Chapter 1.1

INTRODUCTION

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1.1.1 - Program Credits for WinGX

WinGX is an integrated system of publically available (but not necessarily public domain) programs for the analysis and refinement of single crystal X-ray diffraction data. It is primarily focussed on **small molecule crystallography** and has been developed out of the Glasgow GX package (hence its name). Only a few of these original programs remain in ***WinGX***.

A large number of authors worldwide have made their excellent software available to the scientific community through the Internet. The philosophy behind ***WinGX*** is to encapsulate this software in a modern, coherent and user friendly environment.

The following authors are thanked for making their program codes available to the scientific community:

- G. M. Sheldrick - SHELXL,SHELXS, SHELXA, SHELXD and CIF_TABLES
- A. L. Spek - PLATON, PLUTON and LEPAGE
- D. M. Watkin and coworkers - CAMERON
- C. Giacovazzo and coworkers - SIR92
- P. T. Beurskens and coworkers - DIRDIF system
- K. W.Muir and P. R. Mallinson - GX programs GEOM and WTANAL
- (the late) M. Nardelli - PARST and HYDROGEN (CALC-OH)
- (the late) K. Trueblood and coworkers - THMA11/THMA14
- L. Palatinus - SUPERFLIP
- B. Blessing - DREAR suite, SORTAV, UIJXN (ScaleXN)

1.1.2 - File naming conventions in WinGX

All files used and written by ***WinGX*** are of type ASCII unless otherwise stated and may thus be viewed and edited by standard text-editors. Some files have a fixed format (*e.g.* all files with .HKL extention), so some care may be required when editing these. ***WinGX*** can read ASCII files in DOS or UNIX format but will write files in DOS format only.

While *in principle* ***WinGX v1.80*** supports long file names, there is a current restriction to about 255 characters for the fullpath name. The folder (directory) name may contain embedded spaces, but the local filename should not. Most, but not all, files written by ***WinGX*** programs adhere to the old 8.3 DOS standard.

In ***WinGX 1.80***, the program instruction files, e.g. *PARTS.INS* have been renamed <*PROGRAM*>.*INPUT* to avoid confusion with SHELX style .INS files. On starting in a new directory, ***WinGX 1.80*** will check whether such files are present with their old names , and if so they will be automatically renamed.

System files *name.XXX*. A large number of these files are written by ***WinGX*** system programs.

```
 NAME         DESCRIPTION
name.bak --  backup version of name.INS
name.bin --  binary data files written by SIR92 or PLATON (incompatible!)
name.cif --  refinement details in CIF format from SHELXL
name.dat --  raw CAD4 diffractometer file
name.eld --  PLATON/PLUTON style input file with coordinate errors
name.fcf --  CIF listing of Fo vs Fc (or Fo2 vs Fc2) from SHELXL
name.hkl --  principal SHELX reflection file
name.lis --  Text list file from PLATON
name.lpr --  PostScript list file from PLATON
name.ins --  principal model file - input for SHELX  programs
name.omx --  orientation matrix from XCAD4 (also CAD4.matrix)
name.out --  edited SHELX model file written by CAMERON
name.p4p --  Siemens data collection summary file
name.p4t --  raw Siemens diffractometer file
name.par --  space group assignment from PLATON
name.plt --  plotfile from SIR92
name.psi --  raw psi-scan data from CAD4 diffractometer
name.ras --  pseudo PDB file for input to RasMol
name.res --  results file for structure solution and SHELXL refinement
name.spf --  PLATON/PLUTON style input file with coordinate errors
name.st  --  reflection file of standards from XCAD4 for STDANAL
name.sup --  supplementary material tables from GEOM, PLATON
name.tb  --  tables from GEOM
name.tex --  Crystal data summary and publication tables from CIF_TABLES
name.unc --  uncorrected reflection file from XCAD4 for STDANAL
name.xpr --  CAD4 Express data collection summary file
```

It is possible to keep a number of reflection files (with different absorption corrections or other forms of processing) in the same directory. The current reflection file is set using the menu item "Set HKL File" under the Refine menu. All reflection files with .HKL extension are assumed to be SHELX formatted reflection files.

```
name.HKL          --  default (usually uncorrected) reflection file
DELABS.HKL        --  abs. corrected reflection file from DIFABS-PLATON
DIFABS.HKL        --  abs. corrected reflection file from DIFABS
GAUSSIAN.HKL      --  abs. corrected reflection file from GAUSSIAN
ANALYTICAL.HKL    --  abs. corrected reflection file from ANALYTICAL
PSIABS.HKL        --  abs. corrected reflection file from PSIABS
SPHERICAL.HKL     --  abs. corrected reflection file from SPHERICAL
CYLINDRICAL.HKL   --  abs. corrected reflection file from CYLINDRICAL
XABS2.HKL         --  abs. corrected reflection file from XABS2
SHELXA.HKL        --  abs. corrected reflection file from SHELXA
CAMEL_JOCKEY.HKL  --  abs. corrected reflection file from CAMEL JOCKEY
MULTISCAN.HKL     --  abs. corrected reflection file from MULTISCAN
NEEDLE.HKL        --  abs. corrected reflection file from NEEDLE
SQUEEZED.HKL      --  output reflection file from SQUEEZE (PLATON)
DENZOX.HKL        --  output from DENZOX processing of KappaCCD data
SORTAV.HKL        --  reflection data processed and merged with SORTAV
```

System CIF files.

```
absorb.cif    -- results from PLATON-based absorption corrections
archive.cif   -- archive CIF of structural analysis from option ARCHIVE CIF
cifdep.cif    -- CIF for direct CCDC deposition from option CCDC CIF
cifdoc.cif    -- CIF for Acta Cryst. C. from option ACTA-C CIF
difabs.cif    -- results from DIFABS absorption correction (CAD4 version)
difrac.cif    -- diffractometer data in CIF format from DIFRAC
dreduc.cif    -- data reduction summary from XCAD4, PROFIT orIMPORT_KAPPACCD
psi_scan.cif -- results from psi-scan absorption correction
sortav.cif    -- data processing with SORTAV
stdanal.cif   -- decomposition correction summary file from STDANAL
struct.cif    -- basic crystal information written by INITIALISE FILES
xabs2.cif     -- results from XABS2 absorption correction
```

Other system files.

```
*.mpf        --  binary direct-access mapfile written by Fourier programs
sft.lst      --  listing of Fc2/Fo2 in condensed format for deposition
                 or publication
program.LST --  listing file written by most programs - may be printed
wingx.log    --  log file of all WinGX operations
CAD4.matrix       --  orientation matrix from XCAD4
standards.data    --  reflection file of standards from XCAD4 for STDANAL
uncorrected.data --  uncorrected reflection file from XCAD4 for STDANAL
```

1.1.3 - Bugs and errors in WinGX

There is no guarantee that the ***WinGX*** system of programs is free of bugs and errors and LJF accepts no responsibility for any problems arising from errors in these programs.

However, if you find any errors/bugs, I will be very pleased to hear from you. Use the Bug Report Form giving as much detail of the problem, with a sample datafile if appropriate. If you have other queries, please do NOT contact the original authors of the programs directly, but contact me by email louis@chem.gla.ac.uk

1.1.4 - Suggested directory structures in *WinGX* and the JOB PATHS option

The ***WinGX*** system makes a number of assumptions about the way that files are organised.

IT IS STRONGLY RECOMMENDED TO RETAIN THE DEFAULT DIRECTORY NAMES FOR WINGX PROGRAMS AND FILES.

WinGX assumes that you have a main STRUCTURE DIRECTORY (say c:\structur or c:\xray etc) and that all structural analyses are carried out in subdirectories of this, given names such as *name1*, *name2* etc which correspond with the names of files within this subdirectory (i.e that the *JobName* and subdirectory name are the same). With this convention you can use the "change working directory" button on the tool-bar to move easily between structures.

The current *Working Directory*, *Reflection File* and *JobName* are always displayed in the status bars of the main WinGX menu window.
It is also possible to use the JOB PATHS option on the FILES menu to change the working directory explicitly. Use MOVE WORKING DIRECTORY to change the *working directory* and *JobName,* or use NEW JOBNAME to retain the same *working directory,* but change the *JobName*. You can use the BROWSE button to select a new *working directory,* and the *JobName* will be taken from the prefix of a file you select. The menu item CREATE NEW DIRECTORY will create a new DOS directory, but the working directory will be unmoved.

1.1.5 - Operation of programs in WinGX package

WinGX consists of a monolithic kernel with an ever increasing number of external (stand-alone) programs. As new programs are included into the ***WinGX*** system, they will be added as external programs, rather than into the kernel.

Users should be aware that all menu options are intended be executed sequentially, i.e. ***WinGX*** is NOT a multitasking program system. This is because many programs will wish to access or write to the same files, and this would result in chaos in a multitasking environment. As each program (*i.e.* menu option) is initiated, a message appears in main menu ACTIVE MODULE status bar, which indicates a program is running. Some programs do not produce output immediately, but this message will tell you that something is going on. As the program finishes, the message changes to "none". Only at this stage is it possible to start up another program.

Many programs in the ***WinGX*** system, e.g. PLATON, SHELXL97, SIR92 and most of the programs in the Graphics menu are launched as external processes. If these external processes are "locked" then WinGX will not return control to the user until the external process has finished execution (either normally or through a run-time error). It is usually necessary to close all Windows associated with this external process to ensure this happens.

1.1.6 - Space group symbols in the *WinGX* system

The short Herman-Mauguin symbols as described in International Tables Vol A. are used. 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* (in ***WinGX*** files directory). 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 Brown and coworkers.

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. For more details of the conventions used for various settings, see here
WinGX uses the Hall symbol internally, since this is an unambiguous indicator of space group type.

1.1.6.1 - Conventions for space group settings in WinGX

```
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
```

1.1.6.2 Concise Space-Group Symbols

Sydney R. Hall & *Ralf W. Grosse-Kunstleve*

The explicit-origin space group notation proposed by Hall (1981) [1], [2] is based on the minimum number of symmetry operations, in the form of Seitz matrices, needed to uniquely define a space group. The concise unambiguous nature of this notation makes it well suited to handling symmetry in computing and database applications.
The notation has the general form:

$$L\ [N_A^T]_1 \ldots [N_A^T]_p\ V$$

where L is the symbol specifying the lattice translational symmetry (see Table 1), N_A^T identifies the 4x4 Seitz matrix of a symmetry element in the minimum set which defines the space-group symmetry (see Tables 2 3, 4, and 5), and *p* is the number of elements in the set. V is a translation vector which shifts the origin of the generator matrices by fractions of the unit cell lengths **a**, **b** and **c**.
The matrix symbol N_A^T is composed of three parts:
N is the symbol denoting the n-fold order of the rotation matrix (see Tables 3 4, and 5)

A is a superscript symbol denoting the axis of rotation
T is a subscript symbol denoting the translation vector (see Table 2)
Table 6 lists space group notation in several formats. The computer-entry representation of the Hall symbols is listed in column 3. The computer-entry format is the general notation expressed as case insensitive ASCII characters, with the overline (bar) symbol replaced by a minus sign. Column 1 of Table 6 contains the space-group number with an appended code which identifies the non-standard settings. Column 2 contains the full Hermann-Mauguin symbols in computer-entry format with appended codes which identify the origin and cell choice when there are alternatives.

The computer-entry format of the Hall notation contains the rotation-order symbol N as positive integers *1, 2, 3, 4,* or *6* for proper rotations and a negative integers *-1, -2, -3, -4* or *-6* for improper rotations. The *T* translation symbols *1, 2, 3, 4, 5, a, b, c, n, u, v, w, d* are described in Table 2. These translations apply additively (e.g. *ad* signifies a (3/4,1/4,1/4)) translation).

The *A* axis symbols *x, y, z* denote rotations about the axes **a**, **b**, **c**, respectively (see Table 3). The axis symbols " and ' signal rotations about the body-diagonal vectors **a+b** (or alternatively **b+c** or **c+a**) and **a-b** (or alternatively **b-c** or **c-a**) (see Table 4). The axis symbol * always refers to a 3-fold rotation along **a+b+c** (see Table 5).

The origin-shift translation vector **V** has the construction (v_a v_b v_c), where v_a, v_b and v_c denote the shifts in 12^{th}s parallel to the cell edges *a*, *b* and *c*, respectively. $v_a/12$, $v_b/12$ and $v_c/12$ are the coordinates of the unshifted origin in the shifted basis system. The shifted Seitz matrices **S**n' are derived from the unshifted matrices **S**n with the transformation

$$\mathbf{S}n' = \begin{pmatrix} 1 & 0 & 0 & va/12 \\ 0 & 1 & 0 & vb/12 \\ 0 & 0 & 1 & vc/12 \\ 0 & 0 & 0 & 1 \end{pmatrix} * \mathbf{S}n * \begin{pmatrix} 1 & 0 & 0 & -va/12 \\ 0 & 1 & 0 & -vb/12 \\ 0 & 0 & 1 & -vc/12 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Default axes
For most Hall symbols the rotation axes applicable to each N are implied and an explicit axis symbol *A* is not needed. The rules for default axis directions are:
the **first** rotation has an axis direction of **c**
the **second** rotation (if N is 2) has an axis direction of
a if preceded by an N of 2 or 4
a+b if preceded by an N of 3 or 6
the **third** rotation (N is always 3) has an axis direction of
a+b+c

Example matrices

Here are several simple examples of how N_A^T symbols expand to Seitz matrices. The notation -2xc represents an improper 2-fold rotation along **a** and a **c/2** translation:

```
          (-1  0  0   0 )
-2xc  =   ( 0  1  0   0 )
          ( 0  0  1  1/2)
          ( 0  0  0   1 )
```

The notation 3^* represents a 3-fold rotation along **a+b+c**:

```
          ( 0  0  1   0 )
3*    =   ( 1  0  0   0 )
          ( 0  1  0   0 )
          ( 0  0  0   1 )
```

The notation *4vw* represents a 4-fold rotation along **c** (implied) and translation of **b/4** and **c/4**:

```
          ( 0 -1  0   0 )
4vw   =   ( 1  0  0  1/4)
          ( 0  0  1  1/4)
          ( 0  0  0   1 )
```

The notation 6_1 2 (0 0 -1) represents a 6_1 screw along **c** and a 2-fold rotation along **a-b**. The translation component 5/6 of the second matrix is the result of the origin shift of **-c/12**:

```
                  ( 1 -1  0   0 )  ( 0 -1  0   0 )
61 2 (0 0 -1) =   ( 1  0  0   0 )  (-1  0  0   0 )
                  ( 0  0  1  1/6)  ( 0  0 -1  5/6)
                  ( 0  0  0   1 )  ( 0  0  0   1 )
```

Table 1. Lattice Symbol L

The lattice symbol L specifies one or more Seitz matrices which are needed to generate the space-group symmetry elements. For noncentrosymmetric lattices the rotation matrices are for *1* (see Table 3). For centrosymmetric lattices the lattice symbols are preceded by a minus sign `-', rotations are *1* and *-1*, and the total number of generator matrices implied by each symbol is twice the number of implied lattice translations.

Non-centrosymmetric symbol	Number of lattice translations	Implied lattice translation(s)
P	1	(0,0,0)
A	2	(0,0,0), (0,1/2,1/2)
B	2	(0,0,0), (1/2,0,1/2)
C	2	(0,0,0), (1/2,1/2,0)
I	2	(0,0,0), (1/2,1/2,1/2)
R	3	(0,0,0), (2/3,1/3,1/3), (1/3,2/3,2/3)
S	3	(0,0,0), (1/3,1/3,2/3), (2/3,2/3,1/3)
T	3	(0,0,0), (1/3,2/3,1/3), (2/3,1/3,2/3)
F	4	(0,0,0), (0,1/2,1/2), (1/2,0,1/2), (1/2,1/2,0)

The unusual lattice symbols S and T are necessary to allow for obverse and reverse settings for all of 3*x*, 3*y*, and 3*z*, respectively. Table 1.1. summarizes the relationsships.

Table 1.1.	**Lattice symbol**		
Unique axis	R	S	T
3*z*	obverse	–	reverse
3*y*	reverse	obverse	–
3*x*	–	reverse	obverse

Table 2. Translation symbol *T*

The symbol T specifies the translation elements of a Seitz matrix. Alphabetical symbols (column 1 below) specify translations along a fixed direction. Numerical symbols (column 3 below) specify translations as a fraction of the rotation order N, and in the direction of the implied or explicitly defined axis.

Translation symbol	**Translation vector**	**Subscript symbol**	**Fractional translation**
a	1/2,0,0	*1* in 3_1	1/3
b	0,1/2,0	*2* in 3_2	2/3
c	0,0,1/2	*1* in 4_1	1/4
n	1/2,1/2,1/2	*3* in 4_3	3/4
u	1/4,0,0	*1* in 6_1	1/6
v	0,1/4,0	*2* in 6_2	1/3
w	0,0,1/4	*4* in 6_4	2/3
d	1/4,1/4,1/4	*5* in 6_5	5/6

Table 3. Rotation matrices for principal axes

The 3x3 matrices for proper rotations along the three principal unit-cell directions. The matrices for improper rotations (*-1*, *-2*, *-3*, *-4* and *-6*) are identical except that the signs are reversed.

Rotation Order:	1	2	3	4	6
Symbol					
Axis *A*					
	(1 0 0)	(1 0 0)	(1 0 0)	(1 0 0)	(1 0 0)
a *x*	(0 1 0)	(0 -1 0)	(0 0 -1)	(0 0 -1)	(0 1 -1)
	(0 0 1)	(0 0 -1)	(0 1 -1)	(0 1 0)	(0 1 0)
	(1 0 0)	(-1 0 0)	(-1 0 1)	(0 0 1)	(0 0 1)
b *y*	(0 1 0)	(0 1 0)	(0 1 0)	(0 1 0)	(0 1 0)
	(0 0 1)	(0 0 -1)	(-1 0 0)	(-1 0 0)	(-1 0 1)
	(1 0 0)	(-1 0 0)	(0 -1 0)	(0 -1 0)	(1 -1 0)
c *z*	(0 1 0)	(0 -1 0)	(1 -1 0)	(1 0 0)	(1 0 0)
	(0 0 1)	(0 0 1)	(0 0 1)	(0 0 1)	(0 0 1)

Table 4. Rotation matrices for face-diagonal axes

The symbols for face-diagonal 2-fold rotations are 2' and 2". The face-diagonal axis direction is determined by the axis of the preceding rotation N^x, N^y or N^z. Note that the single quote symbol ' is the default and may be omitted.

Preceding rotation:	Nx		Ny		Nz	
Notation:	2'	2"	2'	2"	2'	2"
Axis:	**b−c**	**b+c**	**a−c**	**a+c**	**a−b**	**a+b**
	(−1 0 0)	(−1 0 0)	(0 0 −1)	(0 0 1)	(0 −1 0)	(0 1 0)
	(0 0 −1)	(0 0 1)	(0 −1 0)	(0 −1 0)	(−1 0 0)	(1 0 0)
	(0 −1 0)	(0 1 0)	(−1 0 0)	(1 0 0)	(0 0 −1)	(0 0 −1)

Table 5. Rotation matrix for the body-diagonal axis

The symbol for the 3-fold rotation in the **a+b+c** direction is 3^*. Note that for cubic space groups the body-diagonal axis is implied, and the asterisk * may be omitted.

Axis	*Notation*	
		(0 0 1)
a+b+c	3*	(1 0 0)
		(0 1 0)

Table 6. Concise space-group symbols

The codes appended to space-group numbers listed in column 1 of Table 6 identify the relationship of the symmetry elements to the crystal cell. The appended codes are separated from the space-group number by a colon. When a code is omitted the first listed choice applies.

Monoclinic	code =	*<unique axis><cell choice>*
Unique axis choices(+		b −b c −c a −a
Cell choices(+		1 2 3
Orthorhombic	code =	*<origin choice><setting>*
Origin choices		1 2
Setting choices(+		abc ba−c cab −cba bca a−cb
Tetragonal, Cubic	code =	*<origin choice>*
Origin choices		1 2
Trigonal	code =	*<cell choice>*
Cell choices		H (hex) R (rhomb)

(+ cf. IT Vol. A 1983 Table 4.3.1

Number	**Hermann−Mauguin**	**Hall**
1	P 1	P 1
2	P −1	−P 1

3:b	P 1 2 1	P 2y
3:c	P 1 1 2	P 2
3:a	P 2 1 1	P 2x
4:b	P 1 21 1	P 2yb
4:c	P 1 1 21	P 2c
4:a	P 21 1 1	P 2xa
5:b1	C 1 2 1	C 2y
5:b2	A 1 2 1	A 2y
5:b3	I 1 2 1	I 2y
5:c1	A 1 1 2	A 2
5:c2	B 1 1 2	B 2
5:c3	I 1 1 2	I 2
5:a1	B 2 1 1	B 2x
5:a2	C 2 1 1	C 2x
5:a3	I 2 1 1	I 2x
6:b	P 1 m 1	P -2y
6:c	P 1 1 m	P -2
6:a	P m 1 1	P -2x
7:b1	P 1 c 1	P -2yc
7:b2	P 1 n 1	P -2yac
7:b3	P 1 a 1	P -2ya
7:c1	P 1 1 a	P -2a
7:c2	P 1 1 n	P -2ab
7:c3	P 1 1 b	P -2b
7:a1	P b 1 1	P -2xb
7:a2	P n 1 1	P -2xbc
7:a3	P c 1 1	P -2xc
8:b1	C 1 m 1	C -2y
8:b2	A 1 m 1	A -2y
8:b3	I 1 m 1	I -2y
8:c1	A 1 1 m	A -2
8:c2	B 1 1 m	B -2
8:c3	I 1 1 m	I -2
8:a1	B m 1 1	B -2x
8:a2	C m 1 1	C -2x
8:a3	I m 1 1	I -2x
9:b1	C 1 c 1	C -2yc
9:b2	A 1 n 1	A -2yac
9:b3	I 1 a 1	I -2ya
9:-b1	A 1 a 1	A -2ya
9:-b2	C 1 n 1	C -2ybc
9:-b3	I 1 c 1	I -2yc
9:c1	A 1 1 a	A -2a
9:c2	B 1 1 n	B -2bc
9:c3	I 1 1 b	I -2b
9:-c1	B 1 1 b	B -2b
9:-c2	A 1 1 n	A -2ac
9:-c3	I 1 1 a	I -2a
9:a1	B b 1 1	B -2xb
9:a2	C n 1 1	C -2xbc
9:a3	I c 1 1	I -2xc
9:-a1	C c 1 1	C -2xc
9:-a2	B n 1 1	B -2xbc
9:-a3	I b 1 1	I -2xb
10:b	P 1 2/m 1	-P 2y
10:c	P 1 1 2/m	-P 2
10:a	P 2/m 1 1	-P 2x
11:b	P 1 21/m 1	-P 2yb
11:c	P 1 1 21/m	-P 2c
11:a	P 21/m 1 1	-P 2xa
12:b1	C 1 2/m 1	-C 2y
12:b2	A 1 2/m 1	-A 2y
12:b3	I 1 2/m 1	-I 2y
12:c1	A 1 1 2/m	-A 2
12:c2	B 1 1 2/m	-B 2

12:c3	I 1 1 2/m	-I 2
12:a1	B 2/m 1 1	-B 2x
12:a2	C 2/m 1 1	-C 2x
12:a3	I 2/m 1 1	-I 2x
13:b1	P 1 2/c 1	-P 2yc
13:b2	P 1 2/n 1	-P 2yac
13:b3	P 1 2/a 1	-P 2ya
13:c1	P 1 1 2/a	-P 2a
13:c2	P 1 1 2/n	-P 2ab
13:c3	P 1 1 2/b	-P 2b
13:a1	P 2/b 1 1	-P 2xb
13:a2	P 2/n 1 1	-P 2xbc
13:a3	P 2/c 1 1	-P 2xc
14:b1	P 1 21/c 1	-P 2ybc
14:b2	P 1 21/n 1	-P 2yn
14:b3	P 1 21/a 1	-P 2yab
14:c1	P 1 1 21/a	-P 2ac
14:c2	P 1 1 21/n	-P 2n
14:c3	P 1 1 21/b	-P 2bc
14:a1	P 21/b 1 1	-P 2xab
14:a2	P 21/n 1 1	-P 2xn
14:a3	P 21/c 1 1	-P 2xac
15:b1	C 1 2/c 1	-C 2yc
15:b2	A 1 2/n 1	-A 2yac
15:b3	I 1 2/a 1	-I 2ya
15:-b1	A 1 2/a 1	-A 2ya
15:-b2	C 1 2/n 1	-C 2ybc
15:-b3	I 1 2/c 1	-I 2yc
15:c1	A 1 1 2/a	-A 2a
15:c2	B 1 1 2/n	-B 2bc
15:c3	I 1 1 2/b	-I 2b
15:-c1	B 1 1 2/b	-B 2b
15:-c2	A 1 1 2/n	-A 2ac
15:-c3	I 1 1 2/a	-I 2a
15:a1	B 2/b 1 1	-B 2xb
15:a2	C 2/n 1 1	-C 2xbc
15:a3	I 2/c 1 1	-I 2xc
15:-a1	C 2/c 1 1	-C 2xc
15:-a2	B 2/n 1 1	-B 2xbc
15:-a3	I 2/b 1 1	-I 2xb
16	P 2 2 2	P 2 2
17	P 2 2 21	P 2c 2
17:cab	P 21 2 2	P 2a 2a
17:bca	P 2 21 2	P 2 2b
18	P 21 21 2	P 2 2ab
18:cab	P 2 21 21	P 2bc 2
18:bca	P 21 2 21	P 2ac 2ac
19	P 21 21 21	P 2ac 2ab
20	C 2 2 21	C 2c 2
20:cab	A 21 2 2	A 2a 2a
20:bca	B 2 21 2	B 2 2b
21	C 2 2 2	C 2 2
21:cab	A 2 2 2	A 2 2
21:bca	B 2 2 2	B 2 2
22	F 2 2 2	F 2 2
23	I 2 2 2	I 2 2
24	I 21 21 21	I 2b 2c
25	P m m 2	P 2 -2
25:cab	P 2 m m	P -2 2
25:bca	P m 2 m	P -2 -2
26	P m c 21	P 2c -2
26:ba-c	P c m 21	P 2c -2c
26:cab	P 21 m a	P -2a 2a
26:-cba	P 21 a m	P -2 2a
26:bca	P b 21 m	P -2 -2b

26:a-cb	P m 21 b	P -2b -2
27	P c c 2	P 2 -2c
27:cab	P 2 a a	P -2a 2
27:bca	P b 2 b	P -2b -2b
28	P m a 2	P 2 -2a
28:ba-c	P b m 2	P 2 -2b
28:cab	P 2 m b	P -2b 2
28:-cba	P 2 c m	P -2c 2
28:bca	P c 2 m	P -2c -2c
28:a-cb	P m 2 a	P -2a -2a
29	P c a 21	P 2c -2ac
29:ba-c	P b c 21	P 2c -2b
29:cab	P 21 a b	P -2b 2a
29:-cba	P 21 c a	P -2ac 2a
29:bca	P c 21 b	P -2bc -2c
29:a-cb	P b 21 a	P -2a -2ab
30	P n c 2	P 2 -2bc
30:ba-c	P c n 2	P 2 -2ac
30:cab	P 2 n a	P -2ac 2
30:-cba	P 2 a n	P -2ab 2
30:bca	P b 2 n	P -2ab -2ab
30:a-cb	P n 2 b	P -2bc -2bc
31	P m n 21	P 2ac -2
31:ba-c	P n m 21	P 2bc -2bc
31:cab	P 21 m n	P -2ab 2ab
31:-cba	P 21 n m	P -2 2ac
31:bca	P n 21 m	P -2 -2bc
31:a-cb	P m 21 n	P -2ab -2
32	P b a 2	P 2 -2ab
32:cab	P 2 c b	P -2bc 2
32:bca	P c 2 a	P -2ac -2ac
33	P n a 21	P 2c -2n
33:ba-c	P b n 21	P 2c -2ab
33:cab	P 21 n b	P -2bc 2a
33:-cba	P 21 c n	P -2n 2a
33:bca	P c 21 n	P -2n -2ac
33:a-cb	P n 21 a	P -2ac -2n
34	P n n 2	P 2 -2n
34:cab	P 2 n n	P -2n 2
34:bca	P n 2 n	P -2n -2n
35	C m m 2	C 2 -2
35:cab	A 2 m m	A -2 2
35:bca	B m 2 m	B -2 -2
36	C m c 21	C 2c -2
36:ba-c	C c m 21	C 2c -2c
36:cab	A 21 m a	A -2a 2a
36:-cba	A 21 a m	A -2 2a
36:bca	B b 21 m	B -2 -2b
36:a-cb	B m 21 b	B -2b -2
37	C c c 2	C 2 -2c
37:cab	A 2 a a	A -2a 2
37:bca	B b 2 b	B -2b -2b
38	A m m 2	A 2 -2
38:ba-c	B m m 2	B 2 -2
38:cab	B 2 m m	B -2 2
38:-cba	C 2 m m	C -2 2
38:bca	C m 2 m	C -2 -2
38:a-cb	A m 2 m	A -2 -2
39	A b m 2	A 2 -2c
39:ba-c	B m a 2	B 2 -2c
39:cab	B 2 c m	B -2c 2
39:-cba	C 2 m b	C -2b 2
39:bca	C m 2 a	C -2b -2b
39:a-cb	A c 2 m	A -2c -2c
40	A m a 2	A 2 -2a

40:ba-c	B b m 2	B 2 -2b
40:cab	B 2 m b	B -2b 2
40:-cba	C 2 c m	C -2c 2
40:bca	C c 2 m	C -2c -2c
40:a-cb	A m 2 a	A -2a -2a
41	A b a 2	A 2 -2ac
41:ba-c	B b a 2	B 2 -2bc
41:cab	B 2 c b	B -2bc 2
41:-cba	C 2 c b	C -2bc 2
41:bca	C c 2 a	C -2bc -2bc
41:a-cb	A c 2 a	A -2ac -2ac
42	F m m 2	F 2 -2
42:cab	F 2 m m	F -2 2
42:bca	F m 2 m	F -2 -2
43	F d d 2	F 2 -2d
43:cab	F 2 d d	F -2d 2
43:bca	F d 2 d	F -2d -2d
44	I m m 2	I 2 -2
44:cab	I 2 m m	I -2 2
44:bca	I m 2 m	I -2 -2
45	I b a 2	I 2 -2c
45:cab	I 2 c b	I -2a 2
45:bca	I c 2 a	I -2b -2b
46	I m a 2	I 2 -2a
46:ba-c	I b m 2	I 2 -2b
46:cab	I 2 m b	I -2b 2
46:-cba	I 2 c m	I -2c 2
46:bca	I c 2 m	I -2c -2c
46:a-cb	I m 2 a	I -2a -2a
47	P m m m	-P 2 2
48:1	P n n n:1	P 2 2 -1n
48:2	P n n n:2	-P 2ab 2bc
49	P c c m	-P 2 2c
49:cab	P m a a	-P 2a 2
49:bca	P b m b	-P 2b 2b
50:1	P b a n:1	P 2 2 -1ab
50:2	P b a n:2	-P 2ab 2b
50:1cab	P n c b:1	P 2 2 -1bc
50:2cab	P n c b:2	-P 2b 2bc
50:1bca	P c n a:1	P 2 2 -1ac
50:2bca	P c n a:2	-P 2a 2c
51	P m m a	-P 2a 2a
51:ba-c	P m m b	-P 2b 2
51:cab	P b m m	-P 2 2b
51:-cba	P c m m	-P 2c 2c
51:bca	P m c m	-P 2c 2
51:a-cb	P m a m	-P 2 2a
52	P n n a	-P 2a 2bc
52:ba-c	P n n b	-P 2b 2n
52:cab	P b n n	-P 2n 2b
52:-cba	P c n n	-P 2ab 2c
52:bca	P n c n	-P 2ab 2n
52:a-cb	P n a n	-P 2n 2bc
53	P m n a	-P 2ac 2
53:ba-c	P n m b	-P 2bc 2bc
53:cab	P b m n	-P 2ab 2ab
53:-cba	P c n m	-P 2 2ac
53:bca	P n c m	-P 2 2bc
53:a-cb	P m a n	-P 2ab 2
54	P c c a	-P 2a 2ac
54:ba-c	P c c b	-P 2b 2c
54:cab	P b a a	-P 2a 2b
54:-cba	P c a a	-P 2ac 2c
54:bca	P b c b	-P 2bc 2b
54:a-cb	P b a b	-P 2b 2ab

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55         P b a m       -P 2 2ab
55:cab     P m c b       -P 2bc 2
55:bca     P c m a       -P 2ac 2ac
56         P c c n       -P 2ab 2ac
56:cab     P n a a       -P 2ac 2bc
56:bca     P b n b       -P 2bc 2ab
57         P b c m       -P 2c 2b
57:ba-c    P c a m       -P 2c 2ac
57:cab     P m c a       -P 2ac 2a
57:-cba    P m a b       -P 2b 2a
57:bca     P b m a       -P 2a 2ab
57:a-cb    P c m b       -P 2bc 2c
58         P n n m       -P 2 2n
58:cab     P m n n       -P 2n 2
58:bca     P n m n       -P 2n 2n
59:1       P m m n:1      P 2 2ab -1ab
59:2       P m m n:2     -P 2ab 2a
59:1cab    P n m m:1      P 2bc 2 -1bc
59:2cab    P n m m:2     -P 2c 2bc
59:1bca    P m n m:1      P 2ac 2ac -1ac
59:2bca    P m n m:2     -P 2c 2a
60         P b c n       -P 2n 2ab
60:ba-c    P c a n       -P 2n 2c
60:cab     P n c a       -P 2a 2n
60:-cba    P n a b       -P 2bc 2n
60:bca     P b n a       -P 2ac 2b
60:a-cb    P c n b       -P 2b 2ac
61         P b c a       -P 2ac 2ab
61:ba-c    P c a b       -P 2bc 2ac
62         P n m a       -P 2ac 2n
62:ba-c    P m n b       -P 2bc 2a
62:cab     P b n m       -P 2c 2ab
62:-cba    P c m n       -P 2n 2ac
62:bca     P m c n       -P 2n 2a
62:a-cb    P n a m       -P 2c 2n
63         C m c m       -C 2c 2
63:ba-c    C c m m       -C 2c 2c
63:cab     A m m a       -A 2a 2a
63:-cba    A m a m       -A 2 2a
63:bca     B b m m       -B 2 2b
63:a-cb    B m m b       -B 2b 2
64         C m c a       -C 2bc 2
64:ba-c    C c m b       -C 2bc 2bc
64:cab     A b m a       -A 2ac 2ac
64:-cba    A c a m       -A 2 2ac
64:bca     B b c m       -B 2 2bc
64:a-cb    B m a b       -B 2bc 2
65         C m m m       -C 2 2
65:cab     A m m m       -A 2 2
65:bca     B m m m       -B 2 2
66         C c c m       -C 2 2c
66:cab     A m a a       -A 2a 2
66:bca     B b m b       -B 2b 2b
67         C m m a       -C 2b 2
67:ba-c    C m m b       -C 2b 2b
67:cab     A b m m       -A 2c 2c
67:-cba    A c m m       -A 2 2c
67:bca     B m c m       -B 2 2c
67:a-cb    B m a m       -B 2c 2
68:1       C c c a:1      C 2 2 -1bc
68:2       C c c a:2     -C 2b 2bc
68:1ba-c   C c c b:1      C 2 2 -1bc
68:2ba-c   C c c b:2     -C 2b 2c
68:1cab    A b a a:1      A 2 2 -1ac
68:2cab    A b a a:2     -A 2a 2c
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 68:1-cba  A c a a:1      A 2 2 -1ac
 68:2-cba  A c a a:2     -A 2ac 2c
 68:1bca   B b c b:1      B 2 2 -1bc
 68:2bca   B b c b:2     -B 2bc 2b
 68:1a-cb  B b a b:1      B 2 2 -1bc
 68:2a-cb  B b a b:2     -B 2b 2bc
 69        F m m m       -F 2 2
 70:1      F d d d:1      F 2 2 -1d
 70:2      F d d d:2     -F 2uv 2vw
 71        I m m m       -I 2 2
 72        I b a m       -I 2 2c
 72:cab    I m c b       -I 2a 2
 72:bca    I c m a       -I 2b 2b
 73        I b c a       -I 2b 2c
 73:ba-c   I c a b       -I 2a 2b
 74        I m m a       -I 2b 2
 74:ba-c   I m m b       -I 2a 2a
 74:cab    I b m m       -I 2c 2c
 74:-cba   I c m m       -I 2 2b
 74:bca    I m c m       -I 2 2a
 74:a-cb   I m a m       -I 2c 2
 75        P 4            P 4
 76        P 41           P 4w
 77        P 42           P 4c
 78        P 43           P 4cw
 79        I 4            I 4
 80        I 41           I 4bw
 81        P -4           P -4
 82        I -4           I -4
 83        P 4/m         -P 4
 84        P 42/m        -P 4c
 85:1      P 4/n:1        P 4ab -1ab
 85:2      P 4/n:2       -P 4a
 86:1      P 42/n:1       P 4n -1n
 86:2      P 42/n:2      -P 4bc
 87        I 4/m         -I 4
 88:1      I 41/a:1       I 4bw -1bw
 88:2      I 41/a:2      -I 4ad
 89        P 4 2 2        P 4 2
 90        P 42 1 2       P 4ab 2ab
 91        P 41 2 2       P 4w 2c
 92        P 41 21 2      P 4abw 2nw
 93        P 42 2 2       P 4c 2
 94        P 42 21 2      P 4n 2n
 95        P 43 2 2       P 4cw 2c
 96        P 43 21 2      P 4nw 2abw
 97        I 4 2 2        I 4 2
 98        I 41 2 2       I 4bw 2bw
 99        P 4 m m        P 4 -2
100        P 4 b m        P 4 -2ab
101        P 42 c m       P 4c -2c
102        P 42 n m       P 4n -2n
103        P 4 c c        P 4 -2c
104        P 4 n c        P 4 -2n
105        P 42 m c       P 4c -2
106        P 42 b c       P 4c -2ab
107        I 4 m m        I 4 -2
108        I 4 c m        I 4 -2c
109        I 41 m d       I 4bw -2
110        I 41 c d       I 4bw -2c
111        P -4 2 m       P -4 2
112        P -4 2 c       P -4 2c
113        P -4 21 m      P -4 2ab
114        P -4 21 c      P -4 2n
115        P -4 m 2       P -4 -2
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116	P -4 c 2	P -4 -2c
117	P -4 b 2	P -4 -2ab
118	P -4 n 2	P -4 -2n
119	I -4 m 2	I -4 -2
120	I -4 c 2	I -4 -2c
121	I -4 2 m	I -4 2
122	I -4 2 d	I -4 2bw
123	P 4/m m m	-P 4 2
124	P 4/m c c	-P 4 2c
125:1	P 4/n b m:1	P 4 2 -1ab
125:2	P 4/n b m:2	-P 4a 2b
126:1	P 4/n n c:1	P 4 2 -1n
126:2	P 4/n n c:2	-P 4a 2bc
127	P 4/m b m	-P 4 2ab
128	P 4/m n c	-P 4 2n
129:1	P 4/n m m:1	P 4ab 2ab -1ab
129:2	P 4/n m m:2	-P 4a 2a
130:1	P 4/n c c:1	P 4ab 2n -1ab
130:2	P 4/n c c:2	-P 4a 2ac
131	P 42/m m c	-P 4c 2
132	P 42/m c m	-P 4c 2c
133:1	P 42/n b c:1	P 4n 2c -1n
133:2	P 42/n b c:2	-P 4ac 2b
134:1	P 42/n n m:1	P 4n 2 -1n
134:2	P 42/n n m:2	-P 4ac 2bc
135	P 42/m b c	-P 4c 2ab
136	P 42/m n m	-P 4n 2n
137:1	P 42/n m c:1	P 4n 2n -1n
137:2	P 42/n m c:2	-P 4ac 2a
138:1	P 42/n c m:1	P 4n 2ab -1n
138:2	P 42/n c m:2	-P 4ac 2ac
139	I 4/m m m	-I 4 2
140	I 4/m c m	-I 4 2c
141:1	I 41/a m d:1	I 4bw 2bw -1bw
141:2	I 41/a m d:2	-I 4bd 2
142:1	I 41/a c d:1	I 4bw 2aw -1bw
142:2	I 41/a c d:2	-I 4bd 2c
143	P 3	P 3
144	P 31	P 31
145	P 32	P 32
146:H	R 3:H	R 3
146:R	R 3:R	P 3*
147	P -3	-P 3
148:H	R -3:H	-R 3
148:R	R -3:R	-P 3*
149	P 3 1 2	P 3 2
150	P 3 2 1	P 3 2"
151	P 31 1 2	P 31 2c (0 0 1)
152	P 31 2 1	P 31 2"
153	P 32 1 2	P 32 2c (0 0 -1)
154	P 32 2 1	P 32 2"
155:H	R 32:H	R 3 2"
155:R	R 32:R	P 3* 2
156	P 3 m 1	P 3 -2"
157	P 3 1 m	P 3 -2
158	P 3 c 1	P 3 -2"c
159	P 3 1 c	P 3 -2c
160:H	R 3 m:H	R 3 -2"
160:R	R 3 m:R	P 3* -2
161:H	R 3 c:H	R 3 -2"c
161:R	R 3 c:R	P 3* -2n
162	P -3 1 m	-P 3 2
163	P -3 1 c	-P 3 2c
164	P -3 m 1	-P 3 2"
165	P -3 c 1	-P 3 2"c

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166:H      R -3 m:H      -R 3 2"
166:R      R -3 m:R      -P 3* 2
167:H      R -3 c:H      -R 3 2"c
167:R      R -3 c:R      -P 3* 2n
168        P 6            P 6
169        P 61           P 61
170        P 65           P 65
171        P 62           P 62
172        P 64           P 64
173        P 63           P 6c
174        P -6           P -6
175        P 6/m         -P 6
176        P 63/m        -P 6c
177        P 6 2 2        P 6 2
178        P 61 2 2       P 61 2 (0 0 -1)
179        P 65 2 2       P 65 2 (0 0 1)
180        P 62 2 2       P 62 2c (0 0 1)
181        P 64 2 2       P 64 2c (0 0 -1)
182        P 63 2 2       P 6c 2c
183        P 6 m m        P 6 -2
184        P 6 c c        P 6 -2c
185        P 63 c m       P 6c -2
186        P 63 m c       P 6c -2c
187        P -6 m 2       P -6 2
188        P -6 c 2       P -6c 2
189        P -6 2 m       P -6 -2
190        P -6 2 c       P -6c -2c
191        P 6/m m m     -P 6 2
192        P 6/m c c     -P 6 2c
193        P 63/m c m    -P 6c 2
194        P 63/m m c    -P 6c 2c
195        P 2 3          P 2 2 3
196        F 2 3          F 2 2 3
197        I 2 3          I 2 2 3
198        P 21 3         P 2ac 2ab 3
199        I 21 3         I 2b 2c 3
200        P m -3        -P 2 2 3
201:1      P n -3:1       P 2 2 3 -1n
201:2      P n -3:2      -P 2ab 2bc 3
202        F m -3        -F 2 2 3
203:1      F d -3:1       F 2 2 3 -1d
203:2      F d -3:2      -F 2uv 2vw 3
204        I m -3        -I 2 2 3
205        P a -3        -P 2ac 2ab 3
206        I a -3        -I 2b 2c 3
207        P 4 3 2        P 4 2 3
208        P 42 3 2       P 4n 2 3
209        F 4 3 2        F 4 2 3
210        F 41 3 2       F 4d 2 3
211        I 4 3 2        I 4 2 3
212        P 43 3 2       P 4acd 2ab 3
213        P 41 3 2       P 4bd 2ab 3
214        I 41 3 2       I 4bd 2c 3
215        P -4 3 m       P -4 2 3
216        F -4 3 m       F -4 2 3
217        I -4 3 m       I -4 2 3
218        P -4 3 n       P -4n 2 3
219        F -4 3 c       F -4c 2 3
220        I -4 3 d       I -4bd 2c 3
221        P m -3 m      -P 4 2 3
222:1      P n -3 n:1     P 4 2 3 -1n
222:2      P n -3 n:2    -P 4a 2bc 3
223        P m -3 n      -P 4n 2 3
224:1      P n -3 m:1     P 4n 2 3 -1n
224:2      P n -3 m:2    -P 4bc 2bc 3
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225        F m -3 m      -F 4 2 3
226        F m -3 c      -F 4c 2 3
227:1      F d -3 m:1     F 4d 2 3 -1d
227:2      F d -3 m:2    -F 4vw 2vw 3
228:1      F d -3 c:1     F 4d 2 3 -1cd
228:2      F d -3 c:2    -F 4cvw 2vw 3
229        I m -3 m      -I 4 2 3
230        I a -3 d      -I 4bd 2c 3
```

References

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[2] International Tables Volume B 1994, Section 1.4. *Symmetry in reciprocal space*

1.1.6 - The TextServer

The new version of *WinGX* uses a separate program call the TextServer (executable wgxTextServer.exe) which is started automatically when *WinGX* is started, and is closed automatically when it finishes. Almost all the programs in the WinGX package now use this utility program for displaying text output. The visible Window is identical to those produced in previous versions of WinGX, the only difference is that only ONE text Window is present and all text is directed to this Window. The visible Window may be dismissed at any time - this does not stop the TextServer program. When any program requires text to be displayed, a new instance of a text Window will be opened.

On the File menu, there are options to check whether the TextServer is running (Message Text Server), to start it up again if it has been closed (this should never be needed) and to close it down (again, this should never be needed).

1.1.7 - References for programs and algorithms in the WinGX system

The WinGX system is provided free of charge, but has involved a great deal of work. Please acknowledge the WinGX system (as well as individual programs) in any publication for which this program was used.

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Individual program references (also available from the REFERENCES menu item)

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