Crystallographic Groups, Groupoids, and Orbifolds

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Outline In this note, we first discuss the relationship among crystallographic lattice groups, space groups, and point groups by using a short exact sequence, then in footnotes indicate the classification of those groups. We then introduce screw and glide groupoids as an extension of point groups in a new exact sequence, and list the one-translational-dimension screw and glide groupoids, which require torus and truncated cylinder projection representations in addition to the spherical projection used for point groups. We then briefly discuss the two and three translational dimension groupoids associated with the remaining point groups.

Examples of space groups and their groupoid based nomenclature, which is mainly the extended Hermann-Mauguin international crystallographic nomenclature system plus a specific type of coset decomposition, are then given. Next the crystallographic orbifolds are defined and some application problems associated with orbifolds discussed. Finally, the derivation of what might be called "orbifoldoids" is suggested for future research.

Introduction The International Tables for Crystallography, Volume A, Space Group Symmetry (ITCrA), T. Hahn ed is the standard reference for the crystallographic groups.[2] Much of that information can be reformulated in terms of screw and glide groupoids as used by M.A. Jaswon and M.A. Rose[3]in their concise rederivation of the 230 space groups and 1191 color spaces. The crystallographic groups can also be given a geometric topology interpretation using orbifolds, as described on our website on crystallographic topology.[4] The present note attempts to compare and combine these diverse approaches, and was prepared as lecture notes for an "Orbifolds, Groupoids, and their Applications" workshop[5] held in Bangor, Wales, UK, September 11-15, 2000.

Crystallographic Groups The crystallographic groups are related through the group extension exact sequence

$$0 \to B \to G(3) \to Q \to 1.$$

[1]Oak Ridge National Laboratory is managed and operated by UT-Batelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725.

[2]A useful website for on line space group transformation algebra calculations is the Bilbao Crystallographic Server at: http://www.cryst.ehu.es/cryst

[3]M.A. Jaswon and M.A. Rose "Crystal Symmetry: Theory of Colour Crystallography, "Horwood, 1983.

[4]Crystallographic Topology 101. http://www.ornl.gov/ortep/topology.html

[5]http://www.bangor.ac.uk/ma/news /orbifold/welcome.html

Bravais lattices B is the set of 14 Bravais lattices[6] with five centering types (primitive P, body I, face F, side A/B/C, and rhombohedral R). For the body-centered case ($B = I$), the infinite translation group is $\{Z^3, Z^3 + (1/2, 1/2, 1/2)\}$ with Z^3 the triplet of all integers.

Point Groups The set Q contains the 32 geometric crystal-class point groups[7] which are a subset of the classical finite special orthogonal groups $SO(3)$, except that the groups with 5-fold symmetry elements have been omitted. The point groups are usually visualized using projection onto the 2-sphere S_2 from its center point. The point groups have no translation components.

Space Groups $G(3)$ is the set of 230 geometric space group types, each an infinite group. There are an infinite number of space groups, but the space group types are those with minimum volume unit cell.

Symmorphic Space Groups Of the 230 space group types, 66 are symmorphic (i.e., with no screw or glide operators, thus leaving one common origin point fixed). For the symmorphic cases, we have $Q = G(3)/B$, allowing the use of the direct product $G(3) = Q \otimes B$, but this equality does not hold for the remaining 164 cases. To alleviate this problem Jaswon and Rose introduced the screw and glide groupoids described below.

Groupoids A groupoid[8] has group-like properties but is less restrictive. A groupoid allows any number of origins. A group is a groupoid with one origin.

[6] Bravais lattices (symmetry point groups in parentheses) for the 230 space groups are distributed as follows across the seven crystal classes: triclinic ($\overline{1}$) 2 P; monoclinic ($2/m$) 8 P, 5 C; orthorhombic ($2/m\ 2/m\ 2/m$) 30 P, 15 C, 9 I, 5 F; tetragonal ($4/m\ 2/m\ 2/m$) 49 P, 19 I; trigonal ($\overline{3}\ 1\ 2/m$) 18 P, 7 R; hexagonal($6/m\ 2/m\ 2/m$) 27 P; and cubic ($4/m\ \overline{3},\ 2/m$) 15 P, 11 F, 9 I.

Crystal classes are characterized by the point group symmetry (in parenthesis) of all lattice points surrounding an arbitrary origin lattice point. The Bravais lattice flock of 14 is obtained by combining the trigonal and hexagonal entries.

[7] The distribution of the number of space groups, in parentheses, for each point groups in each crystal classes follows. Triclinic: (1) 1, (1) $\overline{1}$; Monoclinic (3) 2, (4) m, (6) $2/m$; Orthorhombic: (9) 222, (22) $mm2$, (28) $2/m\ 2/m\ 2/m$; Tetragonal: (6) 4, (2) $\overline{4}$, (6) $4/m$, (10) 422, (12) $4mm$, (12) $\overline{4}2m$, (20) $4/m\ 2/m\ 2/m$; Trigonal: (4) 3, (2) $\overline{3}$, (7) 312, (6) $3m1$, (6) $\overline{3}\,1\,2/m$; Hexagonal: (6) 6, (1) $\overline{6}$, (2) $6/m$, (6) 622, (4) $6mm$, (4) $\overline{6}m2$, (6) $6/m\ 2/m\ 2/m$; and Cubic: (5) 23, (7) $2/m\ \overline{3}$, (8) 432, (6) $\overline{4}3m$, (10) $4/m\ \ \overline{3}\ 2/m$.

In these 32 different point groups, the integers $n = 2, 3, 4, 6$ are n-fold rotation axes, and the symbol n/m has a mirror perpendicular to the n-fold rotation axes. A simple m denotes a mirror perpendicular to an implied axis, such as a unit cell axis, which is a function of its position in the point group symbol. The identity operator is 1 and the center of inversion $\overline{1}$. The symbols $\overline{2}$ and $\overline{3}$ represent inversion axes (a line rotation followed by a point inversion), but the $\overline{2}$ symbol is meaningful only with the line segments of orbifolds. $\overline{4}$ is a superposition of 2 and $\overline{2}$ (i.e., $\overline{4}$ has subgroup 2). The $\overline{6}$ symbol is an legacy oddity which means $3/m$. Point group notation examples are discussed later in the broader context of screw and glide groupoids, which include the point groups.

[8] R. Brown, 'From groups to groupoids: a brief survey', Bull. London Math. Soc., 19 (1987) 113-134.

We can have several groups with different origins as components of a groupoid. We can even cut out a piece of an infinite group and define it as a groupoid, and that is what we do for infinite screws and glides by using a modulo(1) function for translations so that a lattice translation cannot occurs within a groupoid set. Consequently, the groupoids are disjoint from the Bravais lattice.

Screw and Glide Groupoids Deviating slightly from the procedure of Jaswon and Rose, we include the point groups in our definition of a set of 186 screw and glide groupoids, Q^*, as $Q^* = G(3)/B$ for all 230 space group types. Thus, we may write

$$0 \rightarrow B \rightarrow G(3) \rightarrow Q^* \rightarrow 1,$$

and use the direct product $G(3) = Q^* \otimes B$ to define all space groups in terms of groupoids and Bravais lattices. Both Q^* and B may have certain rational translation components j/k in their coordinate triplet based on unit-cell axes. For the finite groupoid Q^*, the translation components are restricted to $|j| < k (k = 2, 3, 4, 6)$ by the use of the modulo(1) function relative to a specific origin in Euclidean 3-space, E^3, which as stated previously is the reason why Q^* is a groupoid rather than a group).

Q^* for a specific space group of G(3) is exactly the finite set of coordinate operators listed in the general Wyckoff site of ITCrA, except that the Bravais lattice centering operations are not included.

A systematic generation of space groups from Q, Q^*, P, and B, where $Q \subset Q^*$, and $P \subset B$ is given in the Appendix.

Screw Groups and Screw Groupoids We define an n-fold cyclic group as the set of crystallographic operators

$$\{n\} = \{I, K, K^2, ..., K^{n-1}\}; \;\; K^n = I,$$

and an n_j fold screw as the set

$$\{n_j\} = \{I, T^{j/n}K, T^{2j/n}K^2, ..., T^{(n-1)j/n}K^{n-1}\}; \;\; K^n = I,$$

with the pth operator $T^{(pj)/n}K^p,\ p = 0, 1, ..., n-1$. To form the screw groupoid we change all operators to $T^{((pj/n))modulo(1)}K^p,\ p = 0, 1, ..., n-1$, with T the vector translation of unit length from the origin. An example groupoid set is

$$6_3 = \{I, T^{1/2}6, 6^2, T^{1/2}6^3, 6^4, T^{1/2}6^5\},$$

which has subgroupoids $2_1 = \{I, T^{1/2}6^3\}$ and $3 = \{I, 6^2, 6^4\}$.

Glide Groups and Glide Groupoids A glide is a mirror reflection followed by translation parallel to the mirror. A specific glide reflection is denoted as $A^pB^qC^r(hkl)_m$ with the mirror reflection plane vector normal in covariant coordinates (h k l), and the translation vector p a + q b + r c in contravariant coordinates (p q r) such that the inner product of the two vectors is zero. In crystallography, covariant coordinates refer to reciprocal unit cell axes a^*, b^*, c^*, and contravariant coordinates refer to crystal space unit cell axes a, b, c.

A glide along the a axis (a-glide) may have the following settings in the orthorhombic, tetragonal, and cubic crystal system: $A^{1/2}(001)_m$, $A^{1/2}(010)_m$, $A^{1/2}(011)_m$, and $A^{1/2}(0\overline{1}1)_m$. An n-glide has a designation such as $A^{1/2}B^{1/2}(001)_m$ indicating a translation in the $a+b$ direction. Note that for the glide we obtain the group product $(A^{1/2}B^{1/2}(001)_m)^2 = AB$ which is a lattice translation.

The corresponding glide groupoid uses the unit lattice modulo function to obtain the groupoid product $(A^{1/2}B^{1/2}(001)_m)^2 = I$

Simple Groupoids and Their Subgroupoids The screw groupoids listed below, with their parent point groups in square brackets and all subgroupoids in parentheses, were derived from ITCrA Table 1.4d, which defines the graphical symbols. A single glide (g) without a screw normal to the glide plane will also have translation dimension one in the glide direction.

1. $[2]\ 2_1$
2. $[3]\ 3_1, 3_2$
3. $[4(2)]\ 4_1(2_1), 4_2(2), 4_3(2_1)$
4. $[6(3,2)]\ 6_1(3_1, 2_1), 6_2(3_2, 2), 6_3(3, 2_1), 6_4(3_1, 2), 6_5(3_2, 2_1)$
5. $[2/m(\overline{1})]\ 2_1/m(\overline{1})$
6. $[3/m]$
7. $[4/m(\overline{4}, 2/m, 2, \overline{1})]\ 4_2/m(\overline{4}, 2/m, 2, \overline{1})$,
8. $[6/m(3/m, \overline{3}, 3, 2/m, 2, \overline{1})]\ 6_3/m(3/m, \overline{3}, 3, 2/m, 2_1, \overline{1})$
9. $[n/m : n = 1, 2, 3, 4, 6]\ g, 2/g, 4/g, 2_1/g, 4_2/g$

Planes (m mirror and g glide) in the denominator of lines 5-9 are normal to the axis in the numerator. The translation vector T for line 9 is in the plane pointing in the glide direction. In space groups, glides denoted by g in line 9 will be relabeled a, b, or c if the translation is along a unit cell axis, n if along a diagonal such as the 1 1 0 direction, or d if the glide direction is parallel to an alternating series of primitive and centered Bravais lattice points in orthorhombic-F, tetragonal-I, cubic- F, and cubic-I Bravais lattices. Glide translation imcrements are 1/2 except for d-glides (called diamond glides) which have a translation increment of 1/4.

Geometric Interpretation of Simple Groupoids The vector line segments T of unit length one in the above entries 1-8 may be considered 1-dimensional groupoids with a cylindrical surrounding. The two ends of the line segment are the same point due to the modulo(1) operation. Thus screw entries on lines 1-4 may be considered circles, and those on lines 5-8 may be considered [0:1] intervals with half mirror points at the two end boundaries reflecting the line back into itself.

The glides are more complex in that the groupoid, g must be considered a real projective plane RP^2 cylinder. The translation vector itself is on a real projective plane line RP^1. An important characteristic of a real projective plane circle is its antipodal nature in that any vector in the plane of the circle which intersects the circle is transported half way around the circle and reemitted from the opposite side of the line with the same tangential angle as the angle of incidence. This forms two closed spaces one inside and one outside the circle. In addition, two fold screw axes circles project to antipodal circles.

Groupoids from General Point Groups The groupoids from dihedral, tetrahedral, and octahedral point groups have a series of vectors associated with their individual components. For example the dihedral point group 222 gives rise to three groupoids 222_1, 22_12_1, and $2_12_12_1$. In the third case we have three translation vectors along the three orthogonal screws plus translational vectors of length 1/4 seperating each pair of the three screw axes. The 186 screw and glide groupoids, which include the point groups, are listed in Jaswon and Rose.

Nomenclature Fortunately, screw and glide groupoids are implicit in the extended Hermann-Mauguin international crystallographic space group nomenclature system. We first examine the point group nomenclature since point groups are the basis for the groupoids.

Cubic Point Group Example The ITCrA nomenclature system uses the unit cell axes (a, b, c) as a base for the space group symbols in the triclinic, monoclinic, and orthorhombic crystal classes. However, if certain unit cell axes are related by symmetry, as in the tetragonal, trigonal, hexagonal, and cubic crystal classes, the nomenclature uses subgroups oriented along the three directions of highest but different symmetry called primary, secondary, and tertiary. In all crystal classes, point group can be generated through a direct product of properly oriented subgroups indicated by the three symbols in the international notation (assuming the positions of all elements are known). The tertiary element is sometimes redundant in the group generation.

In the cubic case, the primary, secondary, and tertiary subgroups are oriented along $a, a+b+c$, and $a+b$, but since all three axes are equivalent, coordinates along those directions are expressed as $x, 0, 0; x, x, x$; and $x, x, 0$. The Bravais lattice point group for the cubic crystal class is $\{4/m\ \overline{3}\ 2/m\}$. A geometrical interpretation of this point-group (groupoid) symbol is

(1) $4/m$– 4-fold axes along x, with mirror in xy plane;

(2) $\overline{3}$– 3-fold inversion axes along x, x, x;

(3) $2/m$– 2/m axes along $x, x, 0$.

The $\overline{3}$ axis along x, x, x, positions $4/m$ axes along the $a, b, c, -a, -b$, and $-c$ vectors which also generates an inversion center at the origin. The $4/m$ axes then places $\overline{3}$ axes along all four sign permutations of the $(1, 1, 1)$ axis, and mirrors 45 degrees apart around each axis. A general position x, y, z for point group $\{4/m\,\overline{3}\,2/m\}$ has multiplicity 48.

Orthorhombic Space Group ***Ibam*** (Short symbol $Ibam$, extended symbol $I2/b\ 2/a\ 2/m$, groupoid extended symbol $G(3) = I2_1/b\ 2_1/a\ 2/m$)

This space group is in the orthorhombic crystal system (with unit cell axes a, b, c all different but orthogonal), with body centered Bravais lattice $B = I$, and point group $Q = 2/m\ 2/m\ 2/m$. The screw and glide groupoid symbol $Q^* = G(3)/B = \{2_1/b\, 2_1/a\ 2/m\}$ has the following interpretation:

(a) $2_1/b$ – 2-fold screw axis parallel to a with b-glide plane normal to a,

(b) $2_1/a$ – 2-fold screw axis parallel to b with a-glide plane normal to b, and

(c) $2/m$ – 2-fold axis parallel to c with mirror plane normal to c;

which does not specify the relative positions of the axes and planes. This groupoid combines with primitive (P) and body-centered (I) Bravais lattices to form space groups $Pbam$ and $Ibam$ which have identical entries for their general Wyckoff site coordinates in ITCrA (omitting Bravais lattice translations). However, the different Bravais lattices produce quite different orbit spaces as shown by their special Wyckoff (isometry) sites and space group symmetry drawings in ITCrA.

This groupoid set containing eight operators is expressed in ITCrA matrix notation as,

$$\{x, y, z;\ \overline{x}, \overline{y}, z;\ \overline{x} + 1/2, y + 1/2, \overline{z};\ x + 1/2, \overline{y} + 1/2, \overline{z};$$

$$\overline{x}, \overline{y}, \overline{z};\ x, y, \overline{z};\ x + 1/2, \overline{y} + 1/2, z;\ \overline{x} + 1/2, y + 1/2, z\}$$

relative to origin $2/m$ at $c, c, 2/m$. It also may be written using cosets involving subgroupoid $\{2_1 2_1 2\}$ which has four operators, as

$$\{2_1 2_1 2\} = \{I, A^{1/2}B^{1/2}(100)^{1/2}, A^{1/2}B^{1/2}(010)^{1/2}, (001)^{1/2}\},$$

$$\{2_1/b\, 2_1/a\, 2/m\} = \{2_1 2_1 2\} + J\{2_1 2_1 2\},$$

where J is the inversion operator $(\overline{x}, \overline{y}, \overline{z})$, $A^{1/2}$ denotes translation along a of $1/2$, and (100) denotes rotation about a by $1/2$ cycle, etc. These equations describe the sequential origin shifts and rotation operations of the subgroupoid origin, screws and rotation in the first coset, and the inversion, glides and mirror in the second. A coset decomposition could have been carried out around any index-two normal subgroupoid such as $\{1\ 1\ 2/m\}$ or $\{2/b\ 2/a\ 2\}$, but the above choice of Jaswon and Rose seems more appropriate.

The ITCrA extended symbols for the space groups are $\{P2_1/b\ 2_1/a\ 2/m\}$ and $\{I2/b\ 2/a\ 2/m\}$ because $I222$ is a subgroup of $Ibam$ but $P222$ is not a subgroup of $Pbam$. Consequently, $\{222\}$ is not a subgroupoid of $\{2_1/b\ 2_1/a\ 2/m\}$ This problem arises because space-group subgroups are a function of the Bravais lattice but subgroupoids are not. The short symbols $Pbam$ and $Ibam$ properly depict the glide subgroupoids isomorphism.

Additional Orthorhombic Groupoids The other groupoids with subgroupoid $\{2_1 2_1 2\}$ as given by Jaswon and Rose are:

$$\{2_1/c\, 2_1/c\, 2/n\} = \{2_1 2_1 2\} + A^{1/2}B^{1/2}C^{1/2}J\{2_1 2_1 2\},$$

$$\{2_1/b\, 2_1/c\, 2/m\} = \{2_1 2_1 2\} + A^{1/2}J\{2_1 2_1 2\},$$

$$\{2_1/n\ 2_1/n\ 2/m\} = \{2_1 2_1 2\} + C^{1/2} J\{2_1 2_1 2\},$$
$$\{2_1/m\ 2_1/m\ 2/n\} = \{2_1 2_1 2\} + A^{1/2} B^{1/2} J\{2_1 2_1 2\},$$
$$\{2_1/b\ 2_1/c\ 2/n\} = \{2\ 2_1 2_1\} + C^{1/2} A^{1/2} J\{2\ 2_1 2_1\}.$$

which combine only with the primitive Bravais lattice P to form space groups numbered 56 through 60. However, the resulting space groups do not often have the same origin as those listed in ITCrA, where an inversion center is usually positioned at the origin point.

Orbifolds Orbifolds have received considerable attention in the low-dimensional geometric topology literature and are surveyed in a recent preprint.[9] Orbifolds provide closed space, non-redundant, pictorial and analytic portrayal of crystallographic group symmetry based on orbit space isometries (listed as special Wyckoff sites in ITCrA) which arise from fixed point, rotation axis, and mirror symmetry operators. Orbifolds for point group, Q, plane group, $G(2)$, and space group, $G(3)$, (spherical, Euclidean 2-, and Euclidean 3-orbifolds, respectively), are defined as S^2/Q, $E^2/G(2)$, and $E^3/G(3)$, respectively, with S^2 the 2-sphere and E^n Euclidean n-space. Literature references and orbifold drawings of the orbifolds for all point groups, plane groups, and cubic space groups are shown in Figures 2.3, 2.6, 2.8 and A.1 of Johnson, Burnett, and Dunbar.[10] A new nomenclature system for space groups based on orbifolds has been developed recently by John Conway and coworkers.[11]

If there are no inversion points, rotation axes, or mirrors in a specific $G(3)$, the quotient $E^3/G(3)$ produces an Euclidean 3-manifold (rather than an Euclidean 3-orbifold), with no orbits and thus no orbifold drawing, since screw and glide operators are not explicitly shown in an orbifold drawing. Other Euclidean 3-orbifolds have a sparse singular set which often contains relatively little information. This uneven treatment of the space groups is the reason we are trying to incorporate groupoids.

Orbifoldoids To incorporate screw and glide operators as an enhancement of the point-group's spherical 2-orbifold, we suggest use of the term "orbifoldoid", since there will be significant changes.

Screw and Glide Orbifoldoids The modulo(1) nature of the screw translation along a screw groupoid axis implies that a screw axis parallel to a coordinate axis is a line segment of unit length looped into a circle. For screw

[9] F. Bonahon, Geometric Structures on 3-manifolds, survey to appear in the Handbook of Geometric Topology, R. Daverman, R. Sher eds., Elsevier.
http://math.usc.edu/ fbonahon/Research/Preprints/Preprints.html

[10] C.K. Johnson, M.N. Burnett, and W.D. Dunbar, Crystallographic Topology and its Applications, in Crystallographic Computing 7, eds. P.E. Bourne,and K.D. Watenpaugh, Oxford, In Press, 2000.

[11] J.H. Conway, O. Delgado Friedrichs, D.H. Huson, and W. Thurston, Three-Dimensional Orbifolds and Space Groups http://www.mathematik.uni-bielefeld.de/ huson/papers.html

symbol k_n with $k = 2, 3, 4, 6; n < k$, one (+) transversal of the circle produces a right-handed screw rotation, except when $k > n > k/2$, when it becomes left handed. If the screw is 2-fold the circle is antipodal which often leads to a projective plane underlying topological space.

For symbol k_n/m, the line segment is the interval [0:1] with reversal of direction of travel at each mirror end point. We might call this an antipodal interval.

The next step is to characterize the groupoid quotients $E^1/Q^*(1)$, $E^2/Q^*(2)$, and $E^3/Q^*(3)$, where $Q^*(n)$ denotes those groupoids which have, 1-, 2-, or 3-dimensional screw and glide groupoid translation subspaces. However, more complex spaces than E^n seem to be required.

Orbifold Nomenclature The added orbifoldoid information must in some sense be related to the coupling invariants in the John Conway et al. preprint on an orbifold based space group nomenclature system in which they rederive the space groups by fibration over the 17 base Euclidean 2-orbifolds. However, because of the large quantity of crystallographic results currently available, we prefer to enhanced and clarify the present crystallographically familiar nomenclature system by expanding about the screw and glide groupoids or their orbifoldoids.

APPENDIX: Theorems from Jaswon and Rose

For Q^* a screw and glide groupoid derived from point group Q, translations A, B, C along a primative Bravais lattice P, and I, F, E, R centered lattices, Jaswon and Rose derived the following space group theorems.

Every Bravais lattice has a point-group symmetry with respect to any of its lattice points 0, which is the highest symmetry point group in each of the seven crystal class (holohedral point group). This implies that the primative translation group P must be compatible with the relevant point group Q, expressed as the coupling condition

$$Q_i P_1 Q_i^{-1} = P_2; \quad P_1, P_2 \subset \{P\}, \;\; Q_i \subset \{Q\}, \tag{1}$$

which serves as the foundation for space group theory. For the centered Bravais lattices we have the respective supplementary conditions:

body centered,

$$Q_i A^{1/2} B^{1/2} C^{1/2} Q_i^{-1} = A^{\pm 1/2} B^{\pm 1/2} C^{\pm 1/2} \subset A^{1/2} B^{1/2} C^{1/2} \{P\} \subset \{I\}; \tag{2}$$

face centered,

$$Q_i A^{1/2} B^{1/2} Q_i^{-1} = A^{\pm 1/2} B^{\pm 1/2} \subset \{A^{1/2} B^{1/2},\; B^{1/2} C^{1/2},\; C^{1/2} A^{1/2}\}\{P\} \subset \{F\}; \tag{3}$$

etc., for $B^{1/2} C^{1/2}$ and $C^{1/2} A^{1/2}$,

end centered,

$$Q_i A^{1/2} B^{1/2} Q_i^{-1} = A^{\pm 1/2} B^{\pm 1/2} \subset A^{1/2} B^{1/2} \{P\} \subset \{E\}; \tag{4}$$

and, double centered hexagonal (rhombohedral),

$$Q_i A^{2/3} B^{1/3} C^{1/3} Q_i^{-1} = \{A^{\pm 2/3} B^{\pm 1/3} C^{\pm 1/3}, A^{\pm 1/3} B^{\pm 2/3} C^{\pm 2/3}\}\{P\} \subset \{R\}. \tag{5}$$

Equations 1-5 allow generation of the 66 symmorphic space groups by using the direct product

$$\{G_s\} = \{Q\} \otimes \{P, I, F, E, R\}. \tag{6}$$

Theorem 1 *Given a groupoid $\{Q^*\}$ with the property $\{Q^*\} \Leftrightarrow \{Q\} mod \{P\}$, then $\{Q^*\} \otimes \{P\}$ is a space group if $\{Q\} \otimes \{P\}$ is a space group.*

More generally we write

$$Q_i^* = A^p B^q C^r Q_i; \quad Q_i \subset \{Q\}, \quad \{Q_i^*\} \subset \{Q^*\}; \quad 0 \leq |p|, |q|, |r| < 1 \tag{7}$$

and note that

$$Q_i^* P_1 Q_i^{*-1} = A^p B^q C^r Q_i P_1 Q_i^{-1} C^{-r} B^{-q} A^{-p} = P_2; \qquad P_1, P_2 \subset \{P\} \tag{8}$$

since $\{Q\}$ satisifies the coupling relation (1), the existance of $\{Q^*\} \otimes \{P\}$ follows from (8).

The theory can be extended to centered space groups by virtue of the following theorem.

Theorem 2 *Given a groupoid* $\{Q^*\}$ *with the property* $\{Q^*\} \Leftrightarrow \{Q\} mod \{P\}$ *then* $\{Q^*\} \otimes \{I\}$, $\{Q^*\} \otimes \{F\}$, $\{Q^*\} \otimes \{E\}$, $\{Q^*\} \otimes \{R\}$ *are space groups if, respectively,* $\{Q\} \otimes \{I\}$, *etc., are space groups.*

since, for instance

$$Q_i^* A^{1/2} B^{1/2} C^{1/2} Q_i^{*-1} = A^{\pm 1/2} B^{\pm 1/2} C^{\pm 1/2} \tag{9}$$

if

$$Q_i A^{1/2} B^{1/2} C^{1/2} Q_i^{-1} = A^{\pm 1/2} B^{\pm 1/2} C^{\pm 1/2}. \tag{10}$$

Jaswon and Rose point out that two limitations in this systematic procedure arise in practice.

(1) Most of the resulting space groups from Theorem 2 prove to be redundant, either because they are essentially covered by existing space groups, or because they are equivalent to cognate space groups sharing the same isomorphic properties, e.g. $\{4_2\} \otimes \{I\} = \{4\} \otimes \{I\}$, $\{4_3\} \otimes \{I\} = \{4_1\} \otimes \{I\}$, $\{2_1\} \otimes \{I\} = \{2\} \otimes \{I\}$, $\{3_1\} \otimes \{R\} = \{3\} \otimes \{R\}$, $\{2gg\} \otimes \{E\} = \{2gc\} \otimes \{E\}$. However, $\{a\} \otimes \{I\} \neq \{m\} \otimes \{I\}$, since a glide reflection is distinctly different from a pure reflection.

(2) This systematic procedure does not account for special space groups which fall outside the scope of Theorem 2, e.g. $\{4_1/a\} \otimes \{I\}$ exists even though $\{4_1/a\} \otimes \{P\}$ does not. Similarly, the introduction of diamond glide enables twelve space groups which can not be associated with any primative space lattice.