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Derivation of space groups in mm2, 222 and mmm crystal classes

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Abstract : An algebraic approach is developed to derive space groups using 4×4 Seitz matrices for the crystal classes mm2, 222 and mmm in the orthorhombic system. The advantage of the present method is that it is relatively simple and can be adapted to introduce space groups to beginners. One of the advantages of the present method is that it admits a geometrical visualization of the symmetry elements of space group. The method can easily be extended to other crystal classes in a straight forward way.

Keywords : Space groups, theoretical crystallography.

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1. Introduction

Space groups characterize the symmetry of the structure of crystals. By means of the symmetry operations determined by the space group, the region is multiplied infinitely and fill space completely. The idea behind the derivation of space group is based on the connection between space and point group or crystal class. For any crystal class, one considers in succession the set of symmetry elements in that class with translational subgroup (one of the Bravais lattices) which are possible in the system to which the given crystal class is related. As a result, one obtains the space groups related to that symmetry class.

Space groups are differentiated into two types. In the first type, an operation of point group is combined with the translation of the Bravais lattice. The resulting space group is called the symmorphic space group. The second type of space group arises by replacing some or all rotation axes and reflection planes of symmetry by screw axes and glide reflection planes, respectively. A screw rotation operation is composed of an operation which consists of rotation about an axis of order 2, 3, 4 or 6 with a suitable movement along the direction of

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that axis. Similarly, a glide reflection operation consists of reflection in a plane together with a suitable movement in the plane (for details see International Tables for X-ray Crystallography, Vol. A, 1983). A space group of this type is said to be non-symmorphic space group ; there are 73 symmorphic space groups and 157 non-symmorphic space groups, making a total of 230 space groups.

A space group is composed of a set of symmetry operations in a three dimensional space. They are expressed by 4×4 Seitz matrices or augmented matrices (Seitz 1936, Bradley and Cracknell 1972, Wondratschek 1983) as

$$(\underset{\sim}{S},\underset{\sim}{s})=\left[\begin{array}{ccc:c} S_{11} & S_{12} & S_{13} & s_1 \\ S_{21} & S_{22} & S_{23} & s_2 \\ S_{31} & S_{32} & S_{33} & s_3 \\ \hdashline 0 & 0 & 0 & 1 \end{array}\right]=\{\underset{\sim}{S}\mid\underset{\sim}{s}\}, \tag{1}$$

where $\underset{\sim}{S}$ is the 3×3 matrix representing the rotation part and the column matrix $\underset{\sim}{s}$ the translation part. The form of the matrix depends on the choice of basis vectors and $\underset{\sim}{s}$ also depends on the choice of the origin. The Seitz matrix or the space group operator transforms a point $\underset{\sim}{r}$ to another point $\underset{\sim}{r}'$. The product of two space group operators $\{\underset{\sim}{S}\mid\underset{\sim}{s}\}$ and $\{\underset{\sim}{Q}\mid\underset{\sim}{q}\}$ is another space group operator

$$\{\underset{\sim}{S}\mid\underset{\sim}{s}\}.\{\underset{\sim}{Q}\mid\underset{\sim}{q}\}=\{\underset{\sim}{S}\underset{\sim}{Q}\mid\underset{\sim}{S}\underset{\sim}{q}+\underset{\sim}{s}\}. \tag{2}$$

The operator inverse to a space group $\{\underset{\sim}{S}\mid\underset{\sim}{s}\}$ is

$$\{S\mid s\}^{-1}=\{S^{-1}\mid -S^{-1}s\} \tag{3}$$

and the product of the operators $\{\underset{\sim}{S}\mid\underset{\sim}{s}\}$ and $\{\underset{\sim}{S}\mid\underset{\sim}{s}\}^{-1}$ is equal to $\{\underset{\sim}{I}\mid 0\}$ which is the identity element of the space group. The Seitz matrices form a group in mathematical sense, and the collection of all operators of the type $\{\underset{\sim}{I}\mid\underset{\sim}{t}\}$ form a subgroup, called the translation subgroup of the space group (Wondratschek 1983).

2. The 14 Bravais lattices and 32 point groups

A lattice may be considered as a three-dimensional repetition of a paralleiopiped, called the unit cell, formed by the three basis vectors. It is possible without violating lattice condition, to centre faces or body of the unit cell. These lattices with centred unit cells are called multiply-primitive lattices, whereas lattices with unit cells having eight lattice points on the eight corners are called primitive. Bravais showed that there are fourteen possible lattice types called the Bravais lattices.

A point group is a group of symmetry operations which act at a point 0 (origin) and therefore keep 0 fixed and leave invariant all distances and angles in 3-dimensional Euclidean space. The symmetry operations are rotations and rotations-inversion about axes through 0 or their products. Such products also include reflection planes through 0. There are 32 different crystallographic point groups ; these 32 point groups or alternatively 32 crystal classes can be classified into seven crystal systems or syngonies according to the order of the principal axis. There are five crystal systems for point groups with single principal axis of order 1, 2, 3, 4 or 6

Table 1. The 32 crystal classes and 14 Bravais lattices.

Crystal classes or point groups	Bravais lattice	Symmetry of Bravais lattice	Crystal system	Axes and unit cell
1, $\bar{1}$	P	$\bar{1}$	Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
2, m, 2/m	P, C	2/m	Monoclinic	$a \neq b \neq c$ $\beta \neq 90°$, $\alpha = \gamma = 90°$
222, mm2 mmm	P, C (A, B) I, F	mmm	Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$
4, $\bar{4}$, 4/m 422, 4mm, $\bar{4}$2m, 4/mmm	P, I	4/mmm	Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$
3, $\bar{3}$ 32, 3m, $\bar{3}$m	R	$\bar{3}$m	Trigonal	$a = b = c$ $\alpha = \beta = \gamma \neq 90°$
6, $\bar{6}$, 6/m 622, 6mm $\bar{6}$2m, 6/mmm	P	6/mmm	Hexagonal	$a = b \neq c$ $\alpha = \beta = 90°$ $\gamma = 120°$
23, m3 432, $\bar{4}$3m m3m	P, I, F	m3m	Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90°$

namely the triclinic, monoclinic, trigonal, tetragonal and hexagonal, respectively. There are two more systems, the orthorhombic system which has three mutually perpendicular axes of order 2, and the cubic system which has four triad axes directed towards the vertices of a regular tetrahedron. The 14 Bravais lattices, 32 crystal classes and 7 crystal systems have been listed in Table 1.

In the following, three theorems are presented which are useful in the derivation of space groups.

Theorem 1 :

A two-fold rotation about an axis A followed by a translation perpendicular to the axis, is equivalent to a two-fold rotation in the same sense at half the translation.

Let the two-fold rotation be at A, parallel to c axis

$$2_A=\left[\begin{array}{ccc:c} \bar{1} & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hdashline 0 & 0 & 0 & 1 \end{array}\right]$$

and lattice translation be chosen along $\underset{\sim}{a}$ axis

$$t_1=\left[\begin{array}{ccc:c} 1 & 0 & 0 & t_1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hdashline 0 & 0 & 0 & 1 \end{array}\right]$$

Then

$$2_A.t_1=\left[\begin{array}{ccc:c} \bar{1} & 0 & 0 & t_1 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hdashline 0 & 0 & 0 & 1 \end{array}\right]=2_{A_1}$$

It is a two-fold rotation at A_1 (Figure 1) which is located at half the lattice translation from A. In a similar way, two-fold axes of symmetry are obtained at A_2 and A_3 as a result of translations t_2 and t_1+t_2, respectively.

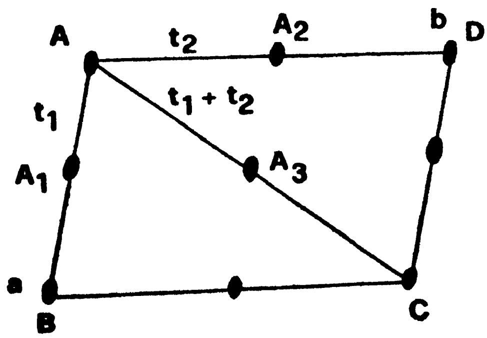

Figure 1. The combination of diad and perpendicular translation.

Theorem 2 :

The combination of two perpendicular glides results in a two-fold rotation (or two fold screw). The position and its being a pure rotation or screw depend on the column matrix $\underset{\sim}{s}_i$ associated with the glides.

Let the two glides be

$$c=\left[\begin{array}{ccc|c} \bar{1} & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right] \text{ and } a=\left[\begin{array}{ccc|c} 1 & 0 & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right]$$

The combination of two glides gives

$$c.a=\left[\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & \frac{1}{2} \\ 0 & 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right]$$

which is a screw diad parallel to $\underset{\sim}{c}$ axis, passing through a point $x=0$, $y=\frac{1}{4}$.

Theorem 3 :

A combination of *C* centred lattice and a diad axis along [001] results in a diad axis parallel to [001] direction, whilst diad axis parallel to [100] and [010] result in screw diad.

Let the Seitz matrix for *C*-centring be

$$C=\left[\begin{array}{ccc|c} 1 & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right]$$

and that for diads along [001], [010] and [100] directions be

$$2_z=\left[\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right],\ 2_y=\left[\begin{array}{ccc|c} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right],$$

$$2_x=\left[\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right]$$

then

$$C.2_z=\left[\begin{array}{ccc:c} \bar{1} & 0 & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 & \frac{1}{2} \\ 0 & 0 & 1 & 0 \\ \hdashline 0 & 0 & 0 & 1 \end{array}\right]=2, \text{ parallel to [001] passing through } x=\tfrac{1}{4},\ y=\tfrac{1}{4}$$

$$C.2_y=\left[\begin{array}{ccc:c} \bar{1} & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & \bar{1} & 0 \\ \hdashline 0 & 0 & 0 & 1 \end{array}\right]=2_1, \text{ parallel to [010] passing through } x=\tfrac{1}{4},\ z=0$$

$$C.2_x=\left[\begin{array}{ccc:c} 1 & 0 & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 & \frac{1}{2} \\ 0 & 0 & \bar{1} & 0 \\ \hdashline 0 & 0 & 0 & 1 \end{array}\right]=2_1, \text{ parallel to [100] passing through } y=\tfrac{1}{4},\ z=0$$

The space groups have been considered by many authors at different levels of complexity (Belov 1957, Buerger 1956, Federov 1891, Schönflies 1923, Sohncke 1879, Seitz 1935a, 1935b, Jensen 1973, Phillips 1971, Weyl 1952, Shubnikov and Koptsik 1974 and Zachariasen 1967). In this paper, an algebraic approach is employed using 4 × 4 augmented matrices, which describe the symmetry of space group in three dimensions. One advantage of this treatment is that one can visualize the effect of two or more successive applications of symmetry operations. The method is relatively simple to apply in the derivation of space groups.

3. Derivation of space groups in crystal class mm2

Space groups based on P-lattice :

The first symbol '*m*' in the crystal class mm2 is the reflection plane 100 and may be represented in space group by any one of the symbols m_x, b_x, c_x or n_x. Similarly second '*m*' 010 plane may be any one of the symbols m_y, a_y, c_y or n_y. According to Theorem 2, the combination of any of the two symmetry elements, taken one from the set 1 and the other from the set 2, gives rise to a diad axis or a diad screw axis depending on if there is a resultant one lattice translation or half lattice translation in the direction of $\underset{\sim}{c}$ axis. Therefore, there are sixteen space group symbols based on primitive lattice. They are Pmm2, Pma2, Pmc2_1, Pmn2_1, Pbm2, Pba2, Pbc2_1, Pbn2_1, Pcm2_1, Pca2_1, Pcc2, Pcn2, Pnm2_1, Pna2_1, Pnc2 and Pnn2. Interchange of $\underset{\sim}{a}$ and $\underset{\sim}{b}$ axes (equivalent ones) will show the equivalence of the symbols, Pmc2_1≡Pcm2_1, Pmn2_1≡Pnm2_1, Pbc2_1≡Pca2_1, Pma2≡Pbm2, Pbn2_1 ≡Pna2_1 and Pcn2≡Pnc2. Hence the unique space groups are ten as Pmm2, Pma2, Pmc2_1, Pmn2_1, Pca2_1, Pcc2, Pcn2, Pba2, Pbn2_1 and Pnn2.

Space groups based on C- and A-centred lattices :

The effect of centring on mirrors and glider has been studied in Table 2. Using the results, we can show the equivalence of the following space groups :

Table 2. Effect of centring in reflection and glide planes.

→/↓	m_x	b_x	c_x	n_x	m_y	a_y	c_y	n_y	m_z	a_z	b_z	n_z
A	$=n_x$	$=c_x$	$=b_x$	$=m_x$	c_y	n_y	m_y	a_y	b_z	n_z	m_z	a_z
B	c_x	n_x	m_x	b_x	$=n_y$	$=c_y$	$=a_y$	$=m_y$	a_z	m_z	n_z	b_z
C	b_x	m_x	n_x	c_x	a_y	m_y	n_y	c_y	$=n_z$	$=b_z$	$=a_z$	$=m_z$
I	n_x	c_x	b_x	m_x	n_y	c_y	a_y	m_y	n_z	b_z	a_z	m_z

Extra planes of symmetry created due to centring are given inside the table. '=' sign means that the planes of symmetry created are coincident with the original plane. Others are shifted from the original ones.

$$\left.\begin{array}{l}\mathrm{Pmm2}\\ \mathrm{Pba2}\\ \mathrm{Pbm2}\\ \mathrm{Pma2}\end{array}\right\}\equiv\mathrm{Cmm2}\qquad \left.\begin{array}{l}\mathrm{Pmc2_1}\\ \mathrm{Pbn2_1}\\ \mathrm{Pbc2_1}\\ \mathrm{Pmn2_1}\end{array}\right\}\equiv\mathrm{Cmc2_1}$$

$$\left.\begin{array}{l}\mathrm{Pcm2_1}\\ \mathrm{Pca2_1}\\ \mathrm{Pnm2_1}\\ \mathrm{Pna2_1}\end{array}\right\}\equiv\mathrm{Ccm2_1}\qquad \left.\begin{array}{l}\mathrm{Pcc2}\\ \mathrm{Pnc2}\\ \mathrm{Pcn2}\\ \mathrm{Pnn2}\end{array}\right\}\equiv\mathrm{Ccc2}$$

Interchange of $\underset{\sim}{a}$ and $\underset{\sim}{b}$ axes shows that Cmc2_1≡Ccm2_1. Thus there are three space groups Cmm2, Cmc2_1 and Ccc2 in C-centred lattice.

Referring to Table 2, we have for A-centring

$$\left.\begin{array}{l}\mathrm{Pmm2}\\ \mathrm{Pmc2_1}\\ \mathrm{Pnc2}\\ \mathrm{Pnm2_1}\end{array}\right\}\equiv\mathrm{Amm2}\qquad \left.\begin{array}{l}\mathrm{Pma2}\\ \mathrm{Pnn2}\\ \mathrm{Pna2_1}\\ \mathrm{Pmn2_1}\end{array}\right\}\equiv\mathrm{Ama2}$$

$$\left.\begin{array}{l}\mathrm{Pba2}\\ \mathrm{Pcn2}\\ \mathrm{Pbn2_1}\\ \mathrm{Pca2_1}\end{array}\right\}\equiv\mathrm{Aba2}\qquad \left.\begin{array}{l}\mathrm{Pbm2}\\ \mathrm{Pcc2}\\ \mathrm{Pcm2_1}\\ \mathrm{Pbc2_1}\end{array}\right\}\equiv\mathrm{Abm2}$$

Four space groups Amm2, Ama2, Aba2 and Abm2 are possible ones based on A-centred lattice.

Space groups based on I-centred lattice :

Referring to Table 2, we have

Pmm2 Pnn2 $Pnm2_1$ $Pmn2_1$	≡Imm2	Pcc2 Pba2 $Pca2_1$ $Pbc2_1$	≡Iba2
Pma2 Pnc2 $Pmc2_1$ $Pna2_1$	≡Ima2	$Pcm2_1$ Pcn2 Pbm2 $Pbn2_1$.	≡Ibm2

Interchange between $\underset{\sim}{a}$ and $\underset{\sim}{b}$ makes the symbols Ima2 and Ibm2 as equivalent. Thus distinct space groups in this case are Imm2 Ima2 and Iba2.

Space groups based on F-centred lattice :

Referring to Table 2, in this case, we conclude that only those arrangements where 100 planes and 010 planes are of the same kind are possible. Fmm2 have glide planes, which are at the same time *c* and *a* (or *b*) planes, parallel to the reflection planes. These reflection planes are also *n* planes. Thus one distinct space group namely Fmm2 is possible in this way. Also in the *F*-centred lattice if the plane 100 had glide of ¼th of the diagonal, then reflection in the second plane 010 would turn the gliding onto the other diagonal. Thus in *F*-lattice there exists a new space group as Fdd2.

4. Derivation of space groups in crystal class 222

We study the general behaviour of two screw diads. Let the two screw diads along *x* and *y* directions be

$$2_x,\ s_1 \left[\begin{array}{ccc:c} 1 & 0 & 0 & s_1 \\ 0 & \bar{1} & 0 & L_1 \\ 0 & 0 & \bar{1} & L_1' \\ \hdashline 0 & 0 & 0 & 1 \end{array}\right]$$

$$2_y,\ s_2 \equiv \left[\begin{array}{ccc:c} \bar{1} & 0 & 0 & L_2 \\ 0 & 1 & 0 & s_2 \\ 0 & 0 & \bar{1} & L_2' \\ \hdashline 0 & 0 & 0 & 1 \end{array}\right]$$

where s_1 and s_2 are zero for rotation and ½ for screw. The combination of $2_x, s_1$ and $2_y, s_2$ is

$$\begin{bmatrix} \bar{1} & 0 & 0 & \vdots & L_2+s_1 \\ 0 & \bar{1} & 0 & \vdots & L_1-s_2 \\ 0 & 0 & 1 & \vdots & L_1'-L_2' \\ \cdots & \cdots & \cdots & \vdots & \cdots \\ 0 & 0 & 0 & \vdots & 1 \end{bmatrix} \equiv 2_z,\ L_1'-L_2'$$

which is a screw or pure diad depending on L_1' and L_2'

Space groups based on primitive lattice.

We may classify the possible combinations as there may be rotation diad axes (i) in all three directions, (ii) in two directions, (iii) in one or (iv) in none; screw axes being present parallel to any of the directions x, y and z not parallelled by the rotation axes. Since x, y and z axes have the same environments, interchange among the axes represents only different orientation of the space group. We thus get the four distinct space groups in this class, viz. P222, P222$_1$, P2$_1$2$_1$2 and P2$_1$2$_1$2$_1$.

Space groups based on C-centred lattice :

Referring to Theorem 3, *C*-centred lattice generates screw diad axes parallel to any rotation diad axes postulated in the [100] and [010] directions but only rotation diad axes in the [001] direction. It follows that C222≡C2$_1$2$_1$2 and C222$_1$≡C2$_1$2$_1$2$_1$. Thus distinct space groups based on *C*-centred lattice are C222 and C222$_1$.

Space groups based on I-centred lattice :

The transformations of *I* space lattice result in the space group I222 possessing screw diad axes, parallel to rotation diad axes. These are mutually intersecting diad and screw diad axes. There is a possibility of another space group based on *I*-centred lattice in which diad axes and screw diad axes are of non-intersecting type. It is denoted by a space group symbol I2$_1$2$_1$2$_1$. Thus, there are two unique space groups viz. I222 and I2$_1$2$_1$2$_1$.

Space groups based on F-centred lattice :

As a result of simultaneous centring *A*-, *B*- and *C*-faces, diad axes result in screw diad axes present in all three directions. Hence F222, F222$_1$, F2$_1$2$_1$2 and F2$_1$2$_1$2$_1$ are equivalent. Thus F222 is the only possible space group.

5. Derivation of space groups in crystal class mmm

In the space groups isomorphous with the crystal class *mmm* and based on primitive lattice, planes parallel to 100 may be *m* planes, *b* planes, *c* planes or *n* planes ; those parallel to 010 may be *m, a, c* or *n* and those parallel to 001 may be *m, a, b* or *n* planes. Thus in total sixty-four combinations can be derived.

Derivation of space groups based on primitive lattice :

The environment of $\underset{\sim}{a}$, $\underset{\sim}{b}$ and $\underset{\sim}{c}$ axes are equivalent. By interchange of $\underset{\sim}{a}$, $\underset{\sim}{b}$ and $\underset{\sim}{c}$ axes, we can see equivalence of few symbols. For example, in the space group Pmma, when x and z are interchanged, Pmma ≡ Pcmm. Thus a total of sixteen unique space groups are Pmmm, Pmma, Pmmn, Pmna, Pbam, Pban, Pbcm, Pbca, Pbcn, Pccm, Pcca Pccn, Pnma, Pnnm, Pnna and Pnnn. The space groups Pmmm and Pnnn have the same symbol in six orientation of axes.

6. Derivation of space groups based on C-centred, I-centred and F-centred lattices

Referring to Table 2, we note that for *C*-lattice, *m* planes parallel to 100 plane are interleaved by *b* planes or *c* planes in this direction are interleaved by *n* planes. The *m* planes parallel to 010 plane results in *a* planes whereas *c* planes are accompanied by *n* planes. The *m* planes parallel to 001 are *n* planes at the same time or *a* planes will also be *b* planes. With these considerations in view, there are six new space groups – Cmmm, Cmma, Cmcm (≡Ccmm), Cmca (≡Ccma), Cccm and Ccca.

For *I*-centred lattice, *m* planes parallel to any of the pinacoids result in *n* planes. Glide planes *a*, *b* or *c* repeats in sets of two kinds. The eight symbols which we can derive will further reduce in number with *I* space lattice. The new space groups are – Immm, Imma, Imaa and Ibca.

For *F*-centred lattice we note that all possible combinations in any direction show a mirror and *n* glide plane. The distribution of symmetry elements has similar pattern parallel to any of the pinacoids. Thus we have only one distinct space group – Fmmm. Also if the plane 100 had a glide, then a reflection in the plane 010 and 001 would turn glide onto the other diagonals. The space group has a symbol Fddd. Thus there are two distinct space groups – Fmmm and Fddd.

7. Conclusions

All space groups in orthorhombic system have been derived. There are 22 space groups in mm2, 9 in 222 and 28 in mmm. There are 59 groups in orthorhombic system. Using the same procedure, space groups in remaining crystal classes can also be derived.

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