	Total number of observations
Integer	Iw	indicator for type of values contained in component SW
Real(Kind=CP), Dimension(:), Allocatable	X	Vector containing a relevant quantity for each observation (x-coordinate ...)
Real(Kind=CP), Dimension(:), Allocatable	Y	Vector containing the observed values
Real(Kind=CP), Dimension(:), Allocatable	Sw	if Iw=0 Vector containing the standard deviation of observations if Iw=1 Weight factors for least squares refinement
Real(Kind=CP), Dimension(:), Allocatable	Yc	Vector containing the calculated values
End Type LSQ_Data_Type		

Defining a derived type encapsulating the observed and calculated data as well as the weighting factors.
It is responsibility of the calling program to allocate the components before calling the Marquardt_Fit subroutine.

CFML_Math_General

General utilities of mathematics for use in Crystallography, Solid State Physics and Chemistry.

Variables

- Err_MathGen
- Err_MathGen_Mess

Functions

Arrays Functions

- Co_Linear
- Co_Prime
- Equal_Matrix
- Equal_Vector
- Euclidean_Norm
- IMaxLoc
- IMinLoc
- Locate
- Modulo_Lat
- Norm
- OuterProd
- Scalar
- Trace
- ZBelong

Scalar Functions

- Factorial
- Negligible
- PGCD
- PPCM
- Pythag

Special Functions

- BessJ0
- BessJ1
- BessJ

Trigonometric Functions

- AcosD
- AsinD
- Atan2D
- AtanD
- CosD
- SinD
- TanD

Subroutines

- Co_Prime_Vector
- Determinant

Fortran Filename

CFML_Math_Gen.f90

CFML_Math_General: Variables

CFML_Math_General: Variables

Logical :: Err_MathGen

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module

CFML_Math_General: Variables

Character (Len=150) :: Err_MathGen_Mess

Variable containing information about the last error occurred in the procedures belonging to this module

CFML_Math_General: Functions

Arrays Functions

CFML_Math_General: Functions

Real Function AcosD (X)

Real(Kind=SP / DP)	**Intent(in)**	X	Value

Elemental function that gives the inverse of cosine in degrees

CFML_Math_General: Functions

Real Function AsinD (X)

Real(Kind=SP / DP)	**Intent(in)**	X	Value

Elemental function that gives the inverse of sine in degrees

CFML_Math_General: Functions

Real Function Atan2D (Y, X)

Real(Kind=SP / DP)	**Intent(in)**	Y	Value
Real(Kind=SP / DP)	**Intent(in)**	X	Value

Elemental function that gives the arctangent of y/x in degrees

CFML_Math_General: Functions

Real Function AtanD (X)

Real(Kind=SP / DP)	**Intent(in)**	X	Value

Elemental function that gives the arctangent in degrees

CFML_Math_General: Functions

Real Function BessJ0 (X)

Real(Kind=CP)	**Intent(in)**	X	Value

Elemental function that gives the value of the Bessel function J0(x)

CFML_Math_General: Functions

Real Function BessJ1 (X)

Real(Kind=CP)	**Intent(in)**	X	Value

Elemental function that gives the value of the Bessel function J1(x)

CFML_Math_General: Functions

Real Function BessJ (N, X)

Integer	**Intent(in)**	N	Order N of the Bessel function
Real(Kind=CP)	**Intent(in)**	X	Value

Returns the value of the Bessel function Jn(x) for any real x and n >= 2

CFML_Math_General: Functions

Logical Function Co_Linear (A, B, N)

Complex, Dimension(:)	**Intent(in)**	A	Vector of dimension N
Complex, Dimension(:)	**Intent(in)**	B	Vector of dimension N
Integer	**Intent(in)**	N	Dimension of A and B vectors

or

Integer, Dimension(:)	**Intent(in)**	A	Vector of dimension N
Integer, Dimension(:)	**Intent(in)**	B	Vector of dimension N
Integer	**Intent(in)**	N	Dimension of A and B vectors

or

Real(Kind=CP), Dimension(:)	**Intent(in)**	A	Vector of dimension N
Real(Kind=CP), Dimension(:)	**Intent(in)**	B	Vector of dimension N

Integer	**Intent(in)**	N	Dimension of A and B vectors

Logical function that returns the **.TRUE.** value if the vectors **A** and **B** are co-linear. That's means that vectors have the same direction.

CFML_Math_General: Functions

Logical Function Co_Prime(V, IMax)

Integer, Dimension(:)	**Intent(in)**	V	Vector of Numbers
Integer	**Intent(in)**	IMax	Maximun prime number to be tested

Provides the value **.TRUE.** if the vector **V** contains co-primes integers: there is no common divisor for all the Integers. Only the first 1000 prime numbers are tested. The value of **IMAX** the the maximum prime number to be tested (**IMAX** <=7919)

CFML_Math_General: Functions

Real Function CosD (X)

Real(Kind=SP / DP)	**Intent(in)**	X	Value

Elemental function that gives the cosine value when the argument is provided in degrees

CFML_Math_General: Functions

Logical Function Equal_Matrix (A, B, N)

Integer, Dimension(:,:)	**Intent(in)**	A	Array of dimension N x N
Integer, Dimension(:,:)	**Intent(in)**	B	Array of dimension N x N
Integer	**Intent(in)**	N	Dimension of A and B arrays

or

Real(Kind=CP), Dimension(:,:)	**Intent(in)**	A	Array of dimension N x N
Real(Kind=CP), Dimension(:,:)	**Intent(in)**	B	Array of dimension N x N
Integer	**Intent(in)**	N	Dimension of A and B arrays

Logical function that returns the **.TRUE.** value if the array **A** is equal to array **B**

CFML_Math_General: Functions

Logical Function Equal_Vector (A, B, N)

Integer, Dimension(:)	**Intent(in)**	A	Vector of dimension N
Integer, Dimension(:)	**Intent(in)**	B	Vector of dimension N
Integer	**Intent(in)**	N	Dimension of A and B vectors

or

Real(Kind=CP), Dimension(:)	**Intent(in)**	A	Vector of dimension N
Real(Kind=CP), Dimension(:)	**Intent(in)**	B	Vector of dimension N
Integer	**Intent(in)**	N	Dimension of A and B vectors

Logical function that returns the **.TRUE.** value if the array **A** is equal to array **B**

CFML_Math_General: Functions

Real Function Euclidean_Norm (N, V)

Integer	**Intent(in)**	N	Dimension of vector X
Real(Kind=CP), Dimension(:)	**Intent(in)**	V	Vector

This function calculates safely the Euclidean norm of a vector:

$$\|\mathbf{v}\| = \sqrt{v_1^2 + v_2^2 + \cdots + v_n^2}$$

CFML_Math_General: Functions

Integer Function Factorial (N)

Integer	**Intent(in)**	N	Value

Returns the factorial of the number N

CFML_Math_General: Functions

Integer / Real Function IMaxLoc (A)

Integer, Dimension(:)	**Intent(in)**	A	Vector of dimension N

or

Real(Kind=CP), Dimension(:)	**Intent(in)**	A	Vector of dimension N

Return the index indicating the position of the maximum value of a vector

CFML_Math_General: Functions

Integer / Real Function IMinLOC (A)

Integer, Dimension(:)	**Intent(in)**	A	Vector of dimension N

or

Real(Kind=CP), Dimension(:)	**Intent(in)**	A	Vector of dimension N

Return the index indicating the position of the minimum value of a vector

CFML_Math_General: Functions

Integer Function Locate (XX, N, X)

Integer, Dimension(:)	**Intent(in)**	XX	Vector of dimension N
Integer	**Intent(in)**	N	Dimension of XX
Integer	**Intent(in)**	X	Value

or

Real(Kind=CP), Dimension(:)	**Intent(in)**	XX	Vector of dimension N
Integer	**Intent(in)**	N	Dimension of XX
Real(Kind=CP)	**Intent(in)**	X	Value

Function for locating the index j of an array **XX(N)** satisfying that **XX(J)** <= **X** < **XX(J+1)**

CFML_Math_General: Functions

Integer / Real Function Modulo_Lat (U)

Integer, Dimension(:)	**Intent(in)**	U	Vector of free dimension

or

Real(Kind=CP), Dimension(:)	**Intent(in)**	U	Vector of free dimension

Return an integer or real vector with components in the interval [0,1)

CFML_Math_General: Functions

Integer / Real Function Norm (X, G)

Integer, Dimension(:)	**Intent(in)**	X	Vector
Real(Kind=CP), Dimension(:,:)	**Intent(in)**	G	Metric array

or

Real(Kind=CP), Dimension(:)	**Intent(in)**	X	Vector
Real(Kind=CP), Dimension(:,:)	**Intent(in)**	G	Metric array

Calculate the norm of a vector using a particular metric

CFML_Math_General: Functions

Logical Function Negligible (V)

Complex	**Intent(in)**	V	Value

or

Real(Kind=CP)	**Intent(in)**	V	Value

Elemental function that provides the value **.TRUE.** if the complex / real number V is less than ***EPS*** value

CFML_Math_General: Functions

Real Function OuterProd (A, B)

Real(Kind=SP / CP), Dimension(:)	**Intent(in)**	A	Vector of free dimension
Real(Kind=SP / CP), Dimension(:)	**Intent(in)**	B	Vector of free dimension

Function that return an array **C** (size(**A**) x size(**B**)) containing the components of the tensorial product of two vectors

CFML_Math_General: Functions

Integer Function PGCD (I, J)

Integer	**Intent(in)**	I	Value
Integer	**Intent(in)**	J	Value

Return the maximum common divisor of two integers

CFML_Math_General: Functions

Integer Function PPCM (I, J)

Integer	**Intent(in)**	I	Value
Integer	**Intent(in)**	J	Value

Return the minimum common multiple of two integers

CFML_Math_General: Functions

Real Function Pythag (A,B)

Real(Kind=SP / DP)	**Intent(in)**	A	Value
Real(Kind=SP / DP)	**Intent(in)**	B	Value

Computes the square root of (A^2 + B^2) without destructive underflow or overflow

CFML_Math_General: Functions

Integer / Real Function Scalar (X, Y, G)

Integer, Dimension(:)	**Intent(in)**	X	Vector
Integer, Dimension(:)	**Intent(in)**	Y	Vector
Real(Kind=CP), Dimension(:,:)	**Intent(in)**	G	Metric array

or

Real(Kind=CP), Dimension(:)	**Intent(in)**	X	Vector
Real(Kind=CP), Dimension(:)	**Intent(in)**	Y	Vector
Real(Kind=CP), Dimension(:,:)	**Intent(in)**	G	Metric array

Return the scalar product of two vectors including metrics

CFML_Math_General: Functions

Real Function SinD (X)

Real(Kind=SP / DP)	**Intent(in)**	X	Value

Elemental function that gives the sine value when the argument is provided in degrees

CFML_Math_General: Functions

Real Function TanD (X)

Real(Kind=SP / DP)	**Intent(in)**	X	Value

Elemental function that give the tangent value when the argument is provided in degrees

CFML_Math_General: Functions

Complex / Integer / Real Function Trace (A)

Complex, Dimension(:,:)	**Intent(in)**	A	Array of dimension N x N

or

Integer, Dimension(:,:)	**Intent(in)**	A	Array of dimension N x N

or

Real(Kind=CP), Dimension(:,:)	**Intent(in)**	A	Array of dimension N x N

Function that provides the trace of a complex/integer or real matrix

CFML_Math_General: Functions

Logical Function Zbelong (V)

Real(Kind=CP), Dimension(:,:)	**Intent(in)**	V	Array of dimension N x N

or

Real(Kind=CP), Dimension(:)	**Intent(in)**	V	Vector of dimension N

or

Real(Kind=CP)	**Intent(in)**	V	Value

Logical function that provides the value **.TRUE.** if a real number, vector or array **V** is close enough (whithin **EPS**) to an integer.

CFML_Math_General: Subroutines

- Co_Prime_Vector
- Determinant
- Diagonalize_SH
- First_Derivative
- In_Sort
- Init_Err_MathGen
- Invert_Matrix
- Linear_Dependent
- LU_Backsub
- LU_Decomp
- MatInv
- Points_in_Line2D
- Rank

Subroutine Co_Prime_Vector (V, Cop, F)

Integer, Dimension (:)	**Intent(in)**	V	Input integer vector
Integer, Dimension (:)	**Intent(out)**	Cop	Co-prime output vector
Integer, Optional	**Intent(out)**	F	Common multiplicative factor

Calculates the co-prime vector (Cop) parallel to the input vector (V)

Subroutine Determinant (A, N, Determ)

Complex, Dimension (:,:)	**Intent(in)**	A	Array (N x N)
Integer	**Intent(in)**	N	Dimension for Square Matrix
Real(Kind=CP)	**Intent(out)**	Determ	Det(Re[A^2]) + Det(Im[A^2])

or

Real(Kind=CP), Dimension (:,:)	**Intent(in)**	A	Array (N x N)
Integer	**Intent(in)**	N	Dimension for Square Matrix
Real(Kind=CP)	**Intent(out)**	Determ	Determinant of A

Subroutine that calculates the determinant of a real or integer square matrix and a pseudo-determinant for the complex square matrix.

NOTE: The calculated value is only useful for linear dependency purposes. It tell us if the complex matrix is singular or not.

Subroutine Diagonalize_SH (A, N, E_Val, E_Vect)

Complex, Dimension (:,:)	**Intent(in)**	A	Array (N x N)
Integer	**Intent(in)**	N	Dimension for Square Matrix
Real(Kind=CP), Dimension (:)	**Intent(out)**	E_Val	Eigen values sorted in descending order
Complex, Dimension (:,:), Optional	**Intent(out)**	E_Vect	Eigenvectors

or

Real(Kind=CP), Dimension (:,:)	**Intent(in)**	A	Array (N x N)
Integer	**Intent(in)**	N	Dimension for Square Matrix
Real(Kind=CP), Dimension (:)	**Intent(out)**	E_Val	Eigen values sorted in descending order
Real(Kind=CP), Dimension (:,:), Optional	**Intent(out)**	E_Vect	Eigenvectors

Procedure for diagonalizes Symmetric/Hermitian matrices.

CFML_Math_General: Subroutines

Subroutine First_Derivative (X, Y, N, D2Y, D1Y)

Real(Kind=CP), Dimension (:)	**Intent(in)**	X	Vector of N points
Real(Kind=CP), Dimension (:)	**Intent(in)**	Y	Y_i=F(X_i)
Integer	**Intent(in)**	N	Dimension of vectors X, Y
Real(Kind=CP), Dimension (:)	**Intent(in)**	D2Y	Vector containing second derivatives at the given points
Real(Kind=CP), Dimension (:)	**Intent(out)**	D1Y	Vector containing first derivatives at the given points

Subroutine that calculates the first derivate values of a vector of N points

CFML_Math_General: Subroutines

Subroutine In_Sort(ID, N, P, Q)

Integer, Dimension (:)	**Intent(in)**	ID	Vector to be sorted
Integer	**Intent(in)**	N	Number items in the vector
Integer, Dimension (:)	**Intent(in)**	P	initial pointer from a previous related call
Integer, Dimension (:)	**Intent(out)**	Q	Final pointer doing the sort of id

Subroutine to order in ascending mode the integer vector ID.

CFML_Math_General: Subroutines

Subroutine Init_Err_MathGen ( )

Subroutine that initializes errors flags in **CFML_Math_General** module.

CFML_Math_General: Subroutines

Subroutine Invert_Matrix (A, B, Singular, Perm)

Real(Kind=CP), Dimension (:,:)	**Intent(in)**	A	input Array
Real(Kind=CP), Dimension (:,:)	**Intent(in)**	B	output array containing A^{-1}
Logical	**Intent(out)**	Singular	**.TRUE.** is the input array is singular
Integer, Dimension (:), Optional	**Intent(out)**	Perm	Hold the row permutation performed during procedure

Subroutine to invert a real matrix using LU decomposition.

CFML_Math_General: Subroutines

Subroutine Linear_Dependent (A, NA, B, NB, MB, Info)

Complex, Dimension (:)	**Intent(in)**	A	input Vector
Integer	**Intent(in)**	NA	Dimension of A
Complex, Dimension (:,:)	**Intent(in)**	B	input Array B(NB,MB)
Integer	**Intent(in)**	NB	Number of rows of B
Integer	**Intent(in)**	MB	Number of columns of B
Integer, Dimension (:), Optional	**Intent(out)**	Info	**.TRUE.** is A is linear dependent

or

Integer, Dimension (:)	**Intent(in)**	A	input Vector
Integer	**Intent(in)**	NA	Dimension of A
Integer, Dimension (:,:)	**Intent(in)**	B	input Array B(NB,MB)
Integer	**Intent(in)**	NB	Number of rows of B
Integer	**Intent(in)**	MB	Number of columns of B
Integer, Dimension (:), Optional	**Intent(out)**	Info	**.TRUE.** is A is linear dependent

or

Real(Kind=CP), Dimension (:)	**Intent(in)**	A	input Vector
Integer	**Intent(in)**	NA	Dimension of A
Real(Kind=CP), Dimension (:,:)	**Intent(in)**	B	input Array B(NB,MB)
Integer	**Intent(in)**	NB	Number of rows of B
Integer	**Intent(in)**	MB	Number of columns of B
Integer, Dimension (:), Optional	**Intent(out)**	Info	**.TRUE.** is A is linear dependent

This subroutine provides a **.TRUE.** value if the vector **A** is linear dependent of the vectors constituting the rows (columns) of the matrix **B.**

The problem is equivalent to determine the rank (in algebraic sense) of the composite matrix C(NB+1,MB)=(B/A) or C(NB,MB+1)=(B|A). In the first case it is supposed that NA = MB and in the second NA = NB and the rank of B is min(NB, MB).

If NA /= NB and NA /= MB an error condition is generated. The function uses floating arithmetic for all types.

NOTE: The actual dimension of vector A should be NA=max(NB,MB).

CFML_Math_General: Subroutines

Subroutine LU_Backsub (A, Indx, B)

Real(Kind=CP), Dimension (:,:)	**Intent(in)**	A		input Array
Integer, Dimension (:)	**Intent(in)**	Indx		Permutation vector returnned by LU_Decomp
Real(Kind=CP), Dimension (:)	**Intent(in out)**	B	in: out:	Right-hand-side vector Solutions of the linear system

Subroutine that solves the set of N linear equations **A** · **X** = **B**
A and Indx are not modified by this routine and can be left in place for successive calls with different right-hand sides B

NOTE: Here the matrix A (N,N) is not as the original matrix A, but rather as its LU decomposition, determined by the routine LU_Decomp.

CFML_Math_General: Subroutines

Subroutine LU_Decomp (A, D, Singular, Indx)

Real(Kind=CP), Dimension (:,:)	**Intent(in out)**	A	in: out:	input Array Matrix U in its upper triangular part (plus diagonal) and in the lower triangular part contains the nontrivial part of matrix L.
Real(Kind=CP)	**Intent(out)**	D		D is output as +/-1 depending on whether the number of row interchanges was even or odd, respectively
Logical	**Intent(out)**	Singular		**.TRUE.** if A is singular
Integer, Dimension (:), Optional	**Intent(out)**	Indx		Permutation vector

Subroutine to make the LU decomposition of an input matrix **A**.

CFML_Math_General: Subroutines

Subroutine MatInv (A, N)

Real(Kind=CP), Dimension (:,:)	**Intent(in out)**	A	in: out:	input Array A^{-1}
Integer	**Intent(in)**	N		Dimension of A

Subroutine for inverting a real square matrix. The input matrix is replaced in output with its inverse

CFML_Math_General: Subroutines

Subroutine Points_in_Line2D(X1, XN, N, XP)

Real(Kind=CP), Dimension (2)	**Intent(in)**	X1	Point 1 in 2D
Real(Kind=CP), Dimension (2)	**Intent(in)**	XN	Point N in 2D
Integer	**Intent(in)**	N	Number of Total points
Real(Kind=CP), Dimension (:)	**Intent(out)**	XP	Vector of N points

Calculate N points belonging to the line defined by X1 and XN with equal distance between them. XP is a vector containing X_1, X_2,.....,X_N points.

CFML_Math_General: Subroutines

Subroutine Rank (A, Tol, R)

Real (Kind=DP /SP), Dimension (:,:)	**Intent(in)**	A	input Array
Real (Kind=DP /SP)	**Intent(in)**	Tol	Tolerance value
Integer	**Intent(out)**	R	Rank of A

Compute the rank (in algebraic sense) of the rectangular matrix **A**.

CFML_Math_General: Subroutines

Subroutine RTan (Y, X, Ang, Deg)

Real(Kind=DP / SP)	**Intent(in)**	Y	Value
Real(Kind=DP / SP)	**Intent(in)**	X	Value
Real(Kind=DP / SP)	**Intent(out)**	Ang	Value
Character (Len=*), Optional	**Intent(in)**	Deg	Value

Returns the arctangent (**Y**/**X**), in the argument **Ang**, in the quadrant where the signs ***sin(Ang)*** and ***cos(Ang)*** are those of **Y** and **X**.
If **Deg** is present, then **Ang** is provided in degrees

CFML_Math_General: Subroutines

Subroutine Second_Derivative (X, Y, N, D2Y)

Real(Kind=CP), Dimension (:)	**Intent(in)**	X	Vector of N points
Real(Kind=CP), Dimension (:)	**Intent(in)**	Y	Y_i=F(X_i)
Integer	**Intent(in)**	N	Dimension of vectors X, Y
Real(Kind=CP), Dimension (:)	**Intent(out)**	D2Y	Vector containing second derivatives at the given points

Computes the second derivate of a vector of N points

CFML_Math_General: Subroutines

Subroutine Set_EPSG (NEW_EPS)

Real(Kind=CP)	**Intent(in)**	NEW_EPS	Value

Sets an internal **EPS** parameters on this module to the value **NEW_EPS**

CFML_Math_General: Subroutines

Subroutine Set_EPSG_Default ( )

Sets the internal **EPS** variable belong to this module to the default value.

Default: (EPS=10^{-5})

CFML_Math_General: Subroutines

Subroutine SmoothingVec (Y, N, NIter, Ys)

Real(Kind=CP), Dimension (:)	**Intent(in out)**	Y	in: out:	input Vector Vector smoothed if YS is not present in the call of this routine
Integer	**Intent(in)**	N		Number of Points
Integer	**Intent(in)**	NIter		Number of Iterations
Real(Kind=CP), Dimension (:), Optional	**Intent(out)**	Ys		If present, Vector smoothed

Smooth a set of values contained in a vector of N points

Subroutine Sort (A, N, Indx)

Integer, Dimension (:)	**Intent(in)**	A	input vector
Integer	**Intent(in)**	N	Dimension of A
Integer, Dimension (:)	**Intent(out)**	Indx	Vector containing the initial index

or

Real(Kind=CP), Dimension (:)	**Intent(in)**	A	input vector
Integer	**Intent(in)**	N	Dimension of A
Integer, Dimension (:)	**Intent(out)**	Indx	Vector containing the initial index

Sort a vector such the **A** (**indx** (j)) is in ascending order for j=1,2,...,N.

Subroutine Sort_Strings (A)

Character (Len=*), Dimension (:)	**Intent(in out)**	A	in: out:	input Vector of Strings Vector of strings ordered

Sorts a vector of strings. The original vector is replaced by the ordered one on output.

Subroutine Spline (X, Y, N, YP1, YPN, Y2)

Real(Kind=CP), Dimension (:)	**Intent(in)**	X	input vector
Real(Kind=CP), Dimension (:)	**Intent(in)**	Y	input vector
Integer	**Intent(in)**	N	Dimension of X and Y
Real(Kind=CP)	**Intent(in)**	YP1	Derivate of Point 1
Real(Kind=CP)	**Intent(in)**	YPN	Derivate of Point N
Real(Kind=CP), Dimension (:)	**Intent(out)**	Y2	Vector containing second derivatives at the given points

Computes the spline of N points

Subroutine Splint (X, Y, Y2, N, Xp, Yp)

Real(Kind=CP), Dimension (:)	**Intent(in)**	X	input vector
Real(Kind=CP), Dimension (:)	**Intent(in)**	Y	input vector Y_i=F(X_i)
Real(Kind=CP), Dimension (:)	**Intent(in)**	Y2	Vector containing second derivatives at the given points
Integer	**Intent(in)**	N	Dimension of X, Y, Y2
Real(Kind=CP)	**Intent(in)**	XP	Point to evaluate
Real(Kind=CP)	**Intent(out)**	YP	interpoled value

Compute the spline interpolation **Yp** at the point **Xp**

CFML_Math_General: Subroutines

Subroutine SVDCMP (A, W, V)

Real (Kind=SP / DP), Dimension (:,:)	**Intent(in out)**	A	in: out:	input Array A(M,N) Matrix U
Real (Kind=SP / DP), Dimension (:)	**Intent(out)**	W		The diagonal matrix of singular values W is output as the N-dimensional vector W
Real (Kind=SP / DP), Dimension (:,:)	**Intent(out)**	V		Array V(N,N)

Compute the computes its singular value decomposition, $\mathbf{A = U \cdot W \cdot V^T}$

CFML_Math_General: Subroutines

Subroutine Swap (A, B, Mask)

Complex / Integer / Real(Kind=CP)	**Intent(in out)**	A	in: out:	A B
Complex / Integer / Real(Kind=CP)	**Intent(in out)**	B	in: out:	B A
Logical, Optional	**Intent(out)**	Mask		**.TRUE.** if it is present

or

Complex / Integer / Real(Kind=CP), Dimension (:)	**Intent(in out)**	A	in: out:	A B
Complex / Integer / Real(Kind=CP), Dimension (:)	**Intent(in out)**	B	in: out:	B A
Logical, Optional	**Intent(out)**	Mask		**.TRUE.** if it is present

or

Complex / Integer / Real(Kind=CP), Dimension (:,:)	**Intent(in out)**	A	in: out:	A B
Complex / Integer / Real(Kind=CP), Dimension (:,:)	**Intent(in out)**	B	in: out:	B A
Logical, Optional	**Intent(out)**	Mask		**.TRUE.** if it is present

Swap the contents of **A** and **B**

CFML_PowderProfiles_CW

Peak profile calculations for constant wavelength

Functions

- Back_To_Back_Exp
- Exponential
- Gaussian
- Hat

Ikeda_Carpenter
Lorentzian
PseudoVoigt
Split_PseudoVoigt
TCH_PVoigt

Subroutines

Back_To_Back_Exp_Der
Exponential_Der
Gaussian_Der
Hat_Der
Ikeda_Carpenter_Der
Lorentzian_Der
PseudoVoigt_Der
Split_PseudoVoigt_Der
TCH_PVoigt_Der

Fortran Filename

CFML_Profile_Functs.f90

CFML_PowderProfiles_CW: Functions

Back_To_Back_Exp
Exponential
Gaussian
Hat
Ikeda_Carpenter
Lorentzian
PseudoVoigt
Split_PseudoVoigt
TCH_PVoigt

CFML_PowderProfiles_CW: Functions

Real Function Back_To_Back_Exp(X, Par)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)= ; PAR(2)=

The Back_to_Back exponentian function is defined as

$$BB(x) = \begin{cases} \frac{1}{2}\frac{\alpha\beta}{\alpha+\beta}\exp(\alpha x) & x < 0 \\ \\ \frac{1}{2}\frac{\alpha\beta}{\alpha+\beta}\exp(-\beta x) & x \geq 0 \end{cases}$$

CFML_PowderProfiles_CW: Functions

Real Function Exponential(X, Par)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=

The exponential function is defined as

$$Exp(x) = \begin{cases} 0 & x < 0 \\ \alpha \exp(-\alpha x) & x \geq 0 \end{cases}$$

CFML_PowderProfiles_CW: Functions

Real Function Gaussian(X, Par)

Real(Kind=CP)	Intent(in)	X	
Real(Kind=CP), Dimension(:)	Intent(in)	Par	PAR(1)=H

The Gaussian function is:

$$G(x) = a_G \exp\left(-b_G x^2\right)$$

$$a_G = \frac{2}{H}\sqrt{\frac{Ln2}{\pi}} \qquad b_G = \frac{4\,Ln2}{H^2}$$

where *H* is the *FWHM*.

CFML_PowderProfiles_CW: Functions

Real Function Hat(X, Par)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=H

The HAT function is defined as

$$Hat(x) = \begin{cases} 1/H & -H/2 < x < H/2 \\ 0 & otherwise \end{cases}$$

CFML_PowderProfiles_CW: Functions

Real Function Ikeda_Carpenter(X, Par)

Real(Kind=CP)	**Intent(in)**	X	

Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)= ; PAR(2)= ; PAR(3)=R

The Ikeda-Carpenter function is for x >0 as

$$IK(x) = \frac{1}{2}\alpha^3\Big[(1-R)x^2\exp(-\alpha x) + \\ +2R\beta\frac{1}{(\alpha-\beta)}\Big\{\exp(-\beta x) - \\ -\exp(-\alpha x)\Big[1+\Big(1+\frac{1}{2}x(\alpha-\beta)\Big)(\alpha-\beta)x\Big]\Big\}\Big]$$

CFML_PowderProfiles_CW: Functions

Real Function Lorentzian(X, Par)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=H

The Lorentzian function is

$$L(x) = \frac{a_L}{1+b_L x^2}$$

$$a_L = \frac{2}{\pi H} \qquad b_L = \frac{4}{H^2}$$

where *H* if the *FWHM*.

CFML_PowderProfiles_CW: Functions

Real Function PseudoVoigt(X, Par)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=H; PAR(2)=

The PseudoVoigt function is

$$pV(x) = \eta L(x) + (1-\eta)G(x) \qquad 0 \le \eta \le 1$$

where *L(x)* and *G(x)* are a Lorentzian and Gaussian functions with the same *FWHM (H)*.

CFML_PowderProfiles_CW: Functions

Real Function Split_PseudoVoigt(X, Par)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=H1; PAR(2)=H2 PAR(3)= 1; PAR(4)= 2

The Split PseudoVoigt is defined as

CFML_PowderProfiles_CW: Functions

Real Function TCH_PVoigt (X, Par)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=H1; PAR(2)=H2 PAR(3)= 1; PAR(4)= 2

The TCH_PVoigt is defined as

CFML_PowderProfiles_CW: Subroutines

- Back_To_Back_Exp_Der
- Exponential_Der
- Gaussian_Der
- Hat_Der
- Ikeda_Carpenter_Der
- Lorentzian_Der
- PseudoVoigt_Der
- Split_PseudoVoigt_Der
- TCH_PVoigt_Der

CFML_PowderProfiles_CW: Subroutines

Subroutine Back_To_Back_Exp_Der (X, Par, BB_Val, DPar)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)= ; PAR(2)=
Real(Kind=CP)	**Intent(out)**	BB_Val	
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	DPar	1=DerX; 2=Der ; 3=Der

Calculation of the value of the function on X and the partial derivate of the function according to the parameters.

CFML_PowderProfiles_CW: Subroutines

Subroutine Exponential_Der (X, Par, Ex_Val, DPar)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=
Real(Kind=CP)	**Intent(out)**	Ex_Val	
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	DPar	1=DerX; 2=Der

Calculation of the value of the function on X and the partial derivate of the function according to the parameters.

CFML_PowderProfiles_CW: Subroutines

Subroutine Gaussian_Der (X, Par, Gauss_Val, DPar)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=H

Real(Kind=CP)	**Intent(out)**	Gauss_Val	
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	DPar	1=DerX; 2=DerH

Calculation of the value of the function on X and the partial derivate of the function according to the parameters.

CFML_PowderProfiles_CW: Subroutines

Subroutine Hat_Der (X, Par, H_Val, DPar)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=H
Real(Kind=CP)	**Intent(out)**	H_Val	
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	DPar	1=DerX; 2=DerH

Calculation of the value of the function on x and the partial derivate of the function according to the parameters.

CFML_PowderProfiles_CW: Subroutines

Subroutine Ikeda_Carpenter_Der(X, Par, IK_Val, DPar)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)= ; PAR(2)= ; PAR(3)=R
Real(Kind=CP)	**Intent(out)**	IK_Val	
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	DPar	1=DerX, 2=Der , 3=Der , 4=DerR

Calculation of the value of the function on X and the partial derivate of the function according to the parameters.

CFML_PowderProfiles_CW: Subroutines

Subroutine Lorentzian_Der (X, Par, Lor_Val, DPar)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=H
Real(Kind=CP)	**Intent(out)**	Lor_Val	
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	DPar	1=DerX, 2=DerH

Calculation of the value of the function on x and the partial derivate of the function according to the parameters

CFML_PowderProfiles_CW: Subroutines

Subroutine PseudoVoigt_Der (X, Par, PV_Val, DPar)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=H; PAR(2)=
Real(Kind=CP)	**Intent(out)**	PV_Val	
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	DPar	1=DerX, 2=DerH, 3=Der

Calculation of the value of the function on X and the partial derivate of the function according to the parameters

CFML_PowderProfiles_CW: Subroutines

Subroutine Split_PseudoVoigt_Der (X, Par, PV_Val, DPar)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=H1; PAR(2)=H2

			PAR(3)= 1; PAR(4)= 2
Real(Kind=CP)	**Intent(out)**	PV_Val	
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	DPar	1=DerX, 2=DerH1, 3=DerH2, 4=Der 1, 5=Der 2

Calculation of the value of the function on x and the partial derivate of the function according to the parameters

CFML_PowderProfiles_CW: Subroutines

Subroutine TCH_PVoigt_Der (X, Par, PV_Val, DPar)

Real(Kind=CP)	**Intent(in)**	X	
Real(Kind=CP), Dimension(:)	**Intent(in)**	Par	PAR(1)=HG; PAR(2)=HL
Real(Kind=CP)	**Intent(out)**	PV_Val	
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	DPar	1=DerX, 2=DerHG, 3=DerHL

Calculation of the value of the function on X and the partial derivate of the function according to the parameters

CFML_PowderProfiles_Finger

Procedures for asymmetry calculations due to axial divergence using the method of Finger, Cox and Jephcoat *(J. Appl. Cryst. (1992), 27, 892)*

Variables

Init_ProfVal

Subroutines

Init_Prof_Val
Prof_Val

Fortran Filename

CFML_Profile_Finger.f90

CFML_PowderProfiles_Finger: Variables

Init_ProfVal

CFML_PowderProfiles_Finger: Variables

LOGICAL :: Init_ProfVal

.TRUE. if the values for the abscissas and weights of the Gauss-Legendre N-point quadrature formula have been precomputed using
routine **Init_Prof_Val** and internally stored.

CFML_PowderProfiles_Finger: Subroutines

Init_Prof_Val

[Prof_Val](#)

CFML_PowderProfiles_Finger: Subroutines

Subroutine Init_Prof_Val( )

Routine that calculate the values for the abscissas and weights of the Gauss-Legendre N-point quadrature formula have been precomputed using routine
Gauleg and the data are stored internally. When this routineis called then the variable [Init_ProfVal](#) is set to .**TRUE**.

CFML_PowderProfiles_Finger: Subroutines

Subroutine Prof_Val (Eta, Gamma, S_L, D_L, TwoTH, TwoTH0, DPrdT, DPrdG, DPrdE, DPrdS, DPrdD, ProfVal, Use_Asym)

Real(Kind=CP)	**Intent(in)**	Eta	Mixing coefficient between Gaussian and Lorentzian
Real(Kind=CP)	**Intent(in)**	Gamma	FWHM
Real(Kind=CP)	**Intent(in)**	S_L	Source width/detector distance
Real(Kind=CP)	**Intent(in)**	D_L	Detector width/detector distance
Real(Kind=CP)	**Intent(in)**	TwoTH	Point at which to evaluate the profile
Real(Kind=CP)	**Intent(in)**	TwoTH0	Two theta value for peak
Real(Kind=CP)	**Intent(out)**	DPrdT	derivative of profile wrt TwoTH0
Real(Kind=CP)	**Intent(out)**	DPrdG	derivative of profile wrt Gamma
Real(Kind=CP)	**Intent(out)**	DPrdE	derivative of profile wrt Eta
Real(Kind=CP)	**Intent(out)**	DPrdS	derivative of profile wrt S_L
Real(Kind=CP)	**Intent(out)**	DPrdD	derivative of profile wrt D_L
Real(Kind=CP)	**Intent(out)**	ProfVal	
Logical	**Intent(in)**	Use_Asym	**.TRUE.** if asymmetry to be used

Return the value of Profile.

NOTE: Asymmetry due to axial divergence using the method of Finger, Cox and Jephcoat, J. Appl. Cryst. 27, 892, 1992.

CFML_PowderProfiles_TOF

This module contains variables and procedures used by programs aiming to handle **T.O.F.** powder diffraction patterns.

Variables

[Deriv_TOF_Type](#)
[LorComp](#)

Functions

[Erfc](#)
[Erfcp](#)

Subroutines

[TOF_Carpenter](#)

TOF_Jorgensen
TOF_Jorgensen_Vondreele

Fortran Filename

CFML_Profile_TOF.f90

CFML_PowderProfiles_TOF: Variables

Deriv_TOF_Type

LorComp

CFML_PowderProfiles_TOF: Variables

	Variable	***Definition***
Type :: Deriv_TOF_Type		
Real(Kind=CP)	Alfa	omega_a DOmega/Dalpha
Real(Kind=CP)	Beta	omega_b DOmega/Dbeta
Real(Kind=CP)	Dt	omega_t DOmega/Ddt (dt=TOFi-TOF(Bragg))
Real(Kind=CP)	Sigma	omega_s DOmega/Dsigma (for tof_Jorgensen function)
Real(Kind=CP)	Gamma	omega_g DOmega/Dgamma (for tof_Jorgensen_VonDreele function)
Real(Kind=CP)	Eta	omega_e DOmega/Deta (for tof_Jorgensen_VonDreele function)
Real(Kind=CP)	Kappa	omega_e DOmega/kappa (for tof_Carpenter function
End Type Deriv_TOF_Type		

CFML_PowderProfiles_TOF: Variables

Logical :: LorComp

This variable is set to **.TRUE.** if there are Lorentzian components

CFML_PowderProfiles_TOF: Functions

Erfc
Erfcp

CFML_PowderProfiles_TOF: Functions

Real Function Erfc(X)

Real(Kind=SP / DP)	**Intent(in)**	X	

Complementary error function

CFML_PowderProfiles_TOF: Functions

Real Function Erfcp(X)

Real(Kind=SP / DP)	**Intent(in)**	X	

Derivate of the complementary error function

CFML_PowderProfiles_TOF: Subroutines

- TOF_Carpenter
- TOF_Jorgensen
- TOF_Jorgensen_Vondreele

CFML_PowderProfiles_TOF: Subroutines

Subroutine TOF_Carpenter (Dt, D, Alfa, Beta, Gamma, Eta, Kappa, TOF_Theta, TOF_Peak, Deriv)

Read(Kind=CP)	**Intent(in)**	Dt	TOF(channel i) -TOF(Bragg position)
Read(Kind=CP)	**Intent(in)**	D	d-spacing of the peak in A
Read(Kind=CP)	**Intent(in)**	Alfa	units microsecs-1
Read(Kind=CP)	**Intent(in)**	Beta	units microsecs-1
Read(Kind=CP)	**Intent(in)**	Gamma	units microsecs
Read(Kind=CP)	**Intent(in)**	Eta	Mixing coefficient calculated using TCH
Read(Kind=CP)	**Intent(in)**	Kappa	Mixing coeficient of the Ikeda-Carpenter function
Read(Kind=CP)	**Intent(in)**	TOF_Theta	This is the value of 2sin(theta)
Read(Kind=CP)	**Intent(out)**	TOF_Peak	
Type(Deriv_TOF_Type), Optional	**Intent(out)**	Deriv	present if derivatives are to be calculated

Calculate Profile of TOF according to Carpenter

CFML_PowderProfiles_TOF: Subroutines

Subroutine TOF_Jorgensen (Dt, Alfa, Beta, Sigma, TOF_Peak, Deriv)

Read(Kind=CP)	**Intent(in)**	Dt	TOF(channel i) -TOF(Bragg position)
Read(Kind=CP)	**Intent(in)**	Alfa	units microsecs^{-1}
Read(Kind=CP)	**Intent(in)**	Beta	units microsecs^{-1}
Read(Kind=CP)	**Intent(in)**	Sigma	units microsecs^{2}
Read(Kind=CP)	**Intent(out)**	TOF_Peak	
Type(Deriv_TOF_Type), Optional	**Intent(out)**	Deriv	present if derivatives are to be calculated

Calculate Profile of TOF according to Jorgensen

CFML_PowderProfiles_TOF: Subroutines

Subroutine TOF_Jorgensen_Vondreele (Dt, Alfa, Beta, Gamma, Eta, TOF_Peak, Deriv)

Read(Kind=CP)	**Intent(in)**	Dt	TOF(channel i) -TOF(Bragg position)
Read(Kind=CP)	**Intent(in)**	Alfa	units microsecs^{-1}
Read(Kind=CP)	**Intent(in)**	Beta	units microsecs^{-1}
Read(Kind=CP)	**Intent(in)**	Gamma	units microsecs
Read(Kind=CP)	**Intent(in)**	Eta	Mixing coefficient calculated using TCH
Read(Kind=CP)	**Intent(out)**	TOF_Peak	
Type(Deriv_TOF_Type), Optional	**Intent(out)**	Deriv	present if derivatives are to be calculated

Calculate Profile of TOF according to Jorgensen_Vondreele

CFML_Random_Generators

Module for random number generation for different distributions

Variables

- Err_Random
- Err_Random_Mess

Subroutines

- Init_Err_Random
- Random_Beta
- Random_Binomial1
- Random_Binomial2
- Random_Cauchy
- Random_ChiSQ
- Random_Exponential
- Random_Gamma
- Random_Gamma1
- Random_Gamma2
- Random_Inv_Gauss
- Random_MVNorm
- Random_Neg_Binomial
- Random_Normal
- Random_Order
- Random_Poisson
- Random_T
- Random_Von_Mises
- Random_Weibull
- Seed_Random_Number

Fortran Filename

CFML_Random.f90

CFML_Random_Generators: Variables

- Err_Random
- Err_Random_Mess

CFML_Random_Generators: Variables

LOGICAL :: Err_Random

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module

CFML_Random_Generators: Variables

Character(Len=150) :: Err_Random_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Random_Generators: Subroutines

- Init_Err_Random
- Random_Beta
- Random_Binomial1
- Random_Binomial2
- Random_Cauchy
- Random_ChiSQ
- Random_Exponential
- Random_Gamma
- Random_Gamma1
- Random_Gamma2
- Random_Inv_Gauss
- Random_MVNorm
- Random_Neg_Binomial
- Random_Normal
- Random_Order
- Random_Poisson
- Random_T
- Random_Von_Mises
- Random_Weibull
- Seed_Random_Number

CFML_Random_Generators: Subroutines

Subroutine Init_Err_Random ( )

Initializes general error variables **Err_Random** and **Err_Random_Mess**

CFML_Random_Generators: Subroutines

Subroutine Random_Beta (AA, BB, First, FN_VAL)

Real(Kind=CP)	**Intent(in)**	AA	Shape parameter from distribution (0 < real)

Real(Kind=CP)	**Intent(in)**	BB	shape parameter from distribution (0 < real)
Logical	**Intent(in)**	First	.TRUE. for the first call
Real(Kind=CP)	**Intent(out)**	FN_VAL	

Generate a random variate in [0,1] from a beta distribution with density proportional to $^{(AA-1)}$ * (1-)$^{(BB-1)}$ using Cheng's log logistic method.

NOTE: Reference to the book from Dagpunar, J. ***Principles of random variate generation,*** Clarendon Press, Oxford, 1988. ISBN 0-19-852202-9

CFML_Random_Generators: Subroutines

Subroutine Random_Binomial1 (N, P, First, Ival)

Integer	**Intent(in)**	N	Number of Bernoulli Trials (1 <= Integer)
Real(Kind=CP)	**Intent(in)**	P	Bernoulli Success Probability (0 <= Real <= 1)
Logical	**Intent(in)**	First	**.TRUE.** for the first call using the current parameter values **.FALSE.** if the values of (n,p) are unchanged from last call
Integer	**Intent(out)**	Ival	

Subroutine that generates a random binomial variate using C.D.Kemp's method. This algorithm is suitable when many random variables are required with the same parameter values for n & p

NOTE: Reference Kemp, C.D. (1986). `A modal method for generating binomial variables", Commun. Statist. - Theor. Meth. 15(3), 805-813.

CFML_Random_Generators: Subroutines

Subroutine Random_Binomial2 (N, PP, First, Ival)

Integer	**Intent(in)**	N	The number of trials in the binomial distribution from which a random deviate is to be generated
Real(Kind=CP)	**Intent(in)**	PP	The probability of an event in each trial of the binomial distribution from which a random deviate is to be generated.
Logical	**Intent(in)**	First	**.TRUE.** for the first call to perform initialization **.FALSE.** for further calls using the same pair of parameter values (N, PP)
Integer	**Intent(out)**	Ival	

Subroutine that generates a single random deviate from a binomial distribution whose number of trials is N and whose probability of an event in each trial is PP.

CFML_Random_Generators: Subroutines

Subroutine Random_Cauchy (FN_VAL)

Real(Kind=CP)	**Intent(out)**	FN_VAL	The probability of an event in each trial of the binomial distribution from which a random deviate is to be generated.

Generates a single random deviate from the standard Cauchy distribution.

CFML_Random_Generators: Subroutines

Subroutine Random_ChiSQ (Ndf, First, FN_VAL)

Integer	**Intent(in)**	Ndf	Integer that represent degree of freedom
Logical	**Intent(in)**	First	**.TRUE.** for the first call using the current parameter values
Real(Kind=CP)	**Intent(out)**	FN_VAL	

Generates a random variate from the chi-squared distribution with **Ndf** degrees of freedom

CFML_Random_Generators: Subroutines

Subroutine Random_Exponential (FN_VAL)

Real(Kind=CP)	**Intent(out)**	FN_VAL	

Generates a random variate in [0,) from a negative exponential distribution with density proportional to exp(-random_exponential), using inversion.

NOTE: Reference to the book from Dagpunar, J. ***Principles of random variate generation,*** Clarendon Press, Oxford, 1988. ISBN 0-19-852202-9

CFML_Random_Generators: Subroutines

Subroutine Random_Gamma (S, First, FN_VAL)

Real(Kind=CP)	**Intent(in)**	S	Shape parameter of distribution (0.0 < real)
Logical	**Intent(in)**	First	**.TRUE.** for the first call using the current parameter values
Real(Kind=CP)	**Intent(out)**	FN_VAL	

Generates a random gamma variate

NOTE: Reference to the book from Dagpunar, J. ***Principles of random variate generation,*** Clarendon Press, Oxford, 1988. ISBN 0-19-852202-9

CFML_Random_Generators: Subroutines

Subroutine Random_Gamma1 (S, First, FN_VAL)

Real(Kind=CP)	**Intent(in)**	S	Shape parameter of distribution (0.0 < real)
Logical	**Intent(in)**	First	**.TRUE.** for the first call using the current parameter values
Real(Kind=CP)	**Intent(out)**	FN_VAL	

Generates a random variate in [0,) from a gamma distribution with density proportional to gamma**(s-1)*exp(-gamma), based upon best's t distribution method.

NOTE: Reference to the book from Dagpunar, J. ***Principles of random variate generation,*** Clarendon Press, Oxford, 1988. ISBN 0-19-852202-9

CFML_Random_Generators: Subroutines

Subroutine Random_Gamma2 (S, First, FN_VAL)

Real(Kind=CP)	**Intent(in)**	S	Shape parameter of distribution (0.0 < real)
Logical	**Intent(in)**	First	**.TRUE.** for the first call using the current parameter values
Real(Kind=CP)	**Intent(out)**	FN_VAL	

Generates a random variate in [0,   ) from a gamma distribution with density proportional to gamma2**(s-1)*exp(-gamma2), using a switching method.

NOTE: Reference to the book from Dagpunar, J. ***Principles of random variate generation,*** Clarendon Press, Oxford, 1988.ISBN 0-19-852202-9

CFML_Random_Generators: Subroutines

Subroutine Random_Inv_Gauss (H, B, First, FN_VAL)

Real(Kind=CP)	**Intent(in)**	H	Parameter of distribution (0 <= real)
Real(Kind=CP)	**Intent(in)**	B	Parameter of distribution (0 <= real)
Logical	**Intent(in)**	First	**.TRUE.** for the first call using the current parameter values
Real(Kind=CP)	**Intent(out)**	FN_VAL	

Generates a random variate in [0,   ) from a reparameterised generalised inverse gaussian (gig) distribution with density proportional to gig**(h-1) * exp(-0.5*b*(gig+1/gig)) using a ratio method.

NOTE: Reference to the book from Dagpunar, J. ***Principles of random variate generation,*** Clarendon Press, Oxford, 1988.ISBN 0-19-852202-9

CFML_Random_Generators: Subroutines

Subroutine Random_MVNorm (N, H, D, F, First, X, Ier)

Integer	**Intent(in)**	N	Number of variates in vector (input,Integer >= 1)
Real(Kind=CP), Dimension(N)	**Intent(in)**	H	Vector of means
Real(Kind=CP), Dimension(N*(N+1)/2)	**Intent(in)**	D	Variance matrix (j> = i)
Real(Kind=CP), Dimension(N*(N+1)/2)	**Intent(in)**	F	Parameter of distribution (0 < real)
Logical	**Intent(in)**	First	**.TRUE.** if this is the first call of the routine or if the distribution has changed since the last call of the routine. **.FALSE.** otherwise
Real(Kind=CP), Dimension(N)	**Intent(out)**	X	Delivered vector

Integer	**Intent(out)**	Ier	= 1 if the input covariance matrix is not +ve definite = 0 otherwise

Generates an n variate random normal vector using a Cholesky decomposition.

NOTE: Reference to the book from Dagpunar, J. ***Principles of random variate generation,*** Clarendon Press, Oxford, 1988. ISBN 0-19-852202-9

CFML_Random_Generators: Subroutines

Subroutine Random_Neg_Binomial (Sk, P, Ival)

Real(Kind=CP)	Intent(in)	Sk	Number of failures required the "power" parameter of the negative binomial (0 < real)
Real(Kind=CP)	Intent(in)	P	Bernoulli success probability (0 < real < 1)
Integer	Intent(out)	Ival	

Generates a random negative binomial variate using unstored inversion and/or the reproductive property.

NOTE: Reference to the book from Dagpunar, J. ***Principles of random variate generation,*** Clarendon Press, Oxford, 1988. ISBN 0-19-852202-9

CFML_Random_Generators: Subroutines

Subroutine Normal (FN_VAL)

Real(Kind=CP)	**Intent(out)**	FN_VAL	

Returns a normally distributed pseudo-random number with zero mean and unit variance. The algorithm uses the ratio of uniforms method of A.J. Kinderman and J.F. Monahan augmented with quadratic bounding curves.

CFML_Random_Generators: Subroutines

Subroutine Random_Order (Order, N)

Integer	**Intent(in)**	N	Number of Integers
Integer, Dimension(N)	**Intent(out)**	Order	Vector of random integers

Generate a random ordering of the Integers 1 ... n.

CFML_Random_Generators: Subroutines

Subroutine Random_Poisson (Mu, Genpoi)

Real(Kind=CP)	**Intent(in)**	Mu	
Integer	**Intent(out)**	Genpoi	

Generates a single random deviate from a Poisson distribution with mean mu.

CFML_Random_Generators: Subroutines

Subroutine Random_T(M, FN_VAL)

Integer	**Intent(in)**	M	Degrees of freedom of distribution (1 <= Integer)
Real(Kind=CP)	**Intent(out)**	FN_VAL	

Generates a random variate from a t distribution using kinderman and monahan's ratio method.

CFML_Random_Generators: Subroutines

Subroutine Random_Von_Mises(K, First, FN_VAL)

Real(Kind=CP)	**Intent(in)**	K	Parameter of the von Mises distribution
Logical	**Intent(in)**	First	set to **.TRUE.** the first time that the subroutine is called
Real(Kind=CP)	**Intent(out)**	FN_VAL	

Generate a Von Mises Distribution

CFML_Random_Generators: Subroutines

Subroutine Random_Weibull(A, FN_VAL)

Real(Kind=CP)	**Intent(in)**	A	
Real(Kind=CP)	**Intent(out)**	FN_VAL	

Generates a random variate from the Weibull distribution with probability density as

$$f(x) = ax^{a-1}e^{-x^a}$$

CFML_Random_Generators: Subroutines

Subroutine Seed_Random_Number (I_Input, I_Output)

Integer, Optional	**Intent(in)**	I_Input	Unit number for input
Integer, Optional	**Intent(in)**	I_Output	Unit number for output

The seed is read from the **I_Input** unit if present and from keyboard if not.
The output messages is directed to **I_Output** unit if it is present or in the screen in default.

CFML_Spherical_Harmonics

Module containing Spherical Harmonics routines

Variables

Err_Spher
Err_Spher_Mess

Functions

Cubic_Harm_Ang

Cubic_Harm_UcVec
Int_Slater_Bessel
Real_Spher_Harm_Ang
Real_Spher_Harm_UcVec
Real_Spher_HarmCharge_UcVec

Subroutines

Init_Err_Spher
Pikout_LJ_Cubic
SphJn

Fortran Filename

CFML_Spher_Harm.f90

CFML_Spherical_Harmonics: Variables

Err_Spher
Err_Spher_Mess

CFML_Spherical_Harmonics: Variables

LOGICAL :: Err_Spher

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module

CFML_Spherical_Harmonics: Variables

Character (Len=150) :: Err_Spher_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Spherical_Harmonics: Functions

Cubic_Harm_Ang
Cubic_Harm_UcVec
Int_Slater_Bessel
Real_Spher_Harm_Ang
Real_Spher_Harm_UcVec
Real_Spher_HarmCharge_UcVec

CFML_Spherical_Harmonics: Functions

Real Function Cubic_Harm_Ang(L, M, THETA, PHI)

Integer	**Intent(in)**	L	
Integer	**Intent(in)**	M	
Real(Kind=CP)	**Intent(in)**	THETA	
Real(Kind=CP)	**Intent(in)**	PHI	

$$K_{lj}(\theta,\varphi) = \sum_{nr} k^{l}_{nrj} y_{\ln r}(\theta,\varphi)$$

Calculation of the cubic harmonics given in Table 3 of reference M.Kara & K. Kurki-Suonio, Acta Cryt. A37, 201 (1981).

NOTE: Only up to tenth order.

CFML_Spherical_Harmonics: Functions

Real Function Cubic_Harm_UcVec(L, M, U)

Integer	**Intent(in)**	L	
Integer	**Intent(in)**	M	
Real(Kind=CP), Dimension(3)	**Intent(in)**	U	

Calculation of the cubic harmonics given in Table 3 of reference M.Kara & K. Kurki-Suonio, Acta Cryt. A37, 201 (1981).

NOTE: Only up to tenth order. A control of errors is included. For **m3m** symmetry, calculations include up to L=20 M=2 using the coefficients from F.M. Mueller and M.G. Priestley, Phys Rev 148, 638 (1966)

CFML_Spherical_Harmonics: Functions

Real Function Int_Slater_Bessel(N, L, Z, S)

Integer	**Intent(in)**	N	
Integer	**Intent(in)**	L	
Real(Kind=CP)	**Intent(in)**	Z	
Real(Kind=CP)	**Intent(in)**	S	

Returns the integral:

$$\int_0^\infty r^{n+2} \exp(-\psi r)\cdot jl(sr)\cdot dr$$

where ***jl*** is the spherical Bessel function of order *l. O*nly -1 <= n and 0 <= l <= n+1

CFML_Spherical_Harmonics: Functions

Real Function Real_Spher_Harm_Ang(L, M, P, Theta, Phi)

Integer	**Intent(in)**	L	index l >= 0
Integer	**Intent(in)**	M	index m <= l
Integer	**Intent(in)**	P	+1: Cosine -1: Sine
Real(Kind=CP)	**Intent(in)**	Theta	Spherical coordinate in degree
Real(Kind=CP)	**Intent(in)**	Phi	Spherical coordinate in degree

Return the value of

$$y_{lm\pm}(\theta,\varphi)=\frac{1}{N_{lm}}P_l^m(\cos\theta)\begin{cases}\cos m\varphi\\ \sin m\varphi\end{cases}$$

where

$$N_{lm}^2=(1+\delta_{m0})\frac{2\pi}{2l+1}\frac{(l+m)!}{(l-m)!}$$

$$P_l^0(z)=P_l(z)=\frac{1}{2^l l!}\frac{d^l}{dz^l}(z^2-1)^l$$

$$P_l^m(z)=(1-z^2)^{m/2}\frac{d^m}{dz^m}P_l(z)$$

NOTE: M.Kara & K. Kurki-Suonio, Acta Cryt. A37, 201 (1981)

CFML_Spherical_Harmonics: Functions

Real Function Real_Spher_Harm_UcVec(L, M, P, U)

Integer	**Intent(in)**	L	index l >= 0
Integer	**Intent(in)**	M	index m <= l
Integer	**Intent(in)**	P	+1: Cosine -1: Sine
Real(Kind=CP), Dimension(3)	**Intent(in)**	U	Unit vector in cartesian coordinates

Return the value of Ylmp(u).

NOTE: M.Kara & K. Kurki-Suonio, Acta Cryt. A37, 201 (1981)

CFML_Spherical_Harmonics: Functions

Real Function Real_Spher_HarmCharge_UcVec(L, M, P, U)

Integer	**Intent(in)**	L	index l >= 0
Integer	**Intent(in)**	M	index m <= l
Integer	**Intent(in)**	P	+1: Cosine -1: Sine
Real(Kind=CP), Dimension(3)	**Intent(in)**	U	Unit vector in cartesian coordinates

Return the value of Clmp Ylmn(u) where Clmp are selected so that Int[abs(Dlmp) dOmega] = 2 -d(l,0)

CFML_Spherical_Harmonics: Subroutines

Init_Err_Spher

- Pikout_LJ_Cubic
- SphJn

CFML_Spherical_Harmonics: Subroutines

Subroutine Init_Err_Spher ( )

Subroutine that initializes errors flags in **CFML_Spherical_Harmonics** module.

CFML_Spherical_Harmonics: Subroutines

Subroutine Pikout_LJ_Cubic(Group, LJ, NCoef, Lun)

Character(Len=*)	**Intent(in)**	Group	
Integer, Dimension(2,11)	**Intent(out)**	LJ	
Integer	**Intent(out)**	NCoef	
Integer, Optional	**Intent(in)**	Lun	

Picking out rules for indices of cubic harmonics for the 5 cubic groups.

NOTE: Only up to tenth order Given in Table 4 of reference M.Kara & K. Kurki-Suonio, Acta Cryt. A37, 201 (1981)

CFML_Spherical_Harmonics: Subroutines

Subroutine SphJn(N, X, NM, JN, DJN)

Integer	**Intent(in)**	N	Order of Jn(x)
Real(Kind=DP)	**Intent(in)**	X	Argument of Jn
Integer	**Intent(out)**	NM	Highest order computed
Real(Kind=DP), Dimension(0:N)	**Intent(out)**	JN	Array with spherical Bessel functions Jn(x)
Real(Kind=DP), Dimension(0:N)	**Intent(out)**	DJN	Array with derivatives Jn'(x)

Compute Spherical Bessel functions Jn(x) and their derivatives

CFML_String_Utilities

Module containing procedures for manipulation of strings with alphanumeric characters

Variables

- Err_String
- Err_String_Mess
- Err_Text_Type
- Ierr_FMT
- Mess_FindFMT

Functions

- Equal_Sets_Text
- L_Case
- Pack_String
- Strip_String

U_Case

Subroutines

CutST
FindFMT
Frac_Trans_1Dig
Frac_Trans_2Dig
Get_BaseName
Get_DirName
Get_Fraction_1Dig
Get_Fraction_2Dig
Get_LogUnit
Get_Separator_Pos
GetNum
GetNum_STD
GetWord
Inc_LineNum
Init_Err_String
Init_FindFMT
Lcase
Number_Lines
NumCol_From_NumFMT
Read_Key_Str
Read_Key_StrVal
Read_Key_Value
Read_Key_ValueSTD
Reading_Lines
SetNum_STD
Ucase

Fortran Filename

CFML_String_Util.f90

CFML_String_Utilities: Variables

Err_Text_Type

Err_String
Err_String_Mess
Ierr_FMT
Mess_FindFMT

CFML_String_Utilities: Variables

	Variable	***Definition***

Type :: Err_Text_Type		
Integer	NLines	Number of lines
Character (Len=132), Dimension(5)	Txt	Error information
End Type Err_Text_Type		

Definition of this special variable used for the **FindFMT** procedure

CFML_String_Utilities: Variables

Logical :: Err_String

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module

CFML_String_Utilities: Variables

Character (Len=150) :: Err_String_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_String_Utilities: Variables

Integer :: Ierr_FMT

This variable contains information about the error on **FindFMT** procedure.

The error code is according to next information:

Code	Meaning
-2	FORTRAN read error
-1	End of file
0	No Error
1	Empty format descriptor (0 field)
2	Data string read error
3	Integer field found real
4	Begged dot, sign or "e" character
5	invalid character in an Integer field
6	invalid field in format descriptor
7	invalid character in a numeric field
8	0 character in current field
9	Format string length exceeded
10	Separator missing
11	incomplete E or D format
12	incomplete number

CFML_String_Utilities: Variables

TYPE (Err_Text_Type) :: Mess_FindFMT

This variable is a text composed of a maximum of 5 lines to inform about position or error in free format reading when **FindFMT** procedure is used

CFML_String_Utilities: Functions

CFML_String_Utilities: Functions

Logical Function Equal_Sets_Text (Text1, N1, Text2, N2)

Character (Len=*), Dimension (:)	**Intent(in)**	Text1	String vector
Integer	**Intent(in)**	N1	Number of lines on TEXT1
Character (Len=*), Dimension (:)	**Intent(in)**	Text2	String vector
Integer	**Intent(in)**	N2	Number of lines on TEXT2

The function is true if the two sets of text have the same lines in whatever order. Two lines are equal only if they have the same length and all their component
characters are equal and in the same order.

CFML_String_Utilities: Functions

Character Function L_Case (Text)

Character (Len=*)	**Intent(in)**	TEXT	String

Function that converts to lower case the **Text** variable

CFML_String_Utilities: Functions

Character Function Pack_String (Text)

Character (Len=*)	**Intent(in)**	Text	String

Function that packs a string. This means that the function provides a string without empty spaces

CFML_String_Utilities: Functions

Character Function Strip_String (String, To_String)

Character (Len=*)	**Intent(in)**	String	String
Character (Len=*)	**Intent(in)**	To_String	Word from where string is cutted

Function that return a string without from **To_String** up the end.

CFML_String_Utilities: Functions

Character Function U_Case (Text)

Character (Len=*)	**Intent(in)**	Text	String

Function that converts to upper case the Text variable

CFML_String_Utilities: Subroutines

CFML_String_Utilities: Subroutines

Subroutine CutST (Line1, Nlong1, Line2, Nlong2)

Character (Len=*)	**Intent(in out)**	Line1	in: out:	input string input string without the first word
Integer, Optional	**Intent(out)**	Nlong1		If present, give the length of LinE1
Character (Len=*), Optional	**Intent(out)**	Line2		If present, the first word of string on input
Integer, Optional	**Intent(out)**	Nlong2		If present, give the length of LinE2

Subroutine that removes the first word of the input String

CFML_String_Utilities: Subroutines

Subroutine FindFMT (Lun, ALine, FMTFields, FMTString, Idebug)

Integer	**Intent(in)**	Lun		Logical unit number
Character (Len=*)	**Intent(in out)**	ALine	in: out:	String to be decoded input string without the first word
Character (Len=*)	**Intent(in)**	FMTFields		Description of the format fields (e.g. IIFIF)
Character (Len=*)	**Intent(out)**	FMTString		format of the line (e.g. (I5,I1,F8.0,I4,F7.0,))

Integer, Optional	**Intent(in)**	Idebug		Logical unit number for writing the input file. If Zero then no writing is performed

This routine emulates the free format data input, according to

READ (***unit***=String1, ***fmt***='(a,i,2f,..)') AString, I1, R1, R2,...

but with additional error checking. Thus, given a description of the expected fields **FindFMT** returns the format of the line to be decoded.

Valid field descriptors are: **I** (Integer), **A** (free A format), 1 to 5 for A1 to A5

NOTE: This routine have an associated an error code **Ierr_FMT**. If ocurrs an error then also an error message is generated and written to the public variable **Mess_FindFMT**

CFML_String_Utilities: Subroutines

Subroutine Frac_Trans_1Dig (V, Charf)

Real(Kind=CP), Dimension(3)	**Intent(in)**	V	Vector
Character (Len=*)	**Intent(out)**	Charf	String

Subroutine returning a string describing a 3D translation vector written in fractional form as quotient of 1-digit Integers with sign.

Example:

input: V= (0.25, -0.4, 0.3333)
output: CHARF="(1/4,-2/5,1/3)"

CFML_String_Utilities: Subroutines

Subroutine Frac_Trans_2Dig (V, Charf)

Real(Kind=CP), Dimension(3)	**Intent(in)**	V	Vector
Character (Len=*)	**Intent(out)**	Charf	String

Subroutine returning a string describing a 3D translation vector written in fractional form as quotient of 2-digit Integers with sign.

Example:

input: V= (0.3, -0.4, -5.5)
output: CHARF="(3/10,-2/5,-11/2)"

CFML_String_Utilities: Subroutines

Subroutine Get_BaseName (Filename, ChSep, Basename)

Character (Len=*)	**Intent(in)**	Filename	input string containing pathname
Character (Len=*)	**Intent(in)**	ChSep	Normally it will be '\' or '.' or '/'
Character (Len=*)	**Intent(out)**	Basename	The final component of the input Pathname

Subroutine returning a base name

Subroutine Get_DirName (Filename, Directory)

Character (Len=*)	**Intent(in)**	Filename	input string containing full path
Character (Len=*)	**Intent(out)**	Directory	String containing only the Path

Subroutine returning the directory for **Filename**

Subroutine Get_Fraction_1Dig (V, Fracc)

Real(Kind=CP)	**Intent(in)**	V	Real number
Character (Len=*)	**Intent(out)**	Fracc	String

Subroutine that gets a string with the most simple fraction that uses single digits in numerator and denominator.

Subroutine Get_Fraction_2Dig (V, Fracc)

Real(Kind=CP)	**Intent(in)**	V	Real number
Character (Len=*)	**Intent(out)**	Fracc	String

Subroutine that gets a string with the most simple fraction that uses up to two digits in numerator and denominator.

Subroutine Get_LogUnit (Lun)

Integer	**Intent(out)**	Lun	First logical unit available

Subroutine providing the number of the first logical unit that is not opened. Useful for getting a logical unit to a file that should be opened on the fly.

Subroutine Get_Separator_Pos (Line, Car, Pos, Ncar)

Character (Len=*)	**Intent(in)**	Line	input String
Character (Len=1)	**Intent(in)**	Car	Separator character
Integer, Dimension(:)	**Intent(out)**	Pos	Vector with positions of *Car* in *Line*
Integer	**Intent(out)**	Ncar	Number of appearance of *Car* in *Line*

Determines the positions of the separator character **Car** in string **Line** and generates the vector **Pos** containing the positions. The number of times the character **Car** appears in **Line** is stored in **Ncar**. The separator **Car** is not counted within substrings of **Line** that are written within quotes.

Example:

```
line =' 23, "List, of, authors", this book, year=1989'
...
call Get_Separator_Pos(line,',',pos,ncar)
...
```

Then this routine provides

POS=(/4, 25, 36, 0, .../)
NCAR=3

CFML_String_Utilities: Subroutines

Subroutine GetNum (Line, Vet, Ivet, Iv)

Character (Len=*)	**Intent(in)**	Line	input String to convert
Real(Kind=CP), Dimension (:)	**Intent(out)**	Vet	Vector of real numbers
Integer, Dimension (:)	**Intent(out)**	Ivet	Vector of Integer numbers
Integer	**Intent(out)**	Iv	Number of numbers in VET / IVET

Subroutine that converts a string to numbers and write on **VET**/**IVET** if real/Integer.
Control of errors is possible by inquiring the global variables **Err_String** and **Err_Mess_String**

CFML_String_Utilities: Subroutines

Subroutine GetNum_STD (Line, Value, STD, Ic)

Character (Len=*)	**Intent(in)**	Line	input String to convert
Real(Kind=CP), Dimension (:)	**Intent(out)**	Value	Vector of real numbers
Real(Kind=CP), Dimension (:)	**Intent(out)**	STD	Vector of standard deviation values
Integer	**Intent(out)**	Ic	Number of of components of vector Value

Subroutine that converts a string to numbers with standard deviation with format: X.FFFF(S). Control of errors is possible by inquiring the global variables **Err_String** and **Err_Mess_String**.

CFML_String_Utilities: Subroutines

Subroutine GetWord (Line, Dire, Iv)

Character (Len=*)	**Intent(in)**	Line	input String to convert
Character (Len=*), Dimension (:)	**Intent(out)**	Dire	Vector of words
Integer	**Intent(out)**	Iv	Number of of components of vector DIRE

Subroutine that determines the number of words in the input string and generates a character vector with separated words.
Control of errors is possible by inquiring the global variables **Err_String** and **Err_Mess_String**

CFML_String_Utilities: Subroutines

Subroutine Inc_LineNum (Line_N)

Integer	**Intent(in)**	Line_N	Number of Lines that need increases

Subroutine that determines increments the current line number used in **FindFMT**

CFML_String_Utilities: Subroutines

Subroutine Init_Err_String ( )

Subroutine that initializes general error variables **Err_String** and **Err_String_Mess**

CFML_String_Utilities: Subroutines

Subroutine Init_FindFMT (NLine)

Integer, Optional	**Intent(in)**	NLine	Number of the line

Subroutine that initializes the subroutine FindMT and Mess_FindFMT is initialized to zero lines. The current line in the file is also to initialized to zero or put to the value NLine if the optional argument is present

CFML_String_Utilities: Subroutines

Subroutine Lcase (Line)

Character (Len=*)	**Intent(in out)**	Line	in: out:	input string input line converted to lower case

Subroutine that converts to lower case the string in the argument

CFML_String_Utilities: Subroutines

Subroutine Number_Lines (Filename, N)

Character (Len=*)	**Intent(in)**	Filename	Name of the input file
Integer	**Intent(out)**	N	Number of lines in the file

Subroutine that gives the number of lines contained in a file. If the file is opened, a rewind command is performed.

CFML_String_Utilities: Subroutines

Subroutine NumCol_From_NumFMT (Text, N_Col)

Character (Len=*)	**Intent(in)**	Text	input format string
Integer	**Intent(out)**	N_Col	Integer number of columns

Subroutine that provides the number of columns spanned by a numeric format field F,I,G,E

CFML_String_Utilities: Subroutines

Subroutine Read_Key_Str (Filevar, Nline_Ini, Nline_End, Keyword, String)

Character (Len=*), Dimension (:)	**Intent(in)**	Filevar		input vector of Strings
Integer	**Intent(in out)**	Nline_Ini	in: out:	initial position to search Current position in search
Integer	**Intent(in)**	Nline_End		Define the final position to search
Character (Len=*)	**Intent(in)**	Keyword		Word to search

Character (**Len**=*)	**Intent**(**out**)	String		Rest of the input string where KEYWORD is contained.

Subroutine that read a string on **Filevar** starting with a particular **Keyword** between lines **Nline_Ini** and **Nline_End**.

CFML_String_Utilities: Subroutines

Subroutine Read_Key_StrVal (Filevar, Nline_Ini, Nline_End, Keyword, String, Vet, Ivet, Iv)

Character (**Len**=*), **Dimension** (:)	**Intent**(**in**)	Filevar		input vector of Strings
Integer	**Intent**(**in out**)	Nline_Ini	in: out:	initial position to search Current position in search
Integer	**Intent**(**in**)	Nline_End		Define the final position to search
Character (**Len**=*)	**Intent**(**in**)	Keyword		Word to search
Character (**Len**=*)	**Intent**(**out**)	String		Rest of the input string where KEYWORD is contained.
Real(**Kind**=CP), **Dimension** (:), **Optional**	**Intent**(**out**)	Vet		Vector for real numbers
Integer, Dimension (:), **Optional**	**Intent**(**out**)	Ivet		Vector for Integer numbers
Integer, Optional	**Intent**(**out**)	Iv		Number of numbers on VET / IVET

Subroutine that read a string on **Filevar** starting with a particular **Keyword** between lines **Nline_Ini** and **Nline_End**. If the string contains numbers they are read and put into **VET** / **IVET**. The variable **String** contains the input string without the **KEYWORD.**

CFML_String_Utilities: Subroutines

Subroutine Read_Key_Value (Filevar, Nline_Ini, Nline_End, Keyword, Vet, Ivet, Iv)

Character (**Len**=*), **Dimension** (:)	**Intent**(**in**)	Filevar		input vector of Strings
Integer	**Intent**(**in out**)	Nline_Ini	in: out:	initial position to search Current position in search
Integer	**Intent**(**in**)	Nline_End		Define the final position to search
Character (**Len**=*)	**Intent**(**in**)	Keyword		Word to search
Real(**Kind**=CP), **Dimension** (:), **Optional**	**Intent**(**out**)	Vet		Vector for real numbers
Integer, Dimension (:), **Optional**	**Intent**(**out**)	Ivet		Vector for Integer numbers
Integer, Optional	**Intent**(**out**)	Iv		Number of numbers on VET / IVET

Subroutine that read parameters on **Filevar** starting with a particular **Keyword** between lines **Nline_Ini** and **Nline_End**. If the string contains numbers they are read and put into **VET** / **IVET**.

CFML_String_Utilities: Subroutines

Subroutine Read_Key_ValueSTD (Filevar, Nline_Ini, Nline_End, Keyword, Vet1, Vet2, Iv)

Character (**Len**=*), **Dimension** (:)	**Intent**(**in**)	Filevar		input vector of Strings
Integer	**Intent**(**in out**)	Nline_Ini	in: out:	initial position to search Current position in search
Integer	**Intent**(**in**)	Nline_End		Define the final position to search

Character (Len=*)	**Intent(in)**	Keyword		Word to search
Real(Kind=CP), Dimension (:)	**Intent(out)**	Vet1		Vector for real numbers
Real(Kind=CP), Dimension (:)	**Intent(out)**	Vet2		Vector for standard deviations numbers
Integer	**Intent(out)**	Iv		Number of numbers on VET1 and VET2

Subroutine that read parameters and standard deviation on **FILEVAR** starting with a particular **KEYWORD** between lines **Nline_Ini** and **Nline_End**.

CFML_String_Utilities: Subroutines

Subroutine Reading_Lines (Filename, Nlines, Filevar)

Character (Len=*)	**Intent(in)**	Filename	Name of the input file
Integer	**Intent(in)**	Nlines	Number of lines to read
Character (Len=*), Dimension(:)	**Intent(out)**	Filevar	String vector

Subroutine that reads **NLines** of the input file and put the information on **Filevar**. If the file was opened, then a rewind command is performed.

CFML_String_Utilities: Subroutines

Subroutine SetNum_STD (Value, STD, Line)

Real(Kind=CP)	**Intent(in)**	Value	Real number
Real(Kind=CP)	**Intent(in)**	STD	Standar deviation
Character (Len=*)	**Intent(out)**	Line	String with format X.FFFF(S)

Subroutine that writes in **Line** a real number with standard deviation between parenthesis

CFML_String_Utilities: Subroutines

Subroutine Ucase (Line)

Character (Len=*)	**Intent(in out)**	Line	in: out:	input string input line converted to upper case

Subroutine that converts to upper case the string in the argument

Level 2

Concept	***Module Name***	***Purpose***
Chemical Tables...	**CFML_Scattering_Chemical_Tables**	Tabulated information about atomic chemical and scattering data
Mathematics...	**CFML_Math_3D**	Simple mathematics general utilities for 3D Systems
Optimization...	**CFML_Optimization_General**	Module implementing several algorithms for global and local optimization
	CFML_Optimization_LSQ	Module implementing Marquard

		algorithm for non-linear least-squares
Patterns...	**CFML_Diffraction_Patterns**	Diffraction Patterns data structures and procedures for reading different powder diffraction formats.
Symmetry Tables...	**CFML_Symmetry_Tables**	Tabulated information on Crystallographic Symmetry

CFML_Diffraction_Patterns

Module containing procedures related with Diffraction Patterns information

Variables

Diffraction_Pattern_Type

Err_DiffPatt
Err_DiffPatt_Mess

Functions

Calc_FWHM_Peak

Subroutines

Allocate_Diffraction_Pattern
Calc_Background
Init_Err_DiffPatt
Purge_Diffraction_Pattern
Read_Background_File
Read_Pattern
Write_Pattern_XYSig

Fortran Filename

CFML_Diffpatt.f90

CFML_Diffraction_Patterns: Variables

Diffraction_Pattern_Type

Err_DiffPatt
Err_DiffPatt_Mess

CFML_Diffraction_Patterns: Variables

	Variable	*Definition*
Type :: Diffraction_Pattern_Type		
Character (Len=180)	Title	Identification of the pattern
Character (Len=20)	Diff_Kind	Type of radiation
Character (Len=20)	Scat_Var	x-space: 2 , TOF, Q, s, d-spacing, sin /
Character (Len=20)	Instr	File type
Character (Len=512)	Filename	File name
Real (Kind=CP)	Xmin	
Real (Kind=CP)	Xmax	
Real (Kind=CP)	Ymin	
Real (Kind=CP)	Ymax	
Real (Kind=CP)	Scal	
Real (Kind=CP)	Monitor	
Real (Kind=CP)	Step	
Real (Kind=CP)	TSsamp	Sample Temperature
Real (Kind=CP)	TSset	Setting Temperature (wished temperature)
Integer	NPts	Number of points
Logical	CT_Step	Constant step
Logical	GY	Logical constants for Graphics
Logical	GYcalc	
Logical	GBgr	
Logical	GSigma	
Logical	AL_X	Logicals for Allocations
Logical	AL_Y	
Logical	AL_Ycalc	
Logical	AL_Bgr	
Logical	AL_Sigma	
Logical	AL_IStat	
Real (Kind=CP), Dimension(3)	Conv	Wavelengths or Dtt1, Dtt2 for converting to Q,d, etc
Real (Kind=CP), Dimension(:), Allocatable	X	Scattering variable (2theta...)
Real (Kind=CP), Dimension(:), Allocatable	Y	Experimental intensity
Real (Kind=CP), Dimension(:), Allocatable	Sigma	observations VARIANCE (it is the square of sigma!)
Integer, Dimension(:), Allocatable	IStat	information about the point "i"
Real (Kind=CP), Dimension(:), Allocatable	Ycalc	Calculated intensity
Real (Kind=CP), Dimension(:), Allocatable	Bgr	Background
End Type Diffraction_Pattern_Type		

Logical :: Err_DiffPatt

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_Diffraction_Patterns: Variables

Character (Len=150) :: Err_DiffPatt_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Diffraction_Patterns: Functions

Calc_FWHM_Peak

CFML_Diffraction_Patterns: Functions

Real Function Calc_FWHM_Peak (Pat, Xi, Yi, Ybi, RLim)

Type(Diffraction_Pattern_Type)	**Intent(in)**	Pat	Pattern profile
Real(Kind=CP)	**Intent(in)**	Xi	X value on point i
Real(Kind=CP)	**Intent(in)**	Yi	Y value on point i
Real(Kind=CP)	**Intent(in)**	Ybi	Y balue for Background on point i
Real(Kind=CP), Optional	**Intent(in)**	Rlim	Limit range in X units to search the point

Function that calculate the FWHM of a peak situated on (*xi,yi*). Then the routine search the Y_m value in the range (xi-rlim, xi+rlim) to obtain the FWHM.
The function return a negative values if an error is ocurred during calculation.

CFML_Diffraction_Patterns: Subroutines

Allocate_Diffraction_Pattern
Calc_Background
Init_Err_DiffPatt
Purge_Diffraction_Pattern
Read_Background_File
Read_Pattern
Write_Pattern_XYSig

CFML_Diffraction_Patterns: Subroutines

Subroutine Allocate_Diffraction_Pattern (Pat, Npts)

Type(Diffraction_Pattern_Type)	**Intent(in out)**	Pat	Pattern
Integer	**Intent(in)**	NPts	Number of points for this Pattern

Allocate the object **Pat** of type Diffraction_Pattern_Type

CFML_Diffraction_Patterns: Subroutines

Subroutine Calc_Background (Pat, Ncyc, Np, Xmin, Xmax)

Type(Diffraction_Pattern_Type)	**Intent(in out)**	Pat	Pattern
Integer	**Intent(in)**	Ncyc	Number of Iterations for Background calculations

Integer	**Intent(in)**	Np	Number of points to define the average
Real(Kind=CP), Optional	**Intent(in)**	Xmin	Lower limit for Background calculation
Real(Kind=CP), Optional	**Intent(in)**	Xmax	Upper limit for Background calculation

Calculate a Background using an iterative process according to Brückner, S. (2000). J. Appl. Cryst., 33, 977-979.

CFML_Diffraction_Patterns: Subroutines

Subroutine Init_Err_DiffPatt ( )

Subroutine that initializes errors flags in **CFML_Diffraction_Patterns** module.

CFML_Diffraction_Patterns: Subroutines

Subroutine Purge_Diffraction_Pattern (Pat, Mode)

Type(Diffraction_Pattern_Type)	**Intent(in out)**	Pat	Pattern
Character (Len=*)	**Intent(in)**	Mode	

Deallocate components of the object **Pat**, of type Diffraction_Pattern_Type depending on the value of the **Mode** string.

At present the following MODE values are available:

MODE	***Value***
DATA	Purge SIGMA, YCALC, BGR, ISTAT
DATAS	Purge YCALC, BGR, ISTAT
RIETV	Purge ISTAT
GRAPH	Purge YCALC, BGR
PRF	Purge SIGMA

CFML_Diffraction_Patterns: Subroutines

Subroutine Read_Background_File (BCK_File, BCK_Mode, Dif_Pat)

Character (Len=*)	**Intent(in)**	BCK_File	Name of the file
Character (Len=*)	**Intent(in)**	BCK_Mode	Options are: POL -> Polynomial INT -> Interpolation
Type(Diffraction_Pattern_Type)	**Intent(in out)**	Dif_Pat	Pattern

Read background from a file

CFML_Diffraction_Patterns: Subroutines

Subroutine Read_Pattern (Filename, Dif_Pat, Mode)

Character (Len=*)	**Intent(in)**	Filename	Name of the file
Type(Diffraction_Pattern_Type)	**Intent(in out)**	Dif_Pat	Pattern
Character (Len=*), Optional	**Intent(in)**	Mode	(Only used for GSAS format)

or

Subroutine Read_Pattern (Filename, Dif_Pat, NumPat, Mode)

Character (Len=*)	**Intent(in)**	Filename	Name of the file
Type(Diffraction_Pattern_Type), Dimension(:)	**Intent(in out)**	Dif_Pat	Pattern
Integer	**Intent(out)**	NumPat	Number of Patterns
Character (Len=*), Optional	**Intent(in)**	Mode	Actual options are: XYSIGMA ISIS GSAS

Read one or several Patterns from a Filename

CFML_Diffraction_Patterns: Subroutines

Subroutine Write_Pattern_XYSig (Filename, Pat)

Character (Len=*)	**Intent(in)**	Filename	Name of the file
Type(Diffraction_Pattern_Type)	**Intent(in)**	Pat	Pattern

Write a pattern in X,Y,Sigma format in file **Filename**

CFML_Math_3D

Simple mathematics general utilities for 3D Systems

Variables

Err_Math3D
Err_Math3D_Mess

Functions

Cross_Product
Determ_A
Determ_V
Invert_A
Polyhedron_Volume
Rotate_OX
Rotate_OY
Rotate_OZ
VecLength

Subroutines

Get_Cart_From_Cylin
Get_Cart_From_Spher
Get_Centroid_Coord

Get_Cylindr_Coord
Get_Plane_From_Points
Get_Spheric_Coord
Init_Err_Math3D
Matrix_DiagEigen
Matrix_Inverse
Resolv_Sist_1x2
Resolv_Sist_1x3
Resolv_Sist_2x2
Resolv_Sist_2x3
Resolv_Sist_3x3
Set_Eps
Set_Eps_Default

Fortran Filename

CFML_Math_3D.f90

CFML_Math_3D: Variables

Err_Math3D
Err_Math3D_Mess

CFML_Math_3D: Variables

Logical :: Err_Math3D

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module

CFML_Math_3D: Variables

Character (Len=150) :: Err_Math3D_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Math_3D: Functions

Cross_Product
Determ_A
Determ_V
Invert_A
Polyhedron_Volume
Rotate_OX
Rotate_OY
Rotate_OZ
VecLength

CFML_Math_3D: Functions

Integer / Real Function Cross_Product(U, V)

Integer, Dimension (3)	**Intent(in)**	U	Vector
Integer, Dimension (3)	**Intent(in)**	V	Vector

or

Real(Kind=SP / DP), Dimension (3)	**Intent(in)**	U	Vector
Real(Kind=SP / DP), Dimension (3)	**Intent(in)**	V	Vector

Calculates the cross product of vectors U and V. All vectors are given in cartesian components.

CFML_Math_3D: Functions

Integer / Real Function Determ_A (A)

Integer, Dimension (3,3)	**Intent(in)**	A	Array

or

Real(Kind=CP), Dimension (3,3)	**Intent(in)**	A	Array

Calculates the determinant of an Integer/real 3x3 matrix

CFML_Math_3D: Functions

Integer / Real Function Determ_V(A, B, C)

Integer, Dimension (3)	**Intent(in)**	A	Vector
Integer, Dimension (3)	**Intent(in)**	B	Vector
Integer, Dimension (3)	**Intent(in)**	C	Vector

or

Real(Kind=CP), Dimension (3)	**Intent(in)**	A	Vector
Real(Kind=CP), Dimension (3)	**Intent(in)**	B	Vector
Real(Kind=CP), Dimension (3)	**Intent(in)**	C	Vector

Calculates the determinant of the components of three vectors

CFML_Math_3D: Functions

Real Function Invert_A (A)

Real(Kind=SP / DP), Dimension (3,3)	**Intent(in)**	A	Array

Calculate de inverse of a real 3x3 matrix. If the routine fails, then a 0.0 matrix is returned.

CFML_Math_3D: Functions

Real Function Polyhedron_Volume(NV, Vert, Cent)

Integer	**Intent(in)**	NV	Number of vertices of Polyhedra

Real(Kind=CP), Dimension (:,:)	**Intent(in)**	Vert	Cartesian coordinates of vertices. First index (1:NV), Second index 3
Real(Kind=CP), Dimension (3)	**Intent(in)**	Cent	Cartesian coordinates for a central point

Procedure to calculate the volume of polyhedral with NV vertices.

Note: It is based on Volcal program of L. W. Finger.

CFML_Math_3D: Functions

Real Function Rotate_OX(X, Angle)

Real(Kind=CP), Dimension (3)	**Intent(in)**	X	Vector
Real(Kind=CP)	**Intent(in)**	Angle	Angle (Degrees)

Rotation a 3D point on X axis about **Angle** degrees

CFML_Math_3D: Functions

Real Function ROTATE_OY(Y, ANGLE)

Real(Kind=CP), Dimension (3)	**Intent(in)**	Y	Vector
Real(Kind=CP)	**Intent(in)**	Angle	Angle (Degrees)

Rotation a 3D point on Y axis about **Angle** degrees

CFML_Math_3D: Functions

Real Function Rotate_OZ (Z, Angle)

Real(Kind=CP), Dimension (3)	**Intent(in)**	Z	Vector
Real(Kind=CP)	**Intent(in)**	Angle	Angle (Degrees)

Rotation a 3D point on Z axis about **Angle** degrees

CFML_Math_3D: Functions

Real Function VecLength(A, B)

Real(Kind=CP), Dimension (3,3)	**Intent(in)**	A	
Real(Kind=CP), Dimension (3)	**Intent(in)**	B	

Length of vector **B** when **A** is the Crystallographic to orthogonal matrix length

CFML_Math_3D: Subroutines

- Get_Cart_From_Cylin
- Get_Cart_From_Spher
- Get_Centroid_Coord
- Get_Cylindr_Coord
- Get_Plane_From_Points
- Get_Spheric_Coord

CFML_Math_3D: Subroutines

Subroutine Get_Cart_From_Cylin (Rho, Phi, Zeta, X0, Mode)

Real(Kind=SP / DP)	**Intent(in)**	Rho	
Real(Kind=SP / DP)	**Intent(in)**	Phi	
Real(Kind=SP / DP)	**Intent(in)**	Zeta	
Real(Kind=SP / DP), Dimension(3)	**Intent(out)**	X0	
Character (Len=*), Optional	**Intent(in)**	Mode	

Determine the Cartesian coordinates from cylindrical coordinates. If Mode='D' the angle phi is provided in Degrees.

CFML_Math_3D: Subroutines

Subroutine Get_Cart_From_Spher (R, Theta, Phi, X0, Mode)

Real(Kind=SP / DP)	**Intent(in)**	R	
Real(Kind=SP / DP)	**Intent(in)**	THETA	
Real(Kind=SP / DP)	**Intent(in)**	PHI	
Real(Kind=SP / DP), Dimension(3)	**Intent(out)**	X0	
Character (Len=*), Optional	**Intent(in)**	MODE	

Determine the Cartesian coordinates from spherical coordinates. If Mode='D' the angle phi is provided in Degrees.

CFML_Math_3D: Subroutines

Subroutine Get_Centroid_Coord (Cn, Atm_Cart, Centroid, Baricenter)

Integer	**Intent(in)**	Cn	Coordination Number
Real(Kind=CP), Dimension(:,:)	**Intent(in)**	Atm_Cart	Cartesian coordinates of atoms
Real(Kind=CP), Dimension(3)	**Intent(out)**	Centroid	Centroid point in Cartesian coordinates
Real(Kind=CP), Dimension(3)	**Intent(out)**	Baricenter	Baricenter point in Cartesian coordinates

Procedure to calculate Centroid and BariCenter of Polyhedral according to Tonci Balic-Zunic (Acta Cryst. B52, 1996, 78-81; Acta Cryst. B54, 1998, 766-773)

CFML_Math_3D: Subroutines

Subroutine Get_Cylindr_Coord (X0, Rho, Phi, Zeta, Mode)

Real(Kind=SP /DP), Dimension(3)	**Intent(in)**	X0	

Real(Kind=SP / DP)	**Intent(out)**	Rho	
Real(Kind=SP / DP)	**Intent(out)**	Phi	
Real(Kind=SP / DP)	**Intent(out)**	Zeta	
Character (Len=*), Optional	**Intent(in)**	Mode	

Determine the cylindrical coordinates from Cartesian coordinates. If Mode='D' the angle phi is provided in Degrees.

CFML_Math_3D: Subroutines

Subroutine Get_Plane_From_Points (P1, P2, P3, A, B, C, D)

Real(Kind=CP), Dimension(3)	**Intent(in)**	P1	
Real(Kind=CP), Dimension(3)	**Intent(in)**	P2	
Real(Kind=CP), Dimension(3)	**Intent(in)**	P3	
Real(Kind=CP)	**Intent(out)**	A	
Real(Kind=CP)	**Intent(out)**	B	
Real(Kind=CP)	**Intent(out)**	C	
Real(Kind=CP)	**Intent(out)**	D	

Calculate the implicit form of a Plane in 3D as   A * X + B * Y + C * Z + D = 0

CFML_Math_3D: Subroutines

Subroutine Get_Spheric_Coord (X0, Ss, Theta, Phi, Mode)

Real(Kind=SP / DP), Dimension(3)	**Intent(in)**	X0	
Real(Kind=SP / DP)	**Intent(in)**	Ss	
Real(Kind=SP / DP)	**Intent(in)**	Theta	
Real(Kind=SP / DP)	**Intent(out)**	Phi	
Character (Len=*), Optional	**Intent(in)**	Mode	

Determine the spheric coordinates from rectangular coordinates. If Mode='D' the angles will be done in Degrees.

CFML_Math_3D: Subroutines

Subroutine Init_Err_Math3D ( )

Subroutine that initializes errors flags in **CFML_Math_3D** module.

CFML_Math_3D: Subroutines

Subroutine Matrix_DiagEigen(A, V, C)

Real(Kind=CP), Dimension(3,3)	**Intent(in)**	A	
Real(Kind=CP), Dimension(3)	**Intent(out)**	V	
Real(Kind=CP), Dimension(3,3)	**Intent(out)**	C	

Diagonalize the matrix **A**, put eigenvalues in **V** and eigenvectors in **C**

CFML_Math_3D: Subroutines

Subroutine Matrix_Inverse(A, B, Ifail)

Real(Kind=CP), Dimension(3,3)	**Intent(in)**	A	input array
Real(Kind=CP), Dimension(3,3)	**Intent(out)**	B	inverse of input array **B=A**$^{-1}$
Integer	**Intent(out)**	Ifail	0: OK 1: Fail

Inverts a 3x3 Matrix

CFML_Math_3D: Subroutines

Subroutine Resolv_Sist_1x2(W, T, TS, X, IX)

Integer, Dimension(2)	**Intent(in)**	W	input vector
Real(Kind=CP)	**Intent(in)**	T	input value
Real(Kind=CP), Dimension(2)	**Intent(out)**	TS	Fixed value of solution
Real(Kind=CP), Dimension(2)	**Intent(out)**	X	Fixed value for x_1 and x_2
Integer, Dimension(2)	**Intent(out)**	IX	1:X 2:Y 3:Z

Resolve the system though the solutions be undetermined

$$W_{11}\, X_1 + W_{12}\, X_2 = T$$

and the solution is

$$X_{sol}(i)=TS(i) + X(i)\ IX(i)$$

CFML_Math_3D: Subroutines

Subroutine Resolv_Sist_1x3(W, T, TS, X, IX)

Integer, Dimension(3)	**Intent(in)**	W	input vector
Real(Kind=CP)	**Intent(in)**	T	input value
Real(Kind=CP), Dimension(3)	**Intent(out)**	TS	Fixed value of solution
Real(Kind=CP), Dimension(3)	**Intent(out)**	X	Fixed value for x_1 ,x_2 and x_3
Integer, Dimension(3)	**Intent(out)**	IX	1:X 2:Y 3:Z

Resolve the system though the solutions be undetermined

$$W_{11}\, X_1 + W_{12}\, X_2 + W_{13}\, X_3 = T$$

and the solution is

$$X_{sol}(i)=TS(i) + X(i)\ IX(i)$$

CFML_Math_3D: Subroutines

Subroutine Resolv_Sist_2x2(W, T, TS, X, IX)

Integer, Dimension(2,2)	**Intent(in)**	W	input vector
Real(Kind=CP), Dimension(2)	**Intent(in)**	T	input value
Real(Kind=CP), Dimension(2)	**Intent(out)**	TS	Fixed value of solution
Real(Kind=CP), Dimension(2)	**Intent(out)**	X	Fixed value for x_1 and x_2
Integer, Dimension(2)	**Intent(out)**	IX	1:X 2:Y 3:Z

Resolve the system though the solutions be undetermined

$W_{11} X_1 + W_{12} X_2 = T_1$

$W_{21} X_1 + W_{22} X_2 = T_2$

and the solution is

$X_{sol}(i)=TS(i) + X(i)\ IX(i)$

CFML_Math_3D: Subroutines

Subroutine Resolv_Sist_2x3(W, T, TS, X, IX)

Integer, Dimension(2,3)	**Intent(in)**	W	input vector
Real(Kind=CP), Dimension(2)	**Intent(in)**	T	input value
Real(Kind=CP), Dimension(3)	**Intent(out)**	TS	Fixed value of solution
Real(Kind=CP), Dimension(3)	**Intent(out)**	X	Fixed value for x_1 ,x_2 and x_3
Integer, Dimension(3)	**Intent(out)**	IX	1:X 2:Y 3:Z

Resolve the system though the solutions be undetermined

$W_{11} X_1 + W_{12} X_2 + W_{13} X_3= T_1$

$W_{21} X_1 + W_{22} X_2 + W_{23} X_3= T_2$

and the solution is

$X_{sol}(i)=TS(i) + X(i)\ IX(i)$

CFML_Math_3D: Subroutines

Subroutine Resolv_Sist_3x3(W, T, TS, X, IX)

Integer, Dimension(3,3)	**Intent(in)**	W	input vector
Real(Kind=CP), Dimension(3)	**Intent(in)**	T	input value
Real(Kind=CP), Dimension(3)	**Intent(out)**	TS	Fixed value of solution
Real(Kind=CP), Dimension(3)	**Intent(out)**	X	Fixed value for x_1 ,x_2 and x_3
Integer, Dimension(3)	**Intent(out)**	IX	1:X 2:Y 3:Z

Resolve the system though the solutions be undetermined

$W_{11} X_1 + W_{12} X_2 + W_{13} X_3= T_1$

$W_{21} X_1 + W_{22} X_2 + W_{23} X_3= T_2$

$W_{31} X_1 + W_{32} X_2 + W_{33} X_3= T_3$

and the solution is

$X_{sol}(i)=TS(i) + X(i)\ IX(i)$

CFML_Math_3D: Subroutines

Subroutine Set_Eps (NewEps)

Real(Kind=CP)	**Intent(in)**	NewEps	

Sets an internal **Eps** variable on **CFML_MATH_3D** module to the value **NewEps**

CFML_Math_3D: Subroutines

Subroutine Set_Eps_Default ( )

Sets the internal **Eps** variable to the default value

Default: 10^{-5}

CFML_Optimization_General

Module containing several algorithms for global and local optimization.

Variables

Opt_Conditions_Type

Err_Optim
Err_Optim_Mess

Subroutines

CG_Quasi_Newton
CSendes_Global
Init_Err_Optim
Init_Opt_Conditions
Local_Min_DFP
Local_Min_Rand
Local_Optimize
Nelder_Mead_Simplex
Set_OptT_Conditions
Write_Optimization_Conditions

Fortran Filename

CFML_Optimization.f90

CFML_Optimization_General: Variables

Opt_Conditions_Type

Err_Optim
Err_Optim_Mess

CFML_Optimization_General: Variables

	Variable	*Definition*
Type :: Opt_Conditions_Type		
Character(Len=20)	Method	String describing the Method
Integer	NMeth	Type of method used
Integer	NPar	Number of free parameters
Integer	MXFun	Maximum number function calls
Integer	IOut	Printing parameter
Integer	Loops	Useful for SIMPLEX method
Integer	IQuad	Useful for SIMPLEX method. If iquad/= 0 fitting to a quadratic
Integer	NFlag	Flag value states which condition caused the exit of the optimization subroutine
Integer	IFun	Total number of function and gradient evaluations
Integer	Iter	Total number of search directions used in the algorithm
Real(Kind=CP)	Eps	Convergence parameter
Real(Kind=CP)	Acc	User supplied estimate of machine accuracy
End Type Opt_Conditions_Type		

Values for **Method** are:

Value	*Description*
Conjugate_Gradient	
BFGS_Quasi_Newton	
Simplex	
DFP_NO_Derivatives	
Global_CSendes	
Local_Random	
UniRandi	

Values for **NMeth** are:

Value	*Description*
0	Conjugate Gradient
1	BFGS method

Values for **IOut** are:

Value	*Description*
0	No printing for Quasi_Newton & Conjugate Gradient Partial printing for Simplex (<0 no printing)
>0	Printing each iout iterations/evaluations

Values for **NFlag** are:

Value	*Description*
0	The algorithm has converged
1	The maximum number of function evaluations have been used
2	The linear search has failed to improve the function value. This is the usual exit if either the function or the gradient is incorrectly coded.
3	The search vector was not a descent direction. This can only be caused by round off, and may suggest that the convergence criterion is too strict.

Values for **Eps** are:

Value	***Description***
10^{-6}	Convergence occurs when the norm of the gradient is less than or equal to EPS times the maximum of one and the norm of the vector X.

Values for **Acc** are:

Value	***Description***
10^{-20}	is a user supplied estimate of machine accuracy. A linear search is unsuccessfully terminated when the norm of the step size becomes smaller than ACC. in practice, ACC=10^{-20} has proved satisfactory. This is the default value.
10^{-6}	For Simplex method the meaning is different (see EPS parameter) and this should be changed to 10^{-6}

This Type has been introduced to simplify the call to optimization procedures. It contains the optimization parameters useful for different algorithms. All Integer components are initialized to zero and the real components are initilized as indicated below.

A variable of this type should be defined by the user and all their input parameters (in) must be provided before calling the procedures. On output from the procedure the (out) items are provided for checking.

CFML_Optimization_General: Variables

Logical :: Err_Optim

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module

CFML_Optimization_General: Variables

Character (Len=150) :: Err_Optim_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Optimization_General: Subroutines

- CG_Quasi_Newton
- CSendes_Global
- Init_Err_Optim
- Init_Opt_Conditions
- Local_Min_DFP
- Local_Min_Rand
- Local_Optimize
- Nelder_Mead_Simplex
- Set_OptT_Conditions
- Write_Optimization_Conditions

CFML_Optimization_General: Subroutines

Subroutine CG_Quasi_Newton (Model_ Funct, N, X, F, G, C, Ipr)

Defined Subroutine Model_Funct		Model_Funct		
Integer	**Intent(in)**	N		The number of variables in the function to be minimized.

Real(Kind=CP), Dimension (N)	**Intent(in out)**	X	in: out:	Must contain an initial estimate supplied by the user X will hold the best estimate to the minimizer obtained
Real(Kind=CP)	**Intent(out)**	F		Contain the lowest value of the object function obtained
Real(Kind=CP), Dimension (N)	**Intent(out)**	G		G =(g(1),...g(n)) will contain the elements of the gradient of F evaluated at the point contained in X=(x(1),...x(N))
Type(Opt_Conditions_Type)	**Intent(in out)**	C		Conditions for the algorithm
Integer, Optional	**Intent(in)**	Ipr		Logical unit for printing if the parameter C%Iout /= 0.

where

Subroutine Model_Funct (N, X, F, G)

Integer	**Intent(in)**	N	Number of free parameters
Real(Kind=CP), Dimension (:)	**Intent(in)**	X	Variables
Real(Kind=CP)	**Intent(out)**	F	Value of Model
Real(Kind=CP), Dimension (:)	**Intent(out)**	G	Gradiente of F

End Subroutine Model_Funct

CG_Quasi_Newton minimizes an unconstrained nonlinear scalar valued function of a vector variable X either by the BFGS variable metric algorithm
or by a beale restarted conjugate gradient algorithm.

(BFGS: Broyden, Fletcher, Goldfarb and Shanno. ACM TRANSACTIONS ON MATHEMATICAL SOFTWARE 6 (DECEMBER 1980), 618-622).

CFML_Optimization_General: Subroutines

Subroutine CSendes_Global(Model_Funct, Mini, Maxi, NParm, NSampl, NSel, NSig, X0, NC, F0, Ipr, Mode)

Defined Subroutine Model_Funct		Model_Funct		Dummy name of the objective function to be optimized
Real(Kind=CP), Dimension (:)	**Intent(in)**	Mini		Vector of length NPARM containing the lower bounds
Real(Kind=CP), Dimension (:)	**Intent(in)**	Maxi	in: out:	Vector of length NPARM containing the upper bounds
Integer	**Intent(in)**	NParm		Number of Parameters
Integer	**Intent(in out)**	NSampl		Number of sample points to be drawn uniformly in one cycle. Suggested value is 100*NPARM
Integer	**Intent(in out)**	NSel		Number of best points selected from the actual sample. The suggested value is twice the expected number of local minima.
Integer	**Intent(in)**	NSig		The accuracy required in the parameter estimates. This convergence criterion is satisfied if on two successive iterations the parameter estimates agree, component by component, to nsig digits. The suggested value is 6.
Real(Kind=CP), Dimension (:,:)	**Intent(in out)**	X0		output matrix (NPARM x NC) containing NC local minimizers found
Integer	**Intent(out)**	NC		Number of different Local Minimizers Found
Real(Kind=CP), Dimension (:)	**Intent(in out)**	F0		output vector of NC objective function values. F0(I) Belongs to the parameters X0(1,I), X0(2,I), ..., X0(NPARM,I)

Integer	**Intent(in)**	Ipr		Printing information
Integer, Optional	**Intent(in)**	Mode		If present the routine LOCAL_Min_DFP is replaced by LOCAL_Min_RAND

where

Subroutine Model_Funct (NParm, X, F)

Integer	Intent(in)	NParm	Number of free parameters
Real(Kind=CP), Dimension (:)	Intent(in)	X	Variables
Real(Kind=CP)	Intent(out)	F	Value of Model

End Subroutine Model_Funct

Global optimization procedure using the Boender-Timmer-Rinnoy Kan algorithm (Local Search Method)

Global optimization is a part of nonlinear optimization, it deals with problems with (possibly) several local minima. The presented method is stochastic (i.e. not deterministic). The framework procedure, the CSendes_Global routine gives a computational evidence, that the best local minimum found is with high probability the global minimum. This routine calls a local search routine, and a routine for generating random numbers.

Let F(X) be a real function of NParm parameters and we are looking for parameter values X(I) from the given intervals [Min(I), MAX(I)] for each I = 1, 2, ..., NPARM. The problem is to determine such a point X*, that the function value F(X) is greater than or equal to F(X*) for every X in the NPARM-dimensional interval specified by Min(I)'s and MAX(I)'s.

CFML_Optimization_General: Subroutines

Subroutine Init_Err_Optim ( )

Subroutine that initializes errors flags in **CFML_Optimization_General** module.

CFML_Optimization_General: Subroutines

Subroutine Init_Opt_Conditions (Opt)

Type(Opt_Conditions_Type)	**Intent(out)**	OPT	Opt Conditions

Initialize the variable **OPT**. Default values are:

Parameter	***Value***
METHOD	SIMPLEX
NMETH	0
NPAR	0
MXFUN	1000
Iout	2000
LOOPS	1
IQUAD	0
NFLAG	0
IFUN	0
ITER	0
EPS	10^{-6}
ACC	10^{-20}

CFML_Optimization_General: Subroutines

Subroutine Local_Min_DFP(Model_Funct, N, X, F, C, Mini, Maxi, Ipr)

Defined Subroutine Model_Funct		Model_Funct		
Integer	**Intent(in)**	N		The number of variables in the function to be minimized.
Real(Kind=CP), Dimension (:)	**Intent(in out)**	X	in: out:	Must contain an initial estimate supplied by the user The Final Parameter Estimates As Determined By Local
Real(Kind=CP)	**Intent(out)**	F		The value of the Function at the final parameter estimates
Type(Opt_Conditions_Type)	**Intent(in out)**	C		Conditions for the algorithm
Real(Kind=CP), Dimension (:)	**Intent(in)**	Mini		Lower bounds of the parameters
Real(Kind=CP), Dimension (:)	**Intent(in)**	Maxi		Upper bounds of the parameters
Integer, Optional	**Intent(in)**	Ipr		Logical unit for printing if the parameter C%Iout /= 0.

Subroutine Model_Funct (N, X, F)

Integer	**Intent(in)**	N	Number of free parameters
Real(Kind=CP), Dimension (:)	**Intent(in)**	X	Variables
Real(Kind=CP)	**Intent(out)**	F	Value of Model

End Subroutine Model_Funct

Provides the minimum of a function of N variables using a Quasic-Newton Method. If there is no stable minimum in the given region the algorithm may fail.

The important parameters for the algorithm are stored in the C-variable on input the components C%Eps and C%MxFun are needed (a call to Init_Opt_Conditions is enough to provide sensible values). On output the component C%ifun is updated.

Subroutine Local_Min_Rand (Model_Funct, N, X, F, C, Mini, Maxi)

Defined Subroutine Model_Funct		Model_Funct		
Integer	**Intent(in)**	N		The number of variables in the function to be minimized.
Real(Kind=CP), Dimension (:)	**Intent(in out)**	X	in: out:	Must contain an initial estimate supplied by the user The Final Parameter Estimates As Determined By Local
Real(Kind=CP)	**Intent(out)**	F		The value of the Function at the final parameter estimates
Type(Opt_Conditions_Type)	**Intent(in out)**	C		Conditions for the algorithm
Real(Kind=CP), Dimension (:), Optional	**Intent(in)**	Mini		Lower bounds of the parameters
Real(Kind=CP), Dimension (:), Optional	**Intent(in)**	Maxi		Upper bounds of the parameters

Subroutine Model_Funct (N, X, F)

Integer	**Intent(in)**	N	Number of free parameters
Real(Kind=CP), Dimension (:)	**Intent(in)**	X	Variables

Real(Kind=CP)	Intent(out)	F	Value of Model

End Subroutine Model_Funct

Subroutine Local_Optimize (Model_Funct, X, F, C, G, Mini, Maxi, V, Ipr)

Defined Subroutine Model_Funct		Model_Funct		
Real(Kind=CP), Dimension (:)	Intent(in out)	X	in: out:	Must contain an initial estimate supplied by the user X will hold the best estimate to the minimizer obtained
Real(Kind=CP)	Intent(out)	F		Contain the lowest value of the object function obtained
Type(Opt_Conditions_Type)	Intent(in out)	C		Conditions for the algorithm
Real(Kind=CP), Dimension (:), Optional	Intent(in out)	G		G =(g(1),...g(n)) will contain the elements of the gradient of F evaluated at the point contained in X=(x(1),...x(N)) For **SIMPLEX** it contains the step values
Real(Kind=CP), Dimension (:), Optional	Intent(in out)	Mini		Lower range
Real(Kind=CP), Dimension (:), Optional	Intent(in out)	Maxi		Upper range
Real(Kind=CP), Dimension (:), Optional	Intent(out)	V		For **SIMPLEX** it contains the sigma of parameters
Integer, Optional	Intent(in)	Ipr		Logical unit for printing if the parameter C%Iout /= 0.

Subroutine Model_Funct (N, X, F, G)

Integer	Intent(in)	N	Number of free parameters
Real(Kind=CP), Dimension (:)	Intent(in)	X	Variables
Real(Kind=CP)	Intent(out)	F	Value of Model
Real(Kind=CP), Dimension (:), Optional	Intent(out)	G	Gradiente of F

End Subroutine Model_Funct

Wraper for selection an optimization method of the function Model_Funct.

The list of free parameters are provided in the vector X (in out), the value of the function F, and eventually the gradient G, are output variables. The optimization conditions in the variable C should be provided for selecting the optimization algorithm

Subroutine Nelder_Mead_Simplerx (Model_Funct, Nop, P, Step, Var, Func, C, Ipr)

Defined Subroutine Model_Funct		Model_Funct		
Integer	Intent(in)	Nop		The number of variables in the function to be minimized.
Real(Kind=CP), Dimension (:)	Intent(in out)	P	in: out:	starting values of parameters final values of parameters
Real(Kind=CP), Dimension (:)	Intent(in out)	Step	in: out:	initial step sizes final step sizes
Real(Kind=CP), Dimension	Intent(out)	Var		Contains the diagonal elements of the inverse of the

(:)				information matrix
Real(Kind=CP)	**Intent(out)**	Func		The function value corresponding to the final parameter values.
Type(Opt_Conditions_Type)	**Intent(in out)**	C		Conditions for the algorithm
Integer, Optional	**Intent(in)**	Ipr		Logical unit for printing if the parameter C%Iout /= 0.

Subroutine Model_Funct (N, X, F, G)

Integer	**Intent(in)**	N	Number of free parameters
Real(Kind=CP), Dimension (:)	**Intent(in)**	X	Variables
Real(Kind=CP)	**Intent(out)**	F	Value of Model
Real(Kind=CP), Dimension (:), Optional	**Intent(out)**	G	Gradiente of F

End Subroutine Model_Funct

Procedure for function minimization using the SIMPLEX method.

Optimization Conditions type with the following components:

Parameter	***Description***
C%MxFun	The maximum number of function evaluations allowed. Say, 20 times the number of parameters
C%IOut	< 0 No printing = 0 Printing of parameter values and the function value after initial evidence of convergence > 0 As for C%Iout = 0 plus progress reports after every C%Iout evaluations, plus printing for the initial simplex
C%Eps	Stopping criterion. The criterion is applied to the standard deviation of the values of FUNC at the points of the simplex
C%Loops	The stopping rule is applied after every NLOOP function evaluations. Normally NLOOP should be slightly greater than NOP, say NLOOP = 2*NOP.
C%IQuad	= 1 If fitting of a quadratic surface is required = 0 If not The fitting of a quadratic surface is strongly recommended, provided that the fitted function is continuous in the vicinity of the minimum. It is often a good indicator of whether a premature termination of the search has occurred.
C%Acc	criterion for expanding the simplex to overcome rounding errors before fitting the quadratic surface. The simplex is expanded so that the function values at the points of the simplex exceed those at the supposed minimum by at least an amount SIMP
IC%NFlag	= 0 for successful termination = 1 If maximum no. of function evaluations exceeded = 2 If information matrix is not +ve semi-definite = 3 if NOP < 1 = 4 if C%LOOPS < 1

Other considerations:

P, **Step** and **Var** (If C%Iquad = 1) must have dimension at least **Nop** in the calling program.

For details, see Nelder & Mead, The Computer JournaL, January 1965. Programmed by D.E.Shaw, CSIRO, Division of Mathematics & Statistics P.O. BOX 218, Lindfield, N.S.W. 2070

CFML_Optimization_General: Subroutines

Subroutine Set_Opt_Conditions (N, File_Lines, Opt)

Integer	**Intent(in)**	N	Logical unit for writing
Character(Len=*), Dimension(:)	**Intent(in)**	File_Lines	info

Type(Opt_Conditions_Type)	**Intent(out)**	Opt	Variable

Get the optimization conditions from a list of text lines obtained from the input file

CFML_Optimization_General: Subroutines

Subroutine Write_Optimization_Conditions (Ipr, C)

Integer	**Intent(in)**	Ipr	Logical unit for writing
Type(Opt_Conditions_Type)	**Intent(in)**	C	Opt Conditions

Subroutine for writing in unit **Ipr** the Opt_Conditions_Type variable **C**

CFML_Optimization_LSQ

Module implementing several algorithms for non-linear least-squares. At present only the Levenberg-Marquardt method is implemented.

There are two high level procedures contained in CFML_Optimization_LSQ based in the Levenberg-Marquardt method. The first procedure,
called Marquardt_Fit, is a simple implementation of the method and the second one is a Fortran 90 version of the MINPACK Fortran 77
LMXXX subroutines, accessible through the general name Levenberg_Marquardt_Fit. The second one is, in principle, more robust for
general LSQ problems.

Variables

Err_LSQ
Err_LSQ_Mess
Info_LSQ_Mess

Functions

FChiSQ

Subroutines

Info_LSQ_Output
Levenberg_Marquardt_Fit
Marquardt_Fit

Fortran Filename

CFML_Optimization.f90

CFML_Optimization_LSQ: Variables

Err_LSQ
Err_LSQ_Mess

Info_LSQ_Mess

CFML_Optimization_LSQ: Variables

Logical :: Err_LSQ

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module

CFML_Optimization_LSQ: Variables

Character (Len=150) :: Err_LSQ_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Optimization_LSQ: Variables

Character (Len=150) :: Info_LSQ_Mess

Character variable containing the information message associated to the exit parameter Info of the Levenberg_Marquardt_Fit procedure.

CFML_Optimization_LSQ: Functions

FChiSQ

CFML_Optimization_LSQ: Functions

Real Function FChiSQ (Nfr, NObs, Y, W, Yc)

Integer	**Intent(in)**	Nfr	
Integer	**Intent(in)**	NObs	
Real(Kind=CP), Dimension (:)	**Intent(in)**	Y	
Real(Kind=CP), Dimension (:)	**Intent(in)**	W	
Real(Kind=CP), Dimension (:)	**Intent(in)**	Yc	

Evaluate reduced ^{2}

CFML_Optimization_LSQ: Subroutines

Info_LSQ_Output
Levenberg_Marquardt_Fit
Marquardt_Fit

CFML_Optimization_LSQ: Subroutines

Subroutine Info_LSQ_Output (Chi2, FL, NObs, X, Y, Yc, W, Lun, C, VS, Out_Obscal)

Real(Kind=CP)	**Intent(in)**	Chi2	Final ^{2}
Real(Kind=CP)	**Intent(in)**	FL	Final Marquardt lambda
Real(Kind=CP)	**Intent(in)**	NObs	Number of data points
Real(Kind=CP), Dimension(:)	**Intent(in)**	X	Array with X of Data points
Real(Kind=CP), Dimension(:)	**Intent(in)**	Y	Array with Y of Data points
Real(Kind=CP), Dimension(:)	**Intent(in)**	Yc	Array with calculated data points

Real(Kind=CP), Dimension(:)	**Intent(in)**	W	Array with weight factors
Integer	**Intent(in)**	Lun	Logical unit for output
Type (LSQ_Conditions_Type)	**Intent(in)**	C	Conditions of the refinement
Type (LSQ_State_Vector_Type)	**Intent(in)**	VS	State vector (parameters of the model)
Character (Len=*), Optional	**Intent(in)**	Out_Obscal	If present the vectors X,Y,Yc, =sqrt(1/w) are output in a file called LM_fit.xy

Subroutine for output information at the end of refinement procedure

CFML_Optimization_LSQ: Subroutines

Subroutine Levenberg_Marquardt_Fit (Model_Funct, M, N, X, FVec, Tol, Info, Iwa)

Defined Subroutine Model_Funct		Model_Funct		Name of the subroutine
Integer	**Intent(in)**	M		Positive number of functions
Integer	**Intent(in)**	N		Positive number of variables (n <= m)
Real(Kind=CP), Dimension(:)	**Intent(in out)**	X	 in: out:	Vector of length N initial estimate of the solution vector Final estimate of the solution vector
Real(Kind=CP), Dimension(:)	**Intent(out)**	FVec		Vector of length M contains the functions evaluated at the output X.
Real(Kind=CP)	**Intent(in)**	Tol		Termination occurs when both the actual and predicted relative reductions in the sum of squares are at most TOL. Therefore, TOL measures the relative error desired in the sum of squares.
Integer	**Intent(out)**	Info	< 0 = 0 = 1 = 2 = 3 = 4 = 5 = 6 = 7	If the user has terminated execution Improper input parameters. Relative error in the sum of squares is at most TOL Algorithm estimates that the relative error between x and the solution is at most tol. Conditions for info = 1 and info = 2 both hold. FVEC is orthogonal to the columns of the jacobian to machine precision. Number of calls to fcn has reached or exceeded maxfev. Tol is too small. no further reduction in the sum of squares is possible. Tol is too small. no further improvement in the approximate solution x is possible.
Integer, Dimension(:)	**Intent(out)**	Iwa		is an Integer work array of length n

or

Subroutine Levenberg_Marquardt_Fit (Model_Funct, M, C, VS, Chi2, InfOut, Residuals)

Defined Subroutine Model_Funct		Model_Funct	Name of the subroutine calculating YC(i) for point X(i)
Integer	**Intent(in)**	M	Number of observations
Type (LSQ_Conditions_Type)	**Intent(in out)**	C	Conditions of refinement
Type (LSQ_State_Vector_Type)	**Intent(in out)**	VS	State vector for the model calculation
Real(Kind=CP)	**Intent(out)**	Chi2	Final reduced Chi-2

Character(Len=*)	**Intent(out)**	InfOut	information about the refinement
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	Residuals	Residuals vector

and

Subroutine Model_Funct (M, N, X, FVec, IFlag)

Integer	**Intent(in)**	M	Number of observations
Integer	**Intent(in)**	N	Number of Free parameters
Real(Kind=CP), Dimension (:)	**Intent(in)**	X	Array with the values of free parameters: X(1:N)
Real(Kind=CP), Dimension (:)	**Intent(in out)**	FVec	Array of residuals FVEC=(y-yc)/sig : FVEC(1:M)
Integer	**Intent(in out)**	IFlag	=1 calculate only FVEC without changing FJAC =2 calculate only FJAC keeping FVEC fixed

End Subroutine Model_Funct

or

Subroutine Levenberg_Marquardt_Fit (Model_Funct, M, N, X, FVec, FJac, Tol, Info, Iwa)

Defined Subroutine Model_Funct		Model_Funct		Name of the subroutine
Integer	**Intent(in)**	M		Positive number of functions
Integer	**Intent(in)**	N		Positive number of variables (n <= m)
Real(Kind=CP), Dimension(:)	**Intent(in out)**	X	 in: out:	Vector of length N initial estimate of the solution vector Final estimate of the solution vector
Real(Kind=CP), Dimension(:)	**Intent(out)**	FVec		Vector of length M contains the functions evaluated at the output X.
Real(Kind=CP), Dimension(:,:)	**Intent(in out)**	FJac		Is an output m by n array. the upper n by n submatrix of fjac contains an upper triangular matrix r with diagonal elements of non increasing magnitude such that $p^t*(jac^t*jac)*p = r^t*r,$ where p is a permutation matrix and jac is the final calculated Jacobian. Column j of p is column ipvt(j) (see below) of the identity matrix. The lower trapezoidal part of fjac contains information generated during the computation of r.
Real(Kind=CP)	**Intent(in)**	Tol		Termination occurs when both the actual and predicted relative reductions in the sum of squares are at most TOL. Therefore, TOL measures the relative error desired in the sum of squares.
Integer	**Intent(out)**	Info	< 0 = 0 = 1 = 2 = 3	If the user has terminated execution Improper input parameters. Relative error in the sum of squares is at most TOL Algorithm estimates that the relative error between x and the solution is at most tol.

			= 4 = 5 = 6 = 7	Conditions for info = 1 and info = 2 both hold. FVEC is orthogonal to the columns of the jacobian to machine precision. Number of calls to fcn has reached or exceeded maxfev. Tol is too small. no further reduction in the sum of squares is possible. Tol is too small. no further improvement in the approximate solution x is possible.
Integer, Dimension(:)	**Intent(out)**	Iwa		is an Integer work array of length n

or

Subroutine Levenberg_Marquardt_Fit (Model_Funct, M, C, VS, Chi2, CalDer, InfOut, Residuals)

Defined Subroutine Model_Funct		Model_Funct	Name of the subroutine calculating YC(i) for point X(i)
Integer	**Intent(in)**	M	Number of observations
Type (LSQ_Conditions_Type)	**Intent(in out)**	C	Conditions of refinement
Type (LSQ_State_Vector_Type)	**Intent(in out)**	VS	State vector for the model calculation
Real(Kind=CP)	**Intent(out)**	Chi2	Final reduced Chi-2
Logical	**Intent(in)**	CalDer	logical (should be .true.) used only for purposes of making unambiguous the generic procedure
Character(Len=*)	**Intent(out)**	InfOut	information about the refinement
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	Residuals	Residuals vector

and

Subroutine Model_Funct (M, N, X, FVec, FJac, IFlag)

Integer	**Intent(in)**	M	Number of observations
Integer	**Intent(in)**	N	Number of Free parameters
Real(Kind=CP), Dimension (:)	**Intent(in)**	X	Array with the values of free parameters: X(1:N)
Real(Kind=CP), Dimension (:)	**Intent(in out)**	FVec	Array of residuals FVEC=(y-yc)/sig : FVEC(1:M)
Real(Kind=CP), Dimension (:,:)	**Intent(out)**	FJac	Jacobian DFVEC/DX(i,j)=DFVEC(i)/DX(j): FJAC(1:m,1:n)
Integer	**Intent(in out)**	IFlag	=1 calculate only FVEC without changing FJAC =2 calculate only FJAC keeping FVEC fixed

End Subroutine Model_Funct

The purpose of this routine is to minimize the sum of the squares of M nonlinear functions in N variables by a modification of the Levenberg-Marquardt algorithm. The user must provide a subroutine which calculates the functions. The Jcobian is then calculated by a forward-difference approximation.

CFML_Optimization_LSQ: Subroutines

Subroutine Marquardt_Fit (Model_Funct, X, Y, W, Yc, NObs, C, VS, Ipr, Chi2, Scroll_Lines)

Defined Subroutine		Model_Funct	Name of the subroutine calculating Yc(i) for point X(i)

Model_Funct			
Real(Kind=CP), Dimension (:)	Intent(in)	X	Vector of x-values
Real(Kind=CP), Dimension (:)	Intent(in)	Y	Vector of observed y-values
Real(Kind=CP), Dimension (:)	Intent(in out)	W	Vector of weights-values (1/variance)
Real(Kind=CP), Dimension (:)	Intent(out)	Yc	Vector of calculated y-values
Integer	Intent(in)	NObs	Number of effective components of X, Y, W, YC
Type (LSQ_Conditions_Type)	Intent(in out)	C	Conditions for the algorithm
Type (LSQ_State_Vector_Type)	Intent(in out)	VS	State vector for the model calculation
Integer	Intent(in)	Ipr	Logical unit for writing
Real(Kind=CP)	Intent(out)	Chi2	Reduced Chi-2
Character(Len=*), Dimension(:), Optional	Intent(out)	Scroll_Lines	If present, part of the output is stored in this text for treatment in the calling program

and

Subroutine Model_Funct (Iv, Xv, Ycalc, Aa, Der)

Integer	Intent(in)	Iv	Number of the component "i"
Real(Kind=CP)	Intent(in)	Xv	Value of X(i)
Real(Kind=CP)	Intent(out)	Ycalc	Value of yc at point x(i)
Real(Kind=CP), Dimension (:)	Intent(in)	Aa	Vector of parameters
Real(Kind=CP), Dimension (:), Optional	Intent(out)	Der	Derivatives of the function w.r.t. free parameters

End Subroutine Model_Funct

or

Subroutine Marquardt_Fit (Model_Funct, D, C, VS, Ipr, Chi2, Scroll_Lines)

Defined Subroutine Model_Funct		Model_Funct	Name of the subroutine calculating YC(i) for point X(i)
Type(LSQ_Data_Type)	Intent(in out)	D	LSQ Data Type
Type (LSQ_Conditions_Type)	Intent(in out)	C	Conditions for the algorithm
Type (LSQ_State_Vector_Type)	Intent(in out)	VS	State vector for the model calculation
Integer	Intent(in)	Ipr	Logical unit for writing
Real(Kind=CP)	Intent(out)	Chi2	Reduced Chi-2
Character(Len=*), Dimension(:), Optional	Intent(out)	Scroll_Lines	If present, part of the output is stored in this text for treatment in the calling program

and

Subroutine Model_Funct (Iv, Xv, Ycalc, VSA, CalDer)

Integer	Intent(in)	Iv	Number of the component "i"
Real(Kind=CP)	Intent(in)	Xv	Value of X(i)
Real(Kind=CP)	Intent(out)	Ycalc	Value of yc at point x(i)
Type (LSQ_State_Vector_Type)	Intent(in out)	VSA	LSQ State vector type
Logical, Optional	Intent(in)	CalDer	If present, derivatives, stored in Vsa%dpv, are

calculated

End Subroutine Model_Funct

Procedure for applying the Levenberg-Marquardt method for Least-Squares.

The user must provide a model function according to the interface above. The model function should use at least some of the public variables of the present module in order to set the derivatives with respect to the model parameters.

For using this routine, the user must provide:

Parameter	***Description***
C%Icyc	Number of cycles
C%Iw	type of weighting scheme
C%Constr	constraint conditions
C%Percent	constraint conditions

Parameter	***Description***
VS%NP	number of model parameters
VS%NamPar	name for all possible parameters of the model
VS%PV	A set of flags values to refine or fix the parameters

The values of all possible refinable parameters are stored in the array VS%PV.

The derivatives must be calculated within Model_Funct, by using the array VS%Der. The actual refined parameters Aa are selected from the larger VS%PV array by the Integer array of flags: VS%Code. A value VS%CODE(j)=1 means that the j-th parameter is to be varied. A value VS%CODE(k)=0 means that the k-th parameter is kept fixed through the refinement cycles.

It is recommended that Model_Funct be stored in a Module. The Integer IV (counter of the loop for all observations for which the subroutine is invoked) is passed because in many cases part of the calculations and derivatives may be calculated only for iv=1 and stored in local variables that should have the SAVE attribute or be private module variables accessible by host association. The only output values of the subroutine are ycalc and Vsa%dpv(:) that vary for each "iv" point. In this version of the algorithm the derivatives with respect to the free parameters in Model_Funct should be calculated before exiting by using the following loop:

```
    vs%dpv=0.0                          !Should be always be initialized for each point
    if (present(calder)) then
       do i=1,vs%np
          if (vs%code(i) == 0) cycle
          vs%dpv(i) = derivative_wrt(i) !symbolic form for calculating the derivative
w.r.t. parameter "i"
       end do                           !at the current point xv (observation "iv")
    end if
```

CFML_Scattering_Chemical_Tables

Tabulated information about atomic chemical and scattering data.

Parameters

- Num_Chen_Info
- Num_Delta_Fp
- Num_Mag_Form

Num_Mag_J2
Num_Mag_J4
Num_Mag_J6
Num_Xray_Form

Variables

Anomalous_SC_Type
Chem_Info_Type
Magnetic_Form_Type
Xray_Form_Type
Xray_Wavelength_Type

Anomalous_SCFac
Chem_Info
Magnetic_Form
Magnetic_J2
Magnetic_J4
Magnetic_J6
Xray_Form
Xray_Wavelengths

Subroutines

Get_Atomic_Mass
Get_ChemSymb
Get_Covalent_Radius
Get_Fermi_Length
Get_Ionic_Radius
Remove_Chem_Info
Remove_Delta_Fp_Fpp
Remove_Magnetic_Form
Remove_Xray_Form
Set_Chem_Info
Set_Delta_Fp_Fpp
Set_Magnetic_Form
Set_Xray_Form

Fortran Filename

CFML_Chem_Scatt.f90

CFML_Scattering_Chemical_Tables: Parameters

Num_Chen_Info
Num_Delta_Fp
Num_Mag_Form

- Num_Mag_J2
- Num_Mag_J4
- Num_Mag_J6
- Num_Xray_Form

CFML_Scattering_Chemical_Tables: Parameters

Integer, Parameter :: Num_Chem_Info=108

Number of total Chem_Info Data

CFML_Scattering_Chemical_Tables: Parameters

Integer, Parameter :: Num_Delta_Fp=98

Number of total F', F'' Data defined in Anomalous_SCFac.

CFML_Scattering_Chemical_Tables: Parameters

Integer, Parameter :: Num_Mag_Form=117

Number of total Magnetic_Form Data

CFML_Scattering_Chemical_Tables: Parameters

Integer, Parameter :: Num_Mag_J2=96

Number of <j2> Magnetic_Form Data defined in Magnetic_J2

CFML_Scattering_Chemical_Tables: Parameters

Integer, Parameter :: Num_Mag_J4=96

Number of <j4> Magnetic_Form Data defined in Magnetic_J4

CFML_Scattering_Chemical_Tables: Parameters

Integer, Parameter :: Num_Mag_J6=38

Number of <j6> Magnetic_Form Data defined in Magnetic_J6

CFML_Scattering_Chemical_Tables: Parameters

Integer, Parameter :: Num_Xray_Form=214

Number of total Xray_Form Data defined in Xray_Form

CFML_Scattering_Chemical_Tables: Variables

- Anomalous_SC_Type
- Chem_Info_Type
- Magnetic_Form_Type
- Xray_Form_Type
- Xray_Wavelength_Type

- Anomalous_SCFac
- Chem_Info
- Magnetic_Form
- Magnetic_J2

CFML_Scattering_Chemical_Tables: Variables

	Variable	***Definition***
Type :: Anomalous_SC_Type		
Character(Len=2)	Symb	Symbol of the Chemical species
Real(Kind=CP), Dimension (5)	Fp	Delta Fp
Real(Kind=CP), Dimension (5)	Fpp	Delta Fpp
End Type Anomalous_SC_Type		

CFML_Scattering_Chemical_Tables: Variables

	Variable	***Definition***
Type :: Chem_Info_Type		
Character(Len=2)	Symb	Symbol of the Chemical species
Character(Len=12)	Name	Name of the Element
Integer	Z	Atomic Number
Real(Kind=CP)	Atwe	Atomic weight
Real(Kind=CP)	RConv	Covalent Radio
Real(Kind=CP)	RWaals	Van der Waals Radio
Real(Kind=CP)	VAtm	Atomic volumen
Integer, Dimension (5)	Oxid	Oxidation State
Real(Kind=CP), Dimension (5)	RIon	Ionic Radio (depending of the oxidation)
Real(Kind=CP)	SCTF	Scattering length Fermi
Real(Kind=CP)	SEDInc	incoherent Scattering Neutron cross-section (barns -> [10^{-24} cm^2])
Real(Kind=CP)	SEA	Neutron Absorption cross-section (barns, for v= 2200m/s, l(A)=3.95/v (km/s))
End Type Chem_Info_Type		

CFML_Scattering_Chemical_Tables: Variables

	Variable	***Definition***
Type :: Magnetic_Form_Type		
Character(Len=4)	Symb	Symbol of the Chemical species
Real(Kind=CP), Dimension (7)	SCTM	Scattering Factors
End Type Magnetic_Form_Type		

CFML_Scattering_Chemical_Tables: Variables

	Variable	***Definition***
Type :: Xray_Form_Type		
Character(Len=4)	Symb	Symbol of the Chemical species
Integer	Z	Atomic Number
Real(Kind=CP), Dimension (4)	A	Coefficients for calculating the X-ray scattering factors
Real(Kind=CP), Dimension (4)	B	f(s) = Sum_{i=1,4} { a(i) exp(-b(i)*s^2) } + c, where s=sin /
Real(Kind=CP)	C	
End Type Xray_Form_Type		

CFML_Scattering_Chemical_Tables: Variables

	Variable	***Definition***
Type :: Xray_Wavelength_Type		
Character(Len=2)	Symb	Symbol of the Chemical species
Real(Kind=CP), Dimension (2)	KAlfa	K-Serie for X-ray
End Type Xray_Wavelength_Type		

CFML_Scattering_Chemical_Tables: Variables

Type(Anomalous_SC_Type), Dimension(:), Allocatable :: Anomalous_SCFac

Table of   F' and   F'' for 5 common radiations according to the items specified in the definition of Anomalous_SC_Type.

The order is the following: 1=Cr, 2=Fe, 3=Cu, 4=Mo, 5=Ag

The actual dimension is defined on Num_Delta_Fp

CFML_Scattering_Chemical_Tables: Variables

Type(Chem_Info_Type), Dimension(:), Allocatable :: Chem_Info

Tabulated chemical data according to the items specified in the definition of Chem_Info_Type.

The total elements are define in Num_Chem_Info

CFML_Scattering_Chemical_Tables: Variables

Type(Magnetic_Form_Type), Dimension(:), Allocatable :: Magnetic_Form

Tabulated magnetic form factor data according to the items specified in the definition of Magnetic_Form_Type.

The number of total elements is defined in Num_Mag_Form

CFML_Scattering_Chemical_Tables: Variables

Type(Magnetic_Form_Type), Dimension(:), Allocatable :: MAGNETIC_J2

Tabulated magnetic form factor J2 data according to the items specified in the definition of Magnetic_Form_Type.

The number of total elements is defined in Num_Mag_J2

CFML_Scattering_Chemical_Tables: Variables

Type(Magnetic_Form_Type), Dimension(:), Allocatable :: MAGNETIC_J4

Tabulated magnetic form factor J4 data according to the items specified in the definition of Magnetic_Form_Type.

The number of total elements is defined in Num_Mag_J4

CFML_Scattering_Chemical_Tables: Variables

Type(Magnetic_Form_Type), Dimension(:), Allocatable :: MAGNETIC_J6

Tabulated magnetic form factor J6 data according to the items specified in the definition of Magnetic_Form_Type.

The number of total elements is defined in Num_Mag_J6

CFML_Scattering_Chemical_Tables: Variables

Type(Xray_Form_Type), Dimension(:), Allocatable :: Xray_Form

Tabulated Xray scattering factor coefficientsaccording to the items specified in the definition of Xray_Form_Type.

The number of total elements is defined in Num_Xray_Form.

CFML_Scattering_Chemical_Tables: Variables

Type(Xray_Wavelength_Type), Dimension(7) :: Xray_Wavelengths

Tabulated K-Series for Xray according to the items specified in the definition of Xray_Wavelength_Type

Symbol	**K_{1}**	**K_{2}**
Cr	2.28988	2.29428
Fe	1.93631	1.94043
Cu	1.54059	1.54431
Mo	0.70932	0.71360
Ag	0.55942	0.56380
Co	1.78919	1.79321
Ni	1.65805	1.66199

CFML_Scattering_Chemical_Tables: Subroutines

- Get_Atomic_Mass
- Get_ChemSymb
- Get_Covalent_Radius
- Get_Fermi_Length

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Get_Atomic_Mass (Atm, Mass)

Character(Len=2)	**Intent(in)**	Atm	Chemical symbol
Real(Kind=CP)	**Intent(out)**	Mass	Atomic mass

Provides the atomic mass given the chemical symbol of the element. in case of problems the returned mass is 0.0

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Get_ChemSymb (Label, ChemSymb, Z)

Character(Len=*)	**Intent(in)**	Label	Atom label
Character(Len=*)	**Intent(out)**	ChemSymb	Chemical Symbol
Integer, Optional	**Intent(out)**	Z	Atomic number

Subroutine to get the chemical symbol from label and optionally the atomic number

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Get_Covalent_Radius (Nam, Rad)

Character(Len=*)	**Intent(in)**	Nam	Chemical Symbol
Real(Kind=CP)	**Intent(out)**	Rad	Covalent radius

Provides the covalent radius given the chemical symbol of the element. in case of problems the returned radius is 1.4 angstroms.

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Get_Fermi_Length (Nam, B)

Character(Len=*)	**Intent(in)**	Nam	Chemical Symbol
Real(Kind=CP)	**Intent(out)**	B	Fermi length

Provides the Fermi length (in 10^{-12} cm) given the chemical symbol of the element. in case of problems the returned Fermi length is 0.0

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Get_Ionic_Radius (Nam, Valence, Rad)

Character(Len=*)	**Intent(in)**	Nam	Chemical symbol
Integer	**Intent(in)**	Valence	Valence value
Real(Kind=CP)	**Intent(out)**	Rad	Ionic radius

Provides the ionic radius given the chemical symbol of the element and the valence as an Integer. in case of problems the returned radius is 0.0

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Remove_Chem_Info ( )

Deallocate Chem_Info variable

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Remove_Delta_Fp_Fpp ( )

Deallocate Anomalous_SCFac variable

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Remove_Magnetic_Form ( )

Deallocate Magnetic_Form variable

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Remove_Xray_Form ( )

Deallocate Xray_Form variable

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Set_Chem_Info ( )

Allocates and loads the Chem_Info variable according to Chem_Info_Type

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Set_Delta_Fp_Fpp ( )

Allocates and loads the Anomalous_SCFac variable according to Anomalous_SC_Type

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Set_Magnetic_Form ( )

Allocates and loads the Magnetic_Form variable according to Magnetic_Form_Type

CFML_Scattering_Chemical_Tables: Subroutines

Subroutine Set_Xray_Form ( )

Allocates and loads the Xray_Form variable according to Xray_Form_Type

CFML_Symmetry_Tables

Tabulated information on Crystallographic Symmetry

Parameters

- BC_D6H
- BC_OH
- DepMat
- IntSymD6H
- IntSymOH
- Kov_D6H
- Kov_OH
- Latt
- Laue_Class
- Ltr_A
- Ltr_B
- Ltr_C
- Ltr_F
- Ltr_I
- Ltr_R
- MagMat
- ML_D6H
- ML_OH
- Mod6
- Point_Group
- Sys_Cry
- X_D6H
- X_OH
- Zak_D6H
- Zak_OH

Variables

- Spgr_Info_Type
- Table_Equiv_Type
- Wyck_Info_Type

- Err_SymTab
- Err_SymTab_Mess
- Spgr_Info
- System_Equiv
- Wyckoff_Info

Subroutines

- Get_Generators
- Remove_Spgr_Info
- Remove_System_Equiv
- Remove_Wyckoff_Info
- Set_Spgr_Info

Set_System_Equiv
Set_Wyckoff_Info

Fortran Filename

CFML_Sym_Table.f90

CFML_Symmetry_Tables: Parameters

- BC_D6H
- BC_OH
- DepMat
- IntSymD6H
- IntSymOH
- Kov_D6H
- Kov_OH
- Latt
- Laue_Class
- Ltr_A
- Ltr_B
- Ltr_C
- Ltr_F
- Ltr_I
- Ltr_R
- MagMat
- ML_D6H
- ML_OH
- Mod6
- Point_Group
- Sys_Cry
- X_D6H
- X_OH
- Zak_D6H
- Zak_OH

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(24), Parameter :: BC_D6H

Bradley & Cracknell Notation for Point Group elements of 6/mmm (D6h)

Order	*Value*	*Order*	*Value*
1	E	**13**	I
2	C+_3	**14**	S-_6
3	C-_3	**15**	S+_6
4	C_2	**16**	s_h
5	C-_6	**17**	S+_3
6	C+_6	**18**	S-_3
7	C'_23	**19**	s_v3

8	C'_21	**20**	s_v1
9	C'_22	**21**	s_v2
10	C`_23	**22**	s_d3
11	C`_21	**23**	s_d1
12	C`_22	**24**	s_d2

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(48), Parameter :: BC_OH

Bradley & Cracknell Notation for Point Group elements of m3m (Oh)

Order	*Value*	*Order*	*Value*	*Order*	*Value*	*Order*	*Value*
1	E	**13**	C_2a	**25**	I	**37**	s_da
2	C_2z	**14**	C_2b	**26**	s_z	**38**	s_db
3	C_2y	**15**	C-_4z	**27**	s_y	**39**	S+_4z
4	C_2x	**16**	C+_4z	**28**	s_x	**40**	S-_4z
5	C+_31	**17**	C-_4x	**29**	S-_61	**41**	S+_4x
6	C+_34	**18**	C_2d	**30**	S-_64	**42**	s_dd
7	C+_33	**19**	C_2f	**31**	S-_63	**43**	d_df
8	C+_32	**20**	C+_4x	**32**	S-_62	**44**	S-_4x
9	C-_31	**21**	C+_4y	**33**	S+_61	**45**	S-_4y
10	C-_33	**22**	C_2c	**34**	S+_63	**46**	s_dc
11	C-_32	**23**	C-_4y	**35**	S+_62	**47**	S+_4y
12	C-_34	**24**	C_2e	**36**	S+_64	**48**	s_de

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(72), Parameter :: DepMat

Magnetic array

Order	*Value*	*Order*	*Value*	*Order*	*Value*
1	(Dx, Dy, Dz)	**25**	(-Dx,-Dy,-Dz)	**49**	(Dx , Dy, Dz)
2	(-Dx,-Dy, Dz)	**26**	(Dx, Dy,-Dz)	**50**	(-Dy, Dx-Dy , Dz)
3	(-Dx, Dy,-Dz)	**27**	(Dx,-Dy, Dz)	**51**	(-Dx+Dy,-Dx , Dz)
4	(Dx,-Dy,-Dz)	**28**	(-Dx, Dy, Dz)	**52**	(-Dx , -Dy, Dz)
5	(Dz, Dx, Dy)	**29**	(-Dz,-Dx,-Dy)	**53**	(Dy,-Dx+Dy, Dz)
6	(Dz,-Dx,-Dy)	**30**	(-Dz, Dx, Dy)	**54**	(Dx-Dy, Dx , Dz)
7	(-Dz,-Dx, Dy)	**31**	(Dz, Dx,-Dy)	**55**	(Dy, Dx ,-Dz)
8	(-Dz, Dx,-Dy)	**32**	(Dz,-Dx, Dy)	**56**	(Dx-Dy, -Dy,-Dz)
9	(Dy, Dz, Dx)	**33**	(-Dy,-Dz,-Dx)	**57**	(-Dx ,-Dx+Dy,-Dz)
10	(-Dy, Dz,-Dx)	**34**	(Dy,-Dz, Dx)	**58**	(-Dy,-Dx ,-Dz)
11	(Dy,-Dz,-Dx)	**35**	(-Dy, Dz, Dx)	**59**	(-Dx+Dy, Dy,-Dz)
12	(-Dy,-Dz, Dx)	**36**	(Dy, Dz,-Dx)	**60**	(Dx , Dx-Dy,-Dz)
13	(Dy, Dx,-Dz)	**37**	(-Dy,-Dx, Dz)	**61**	(-Dx , -Dy,-Dz)
14	(-Dy,-Dx,-Dz)	**38**	(Dy, Dx, Dz)	**62**	(Dy,-Dx+Dy,-Dz)
15	(Dy,-Dx, Dz)	**39**	(-Dy, Dx,-Dz)	**63**	(Dx-Dy,Dx ,-Dz)
16	(-Dy, Dx, Dz)	**40**	(Dy,-Dx,-Dz)	**64**	(Dx , Dy,-Dz)
17	(Dx, Dz,-Dy)	**41**	(-Dx,-Dz, Dy)	**65**	(-Dy, Dx-Dy,-Dz)
18	(-Dx, Dz, Dy)	**42**	(Dx,-Dz,-Dy)	**66**	(-Dx+Dy,-Dx ,-Dz)
19	(-Dx,-Dz,-Dy)	**43**	(Dx, Dz, Dy)	**67**	(-Dy,-Dx , Dz)

20	(Dx,-Dz, Dy)	**44**	(-Dx, Dz,-Dy)	**68**	(-Dx+Dy, Dy, Dz)
21	(Dz, Dy,-Dx)	**45**	(-Dz,-Dy, Dx)	**69**	(Dx , Dx-Dy, Dz)
22	(Dz,-Dy, Dx)	**46**	(-Dz, Dy,-Dx)	**70**	(Dy, Dx , Dz)
23	(-Dz, Dy, Dx)	**47**	(Dz,-Dy,-Dx)	**71**	(Dx-Dy, -Dy, Dz)
24	(-Dz,-Dy,-Dx)	**48**	(Dz, Dy, Dx)	**72**	(-Dx ,-Dx+Dy, Dz)

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(24), Parameter :: IntSymD6H

international Symbols for Point Group elements of 6/mmm (D6h)

Order	*Value*	*Order*	*Value*
1	1	**13**	-1
2	3+ (0, 0, z)	**14**	-3+ (0, 0, z)
3	3- (0, 0, z)	**15**	-3- (0, 0, z)
4	2 (0, 0, z)	**16**	m (x, y, 0)
5	6- (0, 0, z)	**17**	-6- (0, 0, z)
6	6+ (0, 0, z)	**18**	-6+ (0, 0, z)
7	2 (x, x, 0)	**19**	m (x,-x, z)
8	2 (x, 0, 0)	**20**	m (x,2x, z
9	2 (0, y, 0)	**21**	m (2x, x, z)
10	2 (x,-x, 0)	**22**	m (x, x, z)
11	2 (x,2x, 0)	**23**	m (x, 0, z)
12	2 (2x, x, 0)	**24**	m (0, y, z)

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(48), Parameter :: IntSymOH

international Symbols for Point Group elements of m3m (Oh)

Order	*Value*	*Order*	*Value*	*Order*	*Value*	*Order*	*Value*
1	1	**13**	2 (x, x, 0)	**25**	-1	**37**	m (x,-x, z)
2	2 (0, 0, z)	**14**	2 (x,-x, 0)	**26**	m (x, y, 0)	**38**	m (x, x, z)
3	2 (0, y, 0)	**15**	4- (0, 0, z)	**27**	m (x, 0, z)	**39**	-4- (0, 0, z)
4	2 (x, 0, 0)	**16**	4+ (0, 0, z)	**28**	m (0, y, z)	**40**	-4+ (0, 0, z)
5	3+ (x, x, x)	**17**	4- (x, 0, 0)	**29**	-3+ (x, x, x)	**41**	-4- (x, 0, 0)
6	3+ (-x, x,-x)	**18**	2 (0, y, y)	**30**	-3+ (-x, x,-x)	**42**	m (x, y,-y)
7	3+ (x,-x,-x)	**19**	2 (0, y,-y)	**31**	-3+ (x,-x,-x)	**43**	m (x, y, y)
8	3+ (-x,-x, x)	**20**	4+ (x, 0, 0)	**32**	-3+ (-x,-x, x)	**44**	-4+ (x, 0, 0)
9	3- (x, x, x)	**21**	4+ (0, y, 0)	**33**	-3- (x, x, x)	**45**	-4+ (0, y, 0)
10	3- (x,-x,-x)	**22**	2 (x, 0, x)	**34**	-3- (x,-x,-x)	**46**	m (-x, y, x)
11	3- (-x,-x, x)	**23**	4- (0, y, 0)	**35**	-3- (-x,-x, x)	**47**	-4- (0, y, 0)
12	3- (-x, x,-x)	**24**	2 (-x, 0, x)	**36**	-3- (-x, x,-x)	**48**	m (x, y, x)

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(24), Parameter :: Kov_D6H

Kovalev Notation for Point Group elements of 6/mmm (D6h)

Order	Value	Order	Value
1	h1	13	h13
2	h3	14	h15
3	h5	15	h17
4	h4	16	h16
5	h6	17	h18
6	h2	18	h14
7	h11	19	h23
8	h9	20	h21
9	h7	21	h19
10	h8	22	h20
11	h12	23	h24
12	h10	24	h22

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(48), Parameter :: Kov_OH

Kovalev Notation for Point Group elements of m3m (Oh)

Order	Value	Order	Value	Order	Value	Order	Value
1	h1	13	h16	25	h25	37	h40
2	h4	14	h13	26	h28	38	h37
3	h3	15	h15	27	h27	39	h39
4	h2	16	h14	28	h26	40	h38
5	h9	17	h20	29	h33	41	h44
6	h10	18	h18	30	h34	42	h42
7	h12	19	h17	31	h36	43	h41
8	h11	20	h19	32	h35	44	h43
9	h5	21	h24	33	h29	45	h48
10	h7	22	h23	34	h31	46	h47
11	h6	23	h22	35	h30	47	h46
12	h8	24	h21	36	h32	48	h45

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(8), Parameter :: Latt

Lattice Traslations

Order	Value
1	P: { 000 }
2	A: { 000; 0 1/2 1/2 }+
3	B: { 000; 1/2 0 1/2 }+
4	C: { 000; 1/2 1/2 0 }+
5	I: { 000; 1/2 1/2 1/2 }+
6	R: { 000; 2/3 1/3 1/3; 1/3 2/3 2/3 }+
7	F: { 000; 0 1/2 1/2; 1/2 0 1/2; 1/2 1/2 0 }+
8	Z: { 000; Unconventional Z-centering vectors }+

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(16), Parameter :: Laue_Class

Laue symbols

Order	***Value***	***Order***	***Value***
1	-1	**9**	-3m1
2	2/m	**10**	-31m
3	mmm	**11**	6/m
4	4/m	**12**	6/mmm
5	4/mmm	**13**	m-3
6	-3 R	**14**	m-3m
7	-3m R	**15**	m3
8	-3	**16**	m3m

CFML_Symmetry_Tables: Parameters

Real(Kind=CP), Dimension(3,2), Parameter :: Ltr_A

Lattice translations of type A

$$LTR\_A = \begin{pmatrix} 0 & 0 \\ 0 & \tfrac{1}{2} \\ 0 & \tfrac{1}{2} \end{pmatrix}$$

CFML_Symmetry_Tables: Parameters

Real(Kind=CP), Dimension(3,2), Parameter :: Ltr_B

Lattice translations of type B

$$LTR\_B = \begin{pmatrix} 0 & \tfrac{1}{2} \\ 0 & 0 \\ 0 & \tfrac{1}{2} \end{pmatrix}$$

CFML_Symmetry_Tables: Parameters

Real(Kind=CP), Dimension(3,2), Parameter :: Ltr_C

Lattice translations of type C

$$LTR\_C = \begin{pmatrix} 0 & \tfrac{1}{2} \\ 0 & \tfrac{1}{2} \\ 0 & 0 \end{pmatrix}$$

CFML_Symmetry_Tables: Parameters

Real(Kind=CP), Dimension(3,4), Parameter :: Ltr_F

Lattice translations of type F

$$LTR\_F=\begin{pmatrix}0 & 0 & \frac{1}{2} & \frac{1}{2}\\ 0 & \frac{1}{2} & 0 & \frac{1}{2}\\ 0 & \frac{1}{2} & \frac{1}{2} & 0\end{pmatrix}$$

CFML_Symmetry_Tables: Parameters

Real(Kind=CP), Dimension(3,2), Parameter :: Ltr_I

Lattice translations of type I

$$LTR\_I=\begin{pmatrix}0 & \frac{1}{2}\\ 0 & \frac{1}{2}\\ 0 & \frac{1}{2}\end{pmatrix}$$

CFML_Symmetry_Tables: Parameters

Real(Kind=CP), Dimension(3,3), Parameter :: Ltr_R

Lattice translations of type R

$$LTR\_R=\begin{pmatrix}0 & \frac{2}{3} & \frac{1}{3}\\ 0 & \frac{1}{3} & \frac{2}{3}\\ 0 & \frac{1}{3} & \frac{2}{3}\end{pmatrix}$$

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(72), Parameter :: MagMat

Magnetic array

Order	*Value*	*Order*	*Value*	*Order*	*Value*
1	(Mx, My, Mz)	**25**	(-Mx,-My,-Mz)	**49**	(Mx , My, Mz)
2	(-Mx,-My, Mz)	**26**	(Mx, My,-Mz)	**50**	(-My, Mx-My, Mz)
3	(-Mx, My,-Mz)	**27**	(Mx,-My, Mz)	**51**	(-Mx+My,-Mx , Mz)
4	(Mx,-My,-Mz)	**28**	(-Mx, My, Mz)	**52**	(-Mx , -My, Mz)
5	(Mz, Mx, My)	**29**	(-Mz,-Mx,-My)	**53**	(My,-Mx+My, Mz)
6	(Mz,-Mx,-My)	**30**	(-Mz, Mx, My)	**54**	(Mx-My, Mx , Mz)
7	(-Mz,-Mx, My)	**31**	(Mz, Mx,-My)	**55**	(My, Mx ,-Mz)
8	(-Mz, Mx,-My)	**32**	(Mz,-Mx, My)	**56**	(Mx-My, -My,-Mz)
9	(My, Mz, Mx)	**33**	(-My,-Mz,-Mx)	**57**	(-Mx ,-Mx+My,-Mz)
10	(-My, Mz,-Mx)	**34**	(My,-Mz, Mx)	**58**	(-My,-Mx ,-Mz)

11	(My,-Mz,-Mx)	**35**	(-My, Mz, Mx)	**59**	(-Mx+My, My,-Mz)
12	(-My,-Mz, Mx)	**36**	(My, Mz,-Mx)	**60**	(Mx , Mx-My,-Mz)
13	(My, Mx,-Mz)	**37**	(-My,-Mx, Mz)	**61**	(-Mx , -My,-Mz)
14	(-My,-Mx,-Mz)	**38**	(My, Mx, Mz)	**62**	(My,-Mx+My,-Mz)
15	(My,-Mx, Mz)	**39**	(-My, Mx,-Mz)	**63**	(Mx-My, Mx ,-Mz)
16	(-My, Mx, Mz)	**40**	(My,-Mx,-Mz)	**64**	(Mx , My,-Mz)
17	(Mx, Mz,-My)	**41**	(-Mx,-Mz, My)	**65**	(-My, Mx-My,-Mz)
18	(-Mx, Mz, My)	**42**	(Mx,-Mz,-My)	**66**	(-Mx+My,-Mx ,-Mz)
19	(-Mx,-Mz,-My)	**43**	(Mx, Mz, My)	**67**	(-My,-Mx , Mz)
20	(Mx,-Mz, My)	**44**	(-Mx, Mz,-My)	**68**	(-Mx+My, My, Mz)
21	(Mz, My,-Mx)	**45**	(-Mz,-My, Mx)	**69**	(Mx , Mx-My, Mz)
22	(Mz,-My, Mx)	**46**	(-Mz, My,-Mx)	**70**	(My, Mx , Mz)
23	(-Mz, My, Mx)	**47**	(Mz,-My,-Mx)	**71**	(Mx-My, -My, Mz)
24	(-Mz,-My,-Mx)	**48**	(Mz, My, Mx)	**72**	(-Mx ,-Mx+My, Mz)

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(24), Parameter :: ML_D6H

Miller & Love Notation for Point Group elements of 6/mmm (D6h)

Order	***Value***	***Order***	***Value***
1	1	**13**	13
2	3	**14**	15
3	5	**15**	17
4	4	**16**	16
5	6	**17**	18
6	2	**18**	14
7	9	**19**	21
8	7	**20**	19
9	11	**21**	23
10	12	**22**	24
11	10	**23**	22
12	8	**24**	20

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(48), Parameter :: ML_OH

Miller & Love Notation for Point Group elements of m3m (Oh)

Order	***Value***	***Order***	***Value***	***Order***	***Value***	***Order***	***Value***
1	1	**13**	16	**25**	25	**37**	40
2	4	**14**	13	**26**	28	**38**	37
3	3	**15**	15	**27**	27	**39**	39
4	2	**16**	14	**28**	26	**40**	38
5	9	**17**	20	**29**	33	**41**	44
6	10	**18**	18	**30**	34	**42**	42
7	12	**19**	17	**31**	36	**43**	41
8	11	**20**	19	**32**	35	**44**	43
9	5	**21**	24	**33**	29	**45**	48

10	7	**22**	23	**34**	31	**46**	47
11	6	**23**	22	**35**	30	**47**	46
12	8	**24**	21	**36**	32	**48**	45

CFML_Symmetry_Tables: Parameters

Integer, Dimension(36,3,3), Parameter :: Mod6

Matrix types for Rotational Operators in conventional basis.

From 1 to 24 for Oh
From 25 to 36 for D6h

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(39), Parameter :: Point_Group

Point Group Symbols

Order	*Value*	*Order*	*Value*	*Order*	*Value*	*Order*	*Value*
1	1	**13**	4/m	**25**	31m	**37**	432
2	-1	**14**	422	**26**	-31m	**38**	-43m
3	2	**15**	4mm	**27**	6	**39**	m-3m
4	m	**16**	-42m	**28**	-6		
5	2/m	**17**	-4m2	**29**	6/m		
6	222	**18**	4/mmm	**30**	622		
7	mm2	**19**	3	**31**	6mm		
8	m2m	**20**	-3	**32**	-62m		
9	2mm	**21**	32	**33**	-6m2		
10	mmm	**22**	3m	**34**	6/mmm		
11	4	**23**	-3m	**35**	23		
12	-4	**24**	312	**36**	m-3		

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(7), Parameter :: Sys_Cry

System Type

Order	*Value*
1	Triclinic
2	Monoclinic
3	Orthorhombic
4	Tetragonal
5	Rhombohedral
6	Hexagonal
7	Cubic

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(24), Parameter :: X_D6H

Notation for Point Group elements of 6/mmm (D6h)

Order	Value	Order	Value
1	(x , y, z)	13	(-x , -y,-z)
2	(-y, x-y, z)	14	(y,-x+y,-z)
3	(-x+y,-x , z)	15	(x-y, x ,-z)
4	(-x , -y, z)	16	(x , y,-z)
5	(y,-x+y, z)	17	(-y, x-y,-z)
6	(x-y, x , z)	18	(-x+y,-x ,-z)
7	(y, x ,-z)	19	(-y,-x , z)
8	(x-y, -y,-z)	20	(-x+y, y, z)
9	(-x ,-x+y,-z)	21	(x , x-y, z)
10	(-y,-x ,-z)	22	(y, x , z)
11	(-x+y, y,-z)	23	(x-y, -y, z)
12	(x , x-y,-z)	24	(-x ,-x+y, z)

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(48), Parameter :: X_OH

Notation for Point Group elements of m3m (Oh)

Order	Value	Order	Value	Order	Value	Order	Value
1	(x, y, z)	13	(y, x,-z)	25	(-x,-y,-z)	37	(-y,-x, z)
2	(-x,-y, z)	14	(-y,-x,-z)	26	(x, y,-z)	38	(y, x, z)
3	(-x, y,-z)	15	(y,-x, z)	27	(x,-y, z)	39	(-y, x,-z)
4	(x,-y,-z)	16	(-y, x, z)	28	(-x, y, z)	40	(y,-x,-z)
5	(z, x, y)	17	(x, z,-y)	29	(-z,-x,-y)	41	(-x,-z, y)
6	(z,-x,-y)	18	(-x, z, y)	30	(-z, x, y)	42	(x,-z,-y)
7	(-z,-x, y)	19	(-x,-z,-y)	31	(z, x,-y)	43	(x, z, y)
8	(-z, x,-y)	20	(x,-z, y)	32	(z,-x, y)	44	(-x, z,-y)
9	(y, z, x)	21	(z, y,-x)	33	(-y,-z,-x)	45	(-z,-y, x)
10	(-y, z,-x)	22	(z,-y, x)	34	(y,-z, x)	46	(-z, y,-x)
11	(y,-z,-x)	23	(-z, y, x)	35	(-y, z, x)	47	(z,-y,-x)
12	(-y,-z, x)	24	(-z,-y,-x)	36	(y, z,-x)	48	(z, y, x)

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(24), Parameter :: Zak_D6H

Zak Notation for Point Group elements of 6/mmm (D6h)

Order	Value	Order	Value
1	E	13	I
2	C(z)_3	14	S(5z)_6
3	C(2z)_3	15	S(z)_6
4	C_2	16	s(z)
5	C(5z)_6	17	S(z)_3
6	C(z)_6	18	S(2z)_3
7	U(xy)	19	s(xy)

8	U(x)	**20**	s(x)
9	U(y)	**21**	s(y)
10	U(3)	**22**	s(3)
11	U(2)	**23**	s(2)
12	U(1)	**24**	s(1)

CFML_Symmetry_Tables: Parameters

Character(Len=*), Dimension(48), Parameter :: Zak_OH

Zak Notation for Point Group elements of m3m (Oh)

Order	***Value***	***Order***	***Value***	***Order***	***Value***	***Order***	***Value***
1	E	**13**	U(xy)	**25**	I	**37**	s(xy)
2	U(z)	**14**	U(-xy)	**26**	s(z)	**38**	s(-xy)
3	U(y)	**15**	C(3z)_4	**27**	s(y)	**39**	S(z)_4
4	U(x)	**16**	C(z)_4	**28**	s(x)	**40**	S(3z)_4
5	C(xyz)_3	**17**	C(3x)_4	**29**	S(5xyz)_6	**41**	S(x)_4
6	C(-xy-z)_3	**18**	U(yz)	**30**	S(-5xy-z)_6	**42**	s(yz)
7	C(x-y-z)_3	**19**	U(y-z)	**31**	S(5x-y-z)_6	**43**	s(y-z)
8	C(-x-yz)_3	**20**	C(x)_4	**32**	S(-5x-yz)_6	**44**	S(3x)_4
9	C(2xyz)_3	**21**	C(y)_4	**33**	S(xyz)_6	**45**	S(3y)_4
10	C(2x-y-z)_3	**22**	U(xz)	**34**	S(x-y-z)_6	**46**	s(xz)
11	C(2x-yz)_3	**23**	C(3y)_4	**35**	S(-x-yz)_6	**47**	S(y)_4
12	C(-2xy-z)_3	**24**	U(x-z)	**36**	S(-xy-z)_6	**48**	s(x-z)

CFML_Symmetry_Tables: Variables

Spgr_Info_Type
Table_Equiv_Type
Wyck_Info_Type

Err_SymTab
Err_SymTab_Mess
Spgr_Info
System_Equiv
Wyckoff_Info

CFML_Symmetry_Tables: Variables

	Variable	***Definition***
Type :: Spgr_Info_Type		
Integer	N	Number of the Space group according to I.T.
Character (Len=12)	HM	Hermann-Mauguin symbol
Character (Len=16)	Hall	Hall symbol
Integer	Laue	Laue group

Integer	PG	Point group
Integer, Dimension(6)	Asu	Asymmetric unit * 24
Character (Len=5)	Inf_Extra	Extra information
End Type Spgr_Info_Type		

CFML_Symmetry_Tables: Variables

	Variable	*Definition*
Type :: Table_Equiv_Type		
Character (Len=6)	SC	Schoenflies
Character (Len=17)	ML	Miller & Love
Character (Len=18)	KO	Kovalev
Character (Len=32)	BC	Bradley & Cracknell
Character (Len=18)	ZA	Zak
End Type Table_Equiv_Type		

Definition for Equivalences on a Table

CFML_Symmetry_Tables: Variables

	Variable	*Definition*
Type :: Wyck_Info_Type		
Character (Len=12)	HM	Hermann-Mauguin symbol
Integer	NOrbit	Number of orbites
Character (Len=15), Dimension(24)	COrbit	Generator of the orbit
End Type Wyck_Info_Type		

Definition for Wyckoff Positions according to I.T.

CFML_Symmetry_Tables: Variables

Logical :: Err_SymTab

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module

CFML_Symmetry_Tables: Variables

Character (Len=150) :: Err_SymTab_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Symmetry_Tables: Variables

Type(Spgr_Info_Type), Dimension(:) :: Spgr_Info

General information about Space Groups

CFML_Symmetry_Tables: Variables

Type(Table_Equiv_Type), Dimension(:), Allocatable :: System_Equiv

General information about equivalence between Notations

CFML_Symmetry_Tables: Variables

Type(Wyck_Info_Type), Dimension(:), Allocatable :: Wyckoff_Info

General info about Wyckoff Positions on IT

CFML_Symmetry_Tables: Subroutines

- Get_Generators
- Remove_Spgr_Info
- Remove_System_Equiv
- Remove_Wyckoff_Info
- Set_Spgr_Info
- Set_System_Equiv
- Set_Wyckoff_Info

CFML_Symmetry_Tables: Subroutines

Subroutine Get_Generators (Spg, Gener)

Character (Len=*)	**Intent(in)**	Spg	Hermann_Mauguin symbol or number of S.Group
Character (Len=*)	**Intent(out)**	Gener	String with all generators

Provides the string **GENER** containing the list of the generators (as given in the IT Crystallography) corresponding to the space group of symbol **Spg**.
In **Spg** the Hermann-Mauguin symbol or the number of the space group should be given. The calling program is responsible of decoding the string **Gener**. Generator are given in the Jone's Faithful notation and the separator is the symbol ";".

Example:
Space group: R 3 c
GENER= " x+1/3,y+2/3,z+2/3; -y,x-y,z; -y,-x,z+1/2"

CFML_Symmetry_Tables: Subroutines

Subroutine Remove_Spgr_Info( )

Deallocating Spgr_Info Data

CFML_Symmetry_Tables: Subroutines

Subroutine Remove_System_Equiv ( )

Deallocating System_Equiv variable

CFML_Symmetry_Tables: Subroutines

Subroutine Remove_Wyckoff_Info( )

Deallocating Wyckoff_Info variable

CFML_Symmetry_Tables: Subroutines

Subroutine Set_Spgr_Info ( )

Set information on Spgr_Info variable

CFML_Symmetry_Tables: Subroutines

Subroutine Set_System_Equiv( )

Define the conversion table between IT - ML - Kov - BC - Zak

The information given in this file corresponds to that of Table 6 of "Isotropy Subgroups of the 230 Crystallographic Space Groups", by Harold T Stokes and Dorian M Hatch, World Scientific, Singapore (1988).

The transformation operators that take space group elements in the international setting (international Tables of Crystallography, Hahn 1983) to space-groups elements in the Miller and Love (ML, 1967), Kovalev (Kov,1986) Bradley and Cracknell (BC, 1972) and Zak (Zak, 1969) settings.

> In the international setting the basis vectors are always those of the conventional unit cell. in rhombohedral system the primitive basis vectors are in an obverse relationship given by (2/3 1/3 1/3), (-1/3 1/3 1/3) and (-1/3, -2/3 1/3).
> In ML the same basis vectors are chosen except that for rhombohedral system the reverse setting is adopted, so the primitive basis vectors are: t1=(1/3 -1/3 1/3), t2=(1/3, 2/3 1/3) and t3=(2/3 1/3 1/3).
> In Kovalev the a,b,c axes of the coordinate system are along the conventional basis vectors of the lattice, however in the rhombohedral system an hexagonal system is chosen so that the primitive basis vectors are a1=(-1 -1 1/3), a2=(1 0 1/3) and a3=(0 1 1/3).
> In the setting of BC the axes a,b,c of the coordinate system are chosen to be the primitive basis vectors t1,t2,t3 as defined in their book.
> The setting of Zak the basis vectors are as in the international setting, but for rhombohedral system the primitive basis vectors w.r.t. the selected hexagonal coordinate system are given by: (1/3 2/3 1) (1/3 -1/3 1) (-2/3 -1/3 1)

Symmetry and transformation operators of Space Groups can be given as 4 x 4 Seitz matrices or as a character string called Jones Faithful representation. This last representation is that used in this file.

To transform a symmetry operator "gI" in the international setting into a symmetry element "g" in one of the other settings, we simply perform the following operation: g = gT gI gT(-1), where gT is the transformation given tabulated below.

CFML_Symmetry_Tables: Subroutines

Subroutine Set_Wyckoff_Info ( )

Set information on Wyckoff_Info variable

Level 3

Concept	***Module Name***	***Purpose***

Bonds Tables...	**CFML_Bond_Tables**	Contain a simple subroutine providing the list of the usual bonds between atoms
Crystal Metrics...	**CFML_Crystal_Metrics**	Define crystallographic types and to provide automatic crystallographic metrics operations
instrumentation on ILL...	**CFML_ILL_Instrm_Data**	Procedures to access the (single crystals) instrument output data base at ILL
Symmetry information...	**CFML_Crystallographic_Symmetry**	Contain nearly everything needed for handling symmetry in Crystallography.

CFML_Bond_Tables

This module provide the list of the usual bonds between atoms. There are three possible values: simple, double and triple bond

Variables

Bond_Length_Table
Err_Bond
Err_Bond_Mess

Subroutines

Get_Bonds_Table
Init_Err_Bond
Remove_Bonds_Table
Set_Bonds_Table

Fortran Filename

CFML_Bonds_Table.f90

CFML_Bond_Tables: Variables

Bond_Length_Table
Err_Bond
Err_Bond_Mess

CFML_Bond_Tables: Variables

Real, Dimension(: , : , :), Allocatable :: Bond_Length_Table

Global variable holding the bond lengths between different type of atoms. Ordered by Z

Bond_Length_Table(1,:,:) represent the simple bond, while Bond_Length_Table(2,:,:) represent a double bound distances or shorter distances and finally Bond_Length_Table(3,:,:) represents the triple bond distance or the shotest distance.

CFML_Bond_Tables: Variables

Logical :: Err_Bond

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_Bond_Tables: Variables

Character (Len=150) :: Err_Bond_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Bond_Tables: Subroutines

- Get_Bonds_Table
- Init_Err_Bond
- Remove_Bonds_Table
- Set_Bonds_Table

CFML_Bond_Tables: Subroutines

Subroutine Get_Bonds_Table (Symbol1, Symbol2, Bonds)

Character (Len=*)	**Intent(in)**	Symbol 1	Atomic symbol
Character (Len=*)	**Intent(in)**	Symbol 2	Atomic symbol
Real(Kind=CP), Dimension(3)	**Intent(out)**	Bonds	Bonds between Specie1 and Specie 2

or

Subroutine Get_Bonds_Table (Z1, Z2, Bonds)

Integer	**Intent(in)**	Z1	Atomic number for Specie 1
Integer	**Intent(in)**	Z2	Atomic number for Specie 2
Real(Kind=CP), Dimension(3)	**Intent(out)**	Bonds	Bonds between Specie1 and Specie 2

Obtain the typical distances between species of atoms

CFML_Bond_Tables: Subroutines

Subroutine Init_Err_Bond ( )

Subroutine that initializes errors flags in **CFML_Bond_Tables** module.

CFML_Bond_Tables: Subroutines

Subroutine Remove_Bonds_Table ( )

Deallocating Bond_Length_Table variable

CFML_Bond_Tables: Subroutines

Subroutine Set_Bonds_Table ( )

Fills the components of the Bond_Length_Table variable.

CFML_Crystal_Metrics

Module to define Crystallographic types and to provide automatic crystallographic procedures.

Variables

- Crystal_Cell_Type
- Twofold_Axes_Type

- Err_Crys
- Err_Crys_Mess

Functions

- Cart_U_Vector
- Cart_Vector
- Convert_B_Betas
- Convert_B_U
- Convert_Betas_B
- Convert_Betas_U
- Convert_U_B
- Convert_U_Betas
- Rot_Matrix
- U_Equiv

Subroutines

- Change_Setting_Cell
- Get_Conventional_Cell
- Get_Cryst_Family
- Get_Deriv_Orth_Cell
- Get_Primitive_Cell
- Get_Transform_Matrix
- Get_TwoFold_Axes
- Init_Err_Crys
- Niggli_Cell
- Set_Crystal_Cell
- Write_Crystal_Cell

Fortran Filename

CFML_Cryst_Types.f90

CFML_Crystal_Metrics: Variables

Crystal_Cell_Type
Twofold_Axes_Type

Err_Crys
Err_Crys_Mess

CFML_Crystal_Metrics: Variables

	Variable	***Definition***
Type :: Crystal_Cell_Type		
Real (Kind=CP), Dimension(3)	Cell	Lengths of the cell parameters in angstroms
Real (Kind=CP), Dimension(3)	Ang	Angles of the cell parameters in degrees
Real (Kind=CP), Dimension(3)	Cell_STD	Standar deviations of cell parameters
Real (Kind=CP), Dimension(3)	Ang_STD	
Real (Kind=CP), Dimension(3)	RCell	Reciprocal cell parameters
Real (Kind=CP), Dimension(3)	Rang	
Real (Kind=CP), Dimension(3,3)	GD	Direct Metric Tensors
Real (Kind=CP), Dimension(3,3)	GR	Reciprocal Metric Tensors
Real (Kind=CP), Dimension(3,3)	CR_Orth_Cel	P-Matrix transforming Orthonormal basis to direct Crystal cell (as I.T.) (or crystallographic components to cartesian components)
Real (Kind=CP), Dimension(3,3)	Orth_CR_Cel	Cartesian to crystallographic components
Real (Kind=CP), Dimension(3,3)	BL_M	Busing-Levy B-matrix
Real (Kind=CP), Dimension(3,3)	BL_MInv	Inverse Busing-Levy B-matrix
Real (Kind=CP)	CellVol	Direct cell volumes
Real (Kind=CP)	RCellVol	Reciprocal cell volumes
Character(Len=1)	CartType	Cartesian Frame type: 'A' Cartesian Frame has x // a. Other Cartesian Frame has z // c
End Type Crystal_Cell_Type		

CFML_Crystal_Metrics: Variables

	Variable	***Definition***
Type :: Twofold_Axes_Type		
Integer	NTwo	Number of two-fold axes
Real (Kind=CP)	Tol	Angular tolerance (ca 3 degrees)
Real (Kind=CP), Dimension(3,12)	CAxes	Cartesian components of two-fold axes
Integer, Dimension(3,12)	DTwofold	Direct indices of two-fold axes
Integer, Dimension(3,12)	RTwofold	Reciprocal indices of two-fold axes
Integer, Dimension(12)	Dot	Scalar product of reciprocal and direct indices

Real (Kind=CP), Dimension(12)	Cross	Angle between direct and reciprocal axes (< tol)
Real (Kind=CP), Dimension(12)	Maxes	Modulus of the zone axes (two-fold axes) vectors
Real (Kind=CP), Dimension(3)	A	Cartesian components of direct cell parameters
Real (Kind=CP), Dimension(3)	B	
Real (Kind=CP), Dimension(3)	C	
End Type Twofold_Axes_Type		

CFML_Crystal_Metrics: Variables

Logical :: Err_Crys

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_Crystal_Metrics: Variables

Character (Len=150) :: Err_Crys_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Crystal_Metrics: Functions

- Cart_U_Vector
- Cart_Vector
- Convert_B_Betas
- Convert_B_U
- Convert_Betas_B
- Convert_Betas_U
- Convert_U_B
- Convert_U_Betas
- Rot_Matrix
- U_Equiv

CFML_Crystal_Metrics: Functions

Real Function Cart_U_Vector(Code, V, Celda)

Character (Len=*)	**Intent(in)**	Code	D: Direct R: Reciprocal
Real(Kind=CP), Dimension (3)	**Intent(in)**	V	Vector
Type(Crystal_Cell_Type)	**Intent(in)**	Celda	Cell parameters

Convert a vector in crystal space to unitary cartesian components. Return a real vector of Dimension(3)

CFML_Crystal_Metrics: Functions

Real Function Cart_Vector (Code, V, Celda)

Character (Len=*)	**Intent(in)**	Code	D: Direct R: Reciprocal

Real(Kind=CP), Dimension (3)	**Intent(in)**	V	Vector
Type(Crystal_Cell_Type)	**Intent(in)**	Celda	Cell parameters

Convert a vector in crystal space to cartesian components. Return a real vector of Dimension(3)

CFML_Crystal_Metrics: Functions

Real Function Convert_B_Betas(B, Cell)

Real(Kind=CP), Dimension (6)	**Intent(in)**	B	B vector: B_{11} B_{22} B_{33} B_{12} B_{13} B_{23}
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters

Convert Thermal factors from B to . Return a vector of Dimension(6)

CFML_Crystal_Metrics: Functions

Real Function Convert_B_U(B)

Real(Kind=CP), Dimension (6)	**Intent(in)**	B	B vector: B_{11} B_{22} B_{33} B_{12} B_{13} B_{23}

Convert Thermal factors from B to U. Return a vector of Dimension(6)

CFML_Crystal_Metrics: Functions

Real Function Convert_Betas_B(Beta, Cell)

Real(Kind=CP), Dimension (6)	**Intent(in)**	Beta	BETA vector: $_{11}$ $_{22}$ $_{33}$ $_{12}$ $_{13}$ $_{23}$
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters

Convert Thermal factors from to B. Return a vector of Dimension(6)

CFML_Crystal_Metrics: Functions

Real Function Convert_Betas_U (Beta, Cell)

Real(Kind=CP), Dimension (6)	**Intent(in)**	Beta	BETA vector: $_{11}$ $_{22}$ $_{33}$ $_{12}$ $_{13}$ $_{23}$
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters

Convert Thermal factors from to U. Return a vector of Dimension(6)

CFML_Crystal_Metrics: Functions

Real Function Convert_U_B (U)

Real(Kind=CP), Dimension (6)	**Intent(in)**	U	U vector: U_{11} U_{22} U_{33} U_{12} U_{13} U_{23}

Convert Thermal factors from U to B. Return a vector of Dimension(6)

CFML_Crystal_Metrics: Functions

Real Function Convert_U_Betas (U, Cell)

Real(Kind=CP), Dimension (6)	**Intent(in)**	U	U vector: U_{11} U_{22} U_{33} U_{12} U_{13} U_{23}
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters

Convert Thermal factors from U to . Return a vector of Dimension(6)

CFML_Crystal_Metrics: Functions

Real Function Rot_Matrix (U, Phi, Celda)

Real(Kind=CP), Dimension (3)	**Intent(in)**	U	U vector
Real(Kind=CP)	**Intent(in)**	Phi	
Type(Crystal_Cell_Type)	**Intent(in)**	Celda	Cell parameters

Returns the matrix (Gibbs matrix (3,3)) of the active rotation of **Phi** degrees along the **U** direction: R v = v', the vector v is tranformed to vector v' keeping the reference frame unchanged.

If one wants to calculate the components of the vector "v'" in a rotated reference frame it suffices to invoke the function using "-phi". If **Celda** is present, **U** is in **Celda** coordinates, if not **U** is in cartesian coordinates.

CFML_Crystal_Metrics: Functions

Real Function U_Equiv (Cell, TH_U)

Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Real(Kind=CP), Dimension (6)	**Intent(in)**	TH_U	U vector: U_{11} U_{22} U_{33} U_{12} U_{13} U_{23}

Subroutine to obtain the U_{eq} from U's

CFML_Crystal_Metrics: Subroutines

CFML_Crystal_Metrics: Subroutines

Subroutine Change_Setting_Cell (Cell, Mat, CellN, MatKind)

Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell components

Real(Kind=CP), Dimension (3,3)	Intent(in)	Mat	Transformation array
Type(Crystal_Cell_Type)	Intent(out)	CellN	New Cell components
Character (Len=*), Optional	Intent(in)	MatKind	If present and it is IT

Transform the **CELL** object in **CELLN** using the transformation matrix **MAT**

CFML_Crystal_Metrics: Subroutines

Subroutine Get_Conventional_Cell(Twofold, Cell, Tr, Message, Ok)

Type(Twofold_Axes_Type)	Intent(in)	Twofold	
Type(Crystal_Cell_Type)	Intent(out)	Cell	Cell components
Integer, Dimension (3,3)	Intent(out)	Tr	
Character (Len=*)	Intent(out)	Message	
Logical	Intent(out)	Ok	

This subroutine provides the "conventional" (or quasi! being still tested) from the supplied object **Twofold** that has been obtained from a previous call to Get_Twofold_Axes. The conventional unit cell can be deduced from the distribution of two-fold axes in the lattice. The cell produced in this procedure applies some rules for obtaining the conventional cell, for instance in monoclinic lattices (a single two-fold axis) the two-fold axis is along b and the final cell is right handed with a <= c and beta >= 90. It may be A,C or I centred. The convertion to the C-centred setting in the A and I centring, is not attempted. The angular tolerance for accepting a two-fold axis, or higher order axes, as such has been previously set into **Twofold%TOL** component.

CFML_Crystal_Metrics: Subroutines

Subroutine Get_Cryst_Family (Cell, Car_Family, Car_Symbol, Car_System)

Type(Crystal_Cell_Type)	Intent(in)	Cell	Cell components
Character (Len=*)	Intent(out)	Car_Family	
Character (Len=*)	Intent(out)	Car_Symbol	
Character (Len=*)	Intent(out)	Car_System	

Obtain the Crystal Family, Symbol and System from cell parameters

CFML_Crystal_Metrics: Subroutines

Subroutine Get_Deriv_Orth_Cell (CellP, De_OrthCell, CarType)

Type(Crystal_Cell_Type)	Intent(in)	CellP	Cell components
Real(Kind=CP), Dimension (3,3,6)	Intent(out)	De_OrthCell	
Character (Len=*), Optional	Intent(in)	CarType	A:

Subroutine to get derivative matrix of the transformation matrix to orthogonal frame.
Useful for calculations of standard deviations of distances and angles. The specialized subroutine calculating sigmas of distances Distance_And_Sigma is in CFML_Atom_TypeDef.

The output matrices De_OrthCell are the derivatives of, with respect to a(1),b(2),c(3),alpha(4),beta(5) and gamma(6) of the matrix CellP%CR_Orth_CEL.

CFML_Crystal_Metrics: Subroutines

Subroutine Get_Primitive_Cell (Lat_Type, Centered_Cell, Primitive_Cell, Transfm)

Character (Len=*)	**Intent(in)**	Lat_Type	Lattice type: P,A,B,C,I,R or F
Type(Crystal_Cell_Type)	**Intent(in)**	Centered_Cell	Cell components
Type(Crystal_Cell_Type)	**Intent(out)**	Primitive_Cell	
Real(Kind=CP), Dimension (3,3)	**Intent(out)**	Transfm	

Subroutine for getting the primitive cell from a centred cell

Get_Transform_Matrix

Subroutine Get_Transform_Matrix (CellA, CellB, Trm, Ok, Tol)

Type(Crystal_Cell_Type)	**Intent(in)**	CellA	Input Cell
Type(Crystal_Cell_Type)	**Intent(in)**	CellB	Input Cell
Real(Kind=CP), Dimension (3,3)	**Intent(out)**	Trm	Transformation array
Logical	**Intent(out)**	Ok	Flag
Real(Kind=CP), Optional	**Intent(in)**	Tol	Tolerance value

Subroutine for getting the transformation matrix between two primitive unit cells (the range of indices is fixed to -2 to 2)

CFML_Crystal_Metrics: Subroutines

Subroutine Get_Twofold_Axes(CellN, Tol, Twofold)

Type(Crystal_Cell_Type)	**Intent(in)**	CellN	Cell components
Real(Kind=CP)	**Intent(in)**	Tol	Angular tolerance in degrees
Type(Twofold_Axes_Type)	**Intent(out)**	Twofold	

Subroutine for getting the possible two-fold axes (within an angular tolerance **TOL**) existing in the lattice generated by the unit cell **CellN**.
Strictly independed two-fold axes are stored in the variable **Twofold** that is of type Twofold_Axes_Type. The output order of the two-fold axes
is ascending in their modulus. Shorter vectors appears before longer ones. The conditions for a reciprocal or direct row to be a two-fold axis are
discussed by Y. Le Page in J.Appl.Cryst. 15, 255 (1982).

CFML_Crystal_Metrics: Subroutines

Subroutine Init_Err_Crys ( )

Subroutine that initializes errors flags in **CFML_Crystal_Metrics** module.

CFML_Crystal_Metrics: Subroutines

Subroutine Niggli_Cell(AD, Niggli_Point, CellN, Trans)

Real(Kind=CP), Dimension (6)	**Intent(in out)**	AD	Cell parameters as a vector
Real(Kind=CP), Dimension (5), Optional	**Intent(out)**	Niggli_Point	
Type(Crystal_Cell_Type), Optional	**Intent(out)**	CellN	Cell components
Real(Kind=CP), Dimension (3,3), Optional	**Intent(out)**	Trans	

or

Subroutine Niggli_Cell(N_Mat, Niggli_Point, CellN, Trans)

Real(Kind=CP), Dimension (2,3)	**Intent(in out)**	N_Mat	Niggli Matrix
Real(Kind=CP), Dimension (5), Optional	**Intent(out)**	Niggli_Point	
Type(Crystal_Cell_Type), Optional	**Intent(out)**	CellN	Cell components
Real(Kind=CP), Dimension (3,3), Optional	**Intent(out)**	Trans	

or

Subroutine Niggli_Cell(A, B, C, AL, BE, GA, Niggli_Point, CellN, Trans)

Real(Kind=CP)	**Intent(in out)**	A	Cell Parameters
Real(Kind=CP)	**Intent(in out)**	B	
Real(Kind=CP)	**Intent(in out)**	C	
Real(Kind=CP)	**Intent(in out)**	AL	
Real(Kind=CP)	**Intent(in out)**	BE	
Real(Kind=CP)	**Intent(in out)**	GA	
Real(Kind=CP), Dimension (5), Optional	**Intent(out)**	Niggli_Point	
Type(Crystal_Cell_Type), Optional	**Intent(out)**	CellN	Cell components
Real(Kind=CP), Dimension (3,3), Optional	**Intent(out)**	Trans	

or

Subroutine Niggli_Cell(Cell, Niggli_Point, CellN, Ttrans)

Type(Crystal_Cell_Type)	**Intent(in out)**	Cell	Cell parameters
Real(Kind=CP), Dimension (5), Optional	**Intent(out)**	Niggli_Point	
Type(Crystal_Cell_Type), Optional	**Intent(out)**	CellN	Cell components
Real(Kind=CP), Dimension (3,3), Optional	**Intent(out)**	Trans	

or

Subroutine Niggli_Cell(A, B, C, Niggli_Point, CellN, Trans)

Real(Kind=CP), Dimension (3)	**Intent(in out)**	A	Vector in Cartesian components
Real(Kind=CP), Dimension (3)	**Intent(in out)**	B	Vector in Cartesian components
Real(Kind=CP), Dimension (3)	**Intent(in out)**	C	Vector in Cartesian components
Real(Kind=CP), Dimension (5), Optional	**Intent(out)**	Niggli_Point	
Type(Crystal_Cell_Type), Optional	**Intent(out)**	CellN	Cell components
Real(Kind=CP), Dimension (3,3), Optional	**Intent(out)**	Trans	

Calculates the Niggli cell according to information passed in the arguments of the subroutine.

CFML_Crystal_Metrics: Subroutines

Subroutine Set_Crystal_Cell (CellV, Angl, Celda, CarType, SCell, SAngl)

Real(Kind=CP), Dimension (3)	**Intent(in)**	CellV	a,b,c parameters
Real(Kind=CP), Dimension (3)	**Intent(in)**	Angl	Angles for cell
Type(Crystal_Cell_Type)	**Intent(out)**	Celda	Cell components
Character (Len=1), Optional	**Intent(in)**	CarType	Type of Cartesian Frame
Real(Kind=CP), Dimension (3), Optional	**Intent(in)**	SCell	Sigmas of a,b,c parameters
Real(Kind=CP), Dimension (3), Optional	**Intent(in)**	Sangl	Sigmas for angles

Constructs the object **Celda** of type Crystal_Cell_Type

CFML_Crystal_Metrics: Subroutines

Subroutine Write_Crystal_Cell (Celda, Lun)

Type(Crystal_Cell_Type)	**Intent(in)**	Celda	Cell parameters
Integer, Optional	**Intent(in)**	Lun	Unit to write the Cell information

Writes the cell characteristics in a file associated to the logical unit **Lun**

CFML_Crystallographic_Symmetry

This module constains everything needed for handling symmetry in Crystallography.

Part of the information is obtained from tabulated items in the module CFML_Symmetry_Tables. In particular the correspondence of non standard settings Hermann-Mauguin symbols and Hall symbols for space groups. The construction of variables of the public type Space_Group_Type is done by using a variety of algorithms and methods.

Many procedures for handling symmetry (symbolic and algebraic) are provided in this module.

Parameters

- Cubic
- HexaG
- Monoc
- Num_Spgr_Info
- Orthor
- Tetra
- Trigo

Variables

- Space_Group_Type
- Sym_Oper_Type
- Wyck_Pos_Type
- Wyckoff_Type

- Lat_Ch
- Err_Symm
- Err_Symm_Mess
- Hexa

- InLat
- Ltr
- NLat
- SpaceG

Functions

- ApplySO
- Axes_Rotation
- Get_Laue_Num
- Get_Multip_Pos
- Get_Occ_Site
- Get_PointGroup_Num
- Is_New_OP
- Lattice_Trans
- Spgr_Equal
- Sym_Prod

Subroutines

- DecodMatMag
- Get_Centring_Vectors
- Get_Crystal_System
- Get_HallSymb_From_Gener
- Get_Lattice_Type
- Get_Laue_PG
- Get_Laue_Str
- Get_Orbit
- Get_PointGroup_Str
- Get_SO_From_Fix
- Get_SO_From_Gener
- Get_SO_From_Hall
- Get_SO_From_HMS
- Get_Stabilizer
- Get_String_Resolv
- Get_SubOrbits
- Get_SymEl
- Get_SymKov
- Get_SymSymb
- Get_T_SubGroups
- Init_Err_Symm
- Inverse_Symm
- LatSym
- Read_MSymm
- Read_SymTrans_Code
- Read_XSym
- SearchOP
- Set_SpaceGroup
- Set_Spg_Mult_Table
- Setting_Change

- Similar_Transf_SG
- Sym_B_Relations
- Sym_Prod_ST
- Symmetry_Symbol
- Write_SpaceGroup
- Write_Sym
- Write_SymTrans_Code
- Write_Wyckoff
- Wyckoff_Orbit

Fortran Filename

CFML_Symmetry.f90

CFML_Crystallographic_Symmetry: Parameters

- Cubic
- HexaG
- Monoc
- Num_Spgr_Info
- Orthor
- Tetra
- Trigo

CFML_Crystallographic_Symmetry: Parameters

Integer, Parameter :: Cubic=554

Index parameter for Cubic Groups

CFML_Crystallographic_Symmetry: Parameters

Integer, Parameter :: HexaG=527

Index parameter for Hexagonal Groups

CFML_Crystallographic_Symmetry: Parameters

Integer, Parameter :: Monoc=15

Index parameter for Monoclinic Groups

CFML_Crystallographic_Symmetry: Parameters

Integer, Parameter :: Num_Spgr_Info=612

Total number (dimension) of space groups information pieces in Spgr_Info variable

CFML_Crystallographic_Symmetry: Parameters

Integer, Parameter :: Orthor=163

Index parameter for Orthorhombic Groups

CFML_Crystallographic_Symmetry: Parameters

Integer, Parameter :: Tetra=410

Index parameter for Tetragonal Groups

CFML_Crystallographic_Symmetry: Parameters

Integer, Parameter :: Trigo=495

Index parameter for Trigonal Groups

CFML_Crystallographic_Symmetry: Variables

- Space_Group_Type
- Sym_Oper_Type
- Wyck_Pos_Type
- Wyckoff_Type

- Lat_Ch
- Err_Symm
- Err_Symm_Mess
- Hexa
- InLat
- Ltr
- NLat
- SpaceG

CFML_Crystallographic_Symmetry: Variables

	Variable	***Definition***
Type :: Space_Group_Type		
Integer	NumSpg	Number of the Space Group
Character (Len=20)	Spg_Symb	Hermann-Mauguin Symbol
Character (Len=16)	Hall	Hall symbol
Character (Len=12)	CrystalSys	Crystal System
Character (Len=5)	Laue	Laue Class
Character (Len=5)	PG	Point group
Character (Len=5)	Info	Extra information
Character (Len=80)	SG_Setting	information about the SG setting: IT KO ML ZA Standard UnConventional
Logical	Hexa	
Character (Len=1)	Spg_Lat	Lattice type

Character (Len=2)	Spg_LatSy	Lattice type Symbol
Integer	NumLat	Number of lattice points in a cell
Real (Kind=CP), Dimension(3,12)	Latt_Trans	Lattice translations
Character (Len=51)	Bravais	String with Bravais symbol + translations
Character (Len=80)	Centre	information about Centric or Acentric
Integer	Centered	=0 Centric (-1 no at origin) =1 Acentric =2 Centric (-1 at origin)
Real (Kind=CP), Dimension(3)	Centre_Coord	Fractional coordinates of the inversion centre
Integer	NumOPS	Number of reduced set of S.O.
Integer	Multip	Multiplicity of the general position
Integer	Num_Gen	Minimum number of operators to generate the Group
Type (Sym_Oper_Type), Dimension(192)	SymOP	Symmetry operators
Character (Len=40), Dimension(192)	SymOPSymb	Strings form of symmetry operators
Type (Wyckoff_Type)	Wyckoff	Wyckoff information
Real (Kind=CP), Dimension(3,2)	R_ASym_Unit	Asymmetric unit in real space
End Type Space_Group_Type		

CFML_Crystallographic_Symmetry: Variables

	Variable	***Definition***
Type :: Sym_Oper_Type		
Integer, Dimension(3,3)	Rot	Rotational part of Symmetry Operator
Real (Kind=CP), Dimension(3)	Tr	Translational part of Symmetry Operator
End Type Sym_Oper_Type		

CFML_Crystallographic_Symmetry: Variables

	Variable	***Definition***
Type :: Wyck_Pos_Type		
Integer	Mult	Multiplicity
Character (Len=6)	Site	Site Symmetry
Integer	NOrb	Number of elements in the orbit
Character (Len=40)	Orig	Original string
Character (Len=40), Dimension(48)	Str_Orbit	Orbit information
Character (Len=40), Dimension(192)	Extra_Orbit	
End Type Wyck_Pos_Type		

CFML_Crystallographic_Symmetry: Variables

	Variable	*Definition*
Type :: Wyckoff_Type		
Integer	Num_Orbit	Number of Orbits
Type (Wyck_Pos_Type), Dimension(26)	Orbit	Orbit information
End Type Wyckoff_Type		

CFML_Crystallographic_Symmetry: Variables

Character (Len=1) :: Lat_Ch

First character of the space group symbol

CFML_Crystallographic_Symmetry: Variables

Logical :: Err_Symm

This variable is set to **.TRUE.** if an error in procedures belonging to this module.

CFML_Crystallographic_Symmetry: Variables

Character (Len=150) :: Err_Symm_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Crystallographic_Symmetry: Variables

Logical :: Hexa

.FALSE.	Rotational part of symmetry operators belongs to m3m
.TRUE.	Rotational part of symmetry operators belongs to 6/mmm

CFML_Crystallographic_Symmetry: Variables

Integer :: InLat

Ordinal index of the lattice

CFML_Crystallographic_Symmetry: Variables

Real, Dimension(3,10) :: Ltr

Centering Lattice Translations.

Up to 10 lattice centring vectors are allowed. Conventional lattice centring need only 4 vectors

CFML_Crystallographic_Symmetry: Variables

Integer :: NLat

Multiplicity of the lattice

CFML_Crystallographic_Symmetry: Variables

Character (Len=20) :: SpaceG

Space group symbol

CFML_Crystallographic_Symmetry: Functions

CFML_Crystallographic_Symmetry: Functions

Real Function ApplySO(OP, V)

Type(Sym_Oper_Type)	**Intent(in)**	OP	Symmetry Operator Type
Real(Kind=CP), Dimension(3)	**Intent(in)**	V	Point vector

Return a vector of dimension 3. Apply a symmetry operator to a vector

CFML_Crystallographic_Symmetry: Functions

Integer Function Axes_Rotation (R)

Integer, Dimension(3,3)	**Intent(in)**	R	Rotation part of Symmetry Operator

Determine the orden of rotation (valid for all bases). Return a zero if any error occurs.

CFML_Crystallographic_Symmetry: Functions

Integer Function Get_Laue_Num (LaueClass)

Character(Len=*)	**Intent(in)**	LaueClass	Laue Class string

Obtain the ordinal number corresponding to the Laue class symbol according to Laue_Class array. Zero if error is present

CFML_Crystallographic_Symmetry: Functions

Integer Function Get_Multip_Pos (X, Spg)

Real(Kind=CP), Dimension(3)	**Intent(in)**	X	Position vector
Type(Space_Group_Type)	**Intent(in)**	Spg	Space Group

Obtain the multiplicity of a real space point given the space group

CFML_Crystallographic_Symmetry: Functions

Real Function Get_Occ_Site (Pto, Spg)

Real(Kind=CP), Dimension(3)	**Intent(in)**	Pto	Position vector
Type(Space_Group_Type)	**Intent(in)**	Spg	Space Group

Obtain the occupancy factor (site multiplicity/multiplicity) for **Pto**

CFML_Crystallographic_Symmetry: Functions

Integer Function Get_PointGroup_Num(PgName)

Character(Len=*)	**Intent(in)**	PgName	String for PointGroup

Obtain the ordinal number corresponding to the Point Group symbol according to Point_Group array. Zero if Error is present

CFML_Crystallographic_Symmetry: Functions

Logical Function Is_New_OP(OP, N, List_OP)

Type(Sym_Oper_Type)	**Intent(in)**	OP	Symmetry operator
Integer	**Intent(in)**	N	Number of Op in the LIST_OP
Type(Sym_Oper_Type), Dimension(:)	**Intent(in)**	List_OP	List of N symmetry operators

Determine if a symmetry operator is or not in a given list

CFML_Crystallographic_Symmetry: Functions

Logical Function Lattice_Trans (V, Lat)

Real(Kind=CP), Dimension(3)	**Intent(in)**	V	Vector
Character(Len=*)	**Intent(in)**	Lat	Lattice Character

Determine whether a vector is a lattice vector depending on the Bravais lattice.

CFML_Crystallographic_Symmetry: Functions

Logical Function Spgr_Equal (SpaceGroup1, SpaceGroup2)

Type(Space_Group_Type)	**Intent(in)**	SpaceGroup1	Space group
Type(Space_Group_Type)	**Intent(in)**	SpaceGroup2	Space group

Determine if two SpaceGroups are equal

CFML_Crystallographic_Symmetry: Functions

Function Sym_Prod (SymA, SymB, ModLat)

Type(Sym_Oper_Type)	Intent(in)	SymA	Space group

Type(Sym_Oper_Type)	Intent(in)	SymB	Space group
LogicalL, Optional	Intent(in)	ModLat	

Obtain the symmetry operation corresponding to the product of two operators. The return is a variable of type Sym_Oper_Type
If **ModLat**=.true. or it is not present, the translation part of the resulting operator is reduced to have components < 1.0

CFML_Crystallographic_Symmetry: Subroutines

CFML_Crystallographic_Symmetry: Subroutines

Subroutine DecodMatMag (Sim, XYZString)

Integer, **Dimension**(**3**,**3**)	**Intent**(**in**)	Sim	Rotation matrix
Character(**Len**=*)	**Intent**(**out**)	XYZString	String (Mx,My,Mz)

Supplies a string of the form (Mx,My,Mz) for the rotation matrix SIM.

Note: Logical Hexa must be defined.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_Centring_Vectors (L, LatC)

Integer	**Intent**(**in out**)	L	Number of centring vectors
Real(**Kind**=CP), **Dimension**(:,:)	**Intent**(**in out**)	LatC	Centering vectors. Array (3,L)

Subroutine to complete the centring vectors of a centered lattice. It is useful when non-conventional lattices are used.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_Crystal_System (NG, Ss, ISystm, Crys)

Integer	**Intent**(**in**)	NG	Number of Operators (not related by inversion and lattice translations)
Integer, **Dimension**(:,:,:)	**Intent**(**in**)	Ss	Rotation Part (3,3,48)
Integer	**Intent**(**out**)	ISystm	Number for Crystal System according to Sys_Cry
Character(**Len**=**1**)	**Intent**(**out**)	Crys	Symbol of Crystal family

or

Subroutine Get_Crystal_System (NG, Gen, ISsystm, Crys)

Integer	**Intent**(**in**)	NG	Number of Operators (not related by inversion and translations)
Character(**Len**=*), **Dimension**(:)	**Intent**(**in**)	Gen	Jones Faithful form of symmetry operators
Integer	**Intent**(**out**)	ISystm	Number for Crystal System according to SYS_CRY
Character(**Len**=**1**)	**Intent**(**out**)	Crys	Symbol of Crystal family

Obtain the number and string of the Crystal System from a set of operators

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_HallSymb_From_Gener (SpaceGroup, SpaceH)

Type(**Space_Group_Type**)	**Intent**(**in out**)	SpaceGroup	SpaceGroup
Character(**Len**=*)	**Intent**(**out**)	SpaceH	Hall Symbol

Determines the Hall symbol.

In general this routine try to obtain the Hall symbol from generators so you need call Get_SO_From_Gener before and call Set_Spgr_Info.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_Lattice_Type (L, LatC, LatTyp)

Integer	**Intent(in)**	L	Number of centring vectors
Real(Kind=CP), Dimension(:,:)	**Intent(in)**	LatC	Centring vectors. Array (3,11)
Character(Len=*)	**Intent(out)**	LatTyp	Lattice symbol

Subroutine to get the lattice symbol from a set of centring vectors.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_Laue_PG (SpaceGroup, Laue_Car, Point_Car)

Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	Space Group
Character(Len=*)	**Intent (out)**	Laue_Car	String with Laue symbol
Character(Len=*)	**Intent (out)**	Point_Car	String with Point Group symbol

Subroutine to get the information of Laue and Point Group.

Note: Point group determination is only valid for conventional bases

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_Laue_Str (ILaue, Laue_Str)

Integer	**Intent(in)**	ILaue	Ordinal number in Laue_Class
Character(Len=*)	**Intent (out)**	Laue_Str	String with the Laue class

Obtain the string for the Laue class. Control of error is present

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_Orbit (X, Spg, Mult, Orb, Ptr, Str, Prim)

Real(Kind=CP), Dimension(3)	**Intent(in)**	X	Position vector
Type(Space_Group_Type)	**Intent(in)**	Spg	Space Group
Integer	**Intent(out)**	Mult	Multiplicity
Real(Kind=CP), Dimension(:,:)	**Intent(out)**	Orb	List of equivalent positions
Integer, Dimension(:), Optional	**Intent(out)**	Ptr	Pointer to effective symops
Integer, Dimension(:), Optional	**Intent(out)**	Str	Pointer to stabilizer
Character(Len=*), Optional	**Intent(in)**	Prim	If given, only the primitive cell is considered

Obtain the multiplicity and list of equivalent positions (including centring!) modulo Integer lattice translations.

It provides also pointers to the stabilizer and to the symmetry operators changing effectively the position.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_PointGroup_Str (IPG, Str)

Integer	**Intent(in)**	IPG	Ordinal number faccording to Point_Group
Character(Len=*)	**Intent(out)**	Str	String for Point Group

Obtain the string for the Point Group. Error control is present

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_SO_From_Fix (ISystm, ISymCe, IBravl, NG, SS, TS, LatSy, CO, SpaceGen)

Integer	**Intent(out)**	ISystm	Number of the crystalline system 1:T, 2:M, 3:O, 4:T, 5:R-Trg, 6:H, 7:C)
Integer	**Intent(out)**	ISymCe	0: Centric (-1 not at origin) 1: Acentric 2: Centric (-1 at origin)
Integer	**Intent(out)**	IBravl	1:P, 2:A, 3:B, 4:C, 5:I, 6:R, 7:F, 8:Z
Integer	**Intent(in)**	NG	Number of symmetry operators
Integer, Dimension(:,:,:)	**Intent(in)**	SS	Rotation parts of the symmetry operators (3,3,48)
Real(Kind=CP), Dimension(:,:)	**Intent(in)**	TS	Translation parts of the symmetry operators(3,48)
Character(Len=2)	**Intent(out)**	LatSy	Bravais Lattice symbol
Real(Kind=CP), Dimension(3)	**Intent(out)**	CO	Coordinates of origin
Character(Len=1)	**Intent(out)**	SpaceGen	Type of Cell

Determines some of items of the object Space_Group_Type from Fixed symmetry operators given by user.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine GET_SO_FROM_GENER (ISystm, ISymCe, IBravl, NG, SS, TS, LatSy, CO, Num_G, SpaceGen)

Integer	**Intent(out)**	ISystm		Number of the crystalline system 1:T, 2:M, 3:O, 4:T, 5:R-Trg, 6:H, 7:C)
Integer	**Intent(out)**	ISymCe		0: Centric (-1 not at origin) 1: Acentric 2: Centric (-1 at origin)
Integer	**Intent(out)**	IBravl		1:P, 2:A, 3:B, 4:C, 5:I, 6:R, 7:F, 8:Z
Integer	**Intent(in out)**	NG	in: out:	Number of defined generators Number of symmetry operators
Integer, Dimension(:,:,:)	**Intent(in out)**	SS	in: out:	Rotation parts of the given generators (3,3,48) Rotation parts of the symmetry operators
Real(Kind=CP), Dimension(:,:)	**Intent(in out)**	TS	in: out:	Translation parts of the given generators (3,48) Translation parts of the symmetry operators
Character(Len=2)	**Intent(out)**	LatSy		Bravais Lattice symbol
Real(Kind=CP), Dimension(3)	**Intent(out)**	CO		Coordinates of origin
Integer	**Intent(out)**	Num_G		Minimum number of generators
Character(Len=1)	**Intent(out)**	SpaceGen		Type of Cell

Calculates the whole set of symmetry operators from a set of given generators.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_SO_From_Hall (ISystm, ISymCe, IBravl, NG, SS, TS, LatSy, CO, Num_G, Hall)

Integer	Intent(out)	ISsystm		Number of the crystalline system 1:T, 2:M, 3:O, 4:T, 5:R-Trg, 6:H, 7:C)
Integer	Intent(out)	ISymCe		0: Centric (-1 not at origin) 1: Acentric 2: Centric (-1 at origin)
Integer	Intent(out)	IBravl		1:P, 2:A, 3:B, 4:C, 5:I, 6:R, 7:F, 8:Z
Integer	Intent(out)	NG		Number of symmetry operators
Integer, Dimension(:,:,:)	Intent(out)	SS		Rotation parts of the symmetry operators (3,3,48)
Real(Kind=CP), Dimension(:,:)	Intent(out)	TS		Translation parts of the symmetry operators (3,48)
Character(Len=2)	Intent(out)	LatSy		Bravais Lattice symbol
Real(Kind=CP), Dimension(3)	Intent(out)	CO		Coordinates of origin
Integer	Intent(out)	Num_G		Number of generators
Character(Len=20)	Intent(in)	Hall		Hall Space group symbol

Subroutine to get all the information contained in the Hall symbol. This routine to interpret the Hall symbol for a space group.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_SO_From_HMS (ISystm, ISymCe, IBravl, NG, SS, TS, LatSy, SpaceH)

Integer	Intent(out)	ISystm		Number of the crystalline system 1:T, 2:M, 3:O, 4:T, 5:R-Trg, 6:H, 7:C)
Integer	Intent(out)	ISymCe		0: Centric (-1 not at origin) 1: Acentric 2: Centric (-1 at origin)
Integer	Intent(out)	IBravl		1:P, 2:A, 3:B, 4:C, 5:I, 6:R, 7:F, 8:Z
Integer	Intent(out)	NG		Number of symmetry operators
Integer, Dimension(:,:,:)	Intent(out)	SS		Rotation parts of the symmetry operators (3,3,48)
Real(Kind=CP), Dimension(:,:)	Intent(out)	TS		Translation parts of the symmetry operators (3,48)
Character(Len=2)	Intent(out)	LatSy		Bravais Lattice symbol
Character(Len=20)	Intent(in)	SpaceH		H-M Spacegroup symbol

Subroutine to get all the information contained in the H-M symbol. Routine to interpret Hermann-Mauguin symbol for space group

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_Stabilizer (X, Spg, Order, Ptr)

Real(Kind=CP), Dimension(3)	Intent(in)	X		Position vector
Type(Space_Group_Type)	Intent(in)	Spg		Space group
Integer	Intent(out)	Order		Number of sym.op. keeping invariant the position x
Integer, Dimension(:)	Intent(out)	Ptr		Array pointing to the symmetry operators numbers of the stabilizer (point group) of x

Subroutine to obtain the list of symmetry operator of a space group that leaves invariant an atomic position. This subroutine provides a pointer to the symmetry operators of the site point group.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_String_Resolv (T, X, IX, Symb)

Real(Kind=CP), Dimension(3)	**Intent(in)**	T		Traslation part
Real(Kind=CP), Dimension(3)	**Intent(in)**	X		real part of Variable
Integer, Dimension(3)	**Intent(in)**	IX		1:X, 2:Y, 3:Z
Character(Len=*)	**Intent(out)**	Symb		String

Returning a string for point, axes or plane give as written in fractional form from Resolv_Sist procedures in CFML_Math_3D.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_SubOrbits (X, Spg, Ptr, Mult, Orb, Ind, Conv)

Real(Kind=CP), Dimension(3)	**Intent(in)**	X		Position vector
Type(Space_Group_Type)	**Intent(in)**	Spg		Space Group
Integer, Dimension(:)	**Intent(in)**	Ptr		Pointer to symops of a subgroup
Integer	**Intent(out)**	Mult		Multiplicity
Real(Kind=CP), Dimension(:,:)	**Intent(out)**	Orb		List of equivalent positions
Integer, Dimension(:)	**Intent(out)**	Ind		Number of the suborbits
Character(Len=*), Optional	**Intent(in)**	Conv		If present centring transl. are considered

Obtain the multiplicity and list of equivalent positions modulo lattice translations (including centring!) of a position. When symmetry operators of a subgroup of **SPG** is given an index vector **inD** gives the division in subOrbits.

The pointer **PTR** indicates the symmetry operators of **SPG** belonging to the subgroup. The first zero value of **PTR** terminates the search.

If the optional argument **CONV** is given the centring translations are considered. The orbits are formed by all atoms within a conventional unit cell. Otherwise the orbit is formed only with the content of a primitive cell.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_SymEl (Sim, XYZString)

Integer, Dimension(3,3)	**Intent(in)**	Sim	Rotation matrix
Character(Len=*)	**Intent(out)**	XYZString	String (Mx,My,Mz)

Supplies a string with the "symmetry element" (I.T.) for the rotation matrix **SIM**. They correspond to the symbols given in I.T. for space groups Pm3m and P6/mmm.

Note: Logical Hexa must be defined.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_SymKov (Sim, XYZString)

Integer, Dimension(3,3)	**Intent(in)**	SIM	Rotation matrix

Character(Len=*)	**Intent(out)**	XYZString	String (Mx,My,Mz)

Supplies a string with the "symmetry element" (I.T.) for the rotation matrix **SIM**. They correspond to the symbols Kovalev.

Note: Logical Hexa must be defined.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_SymSymb (Sim, Tt, StrSym)

Integer, Dimension(3,3) ***or*** **Real(Kind=CP), Dimension(3,3)**	**Intent(in)**	Sim	Rotational part of the S.O.
Real(Kind=CP), Dimension(3)	**Intent(in)**	Tt	Translational part of the S.O.
Character(Len=*)	**Intent(out)**	StrSym	String in th form X,Y,-Z, ...

Obtain the Jones Faithful representation of a symmetry operator

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Get_T_SubGroups (Spg, SubG, NSG)

Type(Space_Group_Type)	**Intent(in)**	Spg	SpaceGroup
Type(Space_Group_Type), Dimension(:)	**Intent(out)**	SubG	SubGroups
Integer	**Intent(out)**	NSG	Number of SubGroups

Subroutine to obtain the list of all non-trivial *translationengleiche* subgroups (t-subgroups) of a given space group.

The unit cell setting is supposed to be the same as that of the input space group **SPG**. The search of space sub-groups is performed using a systematic combination of the symmetry operators of the group.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Init_Err_Symm ( )

Subroutine that initializes errors flags in **CFML_Crystallographic_Symmetry** module.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Inverse_Symm (R, T, S, U)

Integer, Dimension(3,3)	**Intent(in)**	R	Rotational Part
Real(Kind=CP), Dimension(3)	**Intent(in)**	T	Traslational part
Integer, Dimension(3,3)	**Intent(out)**	S	New Rotational part
Real(Kind=CP), Dimension(3)	**Intent(out)**	U	New traslational part

Calculates the inverse of the symmetry operator (R,t)

CFML_Crystallographic_Symmetry: Subroutines

Subroutine LatSym (Symb, NumL, LatC)

Character(Len=*)	**Intent(in)**	Symb	Space Group H-M/Hall symbol

Integer, Optional	**Intent(in)**	NumL	Number of centring vectors
Real(Kind=CP), Dimension(3,11), Optional	**Intent(in)**	LatC	Centering vectors

Provides the Lattice type of the space group of **SYMB**.

Also gives the index InLat of the lattice, the multiplicity NLat and the fractional lattice translations Ltr and Lat_Ch.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Read_MSymm (Info, Sim, P_Mag)

Character(Len=*)	**Intent(in)**	Info	input string with S.Op. in the form: MSYM u,w,w,p_mag
Integer, Dimension(3,3)	**Intent(out)**	Sim	Rotation matrix
Real(Kind=CP)	**Intent(out)**	P_Mag	Magnetic Phase

Read magnetic symmetry operators in the form U,V,W, etc...

Provides the magnetic rotational matrix and phase associated to a MSYM symbol

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Read_SymTrans_Code (Code, N, Tr)

Character(Len=*)	**Intent(in)**	Code	String to read
Integer	**Intent(out)**	N	Number of Op. S.
Real(Kind=CP), Dimension(3)	**Intent(out)**	Tr	Traslation applied

Read a Code string for reference the symmetry operator and the Traslation applied.

Example: _2.555 : N= 2; TR=(0.0, 0.0, 0.0)
_3.456 : N= 3, TR=(-1.0, 0.0, 1.0)

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Read_XSym (Info, IStart, Sim, Tt)

Character(Len=*)	**Intent(in)**	Info	String with the symmetry symbol in the form: SYMM x,-y+1/2,z
Integer	**Intent(in)**	IStart	Starting index of info to read in
Integer, Dimension(3,3)	**Intent(out)**	Sim	Rotational part of the S.O.
Real(Kind=CP), Dimension(3), Optional	**Intent(out)**	Tt	Traslational part of S.O.

Read symmetry or transformation operators in the form X,Y,Z, etc...

Provides the rotational matrix and translation associated a to SYMM symbol in the Jones Faithful representation.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine SearchOP (Sim, I1, I2, ISL)

Integer, Dimension(3,3)	**Intent(in)**	Sim	Rotation matrix
Integer	**Intent(in)**	I1	index for search
Integer	**Intent(in)**	I2	index for search
Integer	**Intent(out)**	ISL	index of the matrix Mod6(Isl,:,:)=**SIM**

Search the index on MOD6 variable

Matrices of m3m (not hexagonal): I1=1 I2=24
Matrices of 6/mmm (hexagonal): I1=25 I2=36

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Set_SpaceGroup (SpaceGen, SpaceGroup, Gen, NGen, Mode, Force_Hall)

Character(Len=*)	**Intent(in)**	SpaceGen	String with Number, Hall or Hermman-Mauguin
Type(Space_Group_Type)	**Intent(out)**	SpaceGroup	Space Group
Character(Len=*), Dimension(:), Optional	**Intent(in)**	Gen	String Generators
Integer, Optional	**Intent(in)**	NGen	Number of Generators
Character(Len=*), Optional	**Intent(in)**	Mode	Value must be: HMS, ITC, HALL, GEN, FIX
Character(Len=*), Optional	**Intent(in)**	Force_Hall	If present force generation from Hall

Subroutine that construct the object SpaceGroup from the H-M or Hall symbol.

Expand the set of operators including centre of symmetry and non Integer translations for centred cells. If the optional argument **GEN** is given, then **NGEN** and **MODE**="GEN" should be given.

If the optional argument **MODE**="ITC", the space group will be generated using the generators given in the international Tables for the standard setting. in this case the string in SPACEGEN should correspond to the Hermann-Mauguin symbol.

If the optional argument **MODE**="HMS","HALL" is given the string in SPACEGEN should correspond to the desired symbol.

If GEN, NGEN and MODE are not given but FORCE_HALL="F_HALL" is given, the generation of the symmetry operators from the symbol of the space group is according to the Hall symbol even if the provided symbol is of Hermann-Maugin type.

The use of the different options give rise to different ordering of the symmetry operators or different origins and settings for the same space group.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Set_Spg_Mult_Table (Spg, Tab, Complete)

Type(Space_Group_Type)	**Intent(in)**	Spg	String with Number, Hall or Hermman-Mauguin
Integer, Dimension(:,:)	**Intent(out)**	Tab	Table
Logical, Optional	**Intent(in)**	Complete	

Subroutine to construct the multiplication table of the factor group of a space group. Two operators are equal if they differ only in a lattice translation. The multiplication table is a square matrix with Integer numbers corresponding to the ordering of operators in the space group.

If **Complete** is not present, or if **Complete**=**.FALSE.**, we consider only the symmetry operators corresponding to the "primitive" content of the unit cell, so a maximun 48x48 matrix is needed to hold the table in this case. If **Complete** is present and **.TRUE.**, the full table is constructed.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Setting_Change (From_Syst, To_Syst, SpaceGroup, CarR_Sym, ICar_Sym)

Character(Len=2)	**Intent(in)**	From_Syst	Values: IT, ML, KO, BC, ZA
Character(Len=2)	**Intent(in)**	To_Syst	Values: IT, ML, KO, BC, ZA
Type(Space_Group_Type)	**Intent(in out)**	SpaceGroup	Space Group
Character(Len=35)	**Intent(out)**	Car_Sym	
Character(Len=35)	**Intent(out)**	ICar_Sym	

Traslate From From_Syst to To_syst the set of symmetry operators

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Similar_Transf_SG (Mat, Orig, Spg, SpgN, MatKind, Fix_Lat)

Real(Kind=CP), Dimension(3,3)	**Intent(in)**	Mat	Matrix transforming the basis
Real(Kind=CP), Dimension(3)	**Intent(in)**	Orig	Coordinates of the new origin
Type(Space_Group_Type)	**Intent(in)**	Spg	Space Group
Type(Space_Group_Type)	**Intent(out)**	SpgN	Maximum subgroup of SPG
Character(Len=*), Optional	**Intent(in)**	MatKind	Type of the input matrix
Character(Len=*), Optional	**Intent(in)**	Fix_Lat	Fixing Lattice type

Subroutine to construct a space group **SPGN** that is a maximal subgroup of the input space group **SPG** compatible with the transformation of the basis corresponding to the matrix **MAT** and the new origin **ORIG**.

The transformed **SPGN** will have (if it is the case) conventional centring vectors.

If **MATKind** is given and matkind="it"/"IT", the input matrix is given as in international Tables:

(a' b' c') = (a b c) Mat

If **MATKind** is not given or if it is not equal to "it"/"IT" the input matrix is the transpose of the international convention (column matrices for basis vectors).

The new space group is obtained using the properties of conventional Bravais lattices and symmetry operators. Only the symmetry operators of the conventional form are retained to construct the new space group.

If the Hermann-Mauguin symbol is not given, that means it correspond to a special setting. The Hall symbol is always given.

The coordinates of the origin is always given with respect to the (a b c) basis.

If **FIX_LAT** is given a conventional lattice centring, this is fixed irrespective of the centring obtained by applying the similarity transformation. For instance is **FIX_LAT**="P" and the transformation implies new centring vectors or the input group is centred, the generators with fraccional translations are removed from the group. If **FIX_LAT**="A" (or whatever) the program will add the corresponding generators irrespective that the generator is in the original/transformed group.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Sym_B_Relations (OP / Symb, B_Ind, B_Fac)

Integer, Dimension(3,3) ***or***	**Intent(in)**	OP	Rotation Matrix

Character(Len=*)		Symb	Symmetry string
Integer, Dimension(6)	**Intent(out)**	B_Ind	B index
Real(Kind=CP), Dimension(6)	**Intent(out)**	B_Fac	B Factor

Symmetry relations among coefficients of the anisotropic temperature factor.

Order for B is: B_{11} B_{22} B_{33} B_{12} B_{13} B_{23}

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Sym_Prod_St (SymA, SymB, SymAB, ModLat)

Character(Len=*)	**Intent(in)**	SymA	
Character(Len=*)	**Intent(in)**	SymB	
Character(Len=*)	**Intent(out)**	SymAB	
LogicalL, Optional	**Intent(in)**	ModLat	

Obtain the symbol/Op/Matrix+trans of the symmetry operation corresponding to the product of two operators given in the Jone's Faithful(symbol) reprentation or in Symmetry Operator type.

If **ModLat=.TRUE.** or it is not present, the traslation part of the resulting operator is reduced to have components < 1.0

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Symmetry_Symbol (OP, Symb)

Type(Sym_Oper_Type)	**Intent(in)**	OP	Symmetry Operator
Character(Len=*)	**Intent(out)**	Symb	String for the symbol of the symmetry element

or

Subroutine Symmetry_Symbol (S, T, Symb)

Integer, Dimension(3,3)	**Intent(in)**	S	Rotational part
Real(Kind=CP), Dimension(3)	**Intent(in)**	T	Traslational part
Character(Len=*)	**Intent(out)**	Symb	String for the symbol of the symmetry element

or

Subroutine Symmetry_Symbol (Symm, Symb)

Character(Len=*)	**Intent(in)**	Symm	String Symmetry Operator
Character(Len=*)	**Intent(out)**	Symb	String for the symbol of the symmetry element

Obtain the symbol of the symmetry element of the operator Op

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Write_SpaceGroup (SpaceGroup, Iunit, Full)

Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	Space Group
Integer, Optional	**Intent(in)**	Iunit	Write information on IUNIT
Logical, Optional	**Intent(in)**	Full	Full operator or not

Writing in file of logical unit **IUNIT** the characteristics of the space group **SpaceGroup**. Part of the information contained in **SpaceGroup** may be undefined, depending on the tabulated nature of the item.

If **FULL**=**.TRUE.** is present the whole group is output including the symmetry symbol associated to each operator.

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Write_Sym (Lun, Indx, Sim, Tt, P_Mag, Mag)

Integer	**Intent(in)**	Lun	Logical unit of the file to write
Integer	**Intent(in)**	Indx	Ordinal of the current Symm.Operator
Integer, Dimension(3,3)	**Intent(in)**	Sim	Rotational part of the S.O.
Real(Kind=CP), Dimension(3)	**Intent(in)**	Tt	Translation part of the S.O.
Real(Kind=CP)	**Intent(in)**	P_Mag	Magnetic phase of the magnetic S.O.
Logical	**Intent(in)**	Mag	.true. if it is a magnetic S.O.

Writing the reduced set of symmetry operators.

Note: Logical Hexa must be defined (valid for conventional bases)

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Write_SymTrans_Code (N, Tr, Code)

Integer	**Intent(in)**	N	Number of the Symmetry Operator
Real(Kind=CP), Dimension(3)	**Intent(in)**	Tr	Traslational part
Character(Len=*)	**Intent(out)**	Code	String

Write the code string for reference the symmetry operator and the Traslation applied.

Example: N=2; TR=(0.0, 0.0, 0.0) -> CODE=_2.555
N=3; TR=(-1.0, 0.0, 1.0) -> CODE=_3.456

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Write_Wyckoff (Wyckoff, Spg_Name, Lun, Sorting)

Type(Wyckoff_Type)	**Intent(in)**	Wyckoff	Wyckoff Type variable
Character(Len=*)	**Intent(in)**	Spg_Name	Space Group
Integer, Optional	**Intent(in)**	Lun	Unit to write the information
Logical, Optional	**Intent(in)**	Sorting	.true. for sorting list

Print/Write the Wyckoff positions in LUN unit

CFML_Crystallographic_Symmetry: Subroutines

Subroutine Wyckoff_Orbit (SpaceGroup, WyckoffStr, N_Orbit, OrbitStr)

Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	Space Group
Character(Len=*)	**Intent(in)**	WyckoffStr	Representative of the Orbit
Integer	**Intent(out)**	N_Orbit	Unit to write the information
Character(Len=*), Dimension(:)	**Intent(out)**	OrbitStr	.true. for sorting list

Calculation of the Wyckoff positions from the representative element

CFML_ILL_Instrm_Data

Subroutines related to instrument information from ILL

Variables

- Basic_NumC_Type
- Basic_NumI_Type
- Basic_NumR_Type
- Diffractometer_Type
- Generic_Numor_Type
- ILL_Data_Record_Type
- Powder_Numor_Type
- SXTAL_Numor_Type
- SXTAL_Orient_Type

- Current_Instrm
- Current_Orient
- Cycle_Number
- Err_ILLData
- Err_ILLData_Mess
- ILL_Data_Directory
- Instrm_Directory
- Machine_Name
- Year_ILLData

Subroutines

- Allocate_Powder_Numors
- Allocate_SXTAL_Numors
- Define_Uncompress_Program
- Get_Absolute_Data_Path
- Get_Next_YearCycle
- Get_Single_Frame_2D
- Initialize_Data_Directory
- PowderNumor_To_DiffPattern
- Read_Current_Instrm
- Read_Numor_D1B
- Read_Numor_D20
- Read_Powder_Numor
- Read_SXTAL_Numor
- Set_Current_Orient
- Set_Default_Instrument
- Set_ILL_Data_Directory
- Set_Instrm_Directory
- Update_Current_Instrm_UB
- Write_Current_Instrm_Data
- Write_Generic_Numor
- Write_Powder_Numor
- Write_SXTAL_Numor

Fortran Filename

CFML_ILL_instrm_Data.f90

CFML_ILL_Instrm_Data: Variables

- Basic_NumC_Type
- Basic_NumI_Type
- Basic_NumR_Type
- Diffractometer_Type
- Generic_Numor_Type
- ILL_Data_Record_Type
- Powder_Numor_Type
- SXTAL_Numor_Type
- SXTAL_Orient_Type

- Current_Instrm
- Current_Orient
- Cycle_Number
- Err_ILLData
- Err_ILLData_Mess
- ILL_Data_Directory
- Instrm_Directory
- Machine_Name
- Year_ILLData

CFML_ILL_Instrm_Data: Variables

	Variable	***Definition***
Type :: Basic_NumC_Type		
Integer	N	Number of elements
Character(Len=40), Dimension(:), Allocatable	NameVar	Name of the different fields
Character(Len=80), Dimension(:), Allocatable	CValues	String Values
End Type Basic_NumC_Type		

CFML_ILL_Instrm_Data: Variables

	Variable	***Definition***
Type :: Basic_NumI_Type		
Integer	N	Number of elements
Character(Len=40), Dimension(:), Allocatable	NameVar	Name of fields

Integer, Dimension(:), Allocatable	IValues	Integer values
End Type Basic_NumI_Type		

CFML_ILL_Instrm_Data: Variables

	Variable	***Definition***
Type :: Basic_NumR_Type		
Integer	N	Number of elements
Character(Len=40), Dimension(:), Allocatable	NameVar	Name of fields
Real(Kind=CP), Dimension(:), Allocatable	RValues	Real values
End Type Basic_NumR_Type		

CFML_ILL_Instrm_Data: Variables

	Variable	***Definition***
Type :: Diffractometer_Type		
Character(Len=80)	Info	information about the instrument
Character(Len=10)	Name_Inst	Short name of the instrument
Character(Len=15)	Geom	Eulerian_4C, Kappa_4C, Lifting_arm, Powder, Laue,...
Character(Len=6)	BL_Frame	Kind of BL-frame: ***z-up*** or ***z-down***
Character(Len=4)	Dist_Units	distance units: mm, cm, inch
Character(Len=4)	Angl_Units	angle units: rad, deg
Character(Len=30)	Detector_Type	Point, Flat_rect, Cylin_ImPlate, Tube_PSD, ...
Real(Kind=CP)	Dist_Samp_Detector	Dist. to centre for: Point, Flat_rect, Tube_PSD Radius for: Cylin_ImPlate
Real(Kind=CP)	Wave_Min	Minimum wavelength (Laue diffractometers)
Real(Kind=CP)	Wave_Max	Maximum wavelength (Laue diffractometers)
Real(Kind=CP)	Vert	Vertical dimension
Real(Kind=CP)	Horiz	Horizontal dimension
Real(Kind=CP)	AGap	Gap between anodes
Real(Kind=CP)	CGap	Gap between cathodes
Integer	NP_Vert	Number of pixels in vertical direction
Integer	NP_HorizZ	Number of pixels in horizontal direction
Integer	IGeom	1: Bissectrice (PSI=0) 2: Bissecting - HiCHI 3: Normal beam 4: Parallel (PSI=90)
Integer	IPsd	1: Flat 2: Vertically Curved detector (used in D19amd)
Real(Kind=CP), Dimension(3)	E1	Components of e1 in {i,j,k}
Real(Kind=CP), Dimension(3)	E2	Components of e2 in {i,j,k}
Real(Kind=CP), Dimension(3)	E3	Components of e3 in {i,j,k}
Integer	Num_Ang	Number of angular motors

Character(Len=12), Dimension(15)	Ang_Names	Name of angular motors
Real(Kind=CP), Dimension(15,2)	Ang_Limits	Angular limits (up to 15 angular motors)
Real(Kind=CP), Dimension(15)	Ang_Offsets	Angular offsets
Integer	Num_Disp	Number of displacement motors
Character(Len=12), Dimension(10)	Disp_Names	Name of displacement motors
Real(Kind=CP), Dimension(10,2)	Disp_Limits	Displacement limits (up to 15 displacement motors)
Real(Kind=CP), Dimension(10)	Disp_Offsets	Displacement offsets
Real(Kind=CP), Dimension(3)	Det_Offsets	Offsets X,Y,Z of the detector centre
Real(Kind=CP), Allocatable, Dimension(:,:)	Alphas	Efficiency corrections for each pixel
End Type Diffractometer_Type		

CFML_ILL_Instrm_Data: Variables

	Variable	***Definition***
Type :: Generic_Numor_Type		
Integer	Numor	Numor
Character(Len=4)	Instr	instrument on ILL
Character(Len=10)	ExpName	Experimental Name
Character(Len=20)	Date	Date
Character(Len=80)	Title	Title
Type(Basic_NumC_Type)	SampleID	Sample Identification
Type(Basic_NumR_Type)	DiffOpt	Diffractometer Optics and Reactor Parameters
Type(Basic_NumR_Type)	MonMPar	Monochromator Motor Parameters
Type(Basic_NumR_Type)	DiffMPar	Diffractometer Motor Parameters
Type(Basic_NumR_Type)	DetPar	Detector Parameters
Type(Basic_NumI_Type)	DAcFlags	Data Acquisition Control
Type(Basic_NumR_Type)	DAcParam	Data Acquisition Parameters
Type(Basic_NumR_Type)	SampleST	Sample status
Type(Basic_NumI_Type)	ICounts	Counts as Integers
Type(Basic_NumR_Type)	RCounts	Counts as Reals
End Type Generic_Numor_Type		

CFML_ILL_Instrm_Data: Variables

	Variable	***Definition***
Type :: ILL_Data_Record_Type		
Integer	Numor	Data set numor
Integer	NSet_Prime	Set number (groups of 100000 numor)
Integer	NTran	(key2) 0 or numcomp => data transferred?

Character(Len=4)	Inst_CH	instrument name
Character(Len=22)	Date_CH	Measurement date
Character(Len=2)	Fill_CH	(key3) leader
Character(Len=6)	User_CH	User name
Character(Len=6)	LC_CH	Local contact name
Character(Len=72)	TextT_CH	Comentary
Character(Len=8)	Scan_Motor	Principal scan motor name
Integer	NVers	Data version number
Integer	NType	Data type - single/multi/powder
Integer	KCTRL	Data function type
Integer	Manip	Principle scan angle
Integer	NBang	Number of data saved
Integer	NKMes	Pre-calculated number of points
Integer	NPDone	Actual number of points
Integer	JCode	Count on monitor/time
Integer	ICalc	Angle calculation type
Integer	IAnal	Analyser present (D10)
Integer	IMode	2th motor sense (D10)
Integer	ITGV	D19/D9 fast measurement
Integer	IRegul	Temperature monitor function
Integer	IVolt	Voltmeter function
Integer	NAxe	D10 (number of axes)
Integer	NPStart	Point starting no frag. numor (D19/16)
Integer	ILasti	Elastic measurement (D10)
Integer	ISA	Analyser motor sense (D10)
Integer	FLGKIF	Constant ki or kf (D10)
Integer	IH_SQS	D10 sqs variation on h
Integer	IK_SQS	D10 sqs variation on k
Integer	NBSQS	D10 sqs slice number
Integer	NB_Cells	Multi/powder data - number of detectors
Integer	NFree1	Data control (free)
Integer, Dimension(7)	ICDESC	
Real(Kind=CP), Dimension(35)	ValCO	RVAL(1:35)
Real(Kind=CP), Dimension(10)	ValDEF	RVAL(36:45)
Real(Kind=CP), Dimension(5)	ValENV	RVAL(46:50)
End Type ILL_Data_Record_Type		

Definition for Data Record type

CFML_ILL_Instrm_Data: Variables

	Variable	***Definition***
Type :: Powder_Numor_Type		

Integer	Numor	Numor
Integer	Manip	Principle scan angle
Integer	ICalc	Angle calculation type
Character(Len=32)	Header	User, local contact, date
Character(Len=4)	Instrm	Instrument Name
Character(Len=32)	Title	Title
Character(Len=8)	ScanType	Omega, Phi, etc...
Real(Kind=CP), Dimension(5)	Angles	Angles: phi, chi, omega, 2theta(gamma), psi
Real(Kind=CP), Dimension(3)	Scans	Scan start, scan step, scan width
Real(Kind=CP)	Monitor	
Real(Kind=CP)	Time	
Real(Kind=CP)	Wave	wavelength
Real(Kind=CP), Dimension(5)	Conditions	Temp-s.pt,Temp-Regul,Temp-sample,Voltmeter,Mag.field
Integer	NBData	Total number of pixels nx*ny = np_vert*np_horiz
Integer	NFrames	Total number of frames
Integer	NBAng	Total number of angles moved during scan
Integer, Dimension(7)	ICDesc	Integer values
Real(Kind=CP), Dimension(:,:), Allocatable	TMC_Ang	Time,monitor,total counts, angles*1000: To be allocated as Tmc_ang(nbang,nframes)
Real(Kind=CP), Dimension(:,:), Allocatable	Counts	Counts array to be reshaped (np_vert,np_horiz,nframes) in case of 2D detectors. To be allocated as Counts(nbdata,nframes)
End Type Powder_Numor_Type		

CFML_ILL_Instrm_Data: Variables

	Variable	***Definition***
Type :: SXTAL_Numor_Type		
Integer	Numor	Numor
Integer	Manip	Principle scan angle
Integer	ICalc	Angle calculation type
Character(Len=32)	Header	User, local contact, date
Character(Len=32)	Title	Title
Character(Len=8)	ScanType	Omega, Phi, etc
Real(Kind=CP),Dimension(3)	HMin	h,k,l for Omega scans
Real(Kind=CP),Dimension(3)	HMax	
Real(Kind=CP),Dimension(5)	Angles	Phi, Chi, Omega, 2 (Gamma), Psi
Real(Kind=CP),Dimension(3,3)	UB	UB-matrix
Real(Kind=CP),Dimension(3)	DH	delta_h, delta_k, delta_l
Real(Kind=CP),Dimension(3)	Scans	scan start, scan step, scan width
Real(Kind=CP)	Preset	
Real(Kind=CP)	Wave	Wavelength
Real(Kind=CP)	CPL_Fact	Coupling Factor
Real(Kind=CP),Dimension(5)	Conditions	Temp-s.pt,Temp-Regul,Temp-sample,Voltmeter,Mag.fi

		eld
Integer	NBData	Total number of pixels nx*ny = np_vert*np_horiz
Integer	NFrames	Total number of frames
Integer	NBAng	Total number of angles moved during scan
Integer, Dimension(7)	ICDesc	Integer values
Real(Kind=CP), Allocatable, Dimension(:,:)	TMC_Ang	Array (NBANG,NFRAMES) .Time,monitor,total counts, angles*1000
Real(Kind=CP), Allocatable, Dimension(:,:)	Counts	Array ((NBANG,NFRAMES) . To be reshaped (NP_VERT x NP_HORIZ, NFRAMES) in case of 2D detectors
End Type SXTAL_Numor_Type		

Definition for XTAL Numor type

CFML_ILL_Instrm_Data: Variables

	Variable	***Definition***
Type :: SXTAL_Orient_Type		
Real(Kind=CP)	Wave	Wavelength
Real(Kind=CP),Dimension(3,3)	UB	UB matrix in Busing-Levy setting
Real(Kind=CP),Dimension(3,3)	UBInv	inverse of UB-matrix
Real(Kind=CP),Dimension(3,3)	Conv	Conversion matrix to the local setting
End Type SXTAL_Orient_Type		

CFML_ILL_Instrm_Data: Variables

Type(Diffractometer_Type) :: Current_Instrm

Define a **Current_Instrm** variable according to Diffractometer_Type

CFML_ILL_Instrm_Data: Variables

Type(SXTAL_Orient_Type) :: Current_Orient

Define a **Current_Orient** variable according to SXTAL_Orient_Type

CFML_ILL_Instrm_Data: Variables

Integer :: Cycle_Number

Value to give the cycle number of Reactor at ILL

CFML_ILL_Instrm_Data: Variables

Logical :: Err_ILLData

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_ILL_Instrm_Data: Variables

Character (Len=150) :: Err_ILLData_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_ILL_Instrm_Data: Variables

Character(Len=512) :: ILL_Data_Directory

String containing information about the path for data directory for ILL

CFML_ILL_Instrm_Data: Variables

Character(Len=512) :: ILL_Temp_Directory

String containing information about the path for Temporal directory. It is used for uncompress the .Z files

CFML_ILL_Instrm_Data: Variables

Character(Len=512) :: Instrm_Directory

String containing information about the data directory for specific instrument

CFML_ILL_Instrm_Data: Variables

Character(Len=8) :: Machine_Name

String containing information about the instrument name

CFML_ILL_Instrm_Data: Variables

Integer :: Year_ILLData

Variable indicating the year for ILL data

CFML_ILL_Instrm_Data: Subroutines

- Allocate_Powder_Numors
- Allocate_SXTAL_Numors
- Define_Uncompress_Program
- Get_Absolute_Data_Path
- Get_Next_YearCycle
- Get_Single_Frame_2D
- Initialize_Data_Directory
- PowderNumor_To_DiffPattern
- Read_Current_Instrm
- Read_Numor_D1B
- Read_Numor_D20
- Read_Powder_Numor
- Read_SXTAL_Numor
- Set_Current_Orient
- Set_Default_Instrument
- Set_ILL_Data_Directory
- Set_Instrm_Directory
- Update_Current_Instrm_UB
- Write_Current_Instrm_Data
- Write_Generic_Numor

Write_Powder_Numor
Write_SXTAL_Numor

CFML_ILL_Instrm_Data: Subroutines

Subroutine Allocate_Powder_Numors (Num_Max, NData, Num_Ang, NFrames, Num)

Integer	**Intent(in)**	Num_Max	Number of components of the array (dimension of Num)
Integer	**Intent(in)**	NData	Number of pixels of a single frame
Integer	**Intent(in)**	Num_Ang	Number of angles moved simultaneously during the scan
Integer	**Intent(in)**	NFrames	Number of frames (number of scan points)
Type(Powder_Numor_Type), Allocatable, Dimension(:)	**Intent(in out)**	Num	Numor

Subroutine allocating and initializing the array **Num** of type Powder_Numnor_Type

CFML_ILL_Instrm_Data: Subroutines

Subroutine Allocate_SXTAL_Numors (Num_Max, NData, Num_Ang, NFrames, Num)

Integer	**Intent(in)**	Num_Max	Number of components of the array (dimension of Num)
Integer	**Intent(in)**	NData	Number of pixels of a single frame
Integer	**Intent(in)**	Num_Ang	Number of angles moved simultaneously during the scan
Integer	**Intent(in)**	NFrames	Number of frames (number of scan points)
Type(SXTAL_Numor_Type), Allocatable, Dimension(:)	**Intent(in out)**	Num	Numor

Subroutine allocating and initializing the array **Num** of type SXTAL_Numor_Type

CFML_ILL_Instrm_Data: Subroutines

Subroutine Define_Uncompress_Program (ProgName)

Character(Len=*)	**Intent(in)**	ProgName	Name of the uncompress program

Routine that define the ProgName program that you wants to use

CFML_ILL_Instrm_Data: Subroutines

Subroutine Get_Absolute_Data_Path (Numor, Instrm, Path, IYear, ICycle)

Integer	**Intent(in)**	Numor	Numor
Character (Len=*)	**Intent(in)**	Instrm	instrument Name
Character (Len=*)	**Intent(out)**	Path	Absolute Path
Integer, Optional	**Intent(in)**	IYear	Year
Integer, Optional	**Intent(in)**	ICycle	Cycle number

Finds the absolute path to any Numor.

The base directory is set by a call to Initialize_Data_Directory. The procedure then searches for the Numor in the following order:

1. In the subdirectory defined by the year and cycle if passed as arguments to the subroutine (i.e args iyear, icycle).
2. In the subdirectory defined by the year and cycle of the previous call to Get_Absolute_Data_Path (since Numors are likely to be adjacent).
3. In the DATA subdirectory (since likely to process recent data).
4. In the DATA-1 subdirectory (same logic as above)
5. Working from the current year and most recent cycle and working back through cycles and year until the stopping at the first cycle of 1973, when the first data was archived.

Tries to find an uncompress Numor first and then tries to find a compressed Numor (.Z extension). If found the Numor is uncompressed in the a temporary directory if defined (see subroutine Initialize_Data_Directory) or else into the current directory.

CFML_ILL_Instrm_Data: Subroutines

Subroutine Get_Next_YearCycle (YearCycle, Reset_To_Most_Recent)

Character (Len=*)	**Intent(out)**	YearCycle	
Logical, Optional	**Intent(in)**	Reset_To_Most_Recen t	

Works back through the cycles and years, returning the previous YearCycle combination as a 3 character string i.e.

if Year_ILLData = 6 and cycle_number = 5, returns '064'
if Year_ILLData = 6 and cycle_number = 1, returns '057'

The Reset_To_Most_Recent flag allows the Year_ILLData and Cycle_Number to be set to the most recent possible.
If asked for a YearCycle before '731' (first cycle of 1973) then returns " ", since no data was archived before this date.

CFML_ILL_Instrm_Data: Subroutines

Subroutine Get_Single_Frame_2D (NFr, IOrd, SNum, Dat_2D, Appl_Alphas)

Integer	**Intent(in)**	NFr	Frame number
Integer	**Intent(in)**	IOrd	Type of order: 1: D19 Banana 2: D9/D10 3: D19 Flat 4: D20
Type(SXTAL_Numor_Type)	**Intent(in)**	SNum	Numor Object
Real(Kind=CP), Dimension(:,:)	**Intent(out)**	Dat_2D	
Logical, Optional	**Intent(in)**	Appl_Alphas	Efficiency corrections flag

Extracts into the real two-dimensional array **Dat_2D** the counts of the frame number NFr of the Numor object SNum, applying the efficiency corrections depending of the optional argument Appl_Alphas

CFML_ILL_Instrm_Data: Subroutines

Subroutine Initialize_Data_Directory ( )

Initialize the Data directory where data are saved at ILL.

CFML_ILL_Instrm_Data: Subroutines

Subroutine PowderNumor_To_DiffPattern (Numor, Pat)

Type(Powder_Numor_Type)	**Intent(in)**	Numor	Numor Object
Type(Diffraction_Pattern_Type)	**Intent(out)**	Pat	Pattern Object

Pass all information from Numor object to Diffraction Pattern object

CFML_ILL_Instrm_Data: Subroutines

Subroutine Read_Current_Instrm (Filenam)

Character (Len=*)	**Intent(in)**	Filenam	String

Subroutine reading the file Filenam where the characteristics of the current instrument are written. The global Current_Instrm variable is filled after
returning from this subroutine.

CFML_ILL_Instrm_Data: Subroutines

Subroutine Read_Numor_D1B (Fileinfo, N)

Character (Len=*)	**Intent(in)**	Fileinfo	Filename
Type(Powder_Numor_Type)	**Intent(out)**	N	Generic Numor

Subroutine to read a Numor of D1B instrument at ILL

CFML_ILL_Instrm_Data: Subroutines

Subroutine Read_Numor_D20 (Fileinfo, N)

Character (Len=*)	**Intent(in)**	Fileinfo	Filename
Type(Generic_Numor_Type)	**Intent(out)**	N	Generic Numor

Subroutine to read a Numor of D20 instrument at ILL

CFML_ILL_Instrm_Data: Subroutines

Subroutine Read_Powder_Numor (Numor, Instrm, PathDir, SNum, Info)

Integer	**Intent(in)**	Numor	Numor
Character (Len=*)	**Intent(in)**	Instrm	instrument Name
Character (Len=*)	**Intent(in)**	PathDir	Path directory
Tytpe(Powder_Numor_Type)	**Intent(in out)**	SNum	Object
Logical, Optional	**Intent(in)**	Info	

Read the numor **Numor** from the ILL database and construct the object **SNum** of type **Powder_Numor_Type**.

CFML_ILL_Instrm_Data: Subroutines

Subroutine Read_SXTAL_Numor (Numor, Instrm, SNum)

Integer	**Intent(in)**	Numor	Numor
Character (Len=*)	**Intent(in)**	Instrm	Instrument Name
Type(SXTAL_Numor_Type)	**Intent(in out)**	SNum	Object

Read the numor **Numor** from the ILL database and construct the object **SNum** of type SXTAL_Numor_Type.

CFML_ILL_Instrm_Data: Subroutines

Subroutine Set_Current_Orient (Wave, UB, Setting)

Real(Kind=CP)	**Intent(in)**	Wave	Wavelength
Real(Kind=CP), Dimension(3,3)	**Intent(in)**	UB	UB Matrix
Real(Kind=CP), Dimension(3,3), Optional	**Intent(in)**	Setting	Object

Subroutine setting the Current_Orient global variable.
If the final UB matrix is singular an error is raised by putting Err_ILLData=.true. and filling the error message variable Err_ILLData_Mess.

CFML_ILL_Instrm_Data: Subroutines

Subroutine Set_Default_Instrument ( )

Construct the Current_Instrm as a default 4C diffractometer. The UB matrix is set to a real matrix corresponding to a measurement done on D9.
The characteristics of the diffractometer correspond to those of D9.

CFML_ILL_Instrm_Data: Subroutines

Subroutine Set_ILL_Data_Directory (FileDir)

Character (Len=*)	**Intent(in)**	FileDir	Proposed location of ILL data

Assign a new directory to the global public variable ILL_Data_Directory. If the directory doesn't exist the subroutine rises an error condition by putting Err_ILLData=.TRUE. and filling the error message variable Err_ILLData_Mess. If **FileDir** is blank then data are in the current directory.

CFML_ILL_Instrm_Data: Subroutines

Subroutine Set_Instrm_Directory (Working_Dir, Instrm, IYear, ICycle)

Character (Len=*), Optional	**Intent(in)**	Working_Dir	Directory for Numors
Character (Len=*), Optional	**Intent(in)**	Instrm	Name of the instrument
Character (Len=*), Optional	**Intent(in)**	IYear	Year of the Numor
Character (Len=*), Optional	**Intent(in)**	ICycle	Cycle of the Numor

Assign the global public variable: Instrm_Directory.

If Working_Dir was defined, then it is the directory defined for Instrm_Directory. If not, then **Instrm** is used.
When the routine is called using **Instrm** argument, we have two options:

- Using IYear and ICycle arguments: Instrm_Directory= ILL_Data_Directory/YYC/**Instrm/**
- Only with Instrm argument: Instrm_Directory= ILL_Data_Directory/data/**Instrm/**

It is assumed that the subroutine Set_ILL_Data_Directory has already been called.

CFML_ILL_Instrm_Data: Subroutines

Subroutine Update_Current_Instrm_UB (Filenam, UB, Wave)

Character (Len=*)	**Intent(in)**	Filenam	Filename
Read(Kind=CP), Dimension(3,3)	**Intent(in)**	UB	UB Matrix
Read(Kind=CP)	**Intent(in)**	Wave	Wavelength

Subroutine updating the file **Filenam** where the characteristics of the current instrument are written. The global Current_Instrm variable is re-filled with
new values of wavelength and UB-matrix. The file **Filenam** is re-written and the old version is saved with appended extension '.bak'. The Current_Orient global variable is also updated.

CFML_ILL_Instrm_Data: Subroutines

Subroutine Write_Current_Instrm_Data (Lun)

Integer, Optional	**Intent(in)**	Lun	Unit to write

Writes the characteristics of the Current_Instrm instrument in the file of logical unit Lun. If the subroutine is invoked without argument the subroutine outputs the information on the standard output (screen)

CFML_ILL_Instrm_Data: Subroutines

Subroutine Write_Generic_Numor (N, Lun)

Type(Generic_Numor_Type)	**Intent(in)**	Num	Numor object
Integer, Optional	**Intent(in)**	Lun	Unit to write

Writes the characteristics of the Numor objet **Num** of type Generic_Numor_Type in the file of logical unit **Lun**. If the subroutine is invoked without the **Lun** argument the subroutine outputs the information on the standard output (screen)

CFML_ILL_Instrm_Data: Subroutines

Subroutine Write_Powder_Numor (Num, Inst, Lun)

Type(Powder_Numor_Type)	**Intent(in)**	Num	Numor object
Character (Len=*)	**Intent(in)**	Inst	instrumental Name
Integer, Optional	**Intent(in)**	Lun	Unit to write

Writes the characteristics of the numor objet **Num** of type Powder_Numor_Type in the file of logical unit **Lun**. If the subroutine is invoked without the **Lun**
argument the subroutine outputs the information on the standard output (screen)

CFML_ILL_Instrm_Data: Subroutines

Subroutine Write_SXTAL_Numor (Num, Lun)

Type(SXTAL_Numor_Type)	**Intent(in)**	Num	Numor object
Integer, Optional	**Intent(in)**	Lun	Unit to write

Writes the characteristics of the numor objet **Num** of type SXTAL_Numor_Type in the file of logical unit **Lun**. If the subroutine is invoked without the

Lun argument the subroutine outputs the information on the standard output (screen)

Level 4

Concept	*Module Name*	*Purpose*
Atoms...	**CFML_Atom_TypeDef**	Module defining different data structures concerned with atoms
Geometry...	**CFML_Geometric_SXTAL**	Module for geometrical calculations in single crystal instruments
Reflections...	**CFML_Reflections_Utilities**	Procedures handling operation with Bragg reflections

CFML_Atom_TypeDef

Module for Atom Types definitions

Variables

Atom_Type
Atom_List_Type
Atoms_Cell_Type
MAtom_Type
MAtom_List_Type

Err_ATMD
Err_ATMD_Mess

Functions

Equiv_ATM
WRT_Lab

Subroutines

Allocate_Atom_List
Allocate_Atoms_Cell
Allocate_MAtom_List
ATList1_ExtenCell_ATList2
Atom_List_To_Cell
Atom_Uequi_List
Atoms_Cell_To_List
Copy_Atom_List
Deallocate_Atom_List
Deallocate_Atoms_Cell
Deallocate_MAtom_List
Init_Atom_Type

Init_Err_ATMD
Init_MAtom_Type
Merge_Atoms_Peaks
Multi
Write_Atom_List
Write_Atoms_CFL
Write_CFL

Fortran Filename

CFML_Atom_Mod.f90

CFML_Atom_TypeDef: Variables

Atom_Type
Atom_List_Type
Atoms_Cell_Type
MAtom_Type
MAtom_List_Type

Err_ATMD
Err_ATMD_Mess

CFML_Atom_TypeDef: Variables

	Variable	*Definition*
Type :: Atom_Type		
Character (Len=10)	Lab	Label
Character (Len=2)	ChemSymb	Chemical symbol
Character (Len=4)	SFacSymb	Chemical symbol for SF
Logical	Active	Control flag
Integer	Z	Atomic number
Integer	Mult	Multiplicity site
Real (Kind=CP), Dimension(3)	X	Fractional coordinates
Real (Kind=CP), Dimension(3)	X_STD	Standard deviations of X
Real (Kind=CP), Dimension(3)	MX	Multipliers for coordinates (applied to shifts in non-linear LSQ)
Integer, Dimension(3)	LX	Ordinal numbers of LSQ parameters for atomic position
Real (Kind=CP)	Occ	Occupation factor
Real (Kind=CP)	Occ_STD	Standard deviation of OCC
Real (Kind=CP)	MOcc	Multiplier
Integer	LOcc	Ordinal number of LSQ parameter for OCC
Real (Kind=CP)	Biso	Isotropic B-Factor
Real (Kind=CP)	Biso_STD	Standard deviation of BISO

Real (Kind=CP)	MBiso	Multiplier
Integer	LBiso	Ordinal number of LSQ parameter for BISO
Character (Len=4)	UType	Values are: u_ij -> U's b_ij -> B's beta -> 's none
Character (Len=5)	THType	Values are: Isotr -> Isotropic Aniso -> Anisotropic Other
Real (Kind=CP), Dimension(6)	U	Coeff U11,U22,U33,U12,U13,U23
Real (Kind=CP), Dimension(6)	U_STD	Standard deviations of U's
Real (Kind=CP)	Ueq	U equivalent
Real (Kind=CP), Dimension(6)	MU	Multipliers
Integer, Dimension(6)	LU	Ordinal numbers of LSQ parameters
Real (Kind=CP)	Charge	
Real (Kind=CP)	Moment	
Integer, Dimension(5)	Ind	index vector for different purposes
Integer	NVar	Number of additional free variables (used for different purposes)
Real (Kind=CP), Dimension(10)	VarF	Free variables
End Type Atom_Type		

CFML_Atom_TypeDef: Variables

	Variable	***Definition***
Type :: Atom_List_Type		
Integer	NAtoms	Number of Atoms in the List
Type (Atom_Type), Dimension(:), Allocatable	Atom	Atoms information
End Type Atom_List_Type		

CFML_Atom_TypeDef: Variables

	Variable	***Definition***
Type :: Atoms_Cell_Type		
Integer	Nat	Number of Atoms
Character (Len=10), Dimension(:), Allocatable	Noms	Name of Atoms
Real (Kind=CP), Dimension(:,:), Allocatable	XYZ	Fractional coordinates (3, NAT)
Real (Kind=CP), Dimension(:), Allocatable	Charge	

Real (Kind=CP), Dimension(:), Allocatable	Moment	
Real (Kind=CP), Dimension(:,:), Allocatable	VarF	Free Parameters (10, NAT)
Integer, Dimension(:), Allocatable	Neighb	Number of neighbours (NAT)
Integer, Dimension(:,:), Allocatable	Neighb_Atm	Ptr.->neighbour (# in list)(NAT,IDP)
Real (Kind=CP), Dimension(:,:), Allocatable	Distance	Distances (NAT,IDP)
Real (Kind=CP), Dimension(:,:,:), Allocatable	Trans	Lattice translations (3,NAT,IDP)
Integer	NDist	Number of distinct distances
Real (Kind=CP), Dimension(:), Allocatable	DDist	List of distinct distances(NAT*IDP)
Character (Len=8), Dimension(:), Allocatable	DDLab	Labels of atoms at ddist (NAT*IDP)
End Type Atoms_Cell_Type		

CFML_Atom_TypeDef: Variables

	Variable	*Definition*
Type :: MAtom_Type		
Character (Len=10)	Lab	Label
Character (Len=2)	ChemSymb	Chemical symbol
Character (Len=4)	SFacSymb	Chemical symbol for SF
Logical	Active	Control flag
Integer	Z	Atomic number
Integer	Mult	Multiplicity site
Real (Kind=CP), Dimension(3)	X	Fractional coordinates
Real (Kind=CP), Dimension(3)	X_STD	Standard deviations of X
Real (Kind=CP), Dimension(3)	MX	Multiplier parameters of coordinates
Integer, Dimension(3)	LX	Numbers of LSQ parameters for X
Real (Kind=CP)	Occ	Occupation factor
Real (Kind=CP)	Occ_STD	Standard deviation of OCC
Real (Kind=CP)	MOcc	
Integer	LOcc	
Real (Kind=CP)	Biso	Isotropic B-Factor
Real (Kind=CP)	Biso_STD	Standard deviation of BISO
Real (Kind=CP)	MBiso	
Integer	LBiso	
Character (Len=4)	UType	Values are: u_ij -> U's b_ij -> B's beta -> 's none
Character (Len=5)	THType	Values are: Isotr -> Isotropic Aniso -> Anisotropic Other
Real (Kind=CP), Dimension(6)	U	Coeff U11,U22,U33,U12,U13,U23

Real (Kind=CP), Dimension(6)	U_STD	
Real (Kind=CP)	Ueq	U equivalent
Real (Kind=CP), Dimension(6)	MU	
Integer, Dimension(6)	LU	
Real (Kind=CP)	Charge	
Real (Kind=CP)	Moment	
Integer, Dimension(5)	Ind	index vector for different purposes
Integer	NVar	Number of Free parameters
Real (Kind=CP), Dimension(10)	VarF	Free parameters
Integer	NVK	Num. of propag. vectors (excl. -k)
Integer, Dimension(12)	IMat	Num. of the magnetic matrices/irrep set to be applied
Real (Kind=CP), Dimension(3,12)	SKR	Real part of Fourier Coefficient
Real (Kind=CP), Dimension(3,12)	MSKR	Multipliers for the real part of Fourier coefficients
Integer, Dimension(3,12)	LSKR	Numbers in the list of LSQ parameters
Real (Kind=CP), Dimension(3,12)	SKI	Imaginary part of Fourier Coefficient
Real (Kind=CP), Dimension(3,12)	KSKI	Multipliers for the imaginary part of Fourier coefficients
Integer, Dimension(3,12)	LSKI	Numbers in the list of LSQ parameters
Real (Kind=CP), Dimension(12)	MPhas	Magnetic Phase in fractions of 2
Real (Kind=CP), Dimension(12)	MMPhas	Multiplier for the magnetic phase
Integer, Dimension(12)	LMPhas	Numbers in the list of LSQ parameters
Real (Kind=CP), Dimension(12,12)	CBas	Coeff. of the basis functions of IRreps, the second index is 1:nvk
Real (Kind=CP), Dimension(12,12)	MBas	Multiplier for the coeff. of the basis functions of IRreps
Integer, Dimension(12,12)	LBas	Numbers in the list of LSQ parameters
End Type MAtom_Type		

CFML_Atom_TypeDef: Variables

	Variable	***Definition***
Type :: MAtom_List_Type		
Integer	NAtoms	Number of Atoms in the List
Type (MAtom_Type), Dimension(:), Allocatable	Atom	Atoms information
End Type MAtom_List_Type		

CFML_Atom_TypeDef: Variables

Logical :: Err_ATMD

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_Atom_TypeDef: Variables

Character (Len=150) :: Err_ATMD_Mess

This variable contains information about the last error occurred in the procedures belonging to this module.

CFML_Atom_TypeDef: Functions

CFML_Atom_TypeDef: Functions

Logical Function Equiv_ATM (Nam1, Nam2, NameAt)

Character (Len=*)	**Intent(in)**	Nam1	Atom name
Character (Len=*)	**Intent(in)**	Nam2	Atom name
Character (Len=*)	**Intent(in)**	NameAt	String containing atom names

Determine whether the atoms of names **Nam1** and **Nam2** are included in the longer string **NameAt** (constructed by function WRT_Lab.)

CFML_Atom_TypeDef: Functions

Character Function WRT_Lab (Nam1, Nam2)

Character (Len=*)	**Intent(in)**	Nam1	Atom name
Character (Len=*)	**Intent(in)**	Nam2	Atom name

Return a string of length 8 where merging the main part of the labels (before underscore "_") of the atoms Nam1 and Nam2.

CFML_Atom_TypeDef: Subroutines

CFML_Atom_TypeDef: Subroutines

Subroutine Allocate_Atom_List (N, A, Fail)

Integer	**Intent(in)**	N	Number of elements of A
Type(Atom_List_Type)	**Intent(in out)**	A	Objet to be allocated
Logical, Optional	**Intent(out)**	Fail	String containing atom names

Allocation of objet A of type Atom_List_Type.

This subroutine should be called before using an object of type Atom_List_Type.

CFML_Atom_TypeDef: Subroutines

Subroutine Allocate_Atoms_Cell (NAsu, Mul, DMax, Ac)

Integer	**Intent(in)**	NAsu	Number of atoms in asymmetric unit
Integer	**Intent(in)**	Mul	General multiplicity of the Space Group
Real(Kind=CP)	**Intent(in)**	DMax	Maximun distance to be calculated
Type(Atoms_Cell_Type)	**Intent(in out)**	Ac	Object

Allocation of objet AC of type Atoms_Cell_Type.

Ac contains components with allocatable attribute with dimension depending on the input arguments NAsu, Mul and DMax. The variables used for calculating the dimensions are:

NATCEL = NASU * MUL

IDP=NinT(0.74048 * $(DMAX/1.1)^3$)

Note: This subroutine should be called before using the subroutines of this module with dummy arguments of type Atoms_Cell_Type.

CFML_Atom_TypeDef: Subroutines

Subroutine Allocate_MAtom_List (N, A)

Integer	**Intent(in)**	N	Number of elements of A
Type(MAtom_List_Type)	**Intent(in out)**	A	Objet to be allocated

Allocation of objet A of type MAtom_List_Type

Note: This subroutine should be called before using an object of type MAtom_List_Type.

CFML_Atom_TypeDef: Subroutines

Subroutine ATList1_ExtenCell_ATList2 (Spg, A, B, Conven)

Type(Space_Group_Type)	**Intent(in)**	Spg	Space Group information
Type(Atom_List_Type)	**Intent(in)**	A	Atom List (asymmetric unit)
Type(Atom_List_Type)	**Intent(out)**	B	Atom List in unit cell
Logical	**Intent(in)**	Conven	**.TRUE.** for using the whole conventional unit cell

Subroutine to generate atoms in the primitive (Conven=.**FALSE**.) or the conventional unit cell (Conven=.**TRUE**.)

CFML_Atom_TypeDef: Subroutines

Subroutine Atom_List_To_Cell (A, AC)

Type(Atom_List_Type)	**Intent(in)**	A	Atom List
Type(Atoms_Cell_Type)	**Intent(in out)**	Ac	Atoms in CELL

Subroutine to construct an Atoms_Cell_Type object **Ac** from an Atom_List_Type object **A**.

It is supposed that both objects have been previously allocated using the appropriate procedures.

CFML_Atom_TypeDef: Subroutines

Subroutine Atom_Uequi_List (Cell, A)

Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell Variable
Type(Atom_List_Type)	**Intent(in out)**	A	Atom list

Subroutine to obtain the U_{eq} from U_{11} U_{22} U_{33} U_{12} U_{13} U_{23} for **A** object

CFML_Atom_TypeDef: Subroutines

Subroutine Atoms_Cell_To_List (Ac, A)

Type(Atoms_Cell_Type)	**Intent(in)**	Ac	Atoms in CELL
Type(Atom_List_Type)	**Intent(in out)**	A	Atom List

Subroutine to construct an Atom List object A from an Atoms_Cell_Type object **Ac**.

Note: It is supposed that both objects have been previously allocated using the appropriate procedures: direct allocation for **A** and call to Allocate_Atoms_Cell for **Ac**.

CFML_Atom_TypeDef: Subroutines

Subroutine Copy_Atom_List (A, Ac)

Type(Atom_List_Type)	**Intent(in)**	A	Atom List
Type(Atom_List_Type)	**Intent(out)**	Ac	Atom List

Subroutine to copy an atom list to another one

CFML_Atom_TypeDef: Subroutines

Subroutine Deallocate_Atom_List (A)

Type(Atom_List_Type)	**Intent(in out)**	A	Objet to be allocated

Deallocation of objet **A** of type Atom_List_Type.

Note: This subroutine should be after using an object of type Atom_List_Type that is no more needed.

Subroutine Deallocate_Atoms_Cell (Ac)

Type(Atoms_Cell_Type)	**Intent(in out)**	Ac	Objet to be allocated

Deallocation of objet AC of type Atoms_Cell_Type.

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Subroutine Deallocate_MAtom_List (A)

Type(MAtom_List_Type)	**Intent(in out)**	A	Objet to be allocated

Deallocation of objet A of type MAtom_List_Type.

Note: This subroutine should be invoked after using an object of type MAtom_List_Type that is no more needed.

Subroutine Init_Atom_Type (A)

Type(Atom_Type)	**Intent(in out)**	A	Atom Type

initialize the variable A which is the type Atom_Type

Subroutine Init_Err_ATMD ( )

Subroutine that initializes errors flags in **CFML_Atom_TypeDef** module.

Subroutine Init_MAtom_Type (A)

Type(MAtom_Type)	**Intent(in out)**	A	Atom Type

Initialize the variable A which is the type MAtom_Type

Subroutine Merge_Atoms_Peaks (Cell, Atm, NPks, Pks, Grp, NAtm)

Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Atom_List_Type)	**Intent(in)**	Atm	Atom list
Integer	**Intent(in)**	NPks	Number of Peaks on PKS
Real(Kind=CP), Dimension(:,:)	**Intent(in)**	Pks	List of Peaks

Type(Space_Group_Type)	**Intent(in)**	Grp	Space Group information
Type(Atom_List_Type)	**Intent(out)**	NAtm	New Atoms+Peaks List

This routine merge atoms and peaks on a new List.

CFML_Atom_TypeDef: Subroutines

Subroutine Multi (Lun, IPrin, Conven, Spg, A, Ac)

Integer	**Intent(in)**	Lun	Logical Unit for writing
Logical	**Intent(in)**	IPrin	.true. for writing in Lun
Logical	**Intent(in)**	Conven	.true. for using the whole conventional unit cell
Type(Space_Group_Type)	**Intent(in)**	Spg	Space Group information
Type(Atom_List_Type)	**Intent(in out)**	A	Atom List
Type(Atoms_Cell_Type)	**Intent(out)**	Ac	Atoms in unit cell

Subroutine to obtain multiplicities and coordinates of all atoms in the conventional unit cell.

Calculates A%AT(k)%Mult and constructs, partially, the object Ac of type Atoms_Cell_Type. The generated atoms constitute the content of the primitive (Conven=.FALSE.) or the conventional unit cell (Conven=.TRUE.).

CFML_Atom_TypeDef: Subroutines

Subroutine Write_Atom_List (Ats, Level, Lun, Mult, Cell)

Type(Atom_List_Type), Dimension(:)	**Intent(in)**	Ats	Atom list vector
Integer, Optional	**Intent(in)**	Level	Level of printed information
Integer, Optional	**Intent(in)**	Lun	Unit to write
Integer, Optional	**Intent(in)**	Mult	Multiplicity of the general position
Type(Crystal_Cell_Type), Optional	**Intent(in)**	Cell	Transform to thermal parameters

Write the atoms in the asymmetric unit

CFML_Atom_TypeDef: Subroutines

Subroutine Write_Atoms_CFL (Ats, Lun, Cell)

Type(Atom_List_Type), Dimension(:)	**Intent(in)**	Ats	Atom list vector
Integer, Optional	**Intent(in)**	Lun	Unit to write
Type(Crystal_Cell_Type), Optional	**Intent(in)**	Cell	Transform to thermal parameters

Write the atoms in the asymmetric unit for a CFL file

CFML_Atom_TypeDef: Subroutines

Subroutine Write_CFL (Lun, Cell, Spg, Atm)

Integer	**Intent(in)**	Lun	Unit to write
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Space_Group_Type)	**Intent(in)**	Spg	Space group information
Type(Atom_List_Type)	**Intent(in)**	Atm	Atom List

Write a CFL file

CFML_Geometry_SXTAL

Module for making geometrical calculations in Single crystal instruments.

Variables

- PSD_Val_Type
- SXD_Val_Type

- Err_SXTGeom
- Err_SXTGeom_Mess
- PSD
- SXD

Subroutines

- Angs_4C_Bisecting
- CalAng
- Calc_Om_Chi_Phi
- Calc_Psi
- Cell_Fr_Ub
- Chi_Mat
- D19Psd
- Dspace
- Equatorial_Chi_Phi
- FixDnu
- Flat_Cone_VertDet
- GenB
- GenUB
- Get_Angs_NB
- Get_DSpacing_Theta
- Get_GaOmNu_FrChiPhi
- Get_WaveGaNu_FrZ4
- Get_Z1_D9Angls
- Get_Z1_From_Pixel
- Normal
- Normal_Beam_Angles
- Phi_Mat
- PSD_Convert
- Psi_Mat
- RefVec
- S4CNB
- Set_PSD
- SNB4C
- SXDPSD
- Triple
- Z1FrFC
- Z1FrMD

Z1FrNB
Z1FrZ2
Z1FrZ3
Z1FrZ4
Z2FrZ1
Z3FrZ1
Z4FrGN
Z4FrZ1

Fortran Filename

CFML_SXTAL_Geom.f90

Under construction!!!

CFML_Geometry_SXTAL: Variables

PSD_Val_Type
SXD_Val_Type

Err_SXTGeom
Err_SXTGeom_Mess
PSD
SXD

CFML_Geometry_SXTAL: Variables

	Variable	***Definition***
Type :: PSD_Val_Type		
Real (Kind=CP)	XOff	
Real (Kind=CP)	ZOff	
Real (Kind=CP)	Radius	
Real (Kind=CP)	YOff	
Real (Kind=CP)	CGap	
Real (Kind=CP)	AGap	
Integer	NCat	
Integer	Nano	
Integer	IPSD	
End Type PSD_Val_Type		

CFML_Geometry_SXTAL: Variables

	Variable	*Definition*
Type :: SXD_Val_Type		
Real (Kind=CP)	DistMs	
Real (Kind=CP)	DistSd	
Real (Kind=CP)	DimX	
Real (Kind=CP)	DimZ	
Real (Kind=CP)	Xoff	
Real (Kind=CP)	YOff	
Real (Kind=CP)	ZOff	
Real (Kind=CP)	TOff	
Real (Kind=CP)	Velcon	
Integer	NXCel	
Integer	NZCel	
End Type SXD_Val_Type		

CFML_Geometry_SXTAL: Variables

Logical :: Err_SXTGeom

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_Geometry_SXTAL: Variables

Character (Len=150) :: Err_SXTGeom_Mess

This variable contains information about the last error occurred in the procedures belonging to this module.

CFML_Geometry_SXTAL: Variables

Type (PSD_Val_Type) :: PSD

CFML_Geometry_SXTAL: Variables

Type (SXD_Val_Type) :: SXD

CFML_Geometry_SXTAL: Subroutines

- Angs_4C_Bisecting
- CalAng
- Calc_Om_Chi_Phi
- Calc_Psi
- Cell_Fr_Ub
- Chi_Mat
- D19Psd
- Dspace
- Equatorial_Chi_Phi
- FixDnu
- Flat_Cone_VertDet
- GenB
- GenUB

CFML_Geometry_SXTAL: Subroutines

Subroutine Angs_4C_Bisecting (Wave, Z1, Tth, Om, Ch, Ph, Ierr)

Real(Kind=CP)	**Intent(in)**	Wave	Wavelength
Real(Kind=CP), Dimension(3)	**Intent(in)**	Z1	
Real(Kind=CP)	**Intent(out)**	Tth	2Theta
Real(Kind=CP)	**Intent(out)**	Om	Omega
Real(Kind=CP)	**Intent(out)**	Ch	Chi
Real(Kind=CP)	**Intent(out)**	Ph	Phi
Integer	**Intent(out)**	Ierr	Flag for error

Calculate 2-Theta, Omega (=Theta), Chi, Phi to put the vector Z1 in the bisecting diffraction condition.
The reciprocal vector Z1 is given in Cartesian components with respect to the laboratory system. This geometry corresponds to the bisecting Psi=0.

CFML_Geometry_SXTAL: Subroutines

Subroutine CalAng (H, TTheta, Om, Ch, Ph, Ierr, Wav, UBM, Geom)

Real(Kind=CP), Dimension(3)	**Intent(in)**	H	Reflection indices
Real(Kind=CP)	**Intent(out)**	TTheta	2Theta
Real(Kind=CP)	**Intent(out)**	Om	Omega

Real(Kind=CP)	**Intent(out)**	Ch	Chi
Real(Kind=CP)	**Intent(out)**	Ph	Phi
Integer	**Intent(out)**	Ierr	Flag for error
Real(Kind=CP), Optional	**Intent(in)**	Wav	Wavelength
Real(Kind=CP), Dimension(3,3), Optional	**Intent(in)**	UBM	UB Matrix
Integer, Optional	**Intent(in)**	Geom	Geometric definition

This subroutine is a more general variant of Angs_4C_Bisecting.
If the optional arguments are given, the corresponding values are adopted instead of those of the current instrument.

CFML_Geometry_SXTAL: Subroutines

Subroutine Calc_Om_Chi_Phi (Vhkl, VLab1, Psi, UB, Om, Ch, Ph, Ierr)

Real(Kind=CP), Dimension(3)	**Intent(in)**	Vhkl	Vector Indices hkl
Real(Kind=CP), Dimension(3)	**Intent(in)**	VLab1	
Real(Kind=CP)	**Intent(in)**	Psi	Psi
Real(Kind=CP), Dimension(3,3)	**Intent(in)**	UB	UB Matrix
Real(Kind=CP)	**Intent(in out)**	Om	Omega
Real(Kind=CP)	**Intent(in out)**	Ch	Chi
Real(Kind=CP)	**Intent(in out)**	Ph	Phi
Integer	**Intent(out)**	Ierr	Flag for error

Calculate Om, Ch, Ph for diffraction vector at azimuthal angle Psi from the diffraction condition expressed as :

[TZ]=[OM].[CH].[PH].[TS].[PSI]-1   if [R]=[OM].[CH].[PH]

then [R]'=[TZ].[PSI].[TS]-1

The Om, Ch, Ph angles are provided, on input, to calculate the components of the vector VLab1 in the Theta-system for Psi=0
Used only in the procedure Flat_Cone_VertDet.

CFML_Geometry_SXTAL: Subroutines

Subroutine Calc_Psi (Vhkl, VLab1, Om, Ch, Ph, UB, Psi, Ierr)

Real(Kind=CP), Dimension(3)	**Intent(in)**	Vhkl	Vector Indices hkl
Real(Kind=CP), Dimension(3)	**Intent(in)**	VLab1	
Real(Kind=CP)	**Intent(in)**	Om	Omega
Real(Kind=CP)	**Intent(in)**	Ch	Chi
Real(Kind=CP)	**Intent(in)**	Ph	Phi
Real(Kind=CP), Dimension(3,3)	**Intent(in)**	UB	UB Matrix
Real(Kind=CP)	**Intent(out)**	Psi	Psi
Integer	**Intent(out)**	Ierr	Flag for error

Calculate Psi for the reflection Vhkl positioned at Om, Ch and Ph.

The value of Psi is taken to be zero when (the values of Om, Ch, Ph are such that) the reflection H0 lies in the plane of Vhkl and VZ, on the same side of Vhkl as VZ. The reference vectors H0 and VZ are defined in subroutine RefVec. There, the vector VZ is the z-axis of the fixed laboratory system (Busing and Levy Convention, Y along beam, X in positive 2-THETA direction). H0 is (0,0,1) for all VHKL except when VHKL is parallel to (0,0,1), in which case (0,1,0) is chosen.

CFML_Geometry_SXTAL: Subroutines

Subroutine Calc_Fr_UB (UB, Ipr, DCell, RCell)

Real(Kind=CP), Dimension(3,3)	**Intent(in)**	UB	UB Matrix
Integer	**Intent(in)**	Ipr	Flag to print information
Real(Kind=CP), Dimension(6), Optional	**Intent(out)**	DCell	Direct cell parametrs
Real(Kind=CP), Dimension(6), Optional	**Intent(out)**	RCell	Reciprocal cell parameters

Calculate and print cell parameters from UB-matrix

CFML_Geometry_SXTAL: Subroutines

Subroutine Chi_Mat (Chi, Dum)

Real(Kind=CP)	**Intent(in)**	Chi	Chi
Real(Kind=CP), Dimension(3,3)	**Intent(out)**	Dum	

Calculate the Busing and Levy conventional rotation matrix for Chi (in degrees).

CFML_Geometry_SXTAL: Subroutines

Subroutine D19PSD (MPSD, Ga, Nu, Cath, Anod, Ierr)

Integer	**Intent(in)**	MPSD	
Real(Kind=CP)	**Intent(in out)**	Ga	
Real(Kind=CP)	**Intent(in out)**	Nu	
Real(Kind=CP)	**Intent(in out)**	Cath	
Real(Kind=CP)	**Intent(in out)**	Anod	
Integer	**Intent(in out)**	Ierr	

Specifically for D19A bannana detector, 4 X 64 degrees - 16 X 512 cells and vertically curved.

MPSD + VE - Calculate delta GAMMA and NU from the cathode, anode co-ordinates
MPSD - VE - Calculate the anode co-ordinate from NU

Some of the variables making reference to the characteristics of the detector are provisionally stored in a public type(Psd_Val_Type):: PSD

CFML_Geometry_SXTAL: Subroutines

Subroutine DSpace (Wave, Vhkl, Cell, Ds, Th, Ierr)

Real(Kind=CP)	**Intent(in)**	Wave	
Real(Kind=CP), Dimension(3)	**Intent(in)**	Vhkl	
Real(Kind=CP), Dimension(6)	**Intent(in)**	Cell	
Real(Kind=CP)	**Intent(out)**	Ds	
Real(Kind=CP)	**Intent(out)**	Th	
Integer	**Intent(out)**	Ierr	

Calculate d-spacing and theta from cell parameters and wavelength assume triclinic symmetry. The reflection vector Vhkl is provided in reciprocal lattice components

CFML_Geometry_SXTAL: Subroutines

Subroutine Equatorial_Chi_Phi (Z1, Ch, Ph)

Real(Kind=CP), Dimension(3)	**Intent(in)**	Z1	
Real(Kind=CP)	**Intent(out)**	Ch	
Real(Kind=CP)	**Intent(out)**	Ph	

Calculate Chi, Phi to put the vector Z1 in the equatorial plane. The reciprocal vector Z1 is given in Cartesian components with respect to the laboratory system

CFML_Geometry_SXTAL: Subroutines

Subroutine FixDNu (Wave, Z1, Nu, Ch, Ph, Ga, Om, Ierr)

Real(Kind=CP)	**Intent(in)**	Wave	Wavelength
Real(Kind=CP), Dimension(3)	**Intent(in)**	Z1	
Real(Kind=CP)	**Intent(in)**	Nu	Angle
Real(Kind=CP)	**Intent(out)**	Ch	Angle
Real(Kind=CP)	**Intent(out)**	Ph	Angle
Real(Kind=CP)	**Intent(out)**	Ga	Angle
Real(Kind=CP)	**Intent(out)**	Om	Angle
Integer	**Intent(out)**	Ierr	Flag for control error

Calculate a setting Ch, Ph,Ga,Om to put the diffracted beam at Nu.

Ph puts the diffraction vector Z1 into the Chi circle (as for bisecting geometry), Ch brings the vector to the appropriate Nu and Om then positions the beam at Ga.

CFML_Geometry_SXTAL: Subroutines

Subroutine Flat_Cone_VertDet (Wave, Z1, UB, VRho, Rho, Ch, Ph, Ga, Om, Nu, Ierr)

Real(Kind=CP)	**Intent(in)**	Wave	Wavelength
Real(Kind=CP), Dimension(3)	**Intent(in)**	Z1	
Real(Kind=CP), Dimension(3,3)	**Intent(in)**	UB	UB Matrix
Real(Kind=CP), Dimension(3)	**Intent(in out)**	VRho	
Real(Kind=CP)	**Intent(out)**	Rho	Angle
Real(Kind=CP)	**Intent(out)**	Ch	Angle
Real(Kind=CP)	**Intent(out)**	Ph	Angle
Real(Kind=CP)	**Intent(out)**	Ga	Angle
Real(Kind=CP)	**Intent(out)**	Om	Angle
Real(Kind=CP)	**Intent(out)**	Nu	Angle
Integer	**Intent(out)**	Ierr	Flag for control error

Calculate Rho (=Psi) about given rotation vector VRho (and the corresponding angles Om, Ch, Ph) to put the vector Z1 into the flat-cone diffracting position.

CFML_Geometry_SXTAL: Subroutines

Subroutine GenB (C, B)

Type(Crystal_Cell_Type)	**Intent(in)**	C	Crystal Cell object

Real(Kind=CP), Dimension(3,3)	**Intent(out)**	B	

Calculation of B Matrix.

Note: Acta Cryst., 22, (1967), 457-464 (Eq. 3)

CFML_Geometry_SXTAL: Subroutines

Subroutine GenUB (B, H1, H2, H1O, H2O,UB, Ierr)

Real(Kind=CP), Dimension(3,3)	**Intent(in)**	B	Busing-Levy B-matrix
Real(Kind=CP), Dimension(3)	**Intent(in)**	H1	Miller indices
Real(Kind=CP), Dimension(3)	**Intent(in)**	H2	Miller indices
Real(Kind=CP), Dimension(3)	**Intent(in)**	H1O	Components in Lab system
Real(Kind=CP), Dimension(3)	**Intent(in)**	H2O	Components in Lab system
Real(Kind=CP), Dimension(3,3)	**Intent(out)**	UB	UB Matrix
Integer	**Intent(out)**	Ierr	Flag for control error

Given the B matrix, the Miller indices of two reflections, H1 & H2, and the components of these two reflections, H1O & H2O, in the laboratory system, this subroutine provides the matrix UB. Only the direction in the laboratory system of reflections are needed, e.g. H1O and H2O may be unitary vectors or whatever other vector along these directions.

CFML_Geometry_SXTAL: Subroutines

Subroutine Get_Angs_NB (Wave, Z1, Ga, Om, Nu, Ierr)

Real(Kind=CP)	**Intent(in)**	Wave	Wavelength
Real(Kind=CP), Dimension(3)	**Intent(in)**	Z1	
Real(Kind=CP)	**Intent(out)**	Ga	Angle
Real(Kind=CP)	**Intent(out)**	Om	Angle
Real(Kind=CP)	**Intent(out)**	Nu	Angle
Integer	**Intent(out)**	Ierr	Flag for control error

Calculate normal-beam angles Gamma, Omega, Nu to put the vector Z1 into the diffracting condition.

CFML_Geometry_SXTAL: Subroutines

Subroutine Get_DSpacing_Theta (Wave, Z1, Ds, Th, Ierr)

Real(Kind=CP)	**Intent(in)**	Wave	Wavelength
Real(Kind=CP), Dimension(3)	**Intent(in)**	Z1	
Real(Kind=CP)	**Intent(out)**	Ds	Angle
Real(Kind=CP)	**Intent(out)**	Th	Angle
Integer	**Intent(out)**	Ierr	Flag for control error

Calculate D-spacing (real space) and Theta from the length of Z1. The reciprocal vector Z1 is given in Cartesian components with respect to the laboratory system.

If ierr=1 the calculated d-spacing is is fixed to 0.0 as well as theta. This error condition appears when the length of the reciprocal vector Z1 is lower or equal to 0.0001
If ierr=2 the reflection is outside the resolution sphere.

CFML_Geometry_SXTAL: Subroutines

Subroutine Get_GaOmNu_FrChiPhi (Wave, Z1, Ch, Ph, Ga, Om, Nu, Ierr)

Real(Kind=CP)	Intent(in)	Wave	Wavelength
Real(Kind=CP), Dimension(3)	Intent(in)	Z1	
Real(Kind=CP)	Intent(in)	Ch	Angle
Real(Kind=CP)	Intent(in)	Ph	Angle
Real(Kind=CP)	Intent(out)	Ga	Angle
Real(Kind=CP)	Intent(out)	Om	Angle
Real(Kind=CP)	Intent(out)	Nu	Angle
Integer	Intent(out)	Ierr	Flag for control error

Given Chi & Phi, calculate normal-beam angles Gamma, Omega, Nu to put the vector Z1 into the diffraction condition. The reciprocal vector Z1 is given in Cartesian components with respect to the laboratory system.

CFML_Geometry_SXTAL: Subroutines

Subroutine Get_WaveGaNu_FrZ4 (Z4, Wave, Ga, Nu, Ierr)

Real(Kind=CP), Dimension(3)	Intent(in)	Z4	
Real(Kind=CP)	Intent(out)	Wave	Wavelength
Real(Kind=CP)	Intent(out)	Ga	Angle
Real(Kind=CP)	Intent(out)	Nu	Angle
Integer	Intent(out)	Ierr	Flag for control error

Calculate Ga, Nu and wavelength for diffraction vector in Laboratory system

CFML_Geometry_SXTAL: Subroutines

Subroutine Get_Z1_D9Angls (Wave,TTheta, Om, Ch, Ph, Z1)

Real(Kind=CP)	Intent(in)	Wave	Wavelength
Real(Kind=CP)	Intent(in)	TTheta	Wavelength
Real(Kind=CP)	Intent(in)	Om	Angle
Real(Kind=CP)	Intent(in)	Ch	Angle
Real(Kind=CP)	Intent(in)	Ph	Angle
Real(Kind=CP), Dimension(3)	Intent(out)	Z1	Flag for control error

Calculate Z1 from angles for D9 Instrument

CFML_Geometry_SXTAL: Subroutines

Subroutine Get_Z1_From_Pixel (NPx, NPy, SNum, Z1)

Integer	Intent(in)	NPx	Wavelength
Integer	Intent(in)	NPy	Wavelength
Type(SXTAL_Numor_Type)	Intent(in)	SNum	Numor
Real(Kind=CP), Dimension(3)	Intent(out)	Z1	

Calculate Z1 from Numor

CFML_Geometry_SXTAL: Subroutines

Subroutine Normal (V1, Ierr)

Real(Kind=CP), Dimension(3)	**Intent(in out)**	V1	
Integer	**Intent(out)**	Ierr	Error control

Normalise vector V (in Cartesian components)

CFML_Geometry_SXTAL: Subroutines

Subroutine Normal_Beam_Angles (Wav, UB, H, Sig, AnBCal, Ier, Zer)

Real(Kind=CP)	**Intent(in)**	Wav	Wavelength
Real(Kind=CP), Dimension(3,3)	**Intent(in)**	UB	UB Matrix
Real(Kind=CP), Dimension(3)	**Intent(in)**	H	Miller indices of reflection
Integer	**Intent(in out)**	Sig	-1 for negative Gammas
Real(Kind=CP), Dimension (:)	**Intent(out)**	AnBCal	Normal beam angles
Integer	**Intent(in out)**	Ier	Zero correction on input, Error flag on output
Real(Kind=CP), Dimension(3), Optional	**Intent(in)**	Zer	Zero corrections of NB angles in degrees

Calculation of the normal-beam diffraction angles for reflection H from the UB matrix of the crystal.

On input:
Sig : 1/-1 defines the sign for Gamma
If Zer is provided, the calculated angles are corrected for zero shifts

On output:
Angles(calculated) = Angles(theoretical) + zero shifts
AnBCal(1:4) -> Gamma, Omega(NB), Nu, Theta (in degrees)

Error Flag (Ier)
0 -> all angles are calculable
1 -> reflection hors sphere d'Ewald
2 -> reflection dans zone aveugle ==> angle "NU"
3 -> reflection dans zone aveugle ==> angle "GAMMA"
4 -> H,K,L tous les trois nuls

CFML_Geometry_SXTAL: Subroutines

Subroutine Phi_Mat (Phi, Dum)

Real(Kind=CP)	**Intent(in)**	Phi	Phi
Real(Kind=CP), Dimension(3,3)	**Intent(out)**	Dum	

Calculate the Busing and Levy conventional rotation matrix for Phi or Omega. The Phi/Omega angle must be provided in degrees.

CFML_Geometry_SXTAL: Subroutines

Subroutine PSD_Convert (MPSD, Gamm, GamP, Nup, XObs, ZObs, Cath, Anod, Ierr)

Integer	**Intent(in)**	MPSD	
Real(Kind=CP)	**Intent(in)**	Gamm	
Real(Kind=CP)	**Intent(in out)**	GamP	
Real(Kind=CP)	**Intent(in out)**	Nup	
Real(Kind=CP)	**Intent(out)**	XObs	

Real(Kind=CP)	**Intent(out)**	ZObs	
Real(Kind=CP)	**Intent(in out)**	Cath	
Real(Kind=CP)	**Intent(in out)**	Anod	
Integer	**Intent(out)**	Ierr	Flag for Control error

Subroutine for getting Gamma and Nu of a reflections spot (GamP,NuP), given the gamma angle of the detector (GamM) and the pixel values (cath,anod). This is calculated when MPSD > 0, otherwise the inverse calculation is done. In both cases the detector coordinates (xobs,zobs) in mm are also calculated. The caracteristics of the detector are accessed via de global variable PSD of Type(Psd_Val_Type), that should be set by the calling program.

CFML_Geometry_SXTAL: Subroutines

Subroutine Psi_Mat (Psi, Dum)

Real(Kind=CP)	**Intent(in)**	Psi	Psi
Real(Kind=CP), Dimension(3,3)	**Intent(out)**	Dum	

Calculate the Busing and Levy conventional rotation matrix for Psi (in degrees).

CFML_Geometry_SXTAL: Subroutines

Subroutine RefVec (Vhkl, UB, Vs, Vz, Ierr)

Real(Kind=CP), Dimension(3)	**Intent(in)**	Vhkl	Vector
Real(Kind=CP), Dimension(3,3)	**Intent(in)**	UB	UB Matrix
Real(Kind=CP), Dimension(3)	**Intent(out)**	Vs	
Real(Kind=CP), Dimension(3)	**Intent(out)**	Vz	
Integer	**Intent(out)**	Ierr	Error Control flag

Calculate Vs and Vz as reference vectors for defining Psi=0. The B-L convention is that Psi=0 when the reflection hkl is in diffraction position and the c* is in the plane defined by Vhkl and Vz (z-axis of the laboratory system) for all reflections except when Vhkl is parallel to c* in which case the vector b* plays the role of c* in the above prescription. The vector Vhkl is provided with components in the reciprocal lattice.

CFML_Geometry_SXTAL: Subroutines

Subroutine S4CNB (Angl_4C, Angl_NB, Ierr)

Real(Kind=CP), Dimension(4)	**Intent(in)**	Angl_4C	(/2Theta, Omega, chi, Phi/)
Real(Kind=CP), Dimension(3)	**Intent(out)**	Angl_NB	(/Gamma, Omega_NB, Nu/)
Integer	**Intent(out)**	Ierr	Error Control flag 0 -> OK 1 -> calculation of Nu impossible 2 -> calculation of Gamma impossible 3 -> calculation of phi impossible

Conversion of diffraction angles from the geometry 4-Circles to Normal Beam.

CFML_Geometry_SXTAL: Subroutines

Subroutine Set_PSD ( )

Initialize the PSD Object

CFML_Geometry_SXTAL: Subroutines

Subroutine SNB4C (Angl_NB, Angl_4C)

Real(Kind=CP), Dimension(4)	**Intent(in)**	Angl_NB	(/Gamma, Omega_NB, Nu/)
Real(Kind=CP), Dimension(3)	**Intent(out)**	Angl_4C	(/2Theta, Omega, chi, Phi/)

Conversion of diffraction angles from the geometry Normal Beam to 4-Circles.

CFML_Geometry_SXTAL: Subroutines

Subroutine SXDPSD (MPSD, Gamm, Wave, Nup, GamP, XObs, ZObs, XCel, Time, ZCel, Ierr)

Integer	**Intent(in)**	MPSD	
Real(Kind=CP)	**Intent(in)**	Gamm	
Real(Kind=CP)	**Intent(in out)**	Nup	
Real(Kind=CP)	**Intent(in out)**	GamP	
Real(Kind=CP)	**Intent(out)**	XObs	
Real(Kind=CP)	**Intent(out)**	ZObs	
Real(Kind=CP)	**Intent(out)**	XCel	
Real(Kind=CP)	**Intent(out)**	Time	
Real(Kind=CP)	**Intent(out)**	ZCel	
Integer	**Intent(out)**	Ierr	Flag for Control error

The coordinate system adopted, whether the origin is at the moderator, at the sample (called the fixed laboratory system), or at the surface of the PSD when positioned at 0 degrees; is Y parallel to the beam, X in the horizontal plane on the diffraction side, and Z vertical. Hence if neutrons are diffracted to the left, Z is vertically down. The PSD is driven to an angle GamM. When GamM=0, the direct beam strikes a perfectly aligned PSD at its centre C.

Call this point in space A. A is where we define NuP=0, GamP=0. The coordinates of A with respect to the sample are (0, Distsd, 0); and with respect to the moderator are (0, Distms+Distsd, 0). For a mis-aligned detector, the coordinates of A with respect to C are the translational offsets (Xoff, Yoff, Zoff) in mm.

With the PSD at a general position GamM, the point where the direct beam struck it is rotated to O, where now NuP=0, GamP=GamM. For convenience, define a new cartesian system by rotating the axes of the fixed laboratory system about the vertical, such that X is now along the line joining the sample and O on the PSD. In this system, the coordinates of a Bragg peak P with respect to C are (Xobs, 0, Zobs) in mm, or (Xcel, 0, Zcel) in pixels.

Hence the coordinates of P with respect to O, in this system, are:

```
    (x)      (Xobs   + Xoff)
    (y)  =   (Distsd + Yoff)  and: Tan(GamP - GamM) = x/y
    (z)      (Zobs   + Zoff)       Tan(NuP)         = z/SQRT(x*x + y*y)
```

The PSD front surface measures Dimx by Dimy mm, and is divided into Nxcel by Nzcel pixels.

Time is the time coordinate (bin) relative to an elapsed time Toff after the emission of a pulse at the moderator. The effect of moderator thickness on Time is NOT included yet. Distot is the total distance travelled from the moderator to a particular pixel on the PSD surface, in a total time Timtot.

Note: Routine not tested, probably obsolete for present SXD!!!

CFML_Geometry_SXTAL: Subroutines

Subroutine Triple (V1, V2, Tv, Ierr)

Real(Kind=CP), Dimension(3)	**Intent(in out)**	V1	
Real(Kind=CP), Dimension(3)	**Intent(in out)**	V2	
Real(Kind=CP), Dimension(3,3)	**Intent(out)**	Tv	(/ V1, (V1 x V2) x V1, V1 x V2/)
Integer	**Intent(out)**	Ierr	

Construct orthonormal triplet matrix TV

CFML_Geometry_SXTAL: Subroutines

Subroutine Z1FrFC (Wave,TTh, Om, Ch, Ph, Z1)

Real(Kind=CP)	**Intent(in)**	Wave	Wavelength
Real(Kind=CP)	**Intent(in)**	TTh	2 Theta
Real(Kind=CP)	**Intent(in)**	Om	Angle
Real(Kind=CP)	**Intent(in)**	Ch	Angle
Real(Kind=CP)	**Intent(in)**	Ph	Angle
Real(Kind=CP), Dimension(3)	**Intent(out)**	Z1	

Calculate diffraction vector Z1 from TTh, Om, Ch, Ph (Need not be bisecting, but Z4 is assumed to be in the equatorial plane)

CFML_Geometry_SXTAL: Subroutines

Subroutine Z1FrMD (Wave, Ch, Ph, Ga, Om, Nu, Z1)

Real(Kind=CP)	**Intent(in)**	Wave	Wavelength
Real(Kind=CP)	**Intent(in)**	Ch	Angle
Real(Kind=CP)	**Intent(in)**	Ph	Angle
Real(Kind=CP)	**Intent(in)**	Ga	Angle
Real(Kind=CP)	**Intent(in)**	Om	Angle
Real(Kind=CP)	**Intent(in)**	Nu	Angle
Real(Kind=CP), Dimension(3)	**Intent(out)**	Z1	

Calculate diffraction vector Z1 from Ch, Ph, Ga, Om, Nu for a multi-detector. The angles Chi,Phi,Gamma,Omega and Nu for the equatorial plane are Chi, Phi, 2Theta and Omega (Nu=0).

CFML_Geometry_SXTAL: Subroutines

Subroutine Z1FrNB (Wave,Ga, Om, Nu, Z1)

Real(Kind=CP)	**Intent(in)**	Wave	Wavelength
Real(Kind=CP)	**Intent(in)**	Ga	Angle
Real(Kind=CP)	**Intent(in)**	Om	Angle
Real(Kind=CP)	**Intent(in)**	Nu	Angle
Real(Kind=CP), Dimension(3)	**Intent(out)**	Z1	

Calculate diffraction vector Z1 from Ga, Om, Nu, assuming CH=PH=0. This is is the normal beam geometry for a Lifting arm detector or for a PSD with a single Omega axis for the sample.

CFML_Geometry_SXTAL: Subroutines

Subroutine Z1FrZ2 (Z2, Ph, Z1)

Real(Kind=CP), Dimension(3)	**Intent(in)**	Z2	
Real(Kind=CP)	**Intent(in)**	Ph	Angle

Real(Kind=CP), Dimension(3)	**Intent(out)**	Z1	

Calculate

$Z1=Ph^T Z2$

CFML_Geometry_SXTAL: Subroutines

Subroutine Z1FrZ3 (Z3, Ch, Ph, Z1)

Real(Kind=CP), Dimension(3)	**Intent(in)**	Z3	
Real(Kind=CP)	**Intent(in)**	Ch	
Real(Kind=CP)	**Intent(in)**	Ph	
Real(Kind=CP), Dimension(3)	**Intent(out)**	Z1	

Calculate

$Z1=Ph^T Ch^T Z3$

CFML_Geometry_SXTAL: Subroutines

Subroutine Z1FrZ4 (Z4, Om, Ch, Ph, Z1)

Real(Kind=CP), Dimension(3)	**Intent(in)**	Z4	
Real(Kind=CP)	**Intent(in)**	Om	
Real(Kind=CP)	**Intent(in)**	Ch	
Real(Kind=CP)	**Intent(in)**	Ph	
Real(Kind=CP), Dimension(3)	**Intent(out)**	Z1	

Calculate

$Z1=Ph^T Ch^T Om^T Z3$

CFML_Geometry_SXTAL: Subroutines

Subroutine Z2FrZ1 (Z1, Ph, Z2)

Real(Kind=CP), Dimension(3)	**Intent(in)**	Z1	
Real(Kind=CP)	**Intent(in)**	Ph	Angle
Real(Kind=CP), Dimension(3)	**Intent(out)**	Z2	

Calculate

$Z2=Ph\ Z1$

Note: The reciprocal vector Z1 is given in Cartesian components with respect to the laboratory system.

CFML_Geometry_SXTAL: Subroutines

Subroutine Z3FrZ1 (Z1, Ch, Ph, Z3)

Real(Kind=CP), Dimension(3)	**Intent(in)**	Z1	
Real(Kind=CP)	**Intent(in)**	Ch	

Real(Kind=CP)	**Intent(in)**	Ph	
Real(Kind=CP), Dimension(3)	**Intent(out)**	Z3	

Calculate

Z3= Ch Ph Z1

Note: The reciprocal vector Z1 is given in Cartesian components with respect to the laboratory system.

CFML_Geometry_SXTAL: Subroutines

Subroutine Z4FrGN (Wave, Ga, Nu, Z4)

Real(Kind=CP)	**Intent(in)**	Wave	Wavelength
Real(Kind=CP)	**Intent(in)**	Ga	Angle
Real(Kind=CP)	**Intent(in)**	Nu	Angle
Real(Kind=CP), Dimension(3)	**Intent(out)**	Z4	

Calculates diffraction vector of a reflection in the Laboratory system from the angles Ga and Nu.

CFML_Geometry_SXTAL: Subroutines

Subroutine Z4FrZ1 (Z1, Om, Ch, Ph, Z4)

Real(Kind=CP), Dimension(3)	**Intent(in)**	Z1	
Real(Kind=CP)	**Intent(in)**	Om	
Real(Kind=CP)	**Intent(in)**	Ch	
Real(Kind=CP)	**Intent(in)**	Ph	
Real(Kind=CP), Dimension(3)	**Intent(out)**	Z4	

Calculate

Z4= Om Ch Ph Z1

CFML_Reflections_Utilities

Module containing a series of procedures handling operation with Bragg reflections

Variables

Reflect_Type
Reflection_Type
Reflection_List_Type

Err_Refl
Err_Refl_Mess
HKL_Ref_Conditions

Functions

AsU_HKL
Get_HEquiv_AsU
Get_MaxNumRef
HKL_Absent

HKL_Equal
HKL_Equiv
HKL_Mult
HKL_R
HKL_S
Unit_Cart_HKL

Subroutines

HKL_Equiv_List
HKL_Gen
HKL_Gen_SXTAL
HKL_RP
HKL_Uni
Init_Err_Refl
Init_RefList
Search_Extinctions
Write_AsU
Write_RefList_Info

Fortran Filename

CFML_Reflct_Util.f90

CFML_Reflections_Utilities: Variables

Reflect_Type
Reflection_Type
Reflection_List_Type

Err_Refl
Err_Refl_Mess
HKL_Ref_Conditions

CFML_Reflections_Utilities: Variables

	Variable	***Definition***
Type :: Reflect_Type		
Integer, Dimension(3)	H	Indices for reflection (hkl)
Integer	Mult	Multiplicity
Real(Kind=CP)	S	sin /
End Type Reflect_Type		

CFML_Reflections_Utilities: Variables

	Variable	***Definition***
Type :: Reflection_Type		
Integer, Dimension(3)	H	index of reflection (hkl)
Integer	Mult	Multiplicity
Real(Kind=CP)	Fo	Observed Structure Factor
Real(Kind=CP)	Fc	Calculated Structure Factor
Real(Kind=CP)	SFo	Sigma of Fo
Real(Kind=CP)	S	sin /
Real(Kind=CP)	W	Weight
Real(Kind=CP)	Phase	Phase in degrees
Real(Kind=CP)	A	Real part of the Structure Factor
Real(Kind=CP)	B	Imaginary part of the Structure Factor
Real(Kind=CP)	AA	Free parameter
Real(Kind=CP)	BB	Free parameter
End Type Reflection_Type		

CFML_Reflections_Utilities: Variables

	Variable	***Definition***
Type :: Reflection_List_Type		
Integer	NRef	Number of Reflections
Type(Reflection_Type), Dimension(:), Allocatable	Ref	Reflection List
End Type Reflection_List_Type		

CFML_Reflections_Utilities: Variables

Logical :: Err_Refl

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module

CFML_Reflections_Utilities: Variables

Character (Len=150) :: Err_Refl_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Reflections_Utilities: Variables

Character(Len=80), Dimension(58) :: HKL_Ref_Conditions

Reflection conditions for Lattices, glide planes, screw axes

CFML_Reflections_Utilities: Functions

CFML_Reflections_Utilities: Functions

Integer Function AsU_HKL (H, SpaceGroup)

Integer, Dimension(3)	**Intent(in)**	H	
Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	

Obtain an equivalent reflection in asymmetric unit using simple transformation rules for each crystal system.

When these rules are not satisfied the output is the (0,0,0) reflection. For obtaining a reflection within the asymmetric unit given an input reflection
the best is to use the function: Get_HEquiv_AsU

Note: in default , we assumed that F(hkl)=F(-h -k -l).

CFML_Reflections_Utilities: Functions

Integer Function Get_HEquiv_AsU (H, SpaceGroup)

Integer, Dimension(3)	**Intent(in)**	H	
Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	

Provides a reflection equivalent to the input one but within the asymmetric unit

CFML_Reflections_Utilities: Functions

Integer Function Get_MaxNumRef (SinTlMax, VolCell, SinTlMin, Mult)

Real(Kind=CP)	**Intent(in)**	SinTlMax	Maximum sin /
Real(Kind=CP)	**Intent(in)**	VolCell	Direct Cell Volume
Real(Kind=CP), Optional	**Intent(in)**	SinTlMin	Minimum sin /
Integer, Optional	**Intent(in)**	Mult	General Multiplicity

Provides an upper limit of the expected maximum number of reflections up to **SinTlMAX** for a volume **VolCell** of the primitive cell. If the optional argument **SinTlMin** is given, the result is the number of reflections in the interval (**SinTlMin**,**SinTlMax**).

If **Mult** is provided the result is divided by this multiplicity so we obtain the expected number of unique reflections.

CFML_Reflections_Utilities: Functions

Logical Function HKL_Absent (H, SpaceGroup)

Integer / Real(Kind=CP), Dimension(3)	**Intent(in)**	H	
Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	

Returns the value **.TRUE.** if the reflection is absent.

CFML_Reflections_Utilities: Functions

Logical Function HKL_Equal (H, K)

Integer / Real(Kind=CP), Dimension(3)	**Intent(in)**	H	Reflection vector
Integer / Real(Kind=CP), Dimension(3)	**Intent(in)**	K	Reflection vector

Returns the value **.TRUE.** if two reflections are equal.

CFML_Reflections_Utilities: Functions

LOGICAL Function HKL_EQUIV (H, K, SPACEGROUP, FRIEDEL)

Integer / Real(Kind=CP), Dimension(3)	Intent(in)	H	Reflection vector
Integer / Real(Kind=CP), Dimension(3)	Intent(in)	K	Reflection vector
TYPE(SPACE_GROUP_TYPE)	Intent(in)	SPACEGROUP	Space group information
LOGICAL, Optional	Intent(in)	FRIEDEL	

Calculate if two reflections are equivalent

CFML_Reflections_Utilities: Functions

Integer Function HKL_Mult (H, SpaceGroup, Friedel)

Integer / Real(Kind=CP), Dimension(3)	**Intent(in)**	H	Reflection vector
Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	Space group information
Logical, Optional	**Intent(in)**	Friedel	

Calculate the multiplicity of the reflection **H**

CFML_Reflections_Utilities: Functions

Integer / Real Function HKL_R (H, OP)

Integer / Real(Kind=CP), Dimension(3)	**Intent(in)**	H	Reflection vector
Type(Sym_Oper_Type)	**Intent(in)**	OP	Symmetry operator

Calculate the equivalent reflection

CFML_Reflections_Utilities: Functions

Real Function HKL_S (H, CrystalCell)

Integer / Real(Kind=CP), Dimension(3)	**Intent(in)**	H	Reflection vector
Type(Crystal_cell_Type)	**Intent(in)**	CrystalCell	Cell Parameters

Calculate: sin / = 1/(2d)

CFML_Reflections_Utilities: Functions

Real Function UNIT_CART_HKL (H, CRYSTALCELL)

Integer / Real(Kind=CP), Dimension(3)	**Intent(in)**	H	Reflection vector
Type(Crystal_Cell_Type)	**Intent(in)**	CrystalCell	Cell Parameters

Calculate a unitary vector in the cartesian crystal frame along a reciprocal vector hkl (reciprocal lattice)

CFML_Reflections_Utilities: Subroutines

- HKL_Equiv_List
- HKL_Gen
- HKL_Gen_SXTAL
- HKL_RP
- HKL_Uni
- Init_Err_Refl
- Init_RefList
- Search_Extinctions
- Write_AsU
- Write_RefList_Info

CFML_Reflections_Utilities: Subroutines

Subroutine HKL_Equiv_List (H, SpaceGroup, Friedel, Mul, HList)

Integer / Real(Kind=CP), Dimension(3)	**Intent(in)**	H	Reflection
Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	Space group
Logical	**Intent(in)**	Friedel	
Integer	**Intent (out)**	Mul	Multiplicity
Integer / Real(Kind=CP), Dimension(3, SpaceGroup%NumOps*2)	**Intent (out)**	HList	

Calculate the multiplicity of the reflection and the list of all equivalent reflections. Friedel law assumed if **Friedel**=.true.

CFML_Reflections_Utilities: Subroutines

Subroutine HKL_Gen (CrystalCell, SpaceGroup, Friedel, Value1, Value2, Num_Ref, Reflex)

Type(Crystal_Cell_Type)	**Intent(in)**	CrystalCell	Cell Parameters
Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	Space group
Logical	**Intent(in)**	Friedel	If TRUE, Friedel law applied
Real(Kind=CP)	**Intent(in)**	Value1	Range in Sin /
Real(Kind=CP)	**Intent(in)**	Value2	
Integer	**Intent (out)**	Num_Ref	Number of generated reflections
Type(Reflect_Type)	**Intent (out)**	Reflex	List of generated hkl,mult, s

Calculate unique reflections between two values of Sin / . The output is not ordered.

CFML_Reflections_Utilities: Subroutines

Subroutine HKL_Gen_SXTAL (CrystalCell, SpaceGroup, STlMax, Num_Ref, Reflex, Ord)

Type(Crystal_Cell_Type)	**Intent(in)**	CrystalCell	Cell Parameters
Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	Space group
Real(Kind=CP)	**Intent(in)**	STlMax	Maximum Sin /
Integer	**Intent (out)**	Num_Ref	Number of generated reflections
Type(Reflect_Type) ***or*** **Type(Reflection_List_Type)**	**Intent (out)**	Reflex	List of generated hkl,mult, s
Integer, Dimension(3), Optional	**Intent (out)**	Ord	Order for loop of hkl-indices

Calculate all allowed reflections up to a maximum value of Sin / .

The output is not ordered but the user can obtain the reflections generated in a particular way by providing the Integer vector **Ord**, containing a permutation of the three numbers 1,2,3. By default the loop generating the hkl-indices uses the vector **Ord**=(/3,2,1/), this means that the inner loop (more rapidly changing index) is the l-index, then the k-index and finally the h-index.

CFML_Reflections_Utilities: Subroutines

Subroutine HKL_RP (H, Phase, OP, K, PhaseN)

Integer / Real(Kind=CP), Dimension(3)	**Intent(in)**	H	Reflection vector
Real(Kind=CP)	**Intent(in)**	Phase	Phase in Degrees
Type(Sym_Oper_Type)	**Intent(in)**	OP	Symmetry operator
Integer / Real(Kind=CP), Dimension(3)	**Intent (out)**	K	Equivalent reflection vector
Real(Kind=CP)	**Intent (out)**	PhaseN	Phase in Degrees of the equivalent reflection

Calculate the equivalent reflection and Phase

CFML_Reflections_Utilities: Subroutines

Subroutine HKL_Uni (CrystalCell, SpaceGroup, Friedel, Value1, Value2, Code, Num_Ref, Reflex)

Type(Crystal_Cell_Type)	**Intent(in)**	CrystalCell	Cell Parameters
Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	Space group
Logical	**Intent(in)**	Friedel	If TRUE, Friedel law applied
Real(Kind=CP)	**Intent(in)**	Value1	Range in Sin /
Real(Kind=CP)	**Intent(in)**	Value2	
Character(Len=1)	**Intent(in)**	Code	Value: R : d-spacing are input
Integer	**Intent(out)**	Num_Ref	Number of generated reflections

Type(reflect_Type), Dimension(:)
or
Type(Reflection_Type), Dimension(:)
or
Type(Reflection_List_Type), Dimension(:)
	Intent(out)	Reflex	Ordered set of reflections

Calculate unique reflections between two values (Value1,Value2) of Sin /

CFML_Reflections_Utilities: Subroutines

Subroutine Init_Err_Refl ( )

Subroutine that initializes errors flags in **CFML_Reflections_Utilities** module.

CFML_Reflections_Utilities: Subroutines

Subroutine Init_RefList (Reflex, N)

Type(Reflection_List_Type)	**Intent(in)**	Reflex	
Integer, Optional	**Intent(in)**	N	Number of reflections on the List

initialize the Reflection List Variable Reflex

CFML_Reflections_Utilities: Subroutines

Subroutine Search_Extintions (SpaceGroup, Iunit)

Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	Space group
Integer, Optional	**Intent(in)**	Iunit	Unit to write

Write information about the Reflections extintion for SpaceGroup

CFML_Reflections_Utilities: Subroutines

Subroutine Write_AsU (SpaceGroup, Iunit)

Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	Space group
Integer, Optional	**Intent(in)**	Iunit	Unit to write

Write information about the asymmetric unit for reciprocal space.

CFML_Reflections_Utilities: Subroutines

Subroutine Write_RefList_Info (Reflex, Iunit, Mode)

Type(Reflection_List_Type)	**Intent(in)**	Reflex	Reflection list
Integer, Optional	**Intent(in)**	Iunit	Unit to write
Character(Len=*), Optional	**Intent(in)**	Mode	Value: NUC : For Nuclear reflections Rest: X-Ray reflections

Write information about the Reflection List

Level 5

Concept	***Module Name***	***Purpose***
Geometry...	**CFML_Geometry_Calc**	Geometry Calculations
Propagation vectors...	**CFML_Propagation_Vectors**	Procedures handling operations with propagation/modulation vectors
Structure Factors...	**CFML_Structure_Factors**	Structure Factors Calculations

CFML_Geometry_Calc

Routines for Geometry Calculations

Variables

Coordination_Type
Point_List_Type

Coord_Info
Err_Geom
Err_Geom_Mess

Functions

Angle_Dihedral
Angle_Mod
Angle_UV
Coord_Mod
Distance
Matrix_PhiTheChi
Matrix_RX
Matrix_RY
Matrix_RZ

Subroutines

Allocate_Coordination_Type
Allocate_Point_List
Calc_Dist_Angle
Calc_Dist_Angle_Sigma
Deallocate_Coordination_Type
Deallocate_Point_List
Distance_And_Sigma
Get_Euler_From_Fract
Get_PhiTheChi
Get_Transf_List
Init_Err_Geom
P1_Dist
Print_Distances
Set_Orbits_InList
Set_TDist_Coordination
Set_TDist_Partial_Coordination

Fortran Filename

CFML_Geom_Calc.f90

Variables

Coordination_Type
Point_List_Type

Coord_Info
Err_Geom
Err_Geom_Mess

CFML_Geometry_Calc

	Variable	***Definition***
Type :: Coordination_Type		
Integer	NAtoms	Number of atoms
Integer	Max_Coor	Maximum number of connected atoms to a given one
Integer, Dimension(:), Allocatable	Coord_Num	Counter of distances connected to the current atom
Integer, Dimension(:,:), Allocatable	N_CooAtm	Pointer to the ordinal number in the list of the attached atom to the atom given by the first index
Integer, Dimension(:,:), Allocatable	N_Sym	Number of symmetry operator to apply to N_COOATM
Real (Kind=CP), Dimension(:,:),	Dist	List of distances related to an atom

Allocatable		
Real (**Kind=CP**), **Dimension**(:,:), **Allocatable**	S_Dist	List of Sigma(distances)
Real (**Kind=CP**), **Dimension**(:,:,:), **Allocatable**	Tr_Coo	
End Type Coordination_Type		

CFML_Geometry_Calc

	Variable	***Definition***
Type :: Point_List_Type		
Integer	NP	Number of points in list
Character (**Len=12**), **Dimension**(:), **Allocatable**	Nam	Name/label associated to each point
Integer, **Dimension**(:), **Allocatable**	P	Integer pointer for various purposes
Real, **Dimension**(:,:), **Allocatable**	X	Fractional coordinates of points
End Type Point_List_Type		

CFML_Geometry_Calc

Type (Coordination_Type) :: Coord_Info

Coordination information

CFML_Geometry_Calc

Logical :: Err_Geom

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_Geometry_Calc

Character (Len=150) :: Err_Geom_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Geometry_Calc: Functions

- Angle_Dihedral
- Angle_Mod
- Angle_UV
- Coord_Mod
- Distance
- Matrix_PhiTheChi
- Matrix_RX
- Matrix_RY
- Matrix_RZ

CFML_Geometry_Calc: Functions

Real Function Angle_Dihedral (U, V, W)

Real(Kind=CP), Dimension(3)	**Intent(in)**	U	Vector
Real(Kind=CP), Dimension(3)	**Intent(in)**	V	Vector
Real(Kind=CP), Dimension(3)	**Intent(in)**	W	Vector

or

Real Function Angle_Dihedral (RI, RJ, RK, RN)

Real(Kind=CP), Dimension(3)	**Intent(in)**	RI	Vector
Real(Kind=CP), Dimension(3)	**Intent(in)**	RJ	Vector
Real(Kind=CP), Dimension(3)	**Intent(in)**	RK	Vector
Real(Kind=CP), Dimension(3)	**Intent(in)**	RN	Vector

Calculates the dihedral angle between planes U-V and V-W, where vectors U,V,W are given in cartesian components.

Calculates the dihedral angle corresponding to the four points (RI,RJ,RK,RN) given in cartesian components. The definition used for the dihedral angle is the following:

$$\phi(i,j,k,n) = a\cos\left\{ \frac{\left(r_{ij}\times r_{jk}\right)\left(r_{jk}\times r_{kn}\right)}{\left|r_{ij}\times r_{jk}\right|\left|r_{jk}\times r_{kn}\right|} \right\}$$

with this definition the sign of PHI is positive if the vector product

$$\left(r_{ij}\times r_{jk}\right)\times\left(r_{jk}\times r_{kn}\right)$$

is in the same direction as $\boldsymbol{r_{jk}}$, and negative if the direction is opposite.

CFML_Geometry_Calc: Functions

Real Function Angle_Mod (X)

Real(Kind=CP)	**Intent(in)**	X	Value

or

Real(Kind=CP), Dimension(:)	**Intent(in)**	X	Value

Calculates the angle [- ,)

CFML_Geometry_Calc: Functions

Real Function Angle_UV (U,V,G)

Integer, Dimension(:)	**Intent(in)**	U	Vector
Integer, Dimension(:)	**Intent(in)**	V	Vector
Real(Kind=CP), Dimension(:,:), Optional	**Intent(in)**	G	Metric tensor

or

Real(Kind=CP), Dimension(:)	**Intent(in)**	U	Vector
Real(Kind=CP), Dimension(:)	**Intent(in)**	V	Vector
Real(Kind=CP), Dimension(:,:), Optional	**Intent(in)**	G	Vector

Calculates the angle between vectors **U** and **V** given in cartesian components. If **G** is not given cartesian components are assumed.

CFML_Geometry_Calc: Functions

Real Function Coord_Mod (X)

Real(Kind=CP)	**Intent(in)**	X	Value

or

Real(Kind=CP), Dimension(:)	**Intent(in)**	X	Value

Calculates the coordinates between [0,1)

CFML_Geometry_Calc: Functions

Real Function Distance (X0, X1, Cell)

Real(Kind=CP), Dimension(3)	**Intent(in)**	X0	Point
Real(Kind=CP), Dimension(3)	**Intent(in)**	X1	Point
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters

or

Real Function Distance (X0, X1, Code)

Real(Kind=CP), Dimension(3)	**Intent(in)**	X0	Point
Real(Kind=CP), Dimension(3)	**Intent(in)**	X1	Point
Character(Len=*), Optional	**Intent(in)**	Code	Values: C : Cartesian (Default) S : Spherical

Calculate distance between two points.

CFML_Geometry_Calc: Functions

Real Function Matrix_PhiTheChi (Phi, Theta, Chi, Code)

Real(Kind=CP)	**Intent(in)**	Phi	Phi
Real(Kind=CP)	**Intent(in)**	Theta	Theta
Real(Kind=CP)	**Intent(in)**	Chi	Chi
Character(Len=*), Optional	**Intent(in)**	Code	Values: R : Values are in radians (Default) D : Values are in degrees

Calculate the active rotation matrix (3,3) corresponding to the composition of a rotation around Z of angle Chi, followed by a rotation of angle Theta around the Y-axis and a subsequent rotation of angle Phi around z.

The matrix is M = Rz(Phi) . Ry(Theta) . Rz(Chi)

The columns represent the components of the unitary vectors {u,v,w} that may be considered as an alternative orthonormal frame to the canonical {i,j,k}. Applying the matrix M to a point in {i,j,k} gives another point in {i,j,k} obtained by the successive application of the three rotations given above. The transpose (inverse) of the M-matrix, when applied to a point in {i,j,k}, gives the coordinates of the same point referred to the frame {u,v,w}.

CFML_Geometry_Calc: Functions

Real Function Matrix_RX (Ang, Code)

Real(Kind=CP)	**Intent(in)**	Ang	Angle
Character(Len=*), Optional	**Intent(in)**	CODE	Values: R : Values are in radians (Default) D : Values are in degrees

Calculate the active rotation matrix (3,3) corresponding to the positive rotation of an angle around the x-axis.

CFML_Geometry_Calc: Functions

Real Function Matrix_RY (Ang, Code)

Real(Kind=CP)	**Intent(in)**	Ang	Angle
Character(Len=*), Optional	**Intent(in)**	Code	Values: R : Values are in radians (Default) D : Values are in degrees

Calculate the active rotation matrix (3,3) corresponding to the positive rotation of an angle around the y-axis.

CFML_Geometry_Calc: Functions

Real Function Matrix_RZ (Ang, Code)

Real(Kind=CP)	**Intent(in)**	Ang	Angle
Character(Len=*), Optional	**Intent(in)**	Code	Values: R : Values are in radians (Default) D : Values are in degrees

Calculate the active rotation matrix (3,3) corresponding to the positive rotation of an angle around the z-axis.

CFML_Geometry_Calc: Subroutines

CFML_Geometry_Calc: Subroutines

Subroutine Allocate_Coordination_Type (NAsu, NumOPs, DMax, Max_Coor)

Integer	**Intent(in)**	NAsu	Number of atoms in asymmetric unit
Integer	**Intent(in)**	NumOPs	Number of S.O. excluding lattice centerings
Real(Kind=CP)	**Intent(in)**	DMax	Maximun distance to be calculated
Integer	**Intent(out)**	Max_Coor	Maximum coordination allowed

Allocation of variable Coord_Info.

Note: Should be called before using this module.

CFML_Geometry_Calc: Subroutines

Subroutine Allocate_Point_List (N, Pl, Ier)

Integer	**Intent(in)**	N	Dimension for allocating components
Type(Point_List_Type)	**Intent(in out)**	Pl	Type with allocatable components
Integer	**Intent(out)**	Ier	If /= 0 an error occurred

Allocation of an objet of type Point_List_Type

CFML_Geometry_Calc: Subroutines

Subroutine Calc_Dist_Angle (DMax, DAngl, Cell, Spg, A, Lun)

Real(Kind=CP)	**Intent(in)**	DMax	Max. Distance to calculate
Real(Kind=CP)	**Intent(in)**	DAngl	Max. distance for angle calculations
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Space_Group_Type)	**Intent(in)**	Spg	Space group information
Type(Atom_List_Type)	**Intent(in)**	A	Atoms information
Integer, Optional	**Intent(in)**	Lun	Logical Unit for writing

Subroutine to calculate distances and angles, below the prescribed distances DMax and DAngl (angles of triplets at distance below DAngl to an atom), without standard deviations. If DAngl=0.0, no angle calculations are done. Writes results in file (unit=Lun) if Lun is present. Control for error is present.

CFML_Geometry_Calc: Subroutines

Subroutine Calc_Dist_Angle_Sigma (DMax, DAngl, Cell, Spg, A, Lun, Lun_Cons, Lun_CIF)

Real(Kind=CP)	**Intent(in)**	DMax	Max. Distance to calculate
Real(Kind=CP)	**Intent(in)**	DAngl	Max. distance for angle calculations
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Space_Group_Type)	**Intent(in)**	Spg	Space group information
Type(Atom_List_Type)	**Intent(in)**	A	Atoms information
Integer, Optional	**Intent(in)**	Lun	Logical Unit for writing
Integer, Optional	**Intent(in)**	Lun_Cons	Logical unit for writing restraints
Integer, Optional	**Intent(in)**	Lun_CIF	Logical unit for writing CIF file with distances and angles

Subroutine to calculate distances and angles, below the prescribed distances DMax and DAngl (angles of triplets at distance below DAngl to an atom), without standard deviations. If DAngl=0.0, no angle calculations are done. Writes results in file (unit=Lun) if Lun is present. Control for error is present.

CFML_Geometry_Calc: Subroutines

Subroutine Deallocate_Coordination_Type ( )

Deallocation of variable Coord_Info

CFML_Geometry_Calc: Subroutines

Subroutine Deallocate_Point_List (Pl)

Type(Point_List_Type)	**Intent(in out)**	Pl	Type with allocatable components

Deallocation of an objet of type Point_List_Type

CFML_Geometry_Calc: Subroutines

Subroutine Distance_And_Sigma (CellP, Derm, X0, X1, S0, S1, Dis, S)

Type(Crystal_Cell_Type)	**Intent(in)**	CellP	Cell parameters
Real(Kind=CP), Dimension(3,3,6)	**Intent(in)**	Derm	Matrix of derivatives of CELLP%CR_ORTH_CEL
Real(Kind=CP), Dimension(3)	**Intent(in)**	X0	Point vector
Real(Kind=CP), Dimension(3)	**Intent(in)**	X1	Point vector
Real(Kind=CP), Dimension(3)	**Intent(in)**	S0	Sigma of Point Vector
Real(Kind=CP), Dimension(3)	**Intent(in)**	S1	Sigma of Point Vector
Real(Kind=CP)	**Intent(out)**	Dis	Distance
Real(Kind=CP)	**Intent(out)**	S	Sigma of Distance

Calculate de Distance and sigma between two points in fractional coordinates

CFML_Geometry_Calc: Subroutines

Subroutine Get_Euler_From_Fract (X1, X2, X3, MT, Phi, Theta, Chi, EuM, Code)

Real(Kind=CP), Dimension(3)	**Intent(in)**	X1	Point vector
Real(Kind=CP), Dimension(3)	**Intent(in)**	x2	Point vector
Real(Kind=CP), Dimension(3)	**Intent(in)**	X3	Point vector
Real(Kind=CP), Dimension(3,3)	**Intent(in)**	MT	Matrix transforming to Cartesian coordinates

Real(Kind=CP)	**Intent(out)**	Phi	Angle PHI
Real(Kind=CP)	**Intent(out)**	Theta	Angle Theta
Real(Kind=CP)	**Intent(out)**	Chi	Angle CHI
Real(Kind=CP), Dimension(3,3), Optional	**Intent(out)**	EuM	
Character(Len=*), Optional	**Intent(in)**	Code	

Subroutine to obtain the Euler angles (2nd setting) of a Cartesian frame having as origin the point X3, the z-axis along X1-X3 and the XZ plane coincident with the plane generated by the two vectors (X2-X3,X1-X3).

CFML_Geometry_Calc: Subroutines

Subroutine Get_PhiTheChi (MT, Phi, Theta, Chi, Code)

Real(Kind=CP), Dimension(3,3)	**Intent(in)**	MT	Matrix transforming to Cartesian coordinates
Real(Kind=CP)	**Intent(out)**	Phi	Angle PHI
Real(Kind=CP)	**Intent(out)**	Theta	Angle Theta
Real(Kind=CP)	**Intent(out)**	Chi	Angle CHI
Character(Len=*), Optional	**Intent(in)**	Code	Values: R : Radians (Default) D : Degrees

Calculate the Euler Angles corresponding to an orthogonal matrix. The definition of the Euler angles in this case correspond to the active rotation matrix obtained from the composition of a rotation around Z of angle Chi, followed by a rotation of angle Theta around the Y-axis and a subsequent rotation of angle Phi around Z.

The matrix is supposed to be of the form: M = Rz(Phi).Ry(Theta).Rz(Chi)

A checking of the input matrix is given before calculating the angles.

The user must check the logical variable Err_Geom after calling this subroutine. If Err_Geom=.TRUE. it means that the input matrix is not orthogonal.

CFML_Geometry_Calc: Subroutines

Subroutine Get_Transf_List (Trans, OX, PL, NPL, IFail)

Real(Kind=CP), Dimension(3,3)	**Intent(in)**	Trans	Matrix transforming the basis
Real(Kind=CP), Dimension(3)	**Intent(in)**	OX	Coordinates of origin of the new basis
Type(Point_List_Type)	**Intent(in)**	PL	Point list
Type(Point_List_Type)	**Intent(in out)**	NPL	List of transformed points
Integer	**Intent(out)**	IFail	If /=0 matrix inversion failed

Subroutine to get the fractional coordinates of the points of the input list PL in the new transformed cell (a'= trans a) displaced to the new origing OX. The coordinates are generated using only lattice translations. All coordinates are reduced to be between 0.0 and 1.0, so that 0.0 <= x,y,z < 1.0

CFML_Geometry_Calc: Subroutines

Subroutine Init_Err_Geom ( )

Subroutine that initializes errors flags in **CFML_Geometry_Calc** module.

CFML_Geometry_Calc: Subroutines

Subroutine P1_Dist (DMax, Cell, Spg, Ac, Lun)

Real(Kind=CP)	**Intent(in)**	DMax	Max. Distance to calculate
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Space_Group_Type)	**Intent(in)**	Spg	Space group information
Type(Atoms_Cell_Type)	**Intent(in out)**	Ac	Atoms information
Integer, Optional	**Intent(in)**	Lun	Logical Unit for writing

Subroutine calculate distances, below the prescribed distances DMAX, without standard deviations. No symmetry is applied: only lattice translations.

CFML_Geometry_Calc: Subroutines

Subroutine Print_Distances (Lun, DMax, Cell, Spg, A)

Integer	**Intent(in)**	Lun	Logical Unit for writing
Real(Kind=CP)	**Intent(in)**	DMax	Max. Distance to calculate
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Space_Group_Type)	**Intent(in)**	Spg	Space group information
Type(Atom_List_Type)	**Intent(in)**	A	Atoms information

Subroutine to print distances, below the prescribed distances DMax, without standard deviations.

CFML_Geometry_Calc: Subroutines

Subroutine Set_Orbits_InList (Spg, PL)

Type(Space_Group_Type)	**Intent(in)**	Spg	Space group
Type(Point_List_Type)	**Intent(in out)**	PL	Point list

Set up of the Integer pointer PL%P in the object **PL** of type Point_List_Type. Each point is associated with the number of an orbit. This pointer is useful to get the asymmetric unit with respect to the input space group of an arbitrary list of points (atom coordinates).

CFML_Geometry_Calc: Subroutines

Subroutine Set_TDist_Coordination (Max_Coor, DMax, Cell, Spg, A)

Integer	**Intent(in)**	Max_Coor	Maximum expected coordination
Real(Kind=CP)	**Intent(in)**	DMax	Max. Distance to calculate
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Space_Group_Type)	**Intent(in)**	Spg	Space group information
Type(Atom_List_Type)	**Intent(in)**	A	Atoms information

Subroutine to calculate distances, below the prescribed distance **DMax**. Sets up the coordination type: Coord_Info for each atom in the asymmetric unit

The input argument **Max_Coor** is obtained, before calling the present procedure, by a call to Allocate_Coordination_Type with arguments:(A%NAtoms,SPG%Multip,DMax,Max_Coor)

Further calls to this routine do not need a previous call to Allocate_Coordination_Type.

CFML_Geometry_Calc: Subroutines

Subroutine Set_TDist_Partial_Coordination (List, Max_Coor, DMax, Cell, Spg, A)

Integer	**Intent(in)**	List	Modified atom
Integer	**Intent(in)**	Max_Coor	Maximum expected coordination
Real(Kind=CP)	**Intent(in)**	DMax	Max. Distance to calculate
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Space_Group_Type)	**Intent(in)**	Spg	Space group information
Type(Atom_List_Type)	**Intent(in)**	A	Atoms information

Modify the coordination type: Coord_Info for the atoms affected by the change of atom "List"

This routine is a modification of Set_TDist_Coordination to avoid superfluous calculations in global optimization methods. It assumes that Set_TDist_Coordination has previously been called and the object Coord_Info has already been set.

CFML_Propagation_Vectors

Series of procedures handling operation with Propagation vectors

Variables

Group_K_Type

Functions

HK_Equiv
K_Equiv
K_Equiv_Minus_K

Subroutines

K_Star
Write_Group_K

Fortran Filename

CFML_Propagk.f90

CFML_Propagation_Vectors: Variables

Group_K_Type

CFML_Propagation_Vectors: Variables

	Variable	***Definition***

Type :: Group_K_Type

Type(Space_Group_Type)	G0	initial Space group
Integer	NGK	Number of elements of G_k
Logical	K_Equiv_MinusK	**TRUE** if k equiv -k
Integer, Dimension(192)	P	Pointer to operations of G0 that changes/fix k
Integer, Dimension(48,48)	CO	
Integer	NK	Number of star arms
Real(Kind=CP), Dimension(3,24)	StarK	Star of the wave vector k

End Type Group_K_Type

The Integer pointer P is used as follows:

If we defined the object G as -> Group_K_Type

G%P(1:NGK) gives the numeral of the symmetry operators of G%G0 belonging to G_k.

G%P(192:193-NK) gives the numeral of the the symmetry operators of G%G0 that transform the initial k-vector to the other arms of the star.

G%CO(:,KK) gives also the numerals of the the symmetry operators of G%G0 that transform the initial k-vector to the arm kk of the star to the representative of the coset decomposition of G%G0 with respect to G_k.

CFML_Propagation_Vectors: Functions

HK_Equiv
K_Equiv
K_Equiv_Minus_K

CFML_Propagation_Vectors: Functions

Logical Function HK_Equiv (H, K, SpaceGK, Friedel)

Real(Kind=CP), Dimension(3)	Intent(in)	H	
Real(Kind=CP), Dimension(3)	Intent(in)	K	
Type(Group_K_Type)	Intent(in)	SpaceGK	
Logical, Optional	Intent(in)	Friedel	

Calculate if two real reflections are equivalent

CFML_Propagation_Vectors: Functions

Logical Function K_Equiv (H, K, LatTyp)

Real(Kind=CP), Dimension(3)	Intent(in)	H	
Real(Kind=CP), Dimension(3)	Intent(in)	K	
Character (Len=*)	Intent(in)	LatTyp	

Calculate if two k-vectors are equivalent in the sense that **H** is equivalent to **K** if **H-K** belongs to the reciprocal lattice. Only lattice type is needed.

CFML_Propagation_Vectors: Functions

Logical Function K_Equiv_Minus_K (Vec, Lat)

Real(Kind=CP), Dimension(3)	**Intent(in)**	Vec	
Character (Len=*)	**Intent(in)**	Lat	

Determine whether a k-vector is equivalent to -k

CFML_Propagation_Vectors: Subroutines

- K_Star
- Write_Group_K

CFML_Propagation_Vectors: Subroutines

Subroutine K_Star (K, SpaceGroup, GK)

Integer, Dimension(3)	**Intent(in)**	K	
Type(Space_Group_Type)	**Intent(in)**	SpaceGroup	
Type(Group_K_Type)	**Intent(in)**	GK	

Calculate the star of the propagation vector and the group of the vector k.

CFML_Propagation_Vectors: Subroutines

Subroutine Write_Group_K (GK, Lun)

Type(Group_K_Type)	**Intent(in)**	GK	
Integer, Optional	**Intent(in)**	Lun	Logical unit write

Subroutine to write the operators of the propagation vector group and the list of all vectors {k}, belonging to the star of k.

CFML_Structure_Factor_Module

Main module for Structure Factors Calculations

Variables

- Err_SFac
- Err_SFac_Mess

Subroutines

- Calc_HKL_StrFactor
- Calc_StrFactor
- Init_Calc_StrFactors
- Init_Calc_HKL_StrFactors
- Init_Structure_Factors
- Modify_SF
- Structure_Factors
- Write_Structure_Factors

Fortran Filename

CFML_Sfac.f90

CFML_Structure_Factor_Module: Variables

- Err_SFac
- Err_SFac_Mess

CFML_Structure_Factor_Module: Variables

Logical :: Err_SFac

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module

CFML_Structure_Factor_Module: Variables

Character (Len=150) :: Err_SFac_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Structure_Factor_Module: Subroutines

- Calc_HKL_StrFactor
- Calc_StrFactor
- Init_Calc_StrFactors
- Init_Calc_HKL_StrFactors
- Init_Structure_Factors
- Modify_SF
- Structure_Factors
- Write_Structure_Factors

CFML_Structure_Factor_Module: Subroutines

Subroutine Calc_HKL_StrFactor (Mode, Rad, HN, SN, Atm, Grp, SF2, Deriv, Fc)

Character(Len=*)	**Intent(in)**	Mode	Values: S : SXTAL P : Powder
Character(Len=*)	**Intent(in)**	Rad	Radiation: X-rays, Neutrons
Integer	**Intent(in)**	HN	Reflection H
Real(Kind=CP)	**Intent(in)**	SN	(sin /)^2
Type(Atom_List_Type)	**Intent(in)**	Atm	Atoms information
Type(Space_Group_Type)	**Intent(in)**	Grp	Space group information
Real(Kind=CP)	**Intent(out)**	SF2	
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	Deriv	
Complex, Optional	**Intent(out)**	Fc	

Calculate Structure Factor for reflection HN=(hkl) not related with previous lists and derivatives with respect to refined parameters.

This subroutine calculates the form-factors internally without using global tables. The purpose of this procedure is to avoid the use of too much memory in tables.

CFML_Structure_Factor_Module: Subroutines

Subroutine Calc_StrFactor (Mode, Rad, NN, SN, Atm, Grp, SF2, Deriv, Fc)

Character(Len=*)	**Intent(in)**	Mode	Values: S : SXTAL P : Powder
Character(Len=*)	**Intent(in)**	Rad	Radiation: X-rays, Neutrons
Integer	**Intent(in)**	NN	
Real(Kind=CP)	**Intent(in)**	SN	(sin /)^2
Type(Atom_List_Type)	**Intent(in)**	Atm	Atoms information
Type(Space_Group_Type)	**Intent(in)**	Grp	Space group information
Real(Kind=CP)	**Intent(out)**	SF2	
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	Deriv	
Complex, Optional	**Intent(out)**	Fc	

Calculate Structure Factor for reflection NN in the list and derivatives with respect to refined parameters

CFML_Structure_Factor_Module: Subroutines

Subroutine Init_Calc_StrFactors (Reflex, Atm, Grp, Mode, Lambda, Lun)

Type(Reflection_List_Type)	**Intent(in)**	Reflex	Reflection information
Type(Atom_List_Type)	**Intent(in)**	Atm	Atoms information
Type(Space_Group_Type)	**Intent(in)**	Grp	Space group information
Character(Len=*), Optional	**Intent(in)**	Mode	Value: NUC : For Nuclear reflections Rest: X-Ray reflections
Real(Kind=CP), Optional	**Intent(in)**	Lambda	Wavelength
Integer, Optional	**Intent(in)**	Lun	Logical unit for writing scatt-factors

Allocates and initializes arrays for Calc_StrFactor calculations.

Calculations of fixed tables are performed. Should be called before using the subroutine Calc_StrFactor

CFML_Structure_Factor_Module: Subroutines

Subroutine Init_Calc_HKL_StrFactors (Atm, Mode, Lambda, Lun)

Type(Atom_List_Type)	**Intent(in)**	Atm	Atoms information
Character(Len=*), Optional	**Intent(in)**	Mode	Value: NUC : For Nuclear reflections Rest: X-Ray reflections
Real(Kind=CP), Optional	**Intent(in)**	Lambda	Wavelength
Integer, Optional	**Intent(in)**	Lun	Logical unit for writing scatt-factors

Allocates and initializes arrays for hkl - Structure Factors calculations.

No calculation of fixed tables is performed. Should be called before using the subroutine Calc_HKL_StrFactor

CFML_Structure_Factor_Module: Subroutines

Subroutine Init_Structure_Factors (Reflex, Atm, Grp, Mode, Lambda, Lun)

Type(Reflection_List_Type)	**Intent(in out)**	Reflex	Reflection information
Type(Atom_List_Type)	**Intent(in)**	Atm	Atoms information
Type(Space_Group_Type)	**Intent(in)**	Grp	Space group information
Character(Len=*), Optional	**Intent(in)**	Mode	Value: NUC : For Nuclear reflections Rest: X-Ray reflections
Real(Kind=CP), Optional	**Intent(in)**	Lambda	Wavelength
Integer, Optional	**Intent(in)**	Lun	Logical unit write

Allocates and initializes arrays for Structure Factors calculations. A calculation of fixed tables is also performed.

CFML_Structure_Factor_Module: Subroutines

Subroutine Modify_SF (Reflex, Atm, Grp, List, NList, Mode)

Type(Reflection_List_Type)	**Intent(in out)**	Reflex	Reflection information
Type(Atom_List_Type)	**Intent(in)**	Atm	Atoms information
Type(Space_Group_Type)	**Intent(in)**	Grp	Space group information
Integer, Dimension(:)	**Intent(in)**	List	
Integer	**Intent(in)**	NList	
Character(Len=*), Optional	**Intent(in)**	Mode	Value: NUC : For Nuclear reflections Rest: X-Ray reflections

Recalculation of Structure Factors because a list of Atoms parameters were modified.

List variable contains the number of atoms to be changed.

CFML_Structure_Factor_Module: Subroutines

Subroutine Structure_Factors (Atm, Grp, Reflex, Mode, Lambda)

Type(Atom_List_Type)	**Intent(in)**	Atm	Atoms information
Type(Space_Group_Type)	**Intent(in)**	Grp	Space group information
Type(REFLECTION_LIST_TYPE)	**Intent(in out)**	Reflex	Reflection information
Character(Len=*), Optional	**Intent(in)**	Mode	Value: NUC : For Nuclear reflections Rest: X-Ray reflections
Real(Kind=CP), Optional	**Intent(in)**	Lambda	Wavelength

Calculate the Structure Factors from a list of Atoms and a set of reflections.

A call to Init_Structure_Factors is a pre-requisite for using this subroutine.

CFML_Structure_Factor_Module: Subroutines

Subroutine Write_Structure_Factors (Lun, Reflex, Mode)

Integer	**Intent(in)**	Lun	Logical unit write
Type(Reflection_List_Type)	**Intent(in)**	Reflex	Reflection list
Character(Len=*), Optional	**Intent(in)**	Mode	Value: NUC : For Nuclear reflections Rest: X-Ray reflections

Writes in logical unit=Lun the list of structure factors

Level 6

Concept	***Module Name***	***Purpose***
Configurations...	**CFML_BVS_Energy_Calc**	Procedures related to calculations of energy or configuration properties depending on the crystal structure: BVS, Energy,...
Maps...	**CFML_Maps_Calculations**	Procedures related to operations on arrays describing maps
Molecular...	**CFML_Molecular_Crystals**	Types and procedures related to molecules in crystals

CFML_BVS_Energy_Calc

Module containing procedures related to calculations of Energy or Configuration properties depending on the crystal structure: BVS, Energy,....

Parameters

BVS_Anions
BVS_Anions_N
BVS_Anions_Rlon
BVS_Species_N

Variables

Atoms_Conf_List_Type
BVS_Par_Type

BVS_Table
Err_Conf
Err_Conf_Mess

Subroutines

Allocate_Atoms_Conf_List
Calc_BVS
Calc_Map_BVS
Cost_BVS

- Cost_BVS_CoulombRep
- Deallocate_Atoms_Conf_List
- Deallocate_BVS_Table
- Init_Err_Conf
- Set_BVS_Table
- Set_Table_D0_B
- Species_on_List

Fortran Filename

CFML_Conf_Calc.f90

CFML_BVS_Energy_Calc: Parameters

- BVS_Anions
- BVS_Anions_N
- BVS_Anions_RIon
- BVS_Species_N

CFML_BVS_Energy_Calc: Parameters

Character (Len=*), Dimension(BVS_Anions_N) :: BVS_Anions

Anions tabulated in Bond Valence parameters from O'Keefe, Bresse, Brown

Values are:

Order	*Anion*
1	O-2
2	F-1
3	CL-1
4	BR-1
5	I-1
6	S-2
7	SE-2
8	TE-2
9	N-3
10	P-3
11	AS-3
12	H-1
13	O-1
14	SE-1

CFML_BVS_Energy_Calc: Parameters

Integer :: BVS_Anions_N=14

Number of anions tabulated in BV Tables by O'Keefe, Breese, Brown

CFML_BVS_Energy_Calc: Parameters

Real, Dimension(BVS_Anions_N) :: BVS_Anions_RIon

Ionic radii for anions in Bond Valence parameters table

Values are:

Order	***Value***
1	1.40
2	1.19
3	1.67
4	1.95
5	2.16
6	1.84
7	1.98
8	2.21
9	1.71
10	2.12
11	2.22
12	2.08
13	1.35
14	1.80

CFML_BVS_Energy_Calc: Parameters

Integer :: BVS_Species_N=247

Maximum number of species in BVS_Table

CFML_BVS_Energy_Calc: Variables

- Atoms_Conf_List_Type
- BVS_Par_Type

- BVS_Table
- Err_Conf
- Err_Conf_Mess

CFML_BVS_Energy_Calc: Variables

	Variable	***Definition***
Type :: Atoms_Conf_List_Type		
Integer	NAtoms	Total number of atoms in the list
Integer	N_Spec	Number of different species in the list
Integer	N_Anions	Number of anions in the list
Integer	N_Cations	Number of cations in the list
Real (Kind=CP)	Tol	Tolerance(%) for sum of radii conditions
Real (Kind=CP)	TotAtoms	Total number of atoms in the unit cell
Character (Len=4),Dimension(:), Allocatable	Species	Symbol + valence

Real (Kind=CP), Dimension(:), Allocatable	Radius	ionic/atomic radius of species
Type (Atom_Type), Dimension(:), Allocatable	Atom	Atom information
End Type Atoms_Conf_List_Type		

CFML_BVS_Energy_Calc: Variables

	Variable	***Definition***
Type :: BVS_Par_Type		
Character (Len=4)	Symb	Chemical symbol
Real (Kind=CP), Dimension(BVS_Anions_N)	D0	D0 Parameter
Real (Kind=CP), Dimension(BVS_Anions_N)	B_Par	B Parameter
Integer, Dimension(BVS_Anions_N)	RefNum	Integer pointing to the reference paper
End Type BVS_Par_Type		

CFML_BVS_Energy_Calc: Variables

Type (BVS_Par_Type), Dimension(:), Allocatable :: BVS_Table

Global variable containing BVS parameters for calculations. The dimension is defined for the parameter BVS_Species_N

CFML_BVS_Energy_Calc: Variables

Logical :: Err_Conf

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_BVS_Energy_Calc: Variables

Character (Len=150) :: Err_Conf_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_BVS_Energy_Calc: Subroutines

- Allocate_Atoms_Conf_List
- Calc_BVS
- Calc_Map_BVS
- Cost_BVS
- Cost_BVS_CoulombRep
- Deallocate_Atoms_Conf_List
- Deallocate_BVS_Table
- Init_Err_Conf

Set_BVS_Table
Set_Table_D0_B
Species_on_List

CFML_BVS_Energy_Calc: Subroutines

Subroutine Allocate_Atoms_Conf_List (N, A)

Integer	**Intent(in)**	N	Atoms in asymmetric unit
Type(Atoms_Conf_List_Type)	**Intent(in out)**	A	Objet to be allocated

Allocation of objet A of type Atoms_Conf_List_Type. This subroutine should be called before using an object of type Atoms_Conf_List_Type.

CFML_BVS_Energy_Calc: Subroutines

Subroutine Calc_BVS (A, IPr, N_BVSM, BVS_M, FileCod)

Type(Atoms_Conf_List_Type)	**Intent(in)**	A	Atoms information
Integer, Optional	**Intent(in)**	IPr	Logical unit write
Integer, Optional	**Intent(in)**	N_BVSM	Number of modifications
Character (Len=*), Dimension(:), Optional	**Intent(in)**	BVS_M	Text with BVS parameters
Character (Len=*), Optional	**Intent(in)**	FileCod	

Subroutine to calculate Bond-Valence sums.

Before calling this subroutine it is the responsibility of the calling program to make a previous call to Calc_Dist_Angles_Sigma in order to update the internal private variables related to distance/angle calculations.

CFML_BVS_Energy_Calc: Subroutines

Subroutine Calc_Map_BVS (A, Spg, Cell, FileCod, NDimX, NDimY, NDimZ, AtName, DRMax)

Type(Atoms_Conf_List_Type)	**Intent(in)**	A	Atoms information
Type(Space_Group_Type)	**Intent(in)**	Spg	Space group
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Character (Len=*)	**Intent(in)**	FileCod	
Integer	**Intent(in)**	NDimX	Dimension in x-axis for the BVS map
Integer	**Intent(in)**	NDimY	Dimension in y-axis for the BVS map
Integer	**Intent(in)**	NDimZ	Dimension in z-axis for the BVS map
Character (Len=*)	**Intent(in)**	AtName	
Real(Kind=CP)	**Intent(in)**	DRMax	

Calculate a map of BVS values where each point of the grid is determined by a specie representative defined in **AtName**. The BVS value is evaluated into of **DRMax** value. The BVS map is saved in the file called given as FileCod.

CFML_BVS_Energy_Calc: Subroutines

Subroutine Cost_BVS (A, GII, GIC)

Type(Atoms_Conf_List_Type)	**Intent(in)**	A	Atoms information

Real(Kind=CP)	**Intent(out)**	GII	Global instability index
Character (Len=*), Optional	**Intent(in)**	GIC	If present GII_c is put in GII

Subroutine to calculate the Global instability index.

Before calling this subroutine it is the responsibility of the calling program to make a previous call to
Set_TDist_Coordination in order to update the
internal private variables related to distance/angle calculations.

All items corresponding to the bond-valence parameters contained in A have to be properly set before calling this procedure.

Subroutine Cost_BVS_CoulombRep (A, GII, ERep)

Type(Atoms_Conf_List_Type)	**Intent(in)**	A	Atoms information
Real(Kind=CP)	**Intent(out)**	GII	Global instability index
Real(Kind=CP)	**Intent(out)**	ERep	Pseudo Repulsion Coulomb "energy"

Subroutine to calculate the Global instability index Gii_a and a pseudo Coulomb repulsion energy useful to avoid cation-cation and anion-anion overlap when using this cost function for predicting or solving a ionic crystal structure. It was used in the old program PiXSA, by J. Pannetier, J. Bassas-Alsina, J.Rodriguez-Carvajal and V. Caignaert, in "Prediction of Crystal Structures from Crystal Chemistry Rules by Simulated Annealing", Nature 346, 343-345 (1990).

Before calling this subroutine it is the responsibility of the calling program to make a previous call to
Set_TDist_Coordination in order to update the internal Coord_Info variable related to distance and angle calculations.

Subroutine Deallocate_Atoms_Conf_List (A)

Type(Atoms_Conf_List_Type)	**Intent(in out)**	A	Objet to be allocated

De-allocation of objet A of type Atoms_Conf_List_Type. This subroutine should be after using an object of type Atoms_Conf_List_Type that is no more needed.

Subroutine Deallocate_BVS_Table ( )

Deallocating BVS_Table

Subroutine Init_Err_Conf ( )

Subroutine that initializes errors flags in **CFML_BVS_Energy_Calc** module.

Subroutine Set_BVS_Table ( )

Fills the parameters for BVS from O'Keefe, Bresse, Brown in the BVS_Table variable

CFML_BVS_Energy_Calc: Subroutines

Subroutine Set_Table_D0_B (A, N_BVSM, BVS_M)

Type(Atoms_Conf_List_Type)	**Intent(in)**	A	Atoms information
Integer, Optional	**Intent(in)**	N_BVSM	Number of bvs strings with externally provided values
Character (Len=*), Dimension(:), Optional	**Intent(in)**	BVS_M	Text with BVS parameters

Set external values for D0 and B in BVS calculations

CFML_BVS_Energy_Calc: Subroutines

Subroutine Species_on_List (A, Mulg, Tol)

Type(Atoms_Conf_List_Type)	**Intent(in)**	A	Atoms information
Integer, Optional	**Intent(in)**	Mulg	
Real(Kind=CP), Optional	**Intent(in)**	Tol	

Determines the different species in the List and, optionally, sets the tolerance factor for ionic radii conditions and provides "corrected" occupation factors (mult/MulG) when the user is using a multiplier. The general multiplicity of the space group MulG must be provided in such a case. This first free variable of the Atom-type A%ATOMVFREE(1) is set to the corrected occupation. The first atom in the list must completely occupy its site.

CFML_Maps_Calculations

Subroutines related to operations on the array's map

Parameters

Max_Points

Variables

Cube_Info_Type

Cube_Info
Err_Maps
Err_Maps_Mess

Functions

Index_Cube
Vertice_Point
Vertices_Cube
VPoint_in_Cube
VPoint_in_Line
VPoint_in_Square

Subroutines

Calculate_Contour2D
Calculate_Mesh
Init_Err_Maps
Load_ExtendedMap
Load_Section
Search_Peaks
Set_Cube_Info
Statistic_Map

Fortran Filename

CFML_Maps.f90

CFML_Maps_Calculations: Parameters

Max_Points

CFML_Maps_Calculations: Parameters

Integer, Parameter :: Max_Points = 150000

Number of maximum points permitted

CFML_Maps_Calculations: Variables

Cube_Info_Type

Cube_Info
Err_Maps
Err_Maps_Mess

CFML_Maps_Calculations: Variables

	Variable	***Definition***
Type :: Cube_Info_Type		
Integer	NElem	Number of Elemens
Integer	Code	Code of Elements
Integer, Dimension(12)	EdgesS	Code for Edge connections
End Type Cube_Info_Type		

CFML_Maps_Calculations: Variables

Type(Cube_Info_Type), Dimension(0:255) :: Cube_Info

Information of Mesh in a cube

CFML_Maps_Calculations: Variables

Logical :: Err_Maps

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_Maps_Calculations: Variables

Character (Len=150) :: Err_Maps_Mess

This variable contains information about the last error occurred in the procedures belonging to this module.

CFML_Maps_Calculations: Functions

CFML_Maps_Calculations: Functions

Integer Function Index_Cube (IV, MC)

Integer, Dimension(8)	**Intent(in)**	IV	Vertices state On/Off
Logical	**Intent(in)**	MC	If .TRUE. Code for Triangles (128-255), if not give code from 0-127

Return the index for Marching cubes algorithm

CFML_Maps_Calculations: Functions

Real Function Vertice_Point (Code_Edge)

Integer	**Intent(in)**	Code_Edge	

or

Real Function Vertice_Point (Code_Edge, D0, D1, D2, D3, D4, D5, D6, D7, D8, D9)

Integer	**Intent(in)**	Code_Edge	
Real(Kind=CP)	**Intent(in)**	D0	
Real(Kind=CP)	**Intent(in)**	D1	
Real(Kind=CP)	**Intent(in)**	D2	
Real(Kind=CP)	**Intent(in)**	D3	
Real(Kind=CP)	**Intent(in)**	D4	
Real(Kind=CP)	**Intent(in)**	D5	
Real(Kind=CP)	**Intent(in)**	D6	
Real(Kind=CP)	**Intent(in)**	D7	

Real(Kind=CP)	**Intent(in)**	D8	
Real(Kind=CP)	**Intent(in)**	D9	

Return the relative position point from (i,j,k) of V1

Given a binary dataset, linear interpolation is not needed to extract isosurfaces, When a cell edge in a binary dataset has both on and off corners, the midpoint of the edge is the intersection being looked for.

Integer Function Vertices_Cube (Index_Cube)

Integer	**Intent(in)**	Index_Cube	index

Return the state of the 8 vertices of the cube in Marching cubes algorithm

Real Function VPoint_in_Cube (R, S, T, X000, X001, X010, X011, X100, X101, X110, X111)

Real(Kind=CP)	**Intent(in)**	R	
Real(Kind=CP)	**Intent(in)**	S	
Real(Kind=CP)	**Intent(in)**	T	
Real(Kind=CP)	**Intent(in)**	X000	Value of the Point 000
Real(Kind=CP)	**Intent(in)**	X001	Value of the Point 001
Real(Kind=CP)	**Intent(in)**	X010	Value of the Point 010
Real(Kind=CP)	**Intent(in)**	X011	Value of the Point 011
Real(Kind=CP)	**Intent(in)**	X100	Value of the Point 100
Real(Kind=CP)	**Intent(in)**	X101	Value of the Point 101
Real(Kind=CP)	**Intent(in)**	X110	Value of the Point 110
Real(Kind=CP)	**Intent(in)**	X111	Value of the Point 111

Function that interpolate the value into a cube

Diagram:

```
   011--------------111
    |               |
    |               |
    |               |
    |               |
    |               |
   001--------------101


    *---------------*
    |               |
    |               |
    |      rst      |
    |               |
    |               |
    *---------------*


   010--------------110
    |               |
    |               |
    |               |
  |              |
  |              |
000--------------100
```

CFML_Maps_Calculations: Functions

Real Function VPoint_in_Line (R,X0,X1)

Real(Kind=CP)	**Intent(in)**	R	R is distance between the ends points
Real(Kind=CP)	**Intent(in)**	X0	Value of the Point 0
Real(Kind=CP)	**Intent(in)**	X1	Value of the Point 1

Function that interpolate the value

Diagram: 0-----r-----1

CFML_Maps_Calculations: Functions

Real Function VPoint_in_Square (R, S, X00, X01, X10, X11)

Real(Kind=CP)	**Intent(in)**	R	R is distance between the ends points
Real(Kind=CP)	**Intent(in)**	S	
Real(Kind=CP)	**Intent(in)**	X00	Value of the Point 00
Real(Kind=CP)	**Intent(in)**	X01	Value of the Point 01
Real(Kind=CP)	**Intent(in)**	X10	Value of the Point 10
Real(Kind=CP)	**Intent(in)**	X11	Value of the Point 11

Function that interpolate the value on square

Diagram:

```
01------------11
  |      .      |
  |      .      |
  |.....rs......|
  |      .      |
  |      .      |
00------------10
```

CFML_Maps_Calculations: Subroutines

- Calculate_Contour2D
- Calculate_Mesh
- Init_Err_Maps
- Load_ExtendedMap
- Load_Section
- Search_Peaks
- Set_Cube_Info
- Statistic_Map

CFML_Maps_Calculations: Subroutines

Subroutine Calculate_Contour2D(D, ILB, IUB, JLB, JUB, X, Y, Z, NLV, NTP, XYZ)

Real(Kind=CP), Dimension(ILB:IUB, JLB:JUB)	**Intent(in)**	D	Section 2D
Integer	**Intent(in)**	ILB	Lower limit on the first dimension
Integer	**Intent(in)**	IUB	Upper limit on the first dimension
Integer	**Intent(in)**	JLB	Lower limit on the second dimension
Integer	**Intent(in)**	JUB	Upper limit on the second dimension
Real(Kind=CP), Dimension(ILB:IUB)	**Intent(in)**	X	Limits values on X
Real(Kind=CP), Dimension(JLB:JUB)	**Intent(in)**	Y	Limits values on Y
Real(Kind=CP), Dimension(:)	**Intent(in)**	Z	Levels values
Integer	**Intent(in)**	NLV	Number of levels
Integer	**Intent(in out)**	NTP	Number of points
Real(Kind=CP), Dimension(:,:)	**Intent(out)**	XYZ	XY Points

Calculate the Contour 2D of a section

CFML_Maps_Calculations: Subroutines

Subroutine Calculate_Mesh (Rho, NGrid, NLevel, Levels, MC_Method, NPoints, XYZ, Limits, Step)

Real(Kind=CP), Dimension(:,:,:)	**Intent(in)**	Rho	Array
Integer, Dimension(3)	**Intent(in)**	NGrid	Grid dimensions od RHO
Integer	**Intent(in)**	NLevel	Number of levels
Real(Kind=CP), Dimension(NLevel)	**Intent(in)**	Levels	Levels values
Character(Len=*)	**Intent(in)**	MC_Method	Values: TR : Mesh using Triangles Other : Rectangle and triangles
Integer, Dimension(NLevel)	**Intent(out)**	NPoints	Number of points
Real(Kind=CP), Dimension(:,:)	**Intent(out)**	XYZ	Points
Real(Kind=CP), Dimension(2,3), Optional	**Intent(in)**	Limits	Limits
Integer, Dimension(3), Optional	**Intent(in)**	Step	Step to do calculations

Calculate the 3D Contour

CFML_Maps_Calculations: Subroutines

Subroutine Init_Err_Maps ( )

Subroutine that initializes errors flags in **CFML_Maps_Calculations** module.

CFML_Maps_Calculations: Subroutines

Subroutine Load_ExtendedMap (Rho, NGrid, Limits, RhoNew)

Real(Kind=CP), Dimension(:,:,:)	Intent(in)	Rho	Array
Integer, Dimension(3)	Intent(in)	NGrid	Grid dimensions of RHO
Real(Kind=CP), Dimension(2,3)	Intent(in)	Limits	Limits
Real(Kind=CP), Dimension(:,:,:)	Intent(out)	RhoNew	RHO Extended

RhoNew has one dimension more in each dimension that Rho. This routine is useful for 2D representation.

RHO(NX,NY,NZ) -> RHONEW(NX+1,NY+1,NZ+1)

Subroutine Load_Section (Rho, NGrid, IMap, Section, Limits, NGrid2, DMap)

Real(Kind=CP), Dimension(:,:,:)	**Intent(in)**	Rho	Array
Integer, Dimension(3)	**Intent(in)**	NGrid	Grid dimensions of RHO
Integer	**Intent(in)**	IMap	
Integer	**Intent(in)**	Section	
Real(Kind=CP), Dimension(2,2)	**Intent(in)**	Limits	Limits
Real(Kind=CP), Dimension(2)	**Intent(in)**	NGrid2	
Real(Kind=CP), Dimension(:,:)	**Intent(out)**	DMap	Section 2D

Load a particular section of a map according to the new limits. This routine only works with fractional coordinates

Subroutine Search_Peaks (Rho, Grp, Cell, NPFound, Peaks, ABS_Code)

Real(Kind=CP), Dimension(:,:,:)	**Intent(in)**	Rho	Array
Type(Space_Group_Type)	**Intent(in)**	Grp	SpaceGroup
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Integer	**Intent(in out)**	NPFound	Number of Peaks to found
Real(Kind=CP), Dimension(4,NPFound)	**Intent(out)**	Peaks	Peak List
Logical, Optional	**Intent(in)**	ABS_Code	logical to use absolute value on RHO

General procedure to search peaks on Rho

Subroutine Set_Cube_Info ( )

Set values for Cube_Info Variable.

From 0 to 127 the code is defined according the next table.

Code	***Figure***	***Process***
1	Triangle	Pto1 -> Pto2 -> Pto3 -> Pto1
2	Trapezoide	Pto1 -> Pto2 -> Pto3 -> Pto4 -> Pto1
3	Triangle + Trapezoide	Pto1 -> Pto2 -> Pto3 -> Pto1 Pto4 -> Pto5 -> Pto6 -> Pto7 -> Pto4
4	Triangle + Triangle + Trapezoide	Pto1 -> Pto2 -> Pto3 -> Pto1 Pto4 -> Pto5 -> Pto6 -> Pto4 Pto7 -> Pto8 -> Pto9 -> Pto10 -> Pto7
5	Triangle + Line	Pto1 -> Pto2 -> Pto3 -> Pto1 Pto1 -> Pto4
6	Triangle + Triangle + Line	Pto1 -> Pto2 -> Pto3 -> Pto1 Pto4 -> Pto5 -> Pto6 -> Pto4 Pto4 -> Pto7

From 128 to 255 all is defined using triangles.

CFML_Maps_Calculations: Subroutines

Subroutine Statistic_Map (Rho, MaxV, MinV, AveV, SigmaV)

Real(Kind=CP), Dimension(:,:,:)	**Intent(in)**	Rho	Array
Real(Kind=CP)	**Intent(out)**	MaxV	Maximum value of Rho
Real(Kind=CP)	**Intent(out)**	MinV	Minimum value of Rho
Real(Kind=CP)	**Intent(out)**	AveV	Average value of Rho
Real(Kind=CP)	**Intent(out)**	SigmaV	Sigma value of Rho

Some statistic parameters of the map

CFML_Molecular_Crystals

Module to define molecules on Crystals

Variables

Molecule_Type
Molecular_Crystal_Type

Err_Molec
Err_Molec_Mess

Subroutines

Cartesian_To_Fractional
Cartesian_To_Spherical
Cartesian_To_ZMatrix
Empiric_Formula
Fix_Orient_Cartesian
Fix_Reference
Fractional_To_Cartesian
Fractional_To_Spherical
Fractional_To_ZMatrix
Init_Err_Molec
Init_Molecule
MolCrys_To_AtomList
Molec_To_AtomList
Read_Free_Atoms
Read_Molecule
Set_Euler_Matrix
Spherical_To_Cartesian
Spherical_To_Fractional
Spherical_To_ZMatrix
Write_Free_Atoms
Write_Molecular_Crystal
Write_Molecule
ZMatrix_To_Cartesian
ZMatrix_To_Fractional

ZMatrix_To_Spherical

Fortran Filename

CFML_Molecules.f90

CFML_Molecular_Crystals: Variables

Molecule_Type
Molecular_Crystal_Type

Err_Molec
Err_Molec_Mess

CFML_Molecular_Crystals: Variables

	Variable	***Definition***
Type :: Molecule_Type		
Character(Len=80)	Name_Mol	Global name for the molecule
Integer	NAtoms	Number of atoms
Logical	In_XTAL	TRUE if global coordinates xcentre, orient are defined
Logical	Is_EulerMat	TRUE if the Euler Matrix has been set
Logical	Is_Connect	TRUE if the connectivity is correct
Character(Len=1)	Rot_Type	Type of rotational angles E : Conventional Euler angles (alpha,beta,gamma) P : Second variant of Euler angles (default) Polar:(theta,phi,chi)
Character(Len=1)	Coor_Type	Type of internal coordinates C : Cartesian F : Fractional (only if in_XTAL=.TRUE.) S : Spherical Z : Z-Matrix
Character(Len=3)	Therm_Type	Type of thermal factor ISO : No collective motion T : Translational TL : Translational + Librational TLS : Translational + Librational + Correlation
Real(Kind=CP), Dimension(3)	XCentre	Fractional coordinates of the centre
Real(Kind=CP), Dimension(3)	MXCentre	Refinement codes of Fractional coordinates of the centre
Integer, Dimension(3)	LXCentre	Numbers of LSQ parameters for Fractional coordinates of the centre
Real(Kind=CP), Dimension(3)	Orient	Orientation angles (Euler angles or variant ...)
Real(Kind=CP), Dimension(3)	MOrient	Refinement codes of Orientation angles (Euler angles or variant ...)
Integer, Dimension(3)	LOrient	Numbers of LSQ parameters for Orientation angles

		(Euler angles or variant ...)
Real(Kind=CP), Dimension(6)	T_TLS	Translational Thermal factor tensor
Real(Kind=CP), Dimension(6)	MT_TLS	Refinement codes of Translational Thermal factor tensor
Integer, Dimension(6)	IT_TLS	Numbers of LSQ parameters for Translational Thermal factor tensor
Real(Kind=CP), Dimension(6)	L_TLS	Librational Thermal factor tensor
Real(Kind=CP), Dimension(6)	ML_TLS	Refinement codes of Librational Thermal factor tensor
Integer, Dimension(6)	IL_TLS	Numbers of LSQ parameters for Librational Thermal factor tensor
Real(Kind=CP), Dimension(3,3)	S_TLS	TL-correlation Thermal factor
Real(Kind=CP), Dimension(3,3)	MS_TLS	Refinement codes of TL-correlation Thermal factor
Integer, Dimension(3,3)	IS_TLS	Numbers of LSQ parameters for TL-correlation Thermal factor
Real(Kind=CP), Dimension(3,3)	Euler	Euler matrix
Character(Len=6), Dimension(:), Allocatable	AtName	Atom Name
Character(Len=4), Dimension(:), Allocatable	AtSymb	Atom species
Integer, Dimension(:), Allocatable	ATZ	Atomic Number
Integer, Dimension(:,:),Allocatable	Ptr	Pointer to scat.factors (first index -> pattern)
Real(Kind=CP), Dimension(:,:),Allocatable	I_Coor	internal coordinates (d,ang,dang)
Real(Kind=CP), Dimension(:,:),Allocatable	MI_Coor	Refinement codes of internal coordinates
Integer, Dimension(:,:),Allocatable	LI_Coor	Numbers of LSQ parameters for internal coordinates
Real(Kind=CP), Dimension(:), Allocatable	Biso	Isotropic temperature factor
Real(Kind=CP), Dimension(:), Allocatable	MBiso	Refinement codes of Isotropic temperature factor
Integer, Dimension(:), Allocatable	LBiso	Numbers of LSQ parameters for Isotropic temperature factor
Real(Kind=CP), Dimension(:), Allocatable	Occ	Occupation factor
Real(Kind=CP), Dimension(:), Allocatable	MOcc	Refinement codes of Occupation factor
Integer, Dimension(:), Allocatable	LOcc	Numbers of LSQ parameters for Occupation factor
Integer, Dimension(:), Allocatable	NB	Number of neighbours
Integer, Dimension(:,:), Allocatable	InB	index of neighbous
Integer, Dimension(:,:), Allocatable	TB	Type of bonds
Integer, Dimension(:,:), Allocatable	Conn	Conectivity (N1,N2,N3)
End Type Molecule_Type		

CFML_Molecular_Crystals: Variables

	Variable	***Definition***
Type :: Molecular_Crystal_Type		
Integer	N_Free	Number of free atoms
Integer	N_Mol	Number of Molecules
Integer	N_Species	Number of species
Integer	NPat	
Type(Crystal_Cell_Type)	Cell	Cell information

Type(Space_Group_Type)	Spg	Space Group information
Type(Atom_Type), Dimension(:), Allocatable	Atm	Free Atoms
Type(Molecule_Type), Dimension(:), Allocatable	Mol	Molecules
End Type Molecular_Crystal_Type		

CFML_Molecular_Crystals: Variables

Logical :: Err_Molec

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module

CFML_Molecular_Crystals: Variables

Character (Len=150) :: Err_Molec_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Molecular_Crystals: Subroutines

- Cartesian_To_Fractional
- Cartesian_To_Spherical
- Cartesian_To_ZMatrix
- Empiric_Formula
- Fix_Orient_Cartesian
- Fix_Reference
- Fractional_To_Cartesian
- Fractional_To_Spherical
- Fractional_To_ZMatrix
- Init_Err_Molec
- Init_Molecule
- MolCrys_To_AtomList
- Molec_To_AtomList
- Read_Free_Atoms
- Read_Molecule
- Set_Euler_Matrix
- Spherical_To_Cartesian
- Spherical_To_Fractional
- Spherical_To_ZMatrix
- Write_Free_Atoms
- Write_Molecular_Crystal
- Write_Molecule
- ZMatrix_To_Cartesian
- ZMatrix_To_Fractional
- ZMatrix_To_Spherical

CFML_Molecular_Crystals: Subroutines

Subroutine Cartesian_To_Fractional (Molecule, Cell, NewMolecule)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters

Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object

Subroutine to transform the internal coordinates of a molecule from Cartesian coordinates to Fractional coordinates.

If a third argument is present the subroutine creates a new molecule (copy of the old one) with fractional coordinates, preserving the input molecule in Cartesian Coordinates. Otherwise the input molecule is changed on output.

CFML_Molecular_Crystals: Subroutines

Subroutine Cartesian_To_Spherical (Molecule, NewMolecule)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object

Subroutine to transform the internal coordinates of a molecule from Cartesian coordinates to Spherical coordinates.

If a second argument is present the subroutine creates a new molecule (copy of the old one) with spherical coordinates, preserving the input molecule in Cartesian Coordinates. Otherwise the input molecule is changed on output.

CFML_Molecular_Crystals: Subroutines

Subroutine Cartesian_To_ZMatrix (Molecule, NewMolecule, Cell, D_Min, D_Max)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object
Type(Crystal_Cell_Type), Optional	**Intent(in)**	CEell	Cell parameters
Real(Kind=CP), Optional	**Intent(in)**	D_Min	
Real(Kind=CP), Optional	**Intent(in)**	D_Max	

Subroutine to transform the internal coordinates of a molecule from Cartesian coordinates to Z-Matrix.

If a second argument is present the subroutine creates a new molecule (copy of the old one) with Z-matrix, preserving the input molecule in Cartesian Coordinates. Otherwise the input molecule is changed on output.

The input cartesian coordinates may be defined with respect to another internal frame. The final internal frame is that defined for Z-matrices: the x-axis is from the first to the second atom and the x-y plane is formed by the three first atoms. The Euler matrix and the molecular centre in the crystallographic system is changed in consequence.

CFML_Molecular_Crystals: Subroutines

Subroutine Empiric_Formula (Atm / MolCrys / Molecule, Formula, Form_Weight)

Type(Atom_List_Type)
or
Type(Molecular_Crystal_Type)
or
Type(Molecule_Type)
	Intent(in)	Atm
		
		MolCrys
		
		Molecule
			Atom information

Character(Len=*)	**Intent(out)**	Formula	Empiric Formula
Real(Kind=CP), Optional	**Intent(out)**	Form_Weight	

Obtain the Empiric Formula from Atm/Molcrys/Molecule variable

CFML_Molecular_Crystals: Subroutines

Subroutine Fix_Orient_Cartesian (Molecule, NewMolecule, NAtom_O, NAtom_X, NAtom_XY,

Mat)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object
Integer, Optional	**Intent(in)**	NAtom_O	
Integer, Optional	**Intent(in)**	NAtom_Y	
Integer, Optional	**Intent(in)**	NAtom_XY	
Real(Kind=CP), Dimension(3,3), Optional	**Intent(out)**	Mat	

Subroutine to transform the Cartesian coordinates of the molecule choosing which atom is the origin, which define the X axis and which defines the XY Plane

If the second argument is present the subroutine creates a new molecule preserving the input molecule in Cartesian. Otherwise the input molecule is changed on output.

If Natom_0 is absent, then the first atom on the molecule will be the origin.
If Natom_X is absent, then the second atom on the molecule will define the X axis.
If Natom_XY is absent, then the third atom on the molecule will define the XY Plane.

The optional output matrix Mat is the active rotation matrix passing from the old Cartesian frame to the new one. The transpose matrix has served to transform the original Cartesian coordinates.

CFML_Molecular_Crystals: Subroutines

Subroutine Fix_Reference (Molecule, NewMolecule, NAtom_O, NAtom_X, NAtom_XY)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object
Integer, Optional	**Intent(in)**	NAtom_O	
Integer, Optional	**Intent(in)**	NAtom_Y	
Integer, Optional	**Intent(in)**	NAtom_XY	

Subroutine to order the molecule choosing which atom is the origin, which define the X axis and which defines the XY Plane.

If the second argument is present the subroutine creates a new molecule preserving the input molecule in Cartesian. Otherwise the input molecule is changed on output.

If Natom_0 is absent, then the first atom on the molecule will be the origin.
If Natom_X is absent, then the second atom on the molecule will define the X axis.
If Natom_XY is absent, then the third atom on the molecule will define the XY Plane.

CFML_Molecular_Crystals: Subroutines

Subroutine Fractional_To_Cartesian (Molecule, Cell, NewMolecule)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object

Subroutine to transform the Fractional coordinates to Cartesian internal coordinates of a molecule.

If NewMolecule is present the subroutine creates a new molecule (copy of the old one) with cartesian coordinates, preserving the input molecule in fractional. Otherwise the input molecule is changed on output.

CFML_Molecular_Crystals: Subroutines

Subroutine Fractional_To_Spherical (Molecule, Cell, NewMolecule)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object

Subroutine to transform the internal coordinates of a molecule from Fractional coordinates to Spherical coordinates.

If a third argument is present the subroutine creates a new molecule (copy of the old one) with Spherical coordinates, preserving the input molecule in Fractional Coordinates. Otherwise the input molecule is changed on output.

CFML_Molecular_Crystals: Subroutines

Subroutine Fractional_To_ZMatrix (Molecule, Cell, NewMolecule)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object

Subroutine to transform the internal coordinates of a molecule from Fractional coordinates to Zmatrix coordinates.

If a third argument is present the subroutine creates a new molecule (copy of the old one) with Zmatrix coordinates, preserving the input molecule in Fractional Coordinates. Otherwise the input molecule is changed on output.

CFML_Molecular_Crystals: Subroutines

Subroutine Init_Err_Molec ( )

Subroutine that initializes errors flags in **CFML_Molecular_Crystals** module.

CFML_Molecular_Crystals: Subroutines

Subroutine Init_Molecule (Molecule, NAtm)

Type(Molecule_Type)	**Intent(out)**	Molecule	Molecule object
Integer, Optional	**Intent(in)**	NAtm	Number of Atoms

Initialize the Variable Molecule. If NAtm if given the allocate the respective fields depending of this value

CFML_Molecular_Crystals: Subroutines

Subroutine MolCrys_To_AtomList (MolCrys, Atm)

Type(Molecular_Crystal_Type)	**Intent(in)**	MolCrys	Molecule Object
Type(Atom_List_Type)	**Intent(out)**	Atm	Atoms information

Subroutine to pass all information from Molecular_Crystal_Type to Atom_List_Type

CFML_Molecular_Crystals: Subroutines

Subroutine Molec_To_AtomList (Molec, Atm, Coor_Type, Cell)

Type(Molecule_Type)	**Intent(in)**	Molec	Molecule Object
Type(Atom_List_Type)	**Intent(out)**	Atm	Atoms information
Character(Len=*), Optional	**Intent(in)**	Coor_Type	
Type(Crystal_Cell_Type), Optional	**Intent(in)**	Cell	Cell parameters

Subroutine to pass all information from Molecule_Type to Atom_List_Type

Coor_Type determine the type of coordinates parameter in output. In general **Cell** if necessary to obtain on output fractional coordinates or special case for Z-Matrix.

CFML_Molecular_Crystals: Subroutines

Subroutine Read_Free_Atoms (Lun, AtmF, N)

Integer	**Intent(in)**	Lun	Logical unit to be read
Type(Atom_Type), Dimension(:)	**Intent(out)**	AtmF	Free atoms
Integer	**Intent(out)**	N	Free atoms read

Subroutine to read a set of Free Atoms from a file.

The format is:
ATOMS N_Atoms
internal Coordinates for Atoms (N_Atoms Lines): Atom_Name(6) Atom_Specie(4) Coordinates(3) Biso Occ [VARY]

if VARY is present as last option on the internal Coordinates line, then an extra line is read: Codes_Coordinates(3) Code_BIso Code_Occ

CFML_Molecular_Crystals: Subroutines

Subroutine Read_Molecule (Lun, Molecule)

Integer	**Intent(in)**	Lun	Logical unit to be read
Type(Molecule_Type)	**Intent(out)**	Molecule	Molecule Object

or

Subroutine Read_Molecule (File_Dat, N_Ini, N_End, Molecule)

Character(Len=*), Dimension(:)	**Intent(in)**	File_Dat	Name of the File to read
Intent(in)	**Intent(in)**	N_Ini	initial line to be read
Integer	**Intent(in)**	N_End	Last line to be read
Type(Molecule_Type)	**Intent(out)**	Molecule	Molecule Object

Subroutine to read a molecule from a file.

The format of the file is:
   MOLE[X] N_ATOMS MOLECULE_NAME COORDinATES_TYPE

where

Variables	***Definitions***
N_ATOMS	Number of atoms in the molecule definition
MOLECULE_NAME	Name for the molecule
COORDinATES_TYPE	Values are: C : Cartesian coordinates F : Fractional coordinates

S : Spherical coordinates
Z : Z-Matrix coordinates

If keyword **MOLEX** is present, then the next line will be read (6 reals, 2 characters):
MOLECULE_CENTRE(3) MOLECULE_ORIENT(3) ROTATIONAL_ANGLE(1)_TYPE THERMAL_FACTOR_TYPE(3)

where

Variables	***Definitions***
MOLECULE_CENTRE	Coordinate of Center of Molecule
MOLECULE_ORIENT	Angles orientation
ROTATIONAL_ANGLE_TYPE	Values are: E : Conventional Euler angles (alpha, beta, gamma) P : Polar Euler angles (Phi, theta, Chi) (default)
THERMAL_FACTOR_TYPE	Values are: ISO : No collective motion TLS : Traslational + Librational + Correlation TL : Traslational + Librational T : Traslational

According to Thermal Factors, next lines will be read

Thermal Factors	***Definitions***
T	6 Thermal Factors (Line1) + 6 Codes Thermal Factors (Line2)
TL	6 Thermal Factors (Line1) + 6 Codes Thermal Factors (Line2) 6 Thermal Factors (Line3) + 6 Codes Thermal Factors (Line4)
TLS	6 Thermal Factors (Line1) + 6 Codes Thermal Factors (Line2) 6 Thermal Factors (Line3) + 6 Codes Thermal Factors (Line4) 9 Thermal Factors (Line5) + 9 Codes Thermal Factors (Line6)

internal Coordinates for Atoms (N_Atoms Lines):
ATOM_NAME(6) ATOM_SPECIES(4) COORDinATES(3) N1 N2 N3 BISO OCC [VARY]

If VARY is present as last option on the internal Coordinates line, then an extra line is read:
CODES_COORDinATES(3) CODE_BISO(1) CODE_OCC(1)

CFML_Molecular_Crystals: Subroutines

Subroutine Set_Euler_Matrix (RT, Phi, Theta, Chi, Eu)

Character(Len=*)	**Intent(in)**	RT	Values are: E : Conventional Euler angles (alpha, beta, gamma) P : Polar angles
Real(Kind=CP)	**Intent(in)**	Phi	Angle Phi
Real(Kind=CP)	**Intent(in)**	Theta	Angle Theta
Real(Kind=CP)	**Intent(in)**	Chi	Angle Chi
Real(Kind=CP), Dimension(3,3)	**Intent(out)**	Eu	Euler array

Subroutine to obtain the Euler active matrix to transform a point to another point.

For instance the internal coordinates of a molecule can be transformed to absolute positions using columns vectors.

If the Cartesian coordinates of an atom in the molecular frame is the column vector Xm, the cartesian coordinates in the crystal frame X are obtained from: X = Eu Xm

The internal coordinates of a point are obtained from Xm = EuT X.

CFML_Molecular_Crystals: Subroutines

Subroutine Spherical_To_Cartesian (Molecule, NewMolecule)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object

Subroutine to transform the internal coordinates of a molecule from Spherical coordinates to Cartesian coordinates.

If a second argument is present the subroutine creates a new molecule (copy of the old one) with spherical coordinates, preserving the input molecule in Cartesian Coordinates. Otherwise the input molecule is changed on output.

CFML_Molecular_Crystals: Subroutines

Subroutine Spherical_To_Fractional (Molecule, Cell, NewMolecule)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object

Subroutine to transform the internal coordinates of a molecule from Spherical coordinates to Fractional coordinates.

If a third argument is present the subroutine creates a new molecule (copy of the old one) with Fractional coordinates, preserving the input molecule in Spherical Coordinates. Otherwise the input molecule is changed on output.

CFML_Molecular_Crystals: Subroutines

Subroutine Spherical_To_ZMatrix (Molecule, NewMolecule, Cell)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object
Type(Crystal_Cell_Type), Optional	**Intent(in)**	Cell	Cell parameters

Subroutine to transform the internal coordinates of a molecule from Spherical coordinates to Zmatrix coordinates.

If a second argument is present the subroutine creates a new molecule (copy of the old one) with Zmatrix coordinates, preserving the input molecule in Spherical Coordinates. Otherwise the input molecule is changed on output.

CFML_Molecular_Crystals: Subroutines

Subroutine Write_Free_Atoms (AtmF, N, Lun)

Type(Atom_Type), Dimension(:)	**Intent(in)**	AtmF	Free atoms
Integer	**Intent(in)**	N	Free atoms read
Integer, Optional	**Intent(in)**	Lun	Logical unit to be written

Write information about Free Atoms

CFML_Molecular_Crystals: Subroutines

Subroutine Write_Molecular_Crystal (MolCrys, Lun)

Type(Molecular_Crystal_Type)	**Intent(in)**	MolCrys	Molecule
Integer, Optional	**Intent(in)**	Lun	Logical unit to be written

Write information about Molecular Crystal

CFML_Molecular_Crystals: Subroutines

Subroutine Write_Molecule (Molecule, Lun)

Type(Molecule_Type)	**Intent(in)**	Molecule	Molecule
Integer, Optional	**Intent(in)**	Lun	Logical unit to be written

Write information about molecule

CFML_Molecular_Crystals: Subroutines

Subroutine ZMatrix_To_Cartesian (Molecule, NewMolecule)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object

Subroutine to transform the internal coordinates of a molecule from Z-matrix to Cartesian coordinates.

If a second argument is present the subroutine creates a new molecule (copy of the old one) with cartesian coordinates, preserving the input molecule. Otherwise the input molecule is changed on output.

CFML_Molecular_Crystals: Subroutines

Subroutine ZMatrix_To_Fractional (Molecule, Cell, NewMolecule)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell parameters
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object

Subroutine to transform the internal coordinates of a molecule from Z-matrix to Fractional coordinates.

If a third argument is present the subroutine creates a new molecule (copy of the old one) with fractional coordinates, preserving the input molecule in Z-matrix. Otherwise the input molecule is changed on output.

CFML_Molecular_Crystals: Subroutines

Subroutine Spherical_To_ZMatrix_To_Spherical (Molecule, NewMolecule)

Type(Molecule_Type)	**Intent(in out)**	Molecule	Molecule Object
Type(Molecule_Type), Optional	**Intent(out)**	NewMolecule	Molecule Object

Subroutine to transform the internal coordinates of a molecule from Zmatrix coordinates to Spherical coordinates.

If a second argument is present the subroutine creates a new molecule (copy of the old one) with Spherical coordinates, preserving the input molecule in Zmatrix Coordinates. Otherwise the input molecule is changed on output.

Level 7

Concept	*Module Name*	*Purpose*
Formats...	**CFML_IO_Formats**	Procedures for handling different formats for input/output

CFML_IO_Formats

Creation/Conversion for several formats

Variables

- File_List_Type
- Interval_Type
- Job_Info_Type

- Err_Form
- Err_Form_Mess

Subroutines

- File_To_FileList
- Get_Job_Info
- Init_Err_Form
- Read_Atom
- Read_Cell
- Read_CIF_Atom
- Read_CIF_Cell
- Read_CIF_ChemicalName
- Read_CIF_Cont
- Read_CIF_Hall
- Read_CIF_HM
- Read_CIF_Lambda
- Read_CIF_Symm
- Read_CIF_Title
- Read_CIF_Z
- Read_File_Atom
- Read_File_Cell
- Read_File_Lambda
- Read_File_RNGSinTL
- Read_File_Spg
- Read_File_Transf
- Rread_SHX_Atom
- Read_SHX_Cell
- Read_SHX_Cont
- Read_SHX_Fvar
- Read_SHX_Latt
- Read_SHX_Symm
- Read_SHX_Titl
- Read_Uvals
- Readn_Set_XTAL_Structure
- Write_CIF_Ppwder_Profile
- Write_CIF_Template

Write_SHX_Template

Fortran Filename

CFML_Form_CIF.f90

CFML_IO_Formats: Variables

File_List_Type
Interval_Type
Job_Info_Type

Err_Form
Err_Form_Mess

CFML_IO_Formats: Variables

	Variable	*Definition*
Type :: File_List_Type		
Integer	NLines	Number of lines
Character(Len=132), Dimension(:), Allocatable	Line	Lines
End Type File_List_Type		

CFML_IO_Formats: Variables

	Variable	*Definition*
Type :: Interval_Type		
Real (Kind=CP)	MinA	Low limit
Real (Kind=CP)	MaxB	High limit
End Type Interval_Type		

CFML_IO_Formats: Variables

	Variable	*Definition*
Type :: Job_Info_Type		
Character(Len=120)	Title	Title
Integer	Num_Phases	Number of phases
Integer	Num_Patterns	Number of patterns
Integer	Num_CMD	Number of command lines
Character(Len=16), Dimension(:), Allocatable	Patt_Typ	Type of Pattern

Character(Len=128), Dimension(:), Allocatable	Phas_Nam	Name of phases
Character(Len=128), Dimension(:), Allocatable	CMD	Command lines: text for actions
Type(Interval_Type), Dimension(:), Allocatable	Range_STL	Range in sin /
Type(Interval_Type), Dimension(:), Allocatable	Range_Q	Range in 4 *sin /
Type(Interval_Type), Dimension(:), Allocatable	Range_D	Range in d-spacing
Type(Interval_Type), Dimension(:), Allocatable	Range_2Theta	Range in 2 -spacing
Type(Interval_Type), Dimension(:), Allocatable	Range_Energy	Range in Energy
Type(Interval_Type), Dimension(:), Allocatable	Range_TOF	Range in Time of Flight
Type(Interval_Type), Dimension(:), Allocatable	Lambda	Lambda
Real (Kind=CP), Dimension(:), Allocatable	Ratio	ratio $_2$/ $_1$
Real (Kind=CP), Dimension(:), Allocatable	DTT1	d-to-TOF coefficients
Real (Kind=CP), Dimension(:), Allocatable	DTT2	
End Type Job_Info_Type		

CFML_IO_Formats: Variables

Logical :: Err_Form

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_IO_Formats: Variables

Character (Len=150) :: Err_Form_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_IO_Formats: Subroutines

- File_To_FileList
- Get_Job_Info
- Init_Err_Form
- Read_Atom
- Read_Cell
- Read_CIF_Atom
- Read_CIF_Cell
- Read_CIF_ChemicalName
- Read_CIF_Cont
- Read_CIF_Hall
- Read_CIF_HM
- Read_CIF_Lambda
- Read_CIF_Symm

CFML_IO_Formats: Subroutines

Subroutine FILE_To_FileList (File_Dat, File_List)

Character(Len=*), Dimension (:)	**Intent(in)**	File_Dat	input data file
Type(File_List_Type)	**Intent(out)**	File_List	File list structure

Charge an external file to an object of File_List_Type

CFML_IO_Formats: Subroutines

Subroutine Get_Job_Info (File_Dat, I_Ini, I_End, Job_Info)

Character(Len=*), Dimension (:)	**Intent(in)**	File_Dat	input data file
Integer	**Intent(in)**	I_Ini	initial line to explore
Integer	**Intent(in)**	I_End	Final line to explore
Type(Job_Info_Type)	**Intent(out)**	Job_Info	Object to be constructed

Constructor of the object Job_Info_Type.
The arrary of strings File_Dat have to be provided as input. It contains lines corresponding to the input control file.

CFML_IO_Formats: Subroutines

Subroutine Init_Err_Form ( )

Subroutine that initializes errors flags in **CFML_IO_Formats** module.

CFML_IO_Formats: Subroutines

Subroutine Read_Atom (Line, Atomo)

Character(Len=*)	**Intent(in**	Line	input string with ATOM directive

	out)		
Type(Atom_Type)	**Intent(out)**	Atomo	Parameters on variable

Subroutine to read the atom parameters from a given Line it construct the object Atomo of Atom_Type.

CFML_IO_Formats: Subroutines

Subroutine Read_Cell (Line, Celda)

Character(Len=*)	**Intent(in out)**	Line	input string with CELL directive
Real (Kind=CP), Dimension(6)	**Intent(out)**	Celda	Parameters on variable

Subroutine to read the cell parameters from a given Line.

Assumes the string Line has been read from a file and starts with the word CELL, that is removed before reading the values of the parameters.
Control of error is present

CFML_IO_Formats: Subroutines

Subroutine Read_CIF_Atom (Filevar, NLine_Ini, NLine_End, N_Atom, Atm_List)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Integer	**Intent(out)**	N_Atom		Actual number of atoms
Type(Atom_List_Type)	**Intent(out)**	Atm_List		Atom list

Obtaining Atoms parameters from a CIF file. A control error is present.

CFML_IO_Formats: Subroutines

Subroutine Read_CIF_Cell (Filevar, NLine_Ini, NLine_End, Celda, STDCelda)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Real(Kind=CP), Dimension(6)	**Intent(out)**	Celda		Cell parameters
Real(Kind=CP), Dimension(6)	**Intent(out)**	STDCelda		Standar values for cell parameters

Read Cell parameters from CIF file

CFML_IO_Formats: Subroutines

Subroutine Read_CIF_ChemicalName(Filevar, NLine_Ini, NLine_End, ChemName)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information

Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Character(Len=*)	**Intent(out)**	ChemName		Chemical name information

Obtaining Chemical Name from CIF file

CFML_IO_Formats: Subroutines

Subroutine Read_CIF_Cont (Filevar, NLine_Ini, NLine_End, N_Elem_Type, Elem_Type, N_Elem)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Integer	**Intent(out)**	N_Element_Type		Number of different elements
Character(Len=*), Dimension(:)	**Intent(out)**	Element_Type		Element type characters
Real(Kind=CP), Dimension(:), Optional	**Intent(out)**	N_Elem		Number of elements

Obtaining the chemical contents from CIF file

CFML_IO_Formats: Subroutines

Subroutine Read_CIF_Hall(Filevar, NLine_Ini, NLine_End, Spgr_Ha)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Character(Len=*)	**Intent(out)**	Spgr_Ha		Hall symbol

Obtaining the Hall symbol of the Space Group

CFML_IO_Formats: Subroutines

Subroutine Read_CIF_HM (Filevar, NLine_Ini, NLine_End, Spgr_HM)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Character(Len=*)	**Intent(out)**	Spgr_HM		Hermann-Mauguin symbol

Obtaining the Hermann-Mauguin symbol of the Space Group

CFML_IO_Formats: Subroutines

Subroutine Read_CIF_Lambda (Filevar, NLine_Ini, NLine_End, Lambda)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Real(Kind=CP)	**Intent(out)**	Lambda		Lambda value

Obtaining the radiation length on CIF file

CFML_IO_Formats: Subroutines

Subroutine Read_CIF_Symm (Filevar, NLine_Ini, NLine_End, N_Oper, Oper_Symm)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Integer	**Intent(out)**	N_Oper		Number of Operators
Character(Len=*), Dimension(:)	**Intent(out)**	Oper_Symm		Vector with Symmetry Operators

Obtaining Symmetry Operators from CIF file

CFML_IO_Formats: Subroutines

Subroutine Read_CIF_Title (Filevar, NLine_Ini, NLine_End, Title)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Character(Len=*)	**Intent(out)**	Title		Title

Obtaining Title from CIF file

CFML_IO_Formats: Subroutines

Subroutine Read_CIF_Z (Filevar, NLine_Ini, NLine_End, Z)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Integer	**Intent(out)**	Z		Number of molecules on Unit cell

Unit formula from CIF file

Subroutine Read_File_Atom (Filevar, NLine_Ini, NLine_End, Atomos)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search

Type(Atom_List_Type)
or
TYPE(Point_List_Type)
	Intent(out)	Atomos		Atom list / Point list

Subroutine to read an atom (or point) list from a file. **Atomos** should be previously allocated. Control of error is present.

Subroutine Read_File_Cell (Filevar, NLine_Ini, NLine_End, Celda)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search

Real(Kind=CP), Dimension(6)
or
Type(Crystal_Cell_Type)
	Intent(out)	Celda		Cell parameters

Read Cell Parameters from file. Control error is present

Subroutine Read_File_Lambda (Filevar, NLine_Ini, NLine_End, V1, V2, V3)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Real(Kind=CP)	**Intent(out)**	V1		Lambda1 value
Real(Kind=CP)	**Intent(out)**	V2		Lambda2 value
Real(Kind=CP)	**Intent(out)**	V3		Ratio Lambda2/Lambda1

Read wavelengths and ratio from a file

If no value is read, Lambda1=Lambda2=1.54056 Angstroms, ratio=0.0
If only one value is read Lambda1=Lambda2=v1, ratio=0
If only two values are read Lambda1=v1, Lambda2=v2, ratio=0.5

Subroutine Read_File_RNGSinTL (Filevar, NLine_Ini, NLine_End, V1, V2)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Real(Kind=CP)	**Intent(out)**	V1		Lower value in sin /
Real(Kind=CP)	**Intent(out)**	V2		Upper value in sin /

Read range for in sin / [v1,v2]

If only one value is read v1=0 and v2= read value
If the keyword RNGSL is not given in the file, the default values are v1=0.0, v2=1.0

CFML_IO_Formats: Subroutines

Subroutine Read_File_Spg (Filevar, NLine_Ini, NLine_End, Spgr, Sub)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Character(Len=*)	**Intent(out)**	Spgr		Space Group symbol
Character(Len=*), Optional	**Intent(in)**			The space group symbol is a subgroup of an already given space group
Character(Len=*), Optional	**Intent(in)**	Sub		The space group symbol is a subgroup of an already given space group

Reads the card Spgr in Filevar. Control of error is present

CFML_IO_Formats: Subroutines

Subroutine Read_File_Transf (Filevar, NLine_Ini, NLine_End, Transf, Orig)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Real(Kind=CP), Dimension(3,3)	**Intent(out)**	Transf		Transformation array
Real(Kind=CP), Dimension(3)	**Intent(out)**	Orig		

Read transformation matrix for changing the space group or cell setting. First the matrix M is read row by row and then the origin in the old setting is finally read. A single line with 12 real numbers should be given.

Example:

TRANS m11 m12 m13 m21 m22 m33 m31 m32 m33   o1 o2 o3

That's means:

a'=m11 a + m12 b + m13 c
b'=m21 a + m22 b + m23 c
c'=m31 a + m32 b + m33 c

X' = inv(Mt) (X-O)

CFML_IO_Formats: Subroutines

Subroutine Read_SHX_Atom (Filevar, NLine_Ini, NLine_End, N_FVar, FVar, Elem_Type, Celda, Atm_List)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Integer	**Intent(in)**	N_FVar		Number of parameters on FVAR
Real (Kind=CP), Dimension(:)	**Intent(in)**	FVar		Values for FVAR
Character(Len=*), Dimension(:)	**Intent(in)**	Elem_Type		Elements type
Type(Crystal_Cell_Type)	**Intent(in)**	Celda		Cell Parameter
Type(Atom_List_Type)	**Intent(out)**	Atm_List		Atom list

Obtaining Atoms parameters from SHELX files (.ins or .res)

CFML_IO_Formats: Subroutines

Subroutine Read_SHX_Cell (Filevar, NLine_Ini, NLine_End, Celda, STDCelda, Lambda, Z)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Real (Kind=CP), Dimension(6)	**Intent(out)**	Celda		Cell Parameter
Real (Kind=CP), Dimension(6)	**Intent(out)**	STDCelda		Standar deviations for Cell parameters
Real (Kind=CP)	**Intent(out)**	Lambda		Lambda
Integer	**Intent(out)**	Z		Number of molecules on unit cell

Obtaining Cell Parameter from SHELX file

CFML_IO_Formats: Subroutines

Subroutine Read_SHX_Cont (Filevar, NLine_Ini, NLine_End, N_ELEM_TYPE, ELEM_TYPE, N_ELEM)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Integer	**Intent(out)**	N_Elem_Type		Number of different species
Character(Len=*), Dimension(:)	**Intent(out)**	Elem_Type		Character to identify the specie
Integer, Dimension(:), Optional	**Intent(out)**	N_Elem		Number of elements into the same species

Obtaining Chemical contents from SHELX file (.ins or .res)

Subroutine Read_SHX_FVar (Filevar, NLine_Ini, NLine_End, N_FVar, FVar)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Integer	**Intent(out)**	N_FVar		Number of parameters on FVAR
Real (Kind=CP), Dimension(:)	**Intent(out)**	FVar		Values for FVAR

Obtaining FVAR parameters from SHELX file (.ins or .res)

Subroutine Read_SHX_Latt (Filevar, NLine_Ini, NLine_End, Latt)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Integer	**Intent(out)**	Latt		Lattice number

Obtaining lattice from SHELX file (.ins or .res)

Subroutine Read_SHX_Symm (Filevar, NLine_Ini, NLine_End, N_Oper, Oper_Symm)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Integer	**Intent(out)**	N_Oper		Number of Operators
Character(Len=*), Dimension(:)	**Intent(out)**	Oper_Symm		String for Symmetry Operators

Obtaining Symmetry Operators from SHELX file (.ins or .res)

Subroutine Read_SHX_Titl (Filevar, NLine_Ini, NLine_End, Title)

Character(Len=*), Dimension(:)	**Intent(in)**	Filevar		input strings information
Integer	**Intent(in out)**	NLine_Ini	in: out:	Line to beginning search Current line on Filevar
Integer	**Intent(in)**	NLine_End		Line to the End search
Character(Len=*)	**Intent(out)**	Title		Title string

Obtaining Title from SHELX file (.ins or .res)

CFML_IO_Formats: Subroutines

Subroutine Read_UVals (Line, Atomo, ULabel)

Character(Len=*)	Intent(in out)	Line	input string
Type(Atom_Type)	Intent(in out)	Atomo	Parameters on variable
Character(Len=4)	Intent(in)	ULabel	U_ij; B_ij; BETA

Subroutine to read the anisotropic thermal parameters from a given Line it completes the object **Atomo** of type Atom. Assumes the string Line has been read from a file and starts with one of the words (u_ij, b_ij or beta), that is removed before reading the values of the parameters.

CFML_IO_Formats: Subroutines

Subroutine ReadN_Set_XTAL_Structure (Filenam, MolCrys, Mode, IPhase, Job_Info, File_List)

Character(Len=*)	**Intent(in)**	Filenam	Name of File
Type(Molecular_Crystal_Type)	**Intent(out)**	MolCrys	Molecule information
Character(Len=*), Optional	**Intent(in)**	Mode	
Integer, Optional	**Intent(in)**	IPhase	
Type(Jonb_Info_Type), Optional	**Intent(out)**	Job_Info	
Type(File_List_Type), Optional	**Intent(out)**	File_List	

or

Subroutine ReadN_Set_XTAL_Structure (Filenam, Cell, Spg, A, Mode, IPhase, Job_Info, File_List)

Character(Len=*)	**Intent(in)**	Filenam	Name of File
Type(Crystal_Cell_Type)	**Intent(out)**	Cell	Cell Parameters
Type(Space_Group_Type)	**Intent(out)**	Spg	Space Group
Type(Atom_List_Type)	**Intent(out)**	A	Atom List
Character(Len=*), Optional	**Intent(in)**	Mode	
Integer, Optional	**Intent(in)**	IPhase	
Type(Jonb_Info_Type), Optional	**Intent(out)**	Job_Info	
Type(File_List_Type), Optional	**Intent(out)**	File_List	

Subroutine to read an input file and construct the crystal structure in terms of the object MolCrys or Cell, Spg and A. The optional argument IPhase is an integer telling to the program to read the phase number IPhase in the case of the presence of more than one phase. If absent only the first phase is read.

CFML_IO_Formats: Subroutines

Subroutine Write_CIF_Powder_Profile (Filename, Code)

Character(Len=*)	**Intent(in)**	Filename	Name of File
Integer	**Intent(in)**	Code	Values are: 0 Shelxs-Patterson 1 Shelxs-Direct Methods 2 Shelxl-Refinement

Write a CIF Powder profile file

CFML_IO_Formats: Subroutines

Subroutine Write_CIF_Template (Filename, Type_Data, Code)

Character(Len=*)	**Intent(in)**	Filename	Name of File
Integer	**Intent(in)**	Type_Data	0 Single Crystal 1 Powder Data
Integer	**Intent(in)**	Code	Values are: 0 Shelxs-Patterson 1 Shelxs-Direct Methods 2 Shelxl-Refinement

Write a CIF File

CFML_IO_Formats: Subroutines

Subroutine Write_SHX_Template (Filename, Code, Title, Lambda, Z, Celda, Space, Atomos)

Character(Len=*)	**Intent(in)**	Filename	Name of File
Integer	**Intent(in)**	Code	Values are: 0 Shelxs-Patterson 1 Shelxs-Direct Methods 2 Shelxl-Refinement
Character(Len=*)	**Intent(in)**	Title	Title
Real (Kind=CP)	**Intent(in)**	Lambda	Lambda
Integer	**Intent(in)**	Z	
Type(Crystal_Cell_Type)	**Intent(in)**	Celda	Cell parameters
Type(Space_Group_Type)	**Intent(in)**	Space	Space group
Type(Atom_List_Type)	**Intent(in)**	Atomos	Atom List

Write a Shelx File

Level 8

Concept	***Module Name***	***Purpose***
Refinement...	**CFML_Keywords_Code_Parser**	Refinable Codes parser
Magnetic Symmetry...	**CFML_Magnetic_Symmetry**	Procedures handling operations with Magnetic Symmetry and Magnetic Structures
Simulated Annealing...	**CFML_Simulated_Annealing**	Module for Global Optimization using Simulated Annealing

CFML_Keywords_Code_Parser

Module with procedure for Refinable Codes on Parameters

Parameters

Code_Nam
Key_Code

Variables

Angle_Restraint_Type
Distance_Restraint_Type
Torsion_Restraint_Type

Ang_Rest
Dis_Rest
Err_RefCodes
Err_RefCodes_Mess
NP_Cons
NP_Max
NP_Refi
NP_Rest_Ang
NP_Rest_Dis
NP_Rest_Tor
Tor_Rest
V_BCon
V_Bounds
V_List
V_Name
V_Vec
V_Shift

Subroutines

Allocate_RestParam
Allocate_VParam
Get_RestAng_Line
Get_RestDis_Line
Get_RestTor_Line
Init_Err_RefCodes
Init_RefCodes
Read_RefCodes_File
VState_To_AtomsPar
Write_Info_RefCodes
Write_Info_RefParams
Write_Restraints_ObsCalc

Fortran Filename

CFML_Refcodes.f90

CFML_Keywords_Code_Parser: Parameters

CFML_Keywords_Code_Parser: Parameters

Character (Len=*), Dimension(21), Parameter :: CODE_NAM

Variable for treatement codes

Value	***CODE_NAM***
1	X
2	Y
3	Z
4	B
5	OCC
6	B11
7	B22
8	B33
9	B12
10	B13
11	B23
12	Bns
13	XC
14	YC
15	ZC
16	THETA
17	PHI
18	CHI
19	TH_L
20	TH_T
21	TH_S

CFML_Keywords_Code_Parser: Parameters

Character (Len=*), Dimension(8), Parameter :: Key_Code

Key codes defined in the module

Value	***CODE_NAM***
1	XYZ
2	OCC
3	BIS
4	BAN
5	ALL
6	CEN
7	ORI
8	THE

CFML_Keywords_Code_Parser: Variables

CFML_Keywords_Code_Parser: Variables

	Variable	***Definition***
Type :: Angle_Restraint_Type		
Real (Kind=CP)	AObs	Observed angle
Real (Kind=CP)	ACalc	Calculated angle
Real (Kind=CP)	Sigma	Sigma value
Integer, Dimension(8)	P	index vector
Character (Len=8), Dimension(2)	STCode	
End Type Angle_Restraint_Type		

CFML_Keywords_Code_Parser: Variables

	Variable	***Definition***
Type :: Distance_Restraint_Type		
Real (Kind=CP)	DObs	Observed distance
Real (Kind=CP)	DCalc	Calculated distance
Real (Kind=CP)	Sigma	Sigma value
Integer, Dimension(2)	P	index vector
Character (Len=8)	STCode	

End Type Distance_Restraint_Type		

CFML_Keywords_Code_Parser: Variables

	Variable	*Definition*
Type :: Torsion_Restraint_Type		
Real (Kind=CP)	TObs	Observed torsion angle
Real (Kind=CP)	TCalc	Calculated torsion angle
Real (Kind=CP)	Sigma	Sigma value
Integer, Dimension(4)	P	index vector
Character (Len=8), Dimension(3)	STCode	
End Type Torsion_Restraint_Type		

CFML_Keywords_Code_Parser: Variables

Type (Angle_Restraint_Type), Dimension(:), Allocatable :: Ang_Rest

Relations for Angle Restraints

CFML_Keywords_Code_Parser: Variables

Type (Distance_Restraint_Type), Dimension(:), Allocatable :: Dis_Rest

Relations for Distance Restraints

CFML_Keywords_Code_Parser: Variables

Logical :: Err_RefCodes

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_Keywords_Code_Parser: Variables

Character (Len=150) :: Err_RefCodes_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Keywords_Code_Parser: Variables

Integer :: NP_Cons

Number of Constraints relations

CFML_Keywords_Code_Parser: Variables

Integer :: NP_Max

Number of Maximum Parameters to Refine

CFML_Keywords_Code_Parser: Variables

Integer :: NP_Refi

Number of Refinable Parameters

CFML_Keywords_Code_Parser: Variables

Integer :: NP_Rest_Ang

Number of Angle Restraints relations

CFML_Keywords_Code_Parser: Variables

Integer :: NP_Rest_Dis

Number of Distance Restraints relations

CFML_Keywords_Code_Parser: Variables

Integer :: NP_Rest_Tor

Number of Torsion Restraints relations

CFML_Keywords_Code_Parser: Variables

Type (Torsion_Restraint_Type), Dimension(:), Allocatable :: Tor_Rest

Relations for Torsion Angle Restraints

CFML_Keywords_Code_Parser: Variables

Integer, Dimension(:), Allocatable :: V_BCon

Vector of Boundary Conditions

CFML_Keywords_Code_Parser: Variables

Real(Kind=CP), Dimension(:,:), Allocatable :: V_Bounds

Vector of Lower, Upper limits and Step for Parameters

CFML_Keywords_Code_Parser: Variables

Integer, Dimension(:), Allocatable :: V_List

Vector of index point the atom order

CFML_Keywords_Code_Parser: Variables

Character(Len=20), Dimension(:), Allocatable :: V_Name

Vector of Name of Refinable Parameters

CFML_Keywords_Code_Parser: Variables

Real(Kind=CP), Dimension(:), Allocatable :: V_Vec

Vector of Parameters

CFML_Keywords_Code_Parser: Variables

Real(Kind=CP), Dimension(:), Allocatable :: V_Shift

Vector of holding the shift of parameters

CFML_Keywords_Code_Parser: Subroutines

- Allocate_RestParam
- Allocate_VParam
- Get_RestAng_Line
- Get_RestDis_Line
- Get_RestTor_Line
- Init_Err_RefCodes
- Init_RefCodes
- Read_RefCodes_File
- VState_To_AtomsPar
- Write_Info_RefCodes
- Write_Info_RefParams
- Write_Restraints_ObsCalc

CFML_Keywords_Code_Parser: Subroutines

Subroutine Allocate_RestParam (File_Dat)

Type(File_List_Type)	**Intent(out)**	File_Dat	File list structure

Allocate vectors Ang_Rest, Dist_Rest, Tor_Rest

CFML_Keywords_Code_Parser: Subroutines

Subroutine Allocate_VParam (N)

Integer	**Intent(in)**	N	

Allocate vectors V_Vec, V_Bounds, V_Name, V_Bcon, V_Shift, V_list
If N is equal zero it deallocates the vectors

CFML_Keywords_Code_Parser: Subroutines

Subroutine Get_RestAng_Line (Line, FAtom)

Character(Len=*)	**Intent(in)**	Line	input data
Type(Atom_List_Type)	**Intent(in out)**	FAtom	Atom type structure

Get angle restraints relations for Free atoms Type

Example:
```
Angle [sig] At1a At1b At1c At2a At2b At2c....
```

CFML_Keywords_Code_Parser: Subroutines

Subroutine Get_RestDis_Line (Line, FAtom)

Character(Len=*)	**Intent(in)**	Line	input data
Type(Atom_List_Type)	**Intent(in out)**	FAtom	Atom type structure

Get distance restraints relations for Free atoms type

Example:
```
Dist [sig] At1a At1b At2a At2b ...
```

CFML_Keywords_Code_Parser: Subroutines

Subroutine Get_RestTor_Line (Line, FAtom)

Character(Len=*)	**Intent(in)**	Line	input data
Type(Atom_List_Type)	**Intent(in out)**	FAtom	Atom type structure

Get torsion restraints relations for Free atoms type

Example:
```
Torsion [sig] At1a At1b At1c At1d At2a At2b At2c At2d....
```

CFML_Keywords_Code_Parser: Subroutines

Subroutine Init_Err_RefCodes ( )

Subroutine that initializes errors flags in **CFML_Keywords_Code_Parser** module.

CFML_Keywords_Code_Parser: Subroutines

Subroutine Init_RefCodes(FAtom / MolCrys / Molec)

Type(Atom_List_Type)
or
Type(Molecular_Crystal_Type)
or
Type(Molecule_Type)
	Intent(in out)	FAtom
		
		MolCrys
		
		Molec
			Atom type structure

Initialize all refinement codes

CFML_Keywords_Code_Parser: Subroutines

Subroutine Read_RefCodes_File(Filedat, N_Ini, N_End, FAtom / MolCrys / Molec, Spgr)

Type(File_List_Type)	**Intent(in)**	Filedat	File list type
Integer	**Intent(in)**	N_Ini	initial line
Integer	**Intent(in)**	N_End	Final line

Type(Atom_List_Type)
or
Type(Molecular_Crystal_Type)
or
Type(Molecule_Type)
	Intent(in out)	FAtom
		
		MolCrys
		
		Molec
			Atom type structure
			
			Molecular crystal type structure
			
			Molecule type structure

Type(Space_Group_Type)	**Intent(in)**	Spgr	Space group information

Subroutine for treatment of Codes controls taken from FAtom/Molcrys/Molec

CFML_Keywords_Code_Parser: Subroutines

Subroutine VState_To_AtomsPar(FAtom / MolCrys / Molec, Mode)

Type(Atom_List_Type)
or
Type(Molecular_Crystal_Type)
or
Type(Molecule_Type)
	Intent(in out)	FAtom
		
		MolCrys
		
		Molec
			Atom type structure
			
			Molecular crystal type structure
			
			Molecule type structure

Character (Len=*), Optional	**Intent(in)**	Mode	Space group information

Update the values to the variable FAtom/MolCrys/Molec from Vector

CFML_Keywords_Code_Parser: Subroutines

Subroutine Write_Info_RefCodes(FAtom / MolCrys / Molec, IUnit)

Type(Atom_List_Type)
or
Type(Molecular_Crystal_Type)
or
Type(Molecule_Type)
	Intent(in out)	FAtom
		
		MolCrys
		
		Molec
			Atom type structure
			
			Molecular crystal type structure
			
			Molecule type structure

Integer, Optional	**Intent(in)**	IUnit	Unit for output information

Write the information about Refinement Codes

CFML_Keywords_Code_Parser: Subroutines

Subroutine Write_Info_RefParams(IUnit)

Integer, Optional	**Intent(in)**	IUnit	Unit for output information

Write the information about Refinement parameters in file associated with logical unit IUNIT. If no argument is passed the standard output (iunit=6) is used.

CFML_Keywords_Code_Parser: Subroutines

Subroutine Write_Restraints_ObsCalc(A, IUnit)

Type(Atom_List_Type)	**Intent(in)**	A	Atom type structure
Integer, Optional	**Intent(in)**	IUnit	Unit for output information

Write the current values of the "observed" and calculated restraints, as well as the corresponding cost value.

CFML_Magnetic_Symmetry

Series of procedures handling operations with Magnetic Symmetry and Magnetic Structures

Variables

Magnetic_Domain_Type

Magnetic_Group_Type
MagSymm_K_Type
MSym_Oper_Type

Err_MagSym
Err_MagSym_Mess

Functions

ApplyMSO

Subroutines

Init_Err_MagSym
Init_MagSymm_K_Type
ReadN_Set_Magnetic_Structure
Set_Shubnikov_Group
Write_Magnetic_Structure
Write_Shubnikov_Group

Fortran Filename

CFML_MagSymm.f90

CFML_Magnetic_Symmetry: Variables

Magnetic_Domain_Type
Magnetic_Group_Type
MagSymm_K_Type
MSym_Oper_Type

Err_MagSym
Err_MagSym_Mess

CFML_Magnetic_Symmetry: Variables

	Variable	***Definition***
Type :: Magnetic_Domain_Type		
Integer	ND	Number of rotational domains (not counting chiral domains)
Logical	Chir	***.TRUE***. if chirality domains exist
Integer, Dimension(3,3,24)	DMat	Domain matrices to be applied to Fourier Coefficients
Real (Kind=CP), Dimension(2,24)	POP	Populations of domains (sum=1, the second value is /=0 for CHIR=***.TRUE.***)

Real (Kind=CP), Dimension(2,24)	LPOP	Number of the refined parameter
Real (Kind=CP), Dimension(2,24)	MPOP	Refinement codes for populations
End Type Magnetic_Domain_Type		

Magnetic S-domains corresponds to a different magnetic structure obtained from the domain 1 (actual model) by applying a rotational operator to the Fourier coefficients of magnetic moments. This rotational operator corresponds to a symmetry operator of the paramagnetic group that is lost in the ordered state.
Chirality domains are simply obtained by changing the sign of the imaginary components of the Fourier coefficients. For each rotational domain two chiralities domains exist.

CFML_Magnetic_Symmetry: Variables

	Variable	***Definition***
Type :: Magnetic_Group_Type		
Character (Len=30)	Shubnikov	Shubnikov symbol (Hermman-Mauguin + primes)
Type(Space_Group_Type)	Spg	***.TRUE***. if chirality domains exist
Integer, Dimension(192)	TInv	When a component is +1 no time inversion is associated if tinv(i)=-1, the time inversion is associated to operator "i"
End Type Magnetic_Group_Type		

A magnetic group type is adequate when k=(0,0,0). It contains as the second component the crystallographic space group. The first component is the Shubnikov Group symbol and the third component is an Integer vector with values -1 or 1 when time inversion is associated (-1) with the corresponding crystallographic symmetry operator o not (1).

CFML_Magnetic_Symmetry: Variables

	Variable	***Definition***
Type :: MagSymm_K_Type		
Character (Len=31)	MagModel	Name to characterize the magnetic symmetry
Character (Len=1)	Latt	Symbol of the crystallographic lattice
Integer	NIrreps	Number of irreducible representations (max=4, if nirreps /= 0 => nmsym=0)
Integer	NMSym	Number of magnetic operators per crystallographic operator (max=8)
Integer	Centred	=0 centric centre not at origin =1 acentric =2 centric (-1 at origin)
Integer	MCentred	=1 Anti/a-centric Magnetic symmetry = 2 centric magnetic symmetry
Integer	NVK	Number of independent propagation vectors
Real (Kind=CP), Dimension(3,12)	KVec	Propagation vectors
Integer	NumLat	Number of centring lattice vectors
Real (Kind=CP), Dimension(3,4)	Ltr	Centring translations
Integer	NumOps	Reduced number of crystallographic Symm. Op.
Integer	Multip	General multiplicity of the space group
Integer, Dimension(4)	NBas	Number of basis functions per IRREP (if nbas < 0, the corresponding basis is complex).

Integer, Dimension(12,4)	IComp	indicator (0 pure real/ 1 pure imaginary) for coefficients of basis fucntions
Character (Len=40), Dimension(48)	SymOpSymb	Alphanumeric Symbols for SYMM
Type(Sym_Oper_Type), Dimension(48)	SymOp	Crystallographic symmetry operators
Character (Len=40), Dimension(48,8)	MSymOpSymb	Alphanumeric Symbols for MSYMM
Type(Msym_Oper_Type), Dimension(48,8)	MSymOp	Magnetic symmetry operators
Complex (Kind=CP), Dimension(3,12, 48,4)	BasF	Basis functions of the irreps of Gk
End Type MagSymm_K_Type		

Definition of the **MagSymm_K_Type** derived type, encapsulating the information concerning the crystallographic symmetry, propagation vectors and magnetic matrices. Needed for calculating magnetic structure factors.

CFML_Magnetic_Symmetry: Variables

	Variable	***Definition***
Type :: MSym_Oper_Type		
Integer, Dimension(3,3)	Rot	Rotational Part of Symmetry Operator
Real (Kind=CP)	Phas	Phase in fraction of 2
End Type MSym_Oper_Type		

Definition of Magnetic symmetry operator Type

CFML_Magnetic_Symmetry: Variables

Logical :: Err_MagSym

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_Magnetic_Symmetry: Variables

Character (Len=150) :: Err_MagSym_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Magnetic_Symmetry: Functions

ApplyMSO

CFML_Magnetic_Symmetry: Functions

Complex Function ApplyMSO (Op, SK)

Type(MSym_Oper_Type)	**Intent(in)**	Op	Magnetic Symmetry Operator Type
Complex, Dimension(3)	**Intent(in)**	SK	Complex vector

Return a vector of dimension 3. Apply a magnetic symmetry operator to a complex vector: Skp = ApplyMSO(Op,Sk)

CFML_Magnetic_Symmetry: Subroutines

CFML_Magnetic_Symmetry: Subroutines

Subroutine Init_Err_MagSym ( )

Subroutine that initializes errors flags in **CFML_Magnetic_Symmetry** module.

CFML_Magnetic_Symmetry: Subroutines

Subroutine Init_MagSymm_K_Type (MGP)

Type(MagSymm_K_Type)	**Intent(in out)**	MGP	input string with CELL directive

Subroutine to initialize the MagSymm_K_Type variable ***MGP***.

CFML_Magnetic_Symmetry: Subroutines

Subroutine ReadN_Set_Magnetic_Structure (File_CFL, N_Ini, N_End, MGP, AM, SGO, Mag_Dom)

Type(File_List_Type)	**Intent(in)**	File_CFL	input File
Integer	**Intent(in out)**	N_Ini	initial line
Integer	**Intent(in)**	N_End	Final line
Type(MagSymm_K_Type)	**Intent(out)**	MGP	
Type(MAtom_List_Type)	**Intent(out)**	AM	
Type(Magnetic_Group_Type), Optional	**Intent(out)**	SGO	
Type(Magnetic_Domain_Type), Optional	**Intent(out)**	Mag_Dom	

Subroutine for reading and construct the MagSymm_K_Type variable ***MGP***. It is supposed that the CFL file is included in the File_List_Type variable File_CFL.
On output N_Ini, N_End hold the lines with the starting and ending lines with information about a magnetic phase.
Optionally the Magnetic space group (Shubnikov group) may be obtained separately for further use. Magnetic S-domains are also read in case of providing the optional variable Mag_Dom.

CFML_Magnetic_Symmetry: Subroutines

Subroutine Set_Shubnikov_Group (Shubk, SG, MGP)

Character(Len=*)	**Intent(in)**	Shubk	
Type(Magnetic_Group_Type)	**Intent(out)**	SG	

Type(MagSymm_K_Type)	**Intent(in out)**	MGP	

This subroutine is not completed ... it is still in development

CFML_Magnetic_Symmetry: Subroutines

Subroutine Write_Magnetic_Structure (Ipr, MGP, AM, SGO, Mag_Dom)

Integer	**Intent(in)**	Ipr	input unit file
Type(MagSymm_K_Type)	**Intent(out)**	MGP	
Type(MAtom_List_Type)	**Intent(out)**	AM	
Type(Magnetic_Domain_Type), Optional	**Intent(out)**	Mag_Dom	

Subroutine to write out the information about the magnetic symmetry and magnetic structure in unit IPR.

CFML_Magnetic_Symmetry: Subroutines

Subroutine Write_Shubnikov_Group (SG, Iunit)

Type(Magnetic_Group_Type)	**Intent(in)**	SG	
Integer, Optional	**Intent(in)**	Iunit	

Subroutine to write out the information about the Shubnikov_Group

CFML_Simulated_Annealing

Module for Global Optimization using Simulated Annealing.

Currently there is available only a generic Simulated Annealing subroutine. That must be called with the name of a user-supplied subroutine to calculate the cost function as an argument. The calling program must define at least two variables of derived types SimAnn_Conditions_Type and State_Vector_Type respectively.

The generic simulated annealing procedure can use the constant step algorithm or the Corana algorithm depending on the values of the corresponding component of the SimAnn_Conditions_Type user-defined variable.

Parameters

NP_Conf
NP_SAn

Variables

MultiState_Vector_Type
SimAnn_Conditions_Type
State_Vector_Type

Err_SAn
Err_SAn_Mess

Subroutines

SAnn_Opt_MultiConf
Set_SimAnn_Cond
Set_SimAnn_MStateV
Set_SimAnn_StateV
SimAnneal_Gen
SimAnneal_MultiConf
Write_SimAnn_Cond
Write_SimAnn_MStateV
Write_SimAnn_StateV

Fortran Filename

CFML_Optimization_SAn.f90

CFML_Simulated_Annealing: Parameters

NP_Conf
NP_SAn

CFML_Simulated_Annealing: Parameters

Integer, Parameter :: NP_CONF = 30

Maximum number of initial configurations in parallel

CFML_Simulated_Annealing: Parameters

Integer, Parameter :: NP_SAN = 80

Maximum number of parameters in the model

CFML_Simulated_Annealing: Variables

MultiState_Vector_Type
SimAnn_Conditions_Type
State_Vector_Type

Err_SAn
Err_SAn_Mess

CFML_Simulated_Annealing: Variables

	Variable	***Definition***
Type :: MultiState_Vector_Type		
Integer	NPar	Number of parameters of the model

Integer	NConf	Number of configurations
Integer, Dimension (NP_SAn, NP_Conf)	Code	=0 fixed parameter =1 variable parameter
Integer, Dimension (NP_SAn)	Bound	=0 fixed boundaries =1 periodic boundaries
Real (Kind=CP), Dimension (NP_SAn, NP_Conf)	State	Vector State with the current configuration
Real (Kind=CP), Dimension (NP_SAn, NP_Conf)	STP	Step vector (one value for each parameter)
Real (Kind=CP), Dimension (NP_CONF)	Cost	Vector with cost of the different configurations
Real (Kind=CP), Dimension (NP_SAn)	Low	Low-limit value of parameters
Real (Kind=CP), Dimension (NP_SAn)	High	High-limit value of parameters
Real (Kind=CP), Dimension (NP_SAn)	Config	Vector State with the best configuration
Character (Len=15), Dimension (NP_SAn)	NamPar	Name of parameters of the model
End Type MultiState_Vector_Type		

CFML_Simulated_Annealing: Variables

	Variable	***Definition***
Type :: SimAnn_Conditions_Type		
Real (Kind=CP)	T_Ini	initial temperature
Real (Kind=CP)	Anneal	Kirpactrick factor for Annealing
Real (Kind=CP)	Accept	Minimum percentage of accepted configurations
Real (Kind=CP)	Threshold	Good solutions have cost values below this (used in Sann_Opt_MultiConf)
Integer	InitConfig	Flag determining if the first configuration is random or read
Integer	NAlgor	Flag determining if the Corana algorithm is selected (0) or not (/=0)
Integer	NM_Cycl	Number of Cycles per temp in SA searchs
Integer	Num_Temps	Maximum number of temperatures in SA
Integer	Num_Therm	Number of thermalization cycles in SA
Integer	Num_Conf	Number of paralell configurations in SA
Character (Len=60)	Cost_Function_Name	Name of Function
Integer	Seed	If different from zero, holds the seed for random number generator
End Type SimAnn_Conditions_Type		

CFML_Simulated_Annealing: Variables

	Variable	***Definition***

Type :: State_Vector_Type		
Integer	NPar	Number of parameters of the model
Integer, Dimension (NP_SAn)	Code	=0 fixed parameter =1 variable parameter
Integer, Dimension (NP_SAn)	Bound	=0 fixed boundaries =1 periodic boundaries
Real (Kind=CP), Dimension (NP_SAn)	State	Vector State with the current configuration
Real (Kind=CP), Dimension (NP_SAn)	STP	Step vector (one value for each parameter)
Real (Kind=CP), Dimension (NP_SAn)	Low	Low-limit value of parameters
Real (Kind=CP), Dimension (NP_SAn)	High	High-limit value of parameters
Real (Kind=CP), Dimension (NP_SAn)	Config	Vector State with the best configuration
Real (Kind=CP)	Cost	Cost of the best configuration
Character (Len=15), Dimension (NP_SAn)	NamPar	Name of parameters of the model
End Type State_Vector_Type		

CFML_Simulated_Annealing: Variables

Logical :: Err_SAn

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_Simulated_Annealing: Variables

Character (Len=150) :: Err_SAn_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Simulated_Annealing: Subroutines

- SAnn_Opt_MultiConf
- Set_SimAnn_Cond
- Set_SimAnn_MStateV
- Set_SimAnn_StateV
- SimAnneal_Gen
- SimAnneal_MultiConf
- Write_SimAnn_Cond
- Write_SimAnn_MStateV
- Write_SimAnn_StateV

CFML_Simulated_Annealing: Subroutines

Subroutine SAnn_Opt_MultiConf (Model_Funct, C, VS, Ipr, Filesav, FST)

Defined Subroutine Model_Funct		Model_Funct	
Type(SimAnn_Conditions_Type)	**Intent(in out)**	C	
Type(MultiState_Conditions_Type)	**Intent(in out)**	VS	
Integer	**Intent(in)**	Ipr	
Character (Len=*), Optional	**Intent(in)**	Filesav	
Character (Len=*), Optional	**Intent(in)**	FST	

Subroutine Model_Funct (V, Cost)

Real(Kind=CP),Dimension (:)	**Intent(in)**	V	Variables
Real(Kind=CP)	**Intent(out)**	Cost	Value of Model

End Subroutine Model_Funct

If **FST** is present the user need define the next subroutine

Subroutine Write_FST (FST_File, V, Cost)

Character (Len=*)	**Intent(in)**	FST_File	
Real(Kind=CP),Dimension (:)	**Intent(in)**	V	Variables
Real(Kind=CP)	**Intent(in)**	Cost	Value of Model

End Subroutine Write_FST

Multi-Configurational Simulated Annealing with local optimization when a configuration with cost lower than a threshold value is given or when one of the Markov chains stalls

CFML_Simulated_Annealing: Subroutines

Subroutine Set_SimAnn_Cond (File_List, C)

Type(File_List_Type)	**Intent(in)**	File_List	
Type(SimAnn_Conditions_Type)	**Intent(in)**	C	Conditions

Subroutine for reading and set up the SimAnn_Conditions_Type variable ***C***

CFML_Simulated_Annealing: Subroutines

Subroutine Set_SimAnn_MStateV (N, NSol, Con, Bounds, VNam, Vec, VS, Cod)

Integer	**Intent(in)**	N	Number of parameters
Integer	**Intent(in)**	NSol	Number of Solutions
Integer, Dimension (:)	**Intent(in)**	Con	Number of Configurations
Real(Kind=CP), Dimension (:,:)	**Intent(in)**	Bounds	Boundary conditions (1,:)-> Low (2,:) -> High (3,:) -> Step
Character (Len=*), Dimension (:)	**Intent(in)**	VNam	Names of parameters
Real(Kind=CP), Dimension (:)	**Intent(in)**	Vec	initial value of parameters
Type(State_Vector_Type)	**Intent(out)**	VS	initial State vector
Integer, Dimension (:), Optional	**Intent(in)**	Cod	If present, cod(i)=0 fix the "i" parameter

Subroutine for setting up the State_Vector_Type variable ***VS***

CFML_Simulated_Annealing: Subroutines

Subroutine Set_SimAnn_StateV (N, Con, Bounds, VNam, Vec, VS, Cod)

Integer	**Intent(in)**	N	Number of parameters
Integer, Dimension (:)	**Intent(in)**	Con	Number of Configurations
Real(Kind=CP), Dimension (:,:)	**Intent(in)**	Bounds	Boundary conditions (1,:)-> Low (2,:) -> High

			(3,:) -> Step
Character (**Len**=*), **Dimension** (:)	**Intent(in)**	VNam	Names of parameters
Real(Kind=CP), Dimension (:)	**Intent(in)**	Vec	initial value of parameters
Type(State_Vector_Type)	**Intent(out)**	VS	initial State vector
Integer, Dimension (:), **Optional**	**Intent(in)**	Cod	If present, cod(i)=0 fix the "i" parameter

Subroutine for setting up the State_Vector_Type variable ***VS***

CFML_Simulated_Annealing: Subroutines

Subroutine SimAnneal_Gen (Model_Funct, C, VS, Ipr, Filesav, FST)

Defined Subroutine Model_Funct		Model_Funct	
Type(SimAnn_Conditions_Type)	**Intent(in out)**	C	
Type(State_Vector_Type)	**Intent(in out)**	VS	
Integer	**Intent(in)**	Ipr	
Character (**Len**=*), **Optional**	**Intent(in)**	Filesav	
Character (**Len**=*), **Optional**	**Intent(in)**	FST	

Subroutine Model_Funct (V, Cost)

Real(Kind=CP),Dimension (:)	**Intent(in)**	V	Variables
Real(Kind=CP)	**Intent(out)**	Cost	Value of Model

End Subroutine Model_Funct

If FST is present the user need define the next subroutine

Subroutine Write_FST (FST_File, V, Cost)

Character (Len=*)	**Intent(in)**	FST_File	
Real(Kind=CP),Dimension (:)	**Intent(in)**	V	Variables
Real(Kind=CP)	**Intent(in)**	Cost	Value of Model

End Subroutine Write_FST

CFML_Simulated_Annealing: Subroutines

Subroutine SimAnneal_MultiConf (Model_Funct, NSol, C, VS, Ipr, Filesav, FST)

Defined Subroutine Model_Funct		Model_Funct		
Integer	**Intent(in out)**	NSol		
Type(SimAnn_Conditions_Type)	**Intent(in out)**	C		
Type(MultiState_Conditions_Type)	**Intent(in out)**	VS		
Integer	**Intent(in)**	Ipr		
Character (**Len**=*), **Optional**	**Intent(in)**	Filesav		
Character (**Len**=*), **Optional**	**Intent(in)**	FST		

Subroutine Model_Funct (V, Cost)

Real(Kind=CP),Dimension (:)	**Intent(in)**	V	Variables

```
   Real(Kind=CP)                      Intent(out)   Cost        Value of Model
End Subroutine Model_Funct
```

If FST is present the user need define the next subroutine

```
Subroutine Write_FST (FST_File, V, Cost)
   Character (Len=*)                  Intent(in)    FST_File
   Real(Kind=CP),Dimension  (:)       Intent(in)    V           Variables
   Real(Kind=CP)                      Intent(in)    Cost        Value of Model
End Subroutine Write_FST
```

CFML_Simulated_Annealing: Subroutines

Subroutine Write_SimAnn_Cond (Ipr, C)

Integer	**Intent(in)**	Ipr	input unit file
Type(SimAnn_Conditions_Type)	**Intent(in)**	C	SAn Conditions

Subroutine for writing in unit Ipr the SimAnn_Conditions_Type variable C

CFML_Simulated_Annealing: Subroutines

Subroutine Write_SimAnn_MState (Ipr, VS, Text, Cost)

Integer	**Intent(in)**	Ipr	input unit file
Type(State_Vector_Type)	**Intent(in)**	VS	State vector
Character (Len=*)	**Intent(in)**	Text	
Integer, Optional	**Intent(in)**	Cost	

Subroutine for writing in unit Ipr the State_Vector_Type variable VS

CFML_Simulated_Annealing: Subroutines

Subroutine Write_SimAnn_State (Ipr, VS, Text)

Integer	**Intent(in)**	Ipr	input unit file
Type(State_Vector_Type)	**Intent(in)**	VS	State vector
Character (Len=*)	**Intent(in)**	Text	

Subroutine for Writing in unit Ipr the State_Vector_Type VS

Level 9

Concept	***Module Name***	***Purpose***
Magnetic Structure Factors...	**CFML_Magnetic_Structure_Factors**	Magnetic Structure Factors Calculations
Polarymetry	**CFML_Polarimetry**	Procedures to calculate the polarization tensor as measured using CRYOPAD

CFML_Magnetic_Structure_Factors

Main module for Magnetic Structure Factors Calculations

Variables

MagH_Type
MagH_List_Type
MagHD_Type
MagHD_List_Type

Err_MSFac
Err_MSFac_Mess

Subroutines

Calc_Mag_Interaction_Vector
Calc_Magnetic_StrF_MIV
Calc_Magnetic_StrF_MIV_Dom
Gen_Satellites
Init_Err_MSFac
Init_Mag_Structure_Factors
Mag_Structure_Factors
Modify_MSF
Write_Mag_Structure_Factors

Fortran Filename

CFML_Msfac.f90

CFML_Magnetic_Structure_Factors: Variables

MagH_Type
MagH_List_Type
MagHD_Type
MagHD_List_Type

Err_MSFac
Err_MSFac_Mess

CFML_Magnetic_Structure_Factors: Variables

	Variable	***Definition***

Type :: MagH_Type		
Logical	Keqv_Minus	True if k equivalent to -k
Integer	Mult	Multiplicity of the reflection (useful for powder calculations)
Integer	Num_K	number of the propagation vector Vk
Real (Kind=CP)	SignP	+1 for -Vk and -1 for +Vk
Real (Kind=CP)	S	sin /
Real (Kind=CP)	SQMIV	Square of the Magnetic interaction vector
Real (Kind=CP), Dimension (3)	H	H +/- k
Complex (Kind=CP), Dimension (3)	MSF	magnetic structure factor
Complex (Kind=CP), Dimension (3)	MIV	magnetic interaction vector
End Type MagH_Type		

Define the scatering vector vector H+k and the sign -1 for H+k and +1 for H-k.
Includes the magnetic interaction vector MiV = Mper = M

CFML_Magnetic_Structure_Factors: Variables

	Variable	***Definition***
Type :: MagH_List_Type		
Integer	NRef	
Type (MagH_Type), Dimension (:), Allocatable	MH	
End Type MagH_List_Type		

Define a list of magnetic reflections containing the scattering vector, the magnetic structure factor and the magnetic interaction vector.

CFML_Magnetic_Structure_Factors: Variables

	Variable	***Definition***
Type :: MagHD_Type		
Logical	Keqv_Minus	True if k equivalent to -k
Integer	Num_K	number of the propagation vector Vk
Real (Kind=CP)	SignP	+1 for -Vk and -1 for +Vk
Real (Kind=CP)	S	sin /
Real (Kind=CP)	SQAMIV	Square of the Average Magnetic interaction vector
Real (Kind=CP)	SQMIV	Average of the Square of Magnetic interaction vectors
Real (Kind=CP), Dimension (3)	H	H +/- k
Complex (Kind=CP), Dimension (3,2,24)	MSF	Magnetic structure factors of each domain (second dimension for chirality domains)
Complex (Kind=CP), Dimension (3,2,24)	MIV	Magnetic interaction vector of each domain
Complex (Kind=CP), Dimension (3)	AMIV	Average Magnetic interaction vector = 1/nd Sum{ pop(i) Miv(:,i)}

End Type MagHD_Type		

Define the scattering vector vector H+k and the sign -1 for H+k and +1 for H-k.
Includes the average magnetic interaction vector AMiV(:) = 1/nd Sum[i]{ pop(i) Miv(:,i)}
This type should be used whenever magnetic domains are present (single crystal work)

CFML_Magnetic_Structure_Factors: Variables

	Variable	***Definition***
Type :: MagHD_List_Type		
Integer	NRef	
Type (MagHD_Type), Dimension (:), Allocatable	MH	
End Type MagHD_List_Type		

Define a list of magnetic reflections containing the scattering vector, the magnetic structure factor and the magnetic interaction vector for each of the domains.

CFML_Magnetic_Structure_Factors: Variables

Logical :: Err_MSFac

This variable is set to **.TRUE.** if an error occurs in procedures belonging to this module.

CFML_Magnetic_Structure_Factors: Variables

Character (Len=150) :: Err_MSFac_Mess

This variable contains information about the last error occurred in the procedures belonging to this module

CFML_Magnetic_Structure_Factors: Subroutines

- Calc_Mag_Interaction_Vector
- Calc_Magnetic_StrF_MIV
- Calc_Magnetic_StrF_MIV_Dom
- Gen_Satellites
- Init_Err_MSFac
- Init_Mag_Structure_Factors
- Mag_Structure_Factors
- Modify_MSF
- Write_Mag_Structure_Factors

CFML_Magnetic_Structure_Factors: Subroutines

Subroutine Calc_Mag_Interaction (Reflex, Cell, Mode)

Type(MagH_List_Type)	**Intent(in out)**	Reflex		Magnetic reflections list
Type(Crystal_Cell_Type)	**Intent(in)**	Cell		Cell Parameters
Character (Len=*), Optional	**Intent(in)**	Mode		

Calculate the Magnetic interaction vector from Magnetic Structure factors, reflections and cell parameters.
The components are given with respect to the crystallographic unitary direct cell system: {e1,e2,e3}. If Mode is given the components are with respect to the cartesian frame defined in Cell.

CFML_Magnetic_Structure_Factors: Subroutines

Subroutine Calc_Magnetic_STRF_MIV (Cell, MGP, Atm, MH, Mode)

Type(Crystal_Cell_Type)	**Intent(in)**	Cell		Cell Parameters
Type(MagSymm_K_Type)	**Intent(in)**	MGP		
Type(MAtom_List_Type)	**Intent(in out)**	Atm		
Type(MagH_Type)	**Intent(in out)**	MH		
Character (Len=*), Optional	**Intent(in)**	Mode		

Calculate the Magnetic interaction vector from Magnetic Structure factors, reflections and cell parameters.
The components are given with respect to the crystallographic unitary direct cell system: {e1,e2,e3}. If Mode is given the components are with respect to the cartesian frame defined in Cell.

CFML_Magnetic_Structure_Factors: Subroutines

Subroutine Calc_Magnetic_STRF_MIV_Dom (Cell, MGP, Atm, Mag_Dom, MH, Mode)

Type(Crystal_Cell_Type)	**Intent(in)**	Cell		Cell Parameters
Type (MagSymm_K_Type)	**Intent(in)**	MGP		
Type (MAtom_List_Type)	**Intent(in)**	Atm		
Type (Magnetic_Domain_Type)	**Intent(in)**	Mag_Dom		
Type (MagHD_Type)	**Intent(in out)**	MH		
Character (Len=*), Optional	**Intent(in)**	Mode		

Calculate the Magnetic interaction vector from Magnetic Structure factors, reflections and cell parameters.
The components are given with respect to the crystallographic unitary direct cell system: {e1,e2,e3}. If Mode is given the components are with respect to the cartesian frame defined in Cell.

CFML_Magnetic_Structure_Factors: Subroutines

Subroutine Gen_Satellites (Cell, Grp, SMax, H, Ord, Powder)

Type(Crystal_Cell_Type)	**Intent(in)**	Cell		Cell Parameters
Type (MagSymm_K_Type)	**Intent(in)**	Grp		
Real(Kind=CP)	**Intent(in)**	SMax		
Type (MagH_List_Type)	**Intent(in out)**	H		
Logical, Optional	**Intent(in)**	Ord		
Logical, Optional	**Intent(in)**	Powder		

Generates half reciprocal sphere of Integer reflections and add satellites according to the information given in GRP.

CFML_Magnetic_Structure_Factors: Subroutines

Subroutine Init_Err_MSFac ( )

Initialize the errors flags in this Module

CFML_Magnetic_Structure_Factors: Subroutines

Subroutine Init_Mag_Structure_Factors (Reflex, Atm, Grp, Lun)

Type(MagH_List_Type)	**Intent(in)**	Reflex		
Type(MAtom_List_Type)	**Intent(in)**	Atm		
Type(MagSymm_K_Type)	**Intent(in)**	Grp		
Integer, Optional	**Intent(in)**	Lun		output unit

Allocates and initializes arrays for Magnetic Structure Factors calculations. A calculation of fixed tables is also performed.

CFML_Magnetic_Structure_Factors: Subroutines

Subroutine Mag_Structure_Factors (Atm, Grp, Reflex)

Type(MAtom_List_Type)	**Intent(in)**	Atm		
Type(MagSymm_K_Type)	**Intent(in)**	Grp		
Type(MagH_List_Type)	**Intent(in)**	Reflex		

Calculate the Magnetic Structure Factors from a list of magnetic Atoms and a set of reflections.
A call to Init_Mag_Structure_Factors is a pre-requisite for using this subroutine. In any case the subroutine calls Init_Mag_Structure_Factors if SF_initialized=.false.

CFML_Magnetic_Structure_Factors: Subroutines

Subroutine Modify_MSF (Reflex, Atm, Grp, List, NList)

Type(MagH_List_Type)	**Intent(in)**	Reflex		
Type(MAtom_List_Type)	**Intent(in)**	Atm		
Type(MagSymm_K_Type)	**Intent(in)**	Grp		
Integer, Dimension (:)	**Intent(in)**	List		
Integer	**Intent(in)**	NList		

Recalculation of Magnetic Structure Factors because a list of Atoms parameters were modified. The List variable contains the numbers in the list of the atoms to be changed.

CFML_Magnetic_Structure_Factors: Subroutines

Subroutine Write_Structure_Factors (Lun, Reflex, Grp)

Integer	**Intent(in)**	Lun		output unit
Type(MagH_List_Type)	**Intent(in)**	Reflex		
Type(MagSymm_K_Type)	**Intent(in)**	Grp		

Writes in logical unit Lun the list of structure factors contained in the Reflex type information

CFML_Polarimetry

Module for Polarisation calculations

the polar tensor is calculated respect to the coordinate frame defined in the Blume equations (Phys. Rev. Vol. 130 p.1670-1676,1963, see also the definitions below in magn_inter_Vec_PF). As input the nuclear structure factor, the magnetic interaction vector with respect to the crystal frame and the matrices defined in CFML_Crystal_Metrics for the crystal frame are needed.

Variables

- Polar_Calc_Type
- Polar_Calc_List_Type
- Polar_Info_Type
- Polar_Obs_Type
- Polar_Obs_List_Type

Subroutines

- Calc_Polar_Dom
- Set_Polar_Info
- Write_Polar_Info
- Write_Polar_Line

Fortran Filename

CFML_Polar.f90

CFML_Polarimetry: Variables

- Polar_Calc_Type
- Polar_Calc_List_Type
- Polar_Info_Type
- Polar_Obs_Type
- Polar_Obs_List_Type

CFML_Polarimetry: Variables

	Variable	***Definition***
Type :: Polar_Calc_Type		
Real(Kind=CP), Dimension(3)	H	Scattering vector in hkl
Real(Kind=CP), Dimension(3)	SPV	Second vector in Scattering plane apart of scattering vector to define plane
Type(Crystal_Cell_Type)	Cell	Unit Cell of Crystal
Real(Kind=CP)	P	Magnitude of initial polarisation vector
Complex, Dimension(3,2,24)	MIV	Magnetic interaction vector
Complex	NSF	Nuclear structure factor
Real(Kind=CP)	NC	Nuclear scattering contribution
Real(Kind=CP), Dimension(2,24)	MY	Magnetic contribution along y

Real(Kind=CP), Dimension(2,24)	MZ	Magnetic contribution along z
Real(Kind=CP), Dimension(2,24)	RY	Real part of nuclear magnetic interference term along y
Real(Kind=CP), Dimension(2,24)	RZ	Real part of nuclear magnetic interference term along z
Real(Kind=CP), Dimension(2,24)	IY	Imaginary part of nuclear magnetic interference term along y
Real(Kind=CP), Dimension(2,24)	IZ	Imaginary part of nuclear magnetic interference term along z
Real(Kind=CP), Dimension(2,24)	TC	Chiral contribution
Real(Kind=CP), Dimension(2,24)	MM	Magnetic-magnetic interference term
Real(Kind=CP), Dimension(3,2,24)	CS	Three different elastic cross-sections depending on the direction of the initial polar vector
Real(Kind=CP), Dimension(3,3)	PIJ	Polarisation tensor
End Type Polar_Calc_Type		

CFML_Polarimetry: Variables

	Variable	***Definition***
Type :: Polar_Calc_List_Type		
Integer	Nref	Number of reflections
Type(Polar_Calc_Type), Dimension(:), Allocatable	Polari	Calculated Polarisation tensor for the Reflection List
End Type Polar_Calc_List_Type		

CFML_Polarimetry: Variables

	Variable	***Definition***
Type :: Polar_Info_Type		
Real(Kind=CP), Dimension(3)	H	Scattering vector in hkl
Real(Kind=CP), Dimension(3)	SPV	Second vector in Scattering plane apart of scattering vector to define plane
Type(Crystal_Cell_Type)	Cell	Unit Cell of Crystal
Real(Kind=CP)	P	Magnitude of initial polarisation vector
Complex, Dimension(3)	MIV	Magnetic interaction vector
Complex	NSF	Nuclear structure factor
Real(Kind=CP)	NC	Nuclear scattering contribution
Real(Kind=CP)	MY	Magnetic contribution along y
Real(Kind=CP)	MZ	Magnetic contribution along z
Real(Kind=CP)	RY	Real part of nuclear magnetic interference term along y
Real(Kind=CP)	RZ	Real part of nuclear magnetic interference term along z
Real(Kind=CP)	IY	Imaginary part of nuclear magnetic interference

		term along y
Real(Kind=CP)	IZ	Imaginary part of nuclear magnetic interference term along z
Real(Kind=CP)	TC	Chiral contribution
Real(Kind=CP)	MM	Magnetic-magnetic interference term
Real(Kind=CP), Dimension(3)	CS	Three different elastic cross-sections depending on the direction of the initial polar vector
Real(Kind=CP), Dimension(3,3)	PIJ	Polarisation tensor
End Type Polar_Info_Type		

CFML_Polarimetry: Variables

	Variable	***Definition***
Type :: Polar_Obs_Type		
Real(Kind=CP), Dimension(3)	H	Scattering vector in hkl
Real(Kind=CP), Dimension(3,3)	OPIJ	
Real(Kind=CP), Dimension(3,3)	SOPIJ	
End Type Polar_Obs_Type		

CFML_Polarimetry: Variables

	Variable	***Definition***
Type :: Polar_Obs_List_Type		
Integer	Nref	Number of reflections
Type(Polar_Obs_Type), Dimension(:), Allocatable	Polaro	Observed Polarisation tensor for the Reflection List
End Type Polar_Obs_List_Type		

CFML_Polarimetry: Subroutines

- Calc_Polar_Dom
- Set_Polar_Info
- Write_Polar_Info
- Write_Polar_Line

CFML_Polarimetry: Subroutines

Subroutine Calc_Polar_Dom (Cell, H, SPV, Pin, NSF, Mag_Dom, MH, Polari)

Type(Crystal_Cell_Type)	Intent(in)	Cell	Cell Parametrs
Real(Kind=CP), Dimension (3)	Intent(in)	H	Scattering vector in hkl

Real(Kind=CP), Dimension (3)	**Intent(in)**	SPV	Second Scattering plane vector in hkl
Real(Kind=CP)	**Intent(in)**	Pin	Magnitude of initial polarisation
Complex	**Intent(in)**	NSF	Nuclear Scattering Factor
Type(Magnetic_Domain_Type)	**Intent(in)**	Mag_Dom	
Type(MagHD_TYPE)	**Intent(in out)**	MH	Magnetic interaction vector
Type(Polar_Info_Type)	**Intent(out)**	Polari	All information about polarisation in one point hkl

Calculates Polarization matrix for domain case

CFML_Polarimetry: Subroutines

Subroutine Set_Polar_Info (Cell, H, SPV, Pin, NSF, MIV, Polari)

Type(Crystal_Cell_Type)	**Intent(in)**	Cell	Cell Parametrs
Real(Kind=CP), Dimension (3)	**Intent(in)**	H	Scattering vector in hkl
Real(Kind=CP), Dimension (3)	**Intent(in)**	SPV	Second Scattering plane vector in hkl
Real(Kind=CP)	**Intent(in)**	Pin	Magnitude of initial polarisation
Complex	**Intent(in)**	NSF	Nuclear Scattering Factor
Complex, Dimension (3)	**Intent(in)**	MIV	Magnetic interaction vector
Type(Polar_Info_Type)	**Intent(out)**	Polari	All information about polarisation in one point hkl

Initializes the variable **Polari** using the type Polar_Info_Type

CFML_Polarimetry: Subroutines

Subroutine Write_Polar_Info (Polari, Lun, Info)

Type(Polar_Info_Type)	**Intent(in)**	Polari	Polarisation in one point hkl
Integer, Optional	**Intent(in)**	Lun	Unit to write
Character (Len=*), Optional	**Intent(in)**	Info	Values are: P : also print information about coordinate frame C : also print information about crystal B : also print information about both

Outputs the polarisation info type in nice form

CFML_Polarimetry: Subroutines

Subroutine Write_Polar_Line (Polari, Lun)

Type(Polar_Info_Type)	**Intent(in)**	Polari	Polarisation in one point hkl
Integer, Optional	**Intent(in)**	Lun	Unit to write

outputs the polarization info type in line form, so you can write it to a file