technical memorandum

Daresbury Laborator

DL/SCI/TM83T

A SYMMETRY ANALYSIS PACKAGE FOR CRYSTALS, POLYMERS, SLABS AND MOLECULES

by

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DECEMBER, 1991

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ISSN 0144-5677

$ 1 Introduction

In many studies of material properties one requires a detailed understanding of underlying structure. In the literature structural information is usually presented in a compact form consisting of a material's symmetry properties and the fractional coordinates of constituent atoms. We report the development of a prototype computer package **SYM** which performs the following tasks.

1. **Analysis** of symmetry and coordinate information. For instance an entry in the Inorganic Crystal Structures Database [1] may be used as input.
2. **Structural editing** with retention of symmetry information.
3. The **graphical display** of resulting structural data.

As no clear standard for high performance 3D graphics or has yet emerged the current philosophy of **SYM** allows it to be driven via a very simple *user interface* with loose coupling to the graphical back-end via disk-files or UNIX sockets. Support for a variety of graphics systems is thus easily provided; in particular DISPLAY [5] AVS [3] and Explorer [2] are currently supported. The **SYM** package was originally developed to provide symmetry analysis within CRYSTAL [4] and thus all developments of **SYM** are consistent with CRYSTAL.

$ 1.1 Using SYM — A simple example

Before discussing in detail the functionality and usage of **SYM** we present a simple example; the surface reconstruction of the 100 surface of silicon and the subsequent adsorption of a chlorine overlayer. The input lines used to define bulk silicon are listed below.

```
1)      Crystalline Silicon - The Diamond Structure
2)      3  1 0
2a)     80 1
3)      0
4)      0 0 0
5)      227
6)      5.42
7)      1
8)      14  .125  .125   .125
9)      END
```


Let us examine this input line by line;

1. A **title** — any text string
2. The **3** simply states that the system to be defined is three dimensional. The **1** that an information (**INF**) parameter is to be defined; in LINE 2a the 80th parameter (INF(80)) is set equal to 1. The **0**, on line 2, states that no print control parameters are to be defined and thus a LINE 2b is not present.
3. A "dummy" line retained only for consistency with CRYSTAL
4. Some further control parameters — unimportant for now.
5. The 3D space group is number 227 in the international tables. This is the group containing all the operations of the face centred cubic bravais lattice and inversion.
6. a=5.42 Angstrom — the lattice parameter
7. **1** — there is one unique atom in the unit cell
8. **14 .125 etc . . .** – simply the atomic number and fractional coordinates of the atoms in the unit cell
9. END — the end

The above input file is read by SYM from standard input (FORTRAN stream 5) — analysis of the data is written to standard output (FORTRAN stream 6) and a **plot-file** suitable for one of the graphical back-ends is produced. Although SYM may be run "by hand" in this way it is usually used from within a graphical package. For instance, within DISPLAY (which runs only on SGI and IBM workstations) one simply uses the **EDIT STRUCTURE**, **ANALYSE (NEW)** and **ANALYSE (REPLACE)** items on the **SYM** menu and graphical display of structures is automatic. By default the display of the silicon structure we have created will be a simple **ball & stick** representation of the two silicon atoms in the unit cell and a line representation of the cell. Extending the structure using the unit-cell information can usually be handled by the graphics back-end but may also be performed within **SYM**.

To make a **SLAB** representation of the Si(100) surface we add the following lines before the **END** statement.

```
SLAB
1)   1 0 0
2)   2 4
```

where the **SLAB** keyword is followed by two lines of data which are interpreted as follows;

1. **1 0 0** – the Miller indices (h,k,l) of the surface to be cut
2. **2 4** – of the two possible terminations of the Si(100) surface the second is chosen and we request a slab of **4** atomic layers.

Working within DISPLAY one now saves the edited input file to disk and chooses **ANALYSE (REPLACE)**; the analysis is reported to the terminal and the displayed structure is automatically updated to a single 2-dimensional unit cell.

To form the well known 2x1 reconstruction of the Si(100) surface and to adsorb a monolayer of Cl atoms one adds the following cards to the input file.

```
SUPERCELL
2 0 0 1
ATOMDISP
2
1  -0.74  0.    -0.22
2  +0.74  0.    -0.22
ATOMINSE
2
17   0.72    0.00   4.03
17  -2.633    0.00   4.03
```

Perhaps the reader can follow the effects of these lines without too much assistance. **SUPERCELL**, accepts N^2 integers (where N is the dimensionality — which for the SLAB is 2) which define a super-cell structure in terms of the current unit cell. Here a 2x1 cell is formed. To displace two surface atoms one uses **ATOMDISP**; the following lines are firstly the number of atoms to be displaced and then the "atom number" and displacements in Angstrom for the two surface atoms. Each inequivalent atom is assigned a number which may be determined by examination of the analysis sent to the terminal. The displacements given form the well known dimers observed on this surface. Finally **ATOMINSE** is used to insert two extra surface atoms (atomic number 17 => chlorine) which are repeated within the supercell to create a surface adsorbed monolayer.

Other operations which may be applied to a structure include *elastic distortions* and *atom removal*. It is also possible to request symmetry information for the environment of individual atoms and to extract *clusters* from a periodic sample using a simple seed-point and radii algorithm.

We hope that the above discussion gives a "flavour" of what SYM is about and how it works. The particular example was chosen to appeal to a surface scientist

but **SYM** may also be used in molecular, polymeric and bulk crystalline systems. The next section is a more complete guide to the input and functionality of **SYM**.

$ 2 SYM – A User Manual

The structure of the input file is now described in detail. The input lines are grouped according to their function; *general information*, *structural definition* and *structural editing* and a table is devoted to explaining each. Each table contains a list of data lines, the variables specified on the line and some comments or suggestions. The second column of each table contains the input format. Unless otherwise stated all variables are read in free format and the notation used it FORTRAN-like, A for characters, I for integers and F for floating point variables.

$ 2.1 General Information lines

General information consists of a title for labelling purposes (this is passed to the graphical back-end) and some parameters which may be used to control the operation of SYM.

Table 1 The general information lines

LINE	FORMAT	VARIABLE	MEANING AND/OR SUGGESTED VALUES
1	20A4	TITLE	Any String of 80 Characters
2	3I	IDIM	"dimensionality of the system"
			0 molecules
			1 polymers
			2 slabs
			3 crystals
		NUMINF	number of information parameters to be defined
		NUMPRT	number of printing options to be switched on
	— if NUMINF > 0 —		
2a	(2xNUMINF)I	I, INF(I)	Numbered INF parameters and their new values (see Appendix A)
	— if NUMPRT > 0 —		
2b	(2xNUMPRT)I	I, LPR(I)	Numbered LPR parameters and their new values (see Appendix B)
3		Dummy	Line merely for consistency with CRYSTAL

$ 2.2 Structural Definition

These lines are used to provide an initial structure for SYM, the situation is slightly different for the 3D crystal case and this is explained separately in table 3.

Table 2 A structural definition for molecules, polymers and slabs

LINE	FORMAT	VARIABLE	MEANING AND/OR SUGGESTED VALUES
1	I	IGROUP	point or space group of the system (see Appendix C)
2	3F	A, B, γ	minimal set of cell parameters in Angstrom and degrees.
			molecules : *This line is absent*
			polymers . only A is required
			slabs : rectangular lattices require A and B; for square or hexagonal lattices only A is required
3	I	NATIR	number of symmetry unique atoms
4	I, 3F	NAT, X, Y, Z	Atomic number and coordinates of the independant atoms
			molecules & polymers: X,Y,Z in Angstrom
			slabs: X,Y in fractional units, Z in Angstrom

Table 3 A structural definition for 3D crystals

LINE	FORMAT	VARIABLE	MEANING AND/OR SUGGESTED VALUES
1	3I	IFLAGS	IFLAGS=0 : the space-group will be identified by its sequence number (1-230) in the "International Tables for X-ray Crystallography" (ITXC, Appendix C)
			IFLAGS=1 ; the space group will be identified using Hermann-Mauguin notation
		IFHR	hexagonal (IFHR=0) or rhombohedral (IFHR=1) cell definition in rhombohedral systems.
		IFSO	setting of the origin
			IFSO=0 ; origin derived from space group symbol (second setting in ITXC)
			IFSO=1 : standard shift of the origin (first setting in ITXC)
			IFSO > 1 non standard (user defined) shift or the origin
2	I or 16A1	IGROUP or AGROUP	space group as a sequence number or Hermann-Mauguin symbol
	— if IFSO > 1 —		
2a	3I	IX, IY, IZ	non standard shift of the origin in fractional units multiplied by 24
3	6F	A,B,C α, β, γ	minimal set of cell parameters in Angstrom and degrees (lengths before angles)

Table 3 (Continued) A structural definition for 3D crystals

			cubic : A hexagonal : A,C rhombohedral : A,α (rhombohedral cell) or A, C (hexagonal cell) tetragonal: A,C orthorhombic A, B, C monoclinic A, B, C, β (B unique) A, B, C, γ (C unique) A, B, C, α (A unique - non standard) triclinic A,B,C, α, β, γ
4	I	NATIR	number of symmetry unique atoms
5	I, 3F	NAT, X, Y, Z	Atomic number and fractional coordinates of the independant atoms

$ 2.3 Structural Editing

Setting INF (80) > 0 activates the structural editing features of SYM. Each option is used via a keyword and a few lines of control information.

The input lines for the structural editing must be supplied **after** the **structural information** lines (tables 2 and 3). In Table 4 the keywords and their function are summarizesd.

Table 4 The keywords which drive the structural editing package

KEYWORD	MEANING
ATOMSUBS	to substitute atoms of the system
ATOMINSE	to add atoms
ATOMREMO	to remove atoms
ATOMDISP	to displace atoms
SUPERCEL	to create a 3D, 2D or 1D supercell
ELASTIC	to perform elastic distortions
ROTATE	to define a 3D unit cell orthogonal to a selected crystallographic plane (hkl)
SLAB	to cut a slab with the surface layer with indices (hkl), and containing NLAYER atomic layers
ATOMSYMM	to find the point group of each atomic position and the sets of symmetry related atoms
STOP	to stop the program
END	the last line of the editing directives must be an END card.

Notes on Table 4

Note 1. Different sequences of editing directives can be provided (see examples in chapter 3).

Note 2. When a perturbation is created in the system by the options ATOMSUBS, ATOMINSE and ATOMDISP, the point symmetry of the system is usually lower than the original symmetry. The sub-group of the original group is automatically derived by the program. It is however possible to force the system to keep the original symmetry setting INF(87)>0; as a result the perturbation will be propagated under the symmetry of the original point group (see comments below).

Note 3. The input coordinates for the ATOMDISP and/or ATOMINSE directives are, by default, in Angstrom. However, they can be input in fractional units by setting INF(72)>0. This applies only to x and y, in a 2D system; z remains in Angstrom. For the polymer case x is in fractional units, y and z in Angstrom.

Note 4. Remember that INF parameters are set using NUMINF and line 2a) of the general input (section 2.1) .

Table 5 Using the editing directives

CARD	FORMAT	VARIABLE	MEANING AND/OR SUGGESTED VALUES
1	A8	ROTATE	keyword (first column!)
2	3I	h k l	crystallographic indices of the basal plane of the new 3D unit cell
1	A8	SLAB	keyword (first column!)
2	3I	h k l	crystallographic indices of the plane parallel to the surface
3	2I	ISUP	Label of the surface atomic layer
		NLAYER	Number of atomic layers in the slab
1	A8	SUPERCEL	keyword
2	LDIM*LDIM	F	elements of the expansion matrix (LDIM are the dimensions of the system)
1	A8	ATOMSUBS	keyword
2	I	NSOST	number of atoms to be substituted
3	2I	LAB,NAT	label of the atom to substitute, atomic number of the new atom
to			
NSCOST + 3			
1	A8	ATOMINSE	keyword

Table 5 (Continued) Using the editing directives

2	I	NINS	number of atoms to be added
3	I,3F	NAT,X,Y,Z	atomic number and coordinates of the added atom (see note 3 above)
NINS + 3			
1	A8	ATOMREMO	keyword
2	I	NLACUN	number of atoms to be removed
3	NLACUN I	LACUNE (L)	label of the atoms to be eliminated
1	A8	ATOMDISP	keyword
2	I	NDISP	number of atoms to be displaced
3	I, 3F	LAB, DX, DY,DZ	label and increments of the coordinates of the atom to be displaced (see note 3 above)
to			
NDISPL+3			
1	A8	ELASTIC	keyword
2	I	IDEF	1 - equation (1) Appendix D
			2 - equation (2) Appendix D
3	3F	DELTX (1,I)	first row of the (or E) matrix
4	3F	DELTX (2,I)	second row of the matrix
5	3F	DELTX (3,I)	third row of the matrix
1	A8	ATOMSYMM	keyword
			no additional input is required

Notes on Table 5

ROTATE A unit cell is selected with two faces perpendicular to the (hkl) plane (the indices refer to the Bravais lattice of the crystal; the hexagonal lattice is used for the rhombohedral system). The atoms of the unit cell are grouped in sets (atomic layers), according to their z coordinate in the new cartesian frame, with x and y lying in the (hkl) plane. The terminal output lists the atoms of the unit cell in the new Cartesian frame, grouped in layers.

SLAB A unit cell is selected with two faces perpendicular to the (hkl) plane. The atoms are grouped in sets according to their z coordinate. ISUP is the label of the surface atomic layer. NLAYER other layers are stacked below the surface one (lower z coordinate). The final set of atoms belonging to the two dimensional unit cell is printed. The two sided plane group is selected from the 3D symmetry

group of the original crystal structure: the origin is shifted so as to maximize the order of the plane group.

SUPERCELL A supercell is created; the "expansion" is given in input as the elements of a matrix which, applied to the matrix of the translation vectors, defines the new translation matrix. The subgroup of the original symmetry group is defined (all the operators which have a non null translational component are eliminated).

ATOMSUBS, ATOMINSE, ATOMREMO, ATOMDISP With these options it is possible respectively: to substitute the atoms of the system, to insert new atoms, to remove or to display some atoms of the system; the new symmetry group is selected automatically (see INF(87) below). The coordinates are supposed to be in Angstrom; if INF(72)=1 the input coordinates are supposed to be in fractional units.

INF(87)=1 In this case it is possible to generate a perturbation in the system keeping the original symmetry group; as a consequence new atoms are added in all the positions having the same symmetry (for example if one atom is added on the top of a surface, another one will be generated on the other surface, if the symmetry includes a xy symmetry plane) and to substitute or to displace all the atoms belonging to the same set (for example in a slab with two symmetry related atomic layers, the displacement of the atoms of the first is automatically applied to the others).

$ 3 Further Examples

In the following table the lines are labelled to indicate their function; those with label G belong to the general information set (section 2.1). The cards with label T are for structural definition (section 2.2). Sets of lines labelled A to D belong to the editing directives (Table 5).

Example 1 :

A three layer slab of magnesium oxide is created perpendicular to the 001 face. A supercell containing four 2D cells (8 atoms per layer) is then formed. Into this supercell we place a CO molecule above an oxygen atom on each surface of the slab producing a 1:4 CO to surface oxygen ratio. Finally the oxygen atom beneath CO and its first neighbours are allowed to relax; note that only one atom of the star is displaced because the INF(87)=1 option forces the preservation of the point group symmetry which transfers the same displacement to the other atoms of the star.

Table 6 The adsorption of CO molecules on an MgO surface

LINE			COMMENT
1 G	ANALYSIS OF (001) MGO	:	title
2 G	3 3 0	:	IDIM=3 NUMINF=3 NUMPRT=0
3 G	80 1 87 1 72 1	:	INF(80)=1, INF(87)=1
			INF(72)=1 (input in fractionary units)
4 G	5 5 5 5 10	:	tolerances
1 T	0 0 0	:	geometry input
2 T	225	:	space group
3 T	4.21	:	lattice parameter
4 T	2	:	number of atoms
5 T	12 .0 .0 .0	:	atomic number and coordinates
6 T	8 .5 .5 .5	:	
1 A	SLAB	:	keyword
2 A	0 0 1	:	indices of the plane
3 A	1 3	:	ISUP=1, NLAYER=3
1 B	SUPERCEL	:	keyword
2 B	2. 0. 0. 2.	:	expansion matrix
1 C	ATOMINSE	:	keyword

Table 6 (Continued) The adsorption of CO molecules on an MgO surface

LINE			COMMENT
2 C	2	:	NINS=2
3 C	6 0.0 0.0 5.0	:	atomic number and coordinates
4 C	8 0.0 0.0 6.124	:	
1 D	ATOMDISP	:	keyword
2 D	2	:	NDISP=2
3 D	1 -0.01 -0.01 0.1	:	label and increments (frac. units)
4 D	5 0.0 0.0 0.1	:	
1 E	END	:	keyword

Notes on Table 6

Note INF(80)=1 activates the structural editing directives

Note INF(72)=1 the ATOMINSE and ATOMDISP x and y input coordinates are in fractional units

Note INF(87)=1 in the ATOMINSE and ATOMDISP input lines only the coordinates of one atom of a star of symmetry related atoms must be provided, the others are generated by symmetry.

$ 4 Future Developments

The SYM package described in this document has been developed over the past twelve months and will continue to be improved. In the (near) future the following features will be provided

1. A menu driven interface to prepare the input file for SYM and thus avoid the use of directive driven input lines
2. A feedback loop from the 3D graphics to the structural editor enabling the movement and insertion of atoms etc. to be performed with "point-and-click" operations
3. Interfaces to existing structural definition formats used by, for instance, BIODESIGN and BIOSYM

SYM is currently available only on ARCG workstations at Daresbury Laboratory but (subject to details) will be released into the public domain in the (near) future. Tactfully phrased comments and suggestions are most welcome.

Acknowledgments

This work was carried out in the Theory and Computational Science division at Daresbury Laboratory with financial assistance from ICI plc.

Appendix A Information Parameters

About 150 INF parameters may be defined – fortunately the average user will only have call to use the subset in table 7

Table 7 Information parameters

Parameter	Usage
34	cluster creation
36	calculate the special positions in the unit cell
80	activate structural editing options

Appendix B Print Control Parameters

Table 8 print control parameters

Parameter (=N)	Action
1	N stars of direct lattice vectors
2	crystal symmetry operations
3	print special positions (if INF(36) > 0)

Appendix C Group Symmetries used by SYM

The Point Groups

The center of symmetry is supposed to be at the origin; for the rotation groups the principle axis is assumed to be z.

IGROUP	Hermann-Mauguin	Schoenflies
1	1	C_1
2	-1	C_i
3	2 (x)	C_2 (x)
4	2 (y)	C_2 (y)
5	2 (z)	C_2 (z)
6	m (x)	C_s (x)
7	m (y)	C_s (y)
8	m (z)	C_s (z)
9	2/m (x)	C_{2h} (x)
10	2/m (y)	C_{2h} (y)
11	2/m (z)	C_{2h} (z)
12	222	D_2
13	2mm	C_{2v} (x)
14	m2m	C_{2v} (y)
15	mm2	C_{2v} (z)
16	mmm	D_{2h}
17	4	C_4
18	-4	S_4
19	4/m	C_{4h}
20	422	D_4
21	4mm	C_{4v}
22	-42m	D_{2d} (d planes along x+y and x-y)
23	-4m2	D_{2d} (d planes along x and y)
24	4/mmm	D_{4h}
25	3	C_3
26	-3	C_{3i}
27	321	D_3 (one C_2 axis along y)

28	312	D_3 (one C_2 axis along x)
29	3m1	C_{3v} (one v plane along x)
30	31m	C_{3v} (one v plane along y)
31	-3m1	D_{3d} (one d plane along x)
32	-31m	D_{3d} (one d plane along y)
33	6	C_6
34	-6	C_{3h}
35	6/m	C_{6h}
36	622	D_6
37	6mm	C_{6v}
38	-6m2	D_{3h} (one C_2 axis along x)
39	-62m	D_{3h} (one C_2 axis along y)
40	6/mmm	D_{6h}
41	23	T
42	m-3	T_h
43	432	O
44	-43m	T_d
45	m-3m	O_h

The line Groups

Labels of the line groups for describing polymeric systems. The available line groups are a subset of the 230 space groups; the operators are generated by the routines for the space groups (principal axis z) and then rotated by 90° through y, so as to have the polymer axis along x (CRYSTAL convention).

In the table, the first column gives the label to be used in the INPUT card for identifying the line group (IGROUP variable) . The second column gives the "polymer" symbol, for which we use the following convention: x is the first symmetry direction, y the second. The third column gives the Schoenflies symbol. The fourth column gives the Hermann-Mauguin symbol (generally the short one; the full symbol is adopted when the same short symbol could refer to different settings) of the corresponding space group (principal axis z). For both "polymer" and H.M. group names, symbols like -3 stand for $\bar{3}$. The fifth column gives the number of the corresponding space group, according to the ITXC; this number is written in parentheses when the orientation of the symmetry operators does not correspond to the first setting in the ITXC.

IGROUP	"Polymer" symbol (x direction)	Schoenflies	Hermann Mauguin (z direction)	Number of space group
1	P 1	C_1 -1	P 1	1
2	P -1	C_i -1	P -1	2
3	P 2 1 1	C_2 -1	P 1 1 2	(3)
4	P 2_1 1 1	C_2 -2	P 1 1 2_1	(4)
5	P 1 2 1	C_s -1	P 1 2 1	(3)
6	P 1 1 2	C_s -1	P 2 1 1	(3)
7	P m 1 1	C_s -1	P 1 1 m	(6)
8	P 1 m 1	C_s -1	P 1 m 1	(6)
9	P 1 a 1	C_s -2	P 1 c 1	(7)
10	P 1 1 m	C_s -1	P m 1 1	(6)
11	P 1 1 a	C_s -2	P c 1 1	(7)
12	P 2/m 1 1	C_{2h} -1	P 1 1 2/m	(10)
13	P 2_1/m 1 1	C_{2h} -2	P 1 1 2_1/m	(11)
14	P 1 2/m 1	C_{2h} -1	P 1 2/m 1	(10)
15	P 1 2/a 1	C_{2h} -4	P 1 2/c 1	(13)
16	P 1 1 2/m	C_{2h} -1	P 2/m 1 1	(10)
17	P 1 1 2/a	C_{2h} -4	P 2/c 1 1	(13)
18	P 2 2 2	D_2 -2	P 2 2 2	16
19	P 2_1 2 2	C_{2v} -1	P 2 2 2_1	17
20	P 2 m m	C_{2v} -1	P m m 2	25
21	P 2_1 a m	C_{2v} -2	P m c 2_1	26
22	P 2_1m a	C_{2v} -2	P c m 2_1	(26)
23	P 2 a a	C_{2v} -3	P c c 2	27
24	P m 2 m	C_{2v} -1	P m 2 M	(25)
25	P m 2 a	C_{2v} -4	P c 2 m	(28)
26	P m m 2	C_{2v} -1	P 2 m m	(25)
27	P m a 2	C_{2v} -4	P 2 c m	(28)
28	P m m m	D_{2h} -1	P m m m	47
29	P 2/m 2/a 2/a	D_{2h} -3	P c c m	49
30	P 2_1/m 2/m 2/a	D_{2h} -5	P c m m	(51)
31	P 2_1/m 2/a 2/m	D_{2h} -5	P m c m	(51)
32	P 4	C_4 -1	P 4	75
33	P 4_1	C_4 -2	P 4_1	76
34	P 4_2	C_4 -3	P 4_2	77
35	P 4_3	C_4 -4	P 4_3	78

36	P -4	S_4 1	P 4	81
37	P 4/m	C_{4h} 1	P 4/m	83
38	P 4_2/m	C_{4h} -2	P 4_2/m	89
39	P 4 2 2	D_4 -1	P 4 2 2	89
40	P 4_1 2 2	D_4 -3	P 4_1 2 2	91
41	P 4_2 2 2	D_4 -5	P 4_2 2 2	93
42	P 4_3 2 2	D_4 -7	P 4_3 2 2	95
43	P 4 m m	C_{4v} -1	P 4 m m	99
44	P 4_2 a m	C_{4v} -3	P 4_2 c m	101
45	P 4 a a	C_{4v} -5	P 4 c c	103
46	P 4_2 m a	C_{4v} -7	P 4_2 m c	105
47	P -4 2 m	D_{2d} -1	P -4 2 m	111
48	P -4 2 a	D_{2d} -2	P -4 2 c	112
49	P -4 m 2	D_{2d} -5	P -4 m 2	115
50	P -4 a 2	D_{2d} -6	P -4 c 2	116
51	P 4/m m m	D_{4h} -1	P 4/m m m	123
52	P 4/m 2/a 2/a	D_{4h} -2	P 4/m c c	124
53	P 4_2/m 2/m 2/a	D_{4h} -9	P 4_2/m m c	131
54	P 4_2/m 2/a 2/m	D_{4h} -10	P 4_2/m c m	132
55	P 3	C_3 -1	P 3	143
56	P 3_1	C_3 -2	P 3_1	144
57	P 3_2	C_3 -3	P 3_2	145
58	P -3	C_{3i} -1	P -3	147
59	P 3 1 2	D_3 -1	P 3 1 2	149
60	P 3_1 1 2	D_3 -3	P 3_1 1 2	151
61	P 3_2 1 2	D_3 -5	P 3_2 1 2	153
62	P 3 2 1	D_3 -2	P 3 2 1	150
63	P 3_1 2 1	D_3 -4	P 3_1 2 1	152
64	P 3_2 2 1	D_3 -6	P 3_2 2 1	154
65	P 3 m 1	C_{3v} -1	P 3 m 1	156
66	P 3 a 1	C_{3v} -3	P 3 c 1	158
67	P 3 1 m	C_{3v} -2	P 3 1 m	157
68	P 3 1 a	C_{3v} -4	P 3 1 c	159
69	P -3 1 m	D_{3d} -1	P -3 1 m	162
70	P -3 1 a	D_{3d} -2	P -3 1 c	163
71	P -3 m 1	D_{3d} -3	P -3 m 1	164
72	P -3 a 1	D_{3d} -4	P -3 c 1	165

73	P 6	C_6 - 1	P 6	168
74	P 6_1	C_6 -2	P 6_1	169
75	P 6_5	C_6 -3	P 6_5	170
76	P 6_2	C_6 -4	P 6_2	171
77	P 6_4	C_6 -5	P 6_4	172
78	P 6_3	C_6 -6	P 6_3	173
79	P -6	C_{3h} -1	P -6	174
80	P 6/m	C_{6h} -1	P 6/m	175
81	P 6_3/m	C_{6h} -2	P 6_3/m	176
82	P 6 2 2	D_6 -1	P 6 2 2	177
83	P 6_1 2 2	D_6 -2	P 6_1 2 2	178
84	P 6_5 2 2	D_6 -3	P 6_5 2 2	179
85	P 6_2 2 2	D_6 -4	P 6_2 2 2	180
86	P 6_4 2 2	D_6 -5	P 6_4 2 2	181
87	P 6_3 2 2	D_6 -6	P 6_3 2 2	182
88	P 6 m m	C_{6v} -1	P 6 m m	183
89	P 6 a a	C_{6v} -2	P 6 c c	184
90	P 6_3 a m	C_{6v} -3	P 6_3 c m	185
91	P 6_3 m a	C_{6v} -4	P 6_3 m c	186
92	P -6 m a	D_{3h} -1	P -6 m 2	187
93	P -6 a 2	D_{3h} -2	P -6 c 2	188
94	P -6 2 m	D_{3h} -3	P -6 2 m	189
95	P -6 2 a	D_{3h} -4	P -6 2 c	190
96	P 6/m m m	D_{6h} -1	P 6/m m m	191
97	P 6/m 2/a 2/a	D_{6h} -2	P 6/m c c	192
98	P 6_3/m 2/a 2/m	D_{6h} -3	P 6_3/m c m	193
99	P 6_3/m 2/m 2/a	D_{6h} -4	P 6_3/m m c	194

The plane Groups

The two sided plane groups used to describe slab geometries are a subset of the 230 space groups they may be identified by the corresponding space group. The first collumn gives the label to be used, the second collumn gives the Hermann-Mauguin symbol of the space group. The third collumn gives the Schoenflies and the fourth collumn the the number of the corresponding space group. The number of the space group is written in parenthesis when the orientation of the symmetry operations does not correspond to the first setting ot the ITXC.

IGROUP	Hermann Mauguin	Schoenflies	N
	Trigonal Lattices (P)		
1	P 1	C_1 1	1
2	P - 1	C_i -1	2
3	P 1 1 2	C_2 1	(3)
4	P 1 1 m	C_s - 1	(6)
5	P 1 1 a	C_s 2	(7)
6	P 1 1 2/m	C_{2h} -1	(10)
7	P 1 1 2/a	C_{2h} 4	(13)
	Rectangular Lattices (P or C)		
8	P 2 1 1	C_2 -1	(3)
9	P 2_1 1 1	C_2 -2	(4)
10	C 2 1 1	C_2 - 3	(5)
11	P m 1 1	C_s - 1	(6)
12	P b 1 1	C_s - 2	(7)
13	C m 1 1	C_s - 3	(8)
14	P 2/m 1 1	C_{2h} -1	(10)
15	P 2_1/m 1 1	C_{2h} - 2	(11)
16	C 2/m 1 1	C_{2h} -3	(12)
17	P 2/b 1 1	C_{2h} -4	(13)
18	P 2_1/b 1 1	C_{2h} -5	(14)
19	P 2 2 2	D_2 - 1	16
20	P 2 2_1 2	D_2 - 2	(17)
21	P 2_1 2_1 2	D_2 -3	18
22	C 2 2 2	D_2 -6	21
23	P m m 2	C_{2v} - 1	25
24	P m a 2	C_{2v} - 4	28
25	P b a 2	C_{2v} - 8	32
26	C m m 2	C_{2v} - 11	35
27	P 2 m m	C_{2v} - 1	(25)
28	P 2_1 a m	C_{2v} - 2	(26)
29	P 2_1 m a	C_{2v} - 2	(26)
30	P 2 m b	C_{2v} - 4	(28)
31	P 2_1 m n	C_{2v} - 7	(31)
32	P 2 a a	C_{2v} - 3	(27)
33	P 2_1 a b	C_{2v} - 5	(29)
34	P 2 a n	C_{2v} - 6	(30)

35	C 2 m m	C_{2v} - 11	(35)
36	C 2 m b	C_{2v} 15	(39)
37	P m m m	D_{2h} - 1	47
38	P m a m	D_{2h} - 5	(51)
39	P m m a	D_{2h} - 5	51
40	P m m n	D_{2h} - 13	59
41	P b a m	D_{2h} - 9	55
42	P m a a	D_{2h} - 3	(49)
43	P m a n	D_{2h} - 7	(53)
44	P b m a	D_{2h} - 11	(57)
45	P b a a	D_{2h} - 8	(54)
46	P b a n	D_{2h} - 4	50
47	C m m m	D_{2h} - 19	65
48	C m m a	D_{2h} - 21	67
	Square Lattices (P)		
49	P 4	C_4 - 1	75
50	P - 4	S_4 - 1	81
51	P 4/m	C_{4h} - 1	83
52	P 4/n	C_{4h} - 3	85
53	P 4 2 2	D_4 - 1	89
54	P 4 2_1 2	D_4 - 2	90
55	P 4 m m	C_{4v} - 1	99
56	P 4 b m	C_{4v} - 2	100
57	P - 4 2 m	D_{2d} - 1	111
58	P - 4 2_1 m	D_{2d} - 3	113
59	P - 4 m 2	D_{2d} - 5	115
60	P - 4 b 2	D_{2d} - 7	117
61	P 4/m m m	D_{4h} - 1	123
62	P 4/n b m	D_{4h} - 3	125
63	P 4/m b m	D_{4h} - 5	127
64	P 4/n m m	D_{4h} - 7	129
	Hexagonal Lattices (P)		
65	P 3	C_3 - 1	143
66	P - 3	C_{3i} - 1	147
67	P 3 1 2	D_3 - 1	149
68	P 3 2 1	D_3 - 2	150
69	P 3 m 1	C_{3v} - 1	156

70	P 3 1 m	C_{3v} - 2	157
71	P - 3 1 m	D_{3d} - 1	162
72	P 3 a 1	D_{3d} - 3	164
73	P 6	C_6 - 1	168
74	P - 6	C_{3h} - 1	174
75	P 6/m	C_{6h} 1	175
76	P 6 2 2	D_6 - 1	177
77	P 6 m m	C_{6v} - 1	183
78	P - 6 m 2	D_{3h} - 1	187
79	P - 6 2 m	D_{3h} - 3	189
80	P 6/m m m	D_{6h} - 1	191

The Space Groups

The space group labels are according to the ITXC. The symbols are the standard SHORT symbols, for example; P $\bar{6}$ 2 m → P –6 2 m and P 6_3 m → P 63 m. For the groups 221–230 the symbols are according to the 1952 edition of the International Tables *not* to the 1982 edition (group 221: 1952 P m $\bar{3}$ m)

IGROUP	Hermann Mauguin	18	P 21 21 2	36	C M C 21
1	P 1	19	P 21 21 21	37	C C C 2
2	P - 1	20	C 2 2 21	38	A M M 2
3	P 2	21	C 2 2 2	39	A B M 2
4	P 21	22	F 2 2 2	40	A M A 2
5	C 2	23	I 2 2 2	41	A B A 2
6	P M	24	I 21 21 21	42	F M M 2
7	P C	25	P M M 2	43	F D D 2
8	C M	26	P M C 21	44	I M M 2
9	C C	27	P C C 2	45	I B A 2
10	P 2/M	28	P M A 2	46	I M A 2
11	P 21/M	29	P C A 21	47	P M M M
12	C 2/M	30	P N C 2	48	P N N N
13	P 2/C	31	P M N 21	49	P C C M
14	P 21/C	32	P B A 2	50	P B A N
15	C 2/C	33	P N A 21	51	P M M A
16	P 2 2 2	34	P N N 2	52	P N N A
17	P 2 2 21	35	C M M 2	53	P M N A

54	P C C A	91	P 41 2 2	128	P 4/M N C
55	P B A M	92	P 41 21 2	129	P 4/N M M
56	P C C N	93	P 42 2 2	130	P 4/N C C
57	P B C M	94	P 42 21 2	131	P 42/M M C
58	P N N M	95	P 43 2 2	132	P 42/M C M
59	P M M N	96	P 43 21 2	133	P 42/N B C
60	P B C N	97	I 4 2 2	134	P 42/N N M
61	P B C A	98	I 41 2 2	135	P 42/M B C
62	P N M A	99	P 4 M M	136	P 42/M N M
63	C M C M	100	P 4 B M	137	P 42/N M C
64	C M C A	101	P 42 C M	138	P 42/N C M
65	C M M M	102	P 42 N M	139	I 4/M M M
66	C C C M	103	P 4 C C	140	I 4/M C M
67	C M M A	104	P 4 N C	141	I 41/A M D
68	C C C A	105	P 42 M C	142	I 41/A C D
69	F M M M	106	P 42 B C	143	P 3
70	F D D D	107	I 4 M M	144	P 31
71	I M M M	108	I 4 C M	145	P 32
72	I B A M	109	I 41 M D	146	R 3
73	I B C A	110	I 41 C D	147	P -3
74	I M M A	111	P -4 2 M	148	R -3
75	P 4	112	P -4 2 C	149	P 3 1 2
76	P 41	113	P -4 21 M	150	P 3 2 1
77	P 42	114	P -4 21 C	151	P 31 1 2
78	P 43	115	P -4 M 2	152	P 31 2 1
79	I 4	116	P -4 C 2	153	P 32 1 2
80	I 41	117	P -4 B 2	154	P 32 2 1
81	P -4	118	P -4 N 2	156	R 3 2
82	I -4	119	I -4 M 2	157	P 3 M 1
83	P 4/M	120	I -4 C 2	158	P 3 1 M
84	P 42/M	121	I -4 2 M	159	P 3 C 1
85	P 4/N	122	I -4 2 D	160	P 3 1 C
86	P 42/N	123	P 4/M M M	161	R 3 M
87	I 4/M	124	P 4/M C C	162	R 3 C
88	I 41/A	125	P 4/N B M	162	P -3 1 M
89	P 4 2 2	126	P 4/N N C	163	P -3 1 C
90	P 4 21 2	127	P 4/M B M	164	P -3 M 1

165	P 3 C 1	187	P 6 M 2	209	F 4 3 2
166	R 3 M	188	P 6 C 2	210	F 41 3 2
167	R 3 C	189	P 6 2 M	211	I 4 3 2
168	P 6	190	P 6 2 C	212	P 43 3 2
169	P 61	191	P 6/M M M	213	P 41 3 2
170	P 65	192	P 6/M C C	214	I 41 3 2
171	P 62	193	P 63/M C M	215	P -4 3 M
172	P 64	194	P 63/M M C	216	F -4 3 M
173	P 63	195	P 2 3	217	I -4 3 M
174	P -6	196	F 2 3	218	P -4 3 N
175	P 6/M	197	I 2 3	219	F -4 3 C
176	P 63/M	198	P 21 3	220	I -4 3 D
177	P 6 2 2	199	I 21 3	221	P M 3 M
178	P 61 2 2	200	P M 3	222	P N 3 N
179	P 65 2 2	201	P N 3	223	P M 3 N
180	P 62 2 2	202	F M 3	224	P N 3 M
181	P 64 2 2	203	F D 3	225	F M 3 M
182	P 63 2 2	204	I M 3	226	F M 3 C
183	P 6 M M	205	P A 3	227	F D 3 M
184	P 6 C C	206	I A 3	228	F D 3 C
185	P 63 C M	207	P 4 3 2	229	I M 3 M
186	P 63 M C	208	P 42 3 2	230	I A 3 D

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