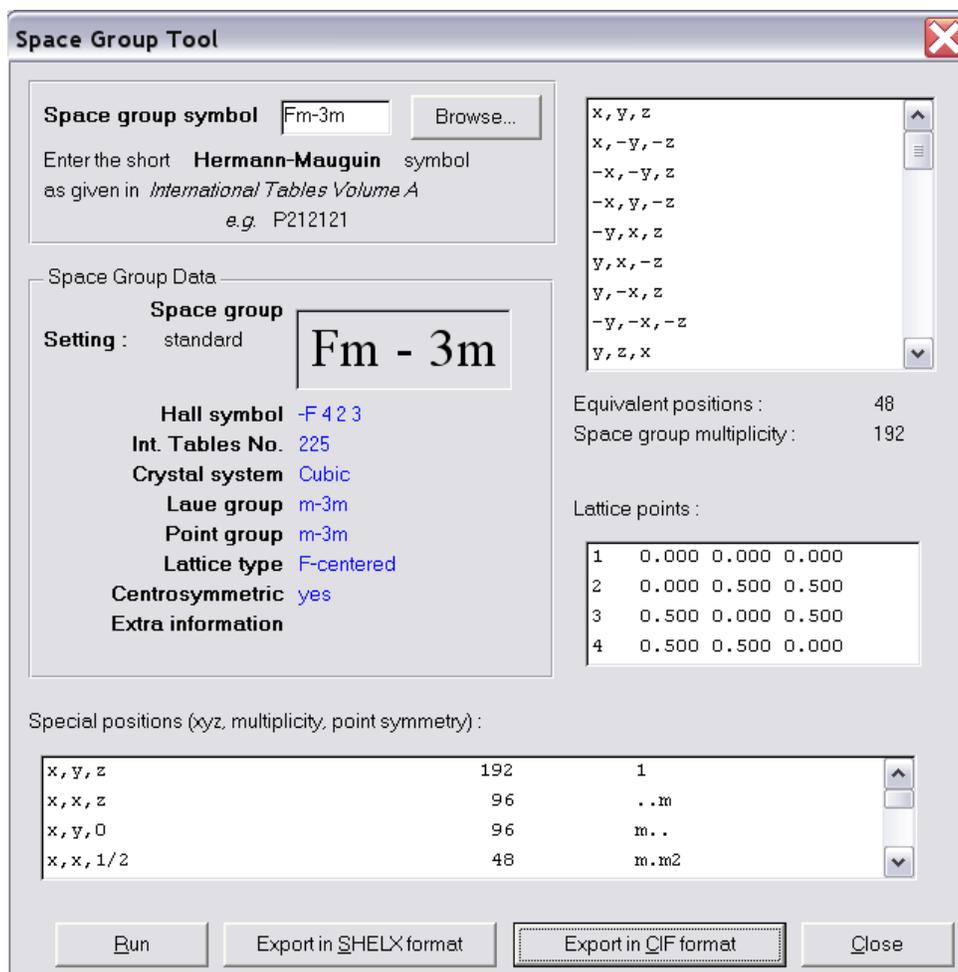# Chapter 2.5

SPACE GROUP TOOL

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The menu item SPACE GROUP TOOL provide information about the space group, including the equivalent positions, when a suitable space group symbol is entered. The following Window opens when this item is selected

The short Herman-Mauguin symbols as described in International Tables Vol A. should be given. The space-group interpreter routine used by WinGX is quite flexible and general. All non-standard settings are acceptable, but centrosymmetric space groups must have the origin coinciding with an inversion centre. The input space group symbol is first checked against the look-up table *SGINFO.DAT*. If no match is found, an error message to this effect is issued. The Herman-Mauguin symbol is then converted to the Hall symbol, and the symmetry matrices derived from this using the GETSPEC routines of Altermatt & Brown.

Clicking the button **Export in SHELX format** causes SHELX style LATT and SYMM instructions to be written to the file SYMM.OUT, for each space group queried. Similarly, clicking the button **Export in CIF format** cause a CIF format entry for that space group to be written out to SYMM.OUT. Only the first 36 operators are listed in the Window, though all will be written to the file.

The character string for the input symbol is case-insensitive. The SHELXTL syntax for subscripts may be used, but is unnecessary. Example syntax is:

```
P21/C    P2(1)/c   P 1 21/c 1  P1121   cmm2    I 4/m m m   P 32 2 1  R-3:h
```

The last example show how you may explicitly specify the setting, for those cases where International Tables allows more then one setting. In this example the space group R-3 on hexagonal axes is indicated.
The conventions used for various settings are :

```
Monoclinic    unique axis b    unique axis c    unique axis a
              abc   c-ba        abc   ba-c       abc   -acb
             ------------      ------------     ------------
cell choice 1  :b1   :-b1        :c1   :-c1       :a1   :-a1
            2  :b2   :-b2        :c2   :-c2       :a2   :-a2
            3  :b3   :-b3        :c3   :-c3       :a3   :-a3

 Orthorhombic   :ba-c    change of basis abc -> ba-c
                :1       origin choice 1
                :2ba-c   origin choice 2, change of basis abc -> ba-c

 Tetragonal     :1       origin choice 1
 & Cubic        :2       origin choice 2

 Trigonal       :h       hexagonal    axes
                :r       rhombohedral axes
```