20.2-05 THE LATTICE PRESERVATION INTO THE DERIVATIVE LATTICES (ISOMORPHIC SUBGROUPS OF p1 AND P1).

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We consider the 2-dimensional space group Γ (p1), a conventional unit cell of which is (A, B). Any isomorphic subgroup γ (p1) may be defined by a unique conventional unit cell (a, b) connected to (A, B) by a suitable triangular transformation matrix S: (a, b) = (A, B)S;

$S = \begin{vmatrix} p_1 & q_1 \\ 0 & p_2 \end{vmatrix}$; p_1, p_2 positive integers; $p_1p_2 = i$ = index of γ with respect to Γ; q_1 integer; $-p_1/2 < q_1 \leqq p_1/2$.

Only a fraction 1/i of the nodes of the lattice-row family ρ [U, V] of Γ is preserved by γ according to these rules: (1) one node out of c_1 nodes is preserved by the lattice row ρ_o which contains the origin lattice point, (2) one lattice row out of i/c_1 lattice rows ρ is preserved in the same way as in the origin lattice row ρ_o, (3) all other lattice rows ρ are not preserved by γ. The preservation rates $1/c_1$ and c_1/i may be related to indices [U, V] in the following way. We define a new conventional unit cell (A°, B°) of Γ and a new conventional unit cell (a°, b°) of γ connected by an appropriate diagonal matrix Δ: $(A°, B°) = (A, B)Q^{-1}$; (a°, b°) = (a, b)P; (a°, b°) = (A°, B°)Δ; $\Delta = QSP = \begin{vmatrix} m_1 & 0 \\ 0 & m_1m_2 \end{vmatrix}$; m_1, m_2 positive integers; $m_1 = GCD(p_1, p_2, q_1)$ [GCD: greatest common divisor]; $m_1^2m_2 = i$; Q, P integer-entry matrices; DetQ = DetP = 1. With respect to (A°, B°) the new indices [U°, V°] of the lattice-row family ρ are given by:

$\begin{vmatrix} U° \\ V° \end{vmatrix} = Q\begin{vmatrix} U \\ V \end{vmatrix}$. It follows that $c_1 = m_1m_2/GCD(m_2, V°)$ and $i/c_1 = m_1GCD(m_2, V°)$. All considerations may be extended to the lattice preservation of rows ρ [U, V, W] of the 3-dimensional space group Γ (P1) (A, B, C) by any isomorphic subgroup γ (P1) (a, b, c):

(a, b, c) = (A, B, C)S; $S = \begin{vmatrix} p_1 & q_1 & r_1 \\ 0 & p_2 & q_2 \\ 0 & 0 & p_3 \end{vmatrix}$; p_1, p_2, p_3 positive integers, $p_1p_2p_3 = i$ = index of γ; q_1, q_2, r_1 integers; $-p_1/2 < q_1 \leqq p_1/2$; $-p_2/2 < q_2 \leqq p_2/2$; $-p_1/2 < r_1 \leqq p_1/2$; $(A°, B°, C°) = (A, B, C)Q^{-1}$; (a°, b°, c°) = (a, b, c)P; (a°, b°, c°) = (A°, B°, C°)Δ;

$\Delta = QSP = \begin{vmatrix} m_1 & 0 & 0 \\ 0 & m_1m_2 & 0 \\ 0 & 0 & m_1m_2m_3 \end{vmatrix}$; m_1, m_2, m_3 positive integers; m_1 is equal to the GCD of the S entries; $m_1^2m_2$ is equal to the GCD of the minors of S; $m_1^3m_2^2m_3 = i$; Q, P integer-entry matrices; DetQ = DetP = 1;

$\begin{vmatrix} U° \\ V° \\ W° \end{vmatrix} = Q\begin{vmatrix} U \\ V \\ W \end{vmatrix}$; $c_1 = m_1m_2m_3/GCD(m_2m_3, V°m_3, W°)$. The preservation of a lattice-plane family π of Γ (P1) by any isomorphic subgroup γ (P1) follows similar rules: (1) one node out of c nodes is preserved by the lattice plane π_o which contains the origin lattice point, (2) one lattice plane out of i/c lattice planes π is preserved as the origin lattice plane π_o, (3) all other planes π are not preserved. With respect to (A°, B°, C°) the new indices (H°, K°, L°) of the family π are given by $(H°, K°, L°) = (H, K, L)Q^{-1}$ and then it results:

$c = m_1^2m_2^2m_3/GCD(H°, K°m_2, L°m_2m_3)$ and

$i/c = m_1GCD(H°, K°m_2, L°m_2m_3)$.

20.2-06 CONDITIONS FOR TYPES OF DIRICHLET PARTITIONS AND OF SPHERE PACKINGS DERIVED FOR CUBIC POINT CONFIGURATIONS.

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Each homogeneous point configuration (set of symmetrically equivalent points) corresponds exactly to one Dirichlet partition (partition of space into Dirichlet domains). In addition it defines uniquely a sphere configuration with the following properties: each point of the configuration is the center of one sphere; all spheres are equal in size; each sphere has contact to at least one other sphere; no spheres overlap. Such a configuration is called a sphere packing if each sphere can be reached from a given one by a chain of spheres in contact.

Within a lattice complex or Wyckoff position with degrees of freedom, several types of sphere configurations and several types of Dirichlet partitions may exist. Normally, the lines which form the boundaries for the types of space partitions do not coincide with those lines which bound the types of sphere configurations. A particular sphere-packing type, therefore, often corresponds to more than one type of Dirichlet partitions, and a particular type of such space partitions often corresponds to several sphere configurations.

The type of sphere configurations (or sphere packings) describes the shortest connections within the framework of a crystal structure.

The corresponding space partition into Dirichlet domains contains all information on the voids within that framework, because all voids together build up a three-dimensional tiling which is dual to that Dirichlet partition. For the description or classification of crystal structures with the aid of anion frameworks, therefore, both aspects have to be taken into account (Koch and Hellner, Z. Kristallogr. (1981) 154, 95).

For all cubic lattice complexes with one or two degrees of freedom, the Dirichlet partitions (Koch, Z. Kristallogr. (1973) 138, 196) and sphere configurations (Fischer, Z. Kristallogr. (1973) 138, 129) are juxtaposed. Examples corresponding to crystal structures will be choosen for presentation.