PROGRAM: CrysCalcon

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This program was used for testing the symmetry procedures of CrysFML. We distribute it as an example of the use of CrysFML and it is useful for simple crystallographic calculations. It is a console program using menus with options to select by the user.

The source code of the program can be found in the CrysFML repository:
http://forge.ill.eu/projects/crysfml/repository
within the subdirectory:
http://forge.ill.eu/projects/crysfml/repository/show/Program_Examples/Cryst_calculator_console

When running the program the following screen appears:

```
     GENERAL CRYSTALLOGRAPHY CALCULATOR

     Principal Menu
 ======================


 [0] Exit

 [1] Space Groups
 [2] Reflections
 [3] Atomistics Calculations
 [4] Chemical Information
 [5] Geometry calculations

 OPTION:
```

The menus of the different options are given below.

Option [1] of Principal Menu

```
    CRYSTRALLOGRAPHIC CALCULATOR

    Space Groups Menu
 ========================


 [0] Back...

 [ 1] Space Group Information (Complete information on the Screen)
 [ 2] List of the full list of Symmetry Operators (File/Screen)
 [ 3] Construct a Space Group from a set of Generators
 [ 4] Hall Symbol from a set of Generators
 [ 5] Comparison of Two Space Groups
 [ 6] Determination of the Laue class and Point Group
 [ 7] Determination of the Symbol for Symmetry Operators
 [ 8] Conversions: IT -> Kovalev, Miller&Love, Zack, etc...
```

Option [2] of Principal Menu

```
    GENERAL CRYSTALLOGRAPHY CALCULATOR

    Reflections Menu
 ========================

 [0] Back...

 [1] Asymmetric Unit in Reciprocal Space
 [2] Change an arbitrary reflection to the Asymmetric Unit
 [3] Systematic Absence of Reflections
 [4] List of Equivalent Reflections
```

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[5] List of unique reflections within a range of S or D (output to a File)
[6] Multiplicity of reflections
```

Option [3] of Principal Menu

```
    GENERAL CRYSTALLOGRAPHY CALCULATOR

    Atomistic Calculations
==============================


[0] Back...

[1] Multiplicity of an atom position
[2] Read a CFL or CIF file to load a crystal structure
[3] Show current structure information
[4] Calculate Ionic Dipolar moment & polarisation of a symmetrized single unit cell
```

Option [4] of Principal Menu

```
    GENERAL CRYSTALLOGRAPHY CALCULATOR

          Chemical Information
       ============================


[0] Back...

[1] International Chemical Table
```

Option [5] of Principal Menu

```
    GENERAL CRYSTALLOGRAPHY CALCULATOR

      Geometrical Calculations Menu
  ====================================


 [0] Back...

 [1] Enter unit cell parameters (or show current cell)
 [2] Zone axis common to two planes
 [3] Angle between two directions in direct space
 [4] Angle between two directions in reciprocal space
 [5] Angle between two directions one reciprocal space and the other in direct space
 [6] Direction in direct space => unitary direction in reciprocal space
 [7] Direction in reciprocal space => unitary direction in direct space
 [8] Basis change matrix => get new unit cell parameters
 [9] Zone axis: list of zone planes and angles,... special angles
[10] Indexing edges of a trapezoidal plane
[11] List of planes intersecting a given one at a particular Zone Axis
[12] Enter Euler Angles Chi, Phi, Theta of frame [u,v,w]
```