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Geometrical Relationships between Nets Mapped on Isomorphic Quotient Graphs: Examples

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The point group of a three-periodic net is generally isomorphic to a subgroup of the automorphism group of its quotient graph. Emphasis is given to the *n*-periodic net of maximal symmetry whose point group is isomorphic to the automorphism group. These characteristic nets, which are unique up to isomorphism, have been determined for the following graphs: $K_3^{(2)}$, $2K_2 \cup 2K_2^{(3)}$, $C_4^{(2)}$, $K_2^{(2)} + K_2^{(2)}$, $K_{2(6),4(3)}$, and AP_4. It is shown that the topology of three-periodic nets admitting these graphs as their quotient graph is generated by orthogonal projection of the net of maximal symmetry. © 1998 Academic Press

I. INTRODUCTION

In the vector method developed by Chung *et al.* (1), three-periodic nets are uniquely characterized by labeled quotient graphs. The labeling of the edges has been proposed to distinguish among nonisomorphic nets which are mapped on isomorphic quotient graphs. This paper explores the geometrical principles which underlie the labeling. The issue is best illustrated by analyzing a two-dimensional example proposed by Klee (2). Consider the planar nets $8^2 \cdot 4$ and $(9^3, 9^2 \cdot 3)$ represented by Fig. 1: both are mapped on the complete graph K_4 but they belong to different topologies and symmetry groups ($p4mm$ and $p3m1$ respectively). Interestingly, Wells (3) had already observed that these nets are obtained by orthogonal projection of the uniform three-periodic net (10, 3)-a (space group $I4_132$) along its four-fold and three-fold axes respectively. Now, we note that the net (10, 3)-a too is mapped on the graph K_4, and moreover that its point group, O, is isomorphic to the automorphism group, S_4, of its quotient graph. The aim of this work is to show that various three-periodic nets which are mapped on isomorphic quotient graphs bear the same property and can be drawn by projection of a unique (up to isomorphism) higher-dimensional net with maximal symmetry.

II. DEFINITIONS AND CONCEPTS

Graph theoretical methods (4) are used throughout the paper. For convenience, we recall some terms previously defined by Chung *et al.* (1). In a three-periodic net, a point lattice is a class of translationally equivalent vertices (atoms). A line lattice, in the same fashion, is a class of translationally equivalent edges (bonds) and is thus associated with a pair of point lattices. The quotient graph of the net is defined in such a way that its vertices and edges map the point and line lattices respectively. It is thus a finite graph that reflects the adjacency relations in the net. Once a unit cell and an origin have been chosen, a labeled quotient graph is obtained by assignment, to each line lattice, of a vector of the translation group, T, of the net. This vector is designated by the three Miller indices that label the cell containing the extremity of an edge which begins in the origin cell and belongs to that line lattice. The labeling uniquely determines the net.

The automorphism group, Aut(G), of the quotient graph G is understood as in (1) to include the exchange of loops and multiple edges when they exist. According to an observation by Klee (2), the factor group of the net is isomorphic to a subgroup of Aut(G).

Let us write as e_i ($i = 1, \dots, n$) the edges of G and $\mathbf{r}_i$ ($h_i\, k_i\, l_i$) the vector that labels the edge e_i. To any closed walk ($e_a e_b \dots e_k$) of G, we associate the sum $\mathbf{s} = \varepsilon_a \mathbf{r}_a + \varepsilon_b \mathbf{r}_b + \dots + \varepsilon_k \mathbf{r}_k$, where ε_i is $+1$ if the edge e_i is taken with the right orientation along the walk and -1 otherwise. Clearly, a closed walk in the quotient graph maps a walk in the net that has both its origin, **O**, and extremity, **E**, in the same point lattice. This shows that the vector $\mathbf{s} = \mathbf{OE}$ defines a translation of the normal translation subgroup of the net: $\mathbf{s} \in T$. In particular, we obtain a mapping of the cycles of G on the translation group T of the net; this mapping induces a linear mapping of the cycle space—defined as a Z-module—in the three-dimensional embedding of the net. For convenience, we extend the cycle space on the field of real numbers and identify *i*) the embedding of the net to

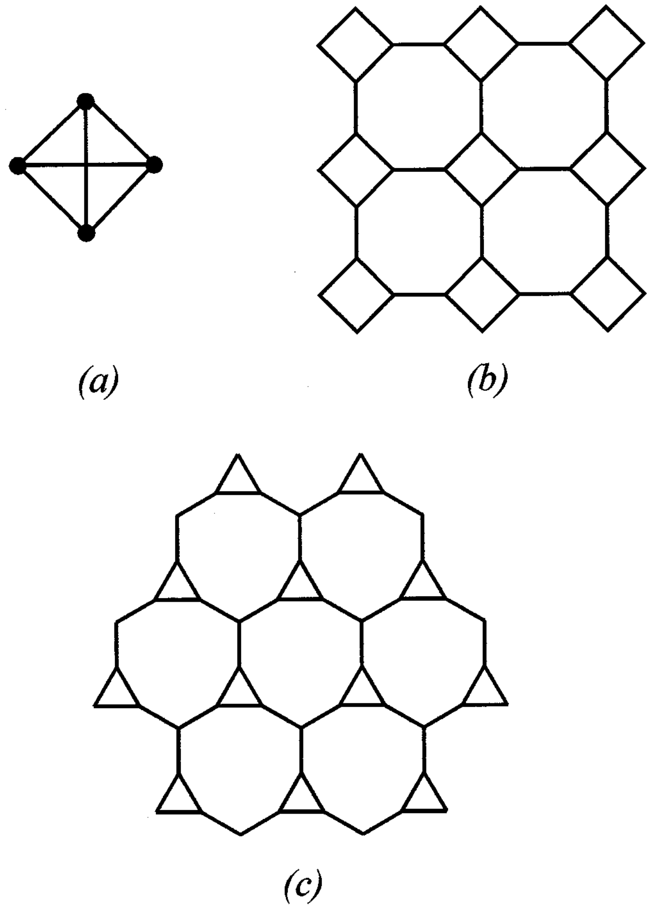

FIG. 1. Two planar net mapped (a) on the complete graph K_4, (b) net $8^2 \cdot 4$, (c) net $(9^3, 9^2 \cdot 3)$.

a subspace of the cycle space and *ii*) the linear mapping with a projection in the cycle space.

It is useful to define the *archetype* N[G] as the net with maximal symmetry which is mapped on the quotient graph G, and embedded in the cycle space. Let v be the cyclomatic number of G, i.e., the dimension of the cycle space: $v = n - p + 1$ (n, p: number of edges and vertices of G). We label the quotient graph with v basis vectors of the cycle space. By extending the results of Chung *et al.* (1), it can be seen that this labeling uniquely defines a net in the cycle space, up to isomorphism. Then we construct a representation of the automorphism group, Aut(G), in the cycle space. The method, based on the permutations of the cycle vectors of G by Aut(G), is illustrated in the next parts of the paper for various examples. In general, it generates a group of unimodular matrices which is thus isomorphic to some v-dimensional crystallographic point group (5). The archetype N[G] is obtained when the basis of the cycle space is suitably chosen so that the point group of the net is isomorphic to the group Aut(G).

III. GRAPH NOMENCLATURE

Figure 2 shows the quotient graphs of some MA_2 nets with tetrahedral coordination, up to four formula units in the primitive cell, and one net with octahedral coordination and two formula units in the primitive cell. As far as possible, we have adopted the conventional nomenclature used in graph theory (4). $K_3^{(2)}$ means the complete graph of three vertices where all edges have been duplicated. $2K_2^{(3)}$ is the juxtaposition of two identical components that are isomorphic to the complete graph of two vertices with triple edges. The union $G_1 \cup G_2$ of two graphs G_1 and G_2 that have the same set of vertices is the graph whose edge set is the reunion of the edges of the two graphs. Thus, $2K_2$ and $2K_2^{(3)}$ are two graphs with four vertices. We consider that their union $2K_2 \cup 2K_2^{(3)}$ is the connected graph represented in Fig. 2. $C_4^{(2)}$ is the cycle with four vertices and double edges. The join $G_1 + G_2$ of two graphs G_1 and G_2 is defined by adding all edges joining them. The join of two identical "double edges" graphs $K_2^{(2)}$ is shown in Fig. 2. $K_{2(6),4(3)}$ symbolizes a bipartite graph in which each of the two

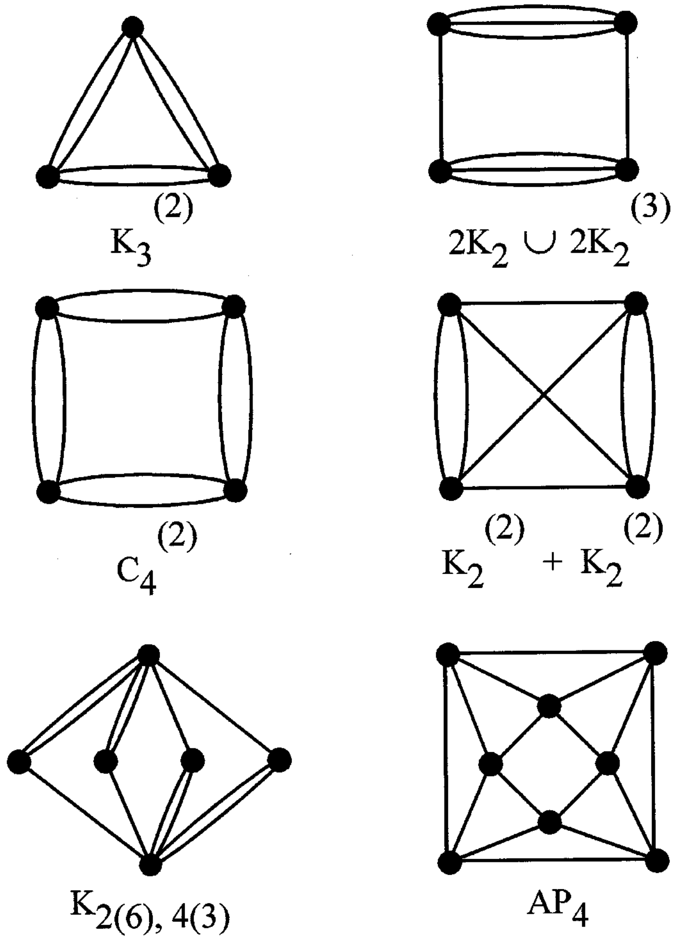

FIG. 2. Nomenclature of some simple graphs.

six-valent vertices is linked at least once to each of the four three-valent vertices. Finally, AP_4 corresponds to the graph of the square antiprism.

IV. $N[K_3^{(2)}]$

The quotient graph, $K_3^{(2)}$, of the quartz net after contraction (elimination of the two-valent vertices) is shown in Fig. 3a. An arbitrary labeling in the cycle space has been chosen. Since its cyclomatic number is $v = 4$, this net provides a simple illustration for the ideas developed above. Among other simple cases are the three-dimensional ones ($v = 3$), such as the (10, 3)-a, ReO_3, and diamond nets which correspond to $N[K_4]$, $N[K_{1,3}^{(2)}]$, and $N[K_2^{(4)}]$ respectively and can be analyzed in the same way.

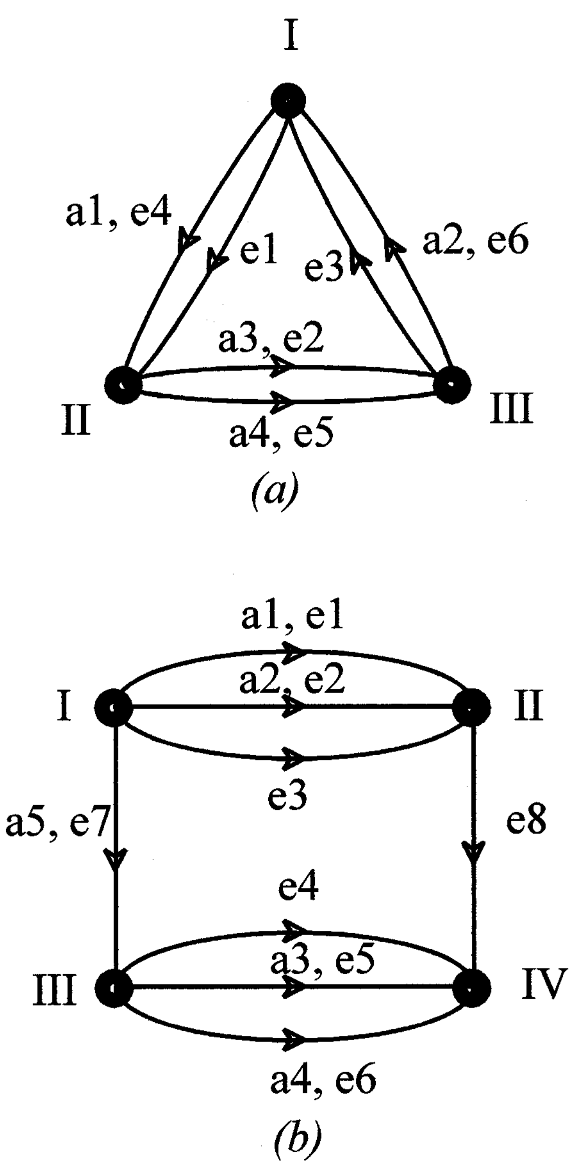

FIG. 3. Labeled quotient graphs: (a) $K_3^{(2)}$; (b) $2K_2 \cup 2K_2^{(3)}$.

We first write the set of *topological relations* [1], which define the basis cycle vectors from the line lattices by using one labeled edge and completing the elementary cycle in G with edges of the spanning tree; each edge is affected by the negative sign when its own direction is opposed to that of the cycle:

$$a_1 = e_4 - e_1,$$

$$a_2 = e_6 - e_3,$$

$$a_3 = e_2 + e_3 + e_1,$$

$$a_4 = e_5 + e_3 + e_1. \qquad [1]$$

We then write the generators of the automorphism group Aut(G) as permutations of the edges; when the orientation of the edge is not preserved, negative signs are used:

E: (e_2, e_5),

C: $(e_1, e_2, e_3)(e_4, e_5, e_6)$,

D: $(e_1, -e_3)(e_4 - e_6)(e_2, -e_2)(e_5, -e_5)$.

The matrices of the generators of the representation of Aut(G) in the cycle space are obtained by determining for each basis cycle vector, the vector mapped after permutation of its edges. For example,

$$C(a_1) = C(e_4 - e_1) = C(e_4) - C(e_1) = e_5 - e_2 = a_4 - a_3.$$

The following matrices are obtained:

$$E := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \qquad C := \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix},$$

$$D := \begin{bmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}.$$

Let us introduce an orthonormal basis α_i, $i = 1, \ldots, 4$ in the cycle space, the transformation matrix P, its transpose P^t and the matrix Z whose entries are the scalar products of the basis vectors a_i.

$$(a_1, \ldots, a_4) = (\alpha_1, \ldots, \alpha_4) \cdot P$$

$$Z = P^t \cdot P$$

We determine the nature of the cycle basis of G in order that the three matrices representing the generators of the automorphism group be isometries by solving Eqs. [2].

$$\mathrm{M}^{t}\cdot \mathrm{Z}\cdot \mathrm{M}=\mathrm{Z} \qquad \mathrm{M}=\mathrm{E},\mathrm{C},\mathrm{D} \tag{2}$$

We obtain:

$$\mathrm{P}=\begin{bmatrix} a & 0 & -\frac{a}{2} & -\frac{a}{2} \\ 0 & a & -\frac{a}{2} & -\frac{a}{2} \\ 0 & 0 & \frac{b}{2} & \frac{b}{2} \\ 0 & 0 & \frac{a}{2} & -\frac{a}{2} \end{bmatrix}.$$

The couple (a,b) corresponds to arbitrary lattice parameters. In the classification of four-dimensional crystallographic groups by Brown *et al.* (5), the net belongs to the cubic orthogonal family; its Bravais type is XVII/IV (Z-centered). In the orthonormal basis, the new matrices for the generators of Aut(G) are

$$\mathrm{E}\alpha:=\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \qquad \mathrm{C}\alpha:=\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix},$$

$$\mathrm{D}\alpha:=\begin{bmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}.$$

It can be seen that these matrices generate the same group as Z-class 25/08/03. In the following equations, the generators following Brown *et al.* (5) are explicitly given from the matrices obtained in this work:

$$\mathrm{A}=\mathrm{X}^{-1}\cdot(\mathrm{C}\alpha^{2}\cdot\mathrm{E}\alpha\cdot\mathrm{C}\alpha\cdot\mathrm{E}\alpha)\cdot\mathrm{X},$$

$$\mathrm{B}=\mathrm{X}^{-1}\cdot(\mathrm{C}\alpha^{2}\cdot\mathrm{E}\alpha\cdot\mathrm{C}\alpha^{2}\cdot\mathrm{E}\alpha\cdot\mathrm{C}\alpha^{2})\cdot\mathrm{X},$$

$$\mathrm{C}=\mathrm{X}^{-1}\cdot(\mathrm{E}\alpha\cdot\mathrm{C}\alpha\cdot\mathrm{E}\alpha\cdot\mathrm{C}\alpha\cdot\mathrm{E}\alpha)\cdot\mathrm{X},$$

$$\mathrm{D}=\mathrm{X}^{-1}\cdot(\mathrm{E}\alpha\cdot\mathrm{C}\alpha\cdot\mathrm{D}\alpha\cdot\mathrm{C}\alpha^{2}\cdot\mathrm{E}\alpha)\cdot\mathrm{X}.$$

Matrix X gives the basis vectors used by Brown *et al.* (5) in our orthonormal basis.

$$\mathrm{X}=\begin{bmatrix} 0 & \frac{a}{2} & \frac{a}{2} & -\frac{a}{2} \\ 0 & \frac{a}{2} & -\frac{a}{2} & \frac{a}{2} \\ b & -\frac{b}{2} & -\frac{b}{2} & \frac{b}{2} \\ 0 & \frac{a}{2} & -\frac{a}{2} & -\frac{a}{2} \end{bmatrix}.$$

On the other hand, the line lattices must verify the topological relations [1] and are related to one another by the permutations of the automorphism group. This allows their calculation in the orthonormal basis:

$$(e_1,\ldots,e_6)=\begin{bmatrix} -\frac{a}{2} & 0 & 0 & \frac{a}{2} & 0 & 0 \\ 0 & 0 & -\frac{a}{2} & 0 & 0 & \frac{a}{2} \\ \frac{b}{6} & \frac{b}{6} & \frac{b}{6} & \frac{b}{6} & \frac{b}{6} & \frac{b}{6} \\ 0 & \frac{a}{2} & 0 & 0 & -\frac{a}{2} & 0 \end{bmatrix}.$$

Let us define $[\mathrm{M},\mathrm{u}(\mathrm{M})]$, the augmented matrix associated to permutation M. We find the vector u(M) by examining the point lattice mapped by the symmetry operation:

$$[\mathrm{E},\mathrm{u}(\mathrm{E})]\cdot\mathrm{I}=\mathrm{I},$$

$$[\mathrm{C},\mathrm{u}(\mathrm{C})]\cdot\mathrm{I}=\mathrm{II},$$

$$[\mathrm{D},\mathrm{u}(\mathrm{D})]\cdot\mathrm{I}=\mathrm{I}.$$

These equations lead to the vectorial system [3], after setting point lattice I at an arbitrary position x (the symbol '$\equiv$' means translationally equivalent).

$$\begin{aligned} \mathrm{u}(\mathrm{E}) &\equiv (1-\mathrm{E})\cdot x, \\ \mathrm{u}(\mathrm{C}) &\equiv e_1+(1-\mathrm{C})\cdot x, \\ \mathrm{u}(\mathrm{D}) &\equiv (1-\mathrm{D})\cdot x. \end{aligned} \tag{3}$$

Let us choose $x=0\,0\,0\,a/2$ in the orthonormal basis so that we find:

$$\begin{aligned} \mathrm{u}(\mathrm{E}) &\equiv 0, \\ \mathrm{u}(\mathrm{C}) &\equiv 2/3\cdot b\cdot\alpha_3 \\ \mathrm{u}(\mathrm{D}) &\equiv 0. \end{aligned} \tag{4}$$

The space group can now be identified as group 25/08/03/003 in the classification of Brown *et al.* (5). For completeness, we repeat the relative coordinates of the point lattices of $\mathrm{N}[\mathrm{K}_3^{(2)}]$ in the cubic orthogonal cell:

I:	0	0	0	1/2	1/2	1/2	1/2	0
II:	1/2	0	1/6	1/2	0	1/2	2/3	0
III:	1/2	0	1/3	0	0	1/2	5/6	0

Moreover, by choosing for the cell parameters $a=\sqrt{(8/3)}$ and $b=2\sqrt{3}$, the distance between nearest neighbors are all equal to unity and all bond angles have the tetrahedral value; each point of the structure is at the center of a regular tetrahedron.

We turn now to the generation of the quartz net by projection of the archetype $\mathrm{N}[\mathrm{K}_3^{(2)}]$. We first note that the matrices D and $E \cdot C \cdot E \cdot C \cdot E$ in Aut(G) generate a subgroup which is isomorphic to the point group D_6. This four-dimensional representation of D_6 is reducible to the sum $A_2 + E_1 + B_2$. From character tables, we know that representations A_2 and E_1 behave as coordinates z and (x, y) respectively. Representation B_2 cannot correspond to any geometrical axis, and must therefore be the kernel of the projection. By using the group-theoretical projection operator [5], in which the summation $\sum$ is extended over all matrices R of the subgroup and $\chi(R)$ is the character in the representation B_2 of the associated symmetry operation in D_6 (6), we find that the vector $\alpha_1 + \alpha_2 - \alpha_4$ behaves as representation B_2.

$$P(B_2) = \sum \chi(R) \cdot R. \qquad [5]$$

It can be verified that the orthogonal projection of the net $N[K_3^{(2)}]$ along this vector onto a three-dimensional subspace generates a net with the linkage pattern of the quartz structure.

V. $N[2K_2^{(3)} \cup 2K_2]$

The quotient graph of the tridymite net is shown in Fig. 3b. The generators of the automorphism group Aut(G) and the topological relations are detailed below.

A: (e_1, e_2),

B: (e_1, e_2, e_3),

C: (e_7, e_8) and $(e_i, -e_i)$ for $i = 1, \ldots, 6$,

D: $(e_1, e_5)(e_2, e_6)(e_3, e_4)(e_7, -e_7)(e_8, -e_8)$,

$$a_1 = e_1 - e_3,$$

$$a_2 = e_2 - e_3,$$

$$a_3 = e_5 - e_4,$$

$$a_4 = e_6 - e_4,$$

$$a_5 = e_7 + e_4 - e_8 - e_3.$$

We list the transformation matrix P (with cell parameters a and b) describing the basis cycle vectors in the orthonormal basis (α), the matrices of the generators of Aut(G), and finally the matrix giving the coordinates of the line lattices equally in the orthonormal basis (α).

$$P = \begin{bmatrix} a & \frac{a}{2} & 0 & 0 & \frac{a}{2} \\ 0 & \frac{a \cdot \sqrt{3}}{2} & 0 & 0 & \frac{a}{2 \cdot \sqrt{3}} \\ 0 & 0 & a & \frac{a}{2} & -\frac{a}{2} \\ 0 & 0 & 0 & \frac{a \cdot \sqrt{3}}{2} & -\frac{a}{2 \cdot \sqrt{3}} \\ 0 & 0 & 0 & 0 & b \end{bmatrix},$$

$$A := \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$B := \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & 0 & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$C := \begin{bmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{bmatrix},$$

$$D := \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{bmatrix},$$

$(e_1, \ldots, e_8) =$

$$\begin{bmatrix} \frac{a}{2} & 0 & -\frac{a}{2} & 0 & 0 & 0 & 0 & 0 \\ -\frac{a}{2 \cdot \sqrt{3}} & \frac{a}{\sqrt{3}} & -\frac{a}{2 \cdot \sqrt{3}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{a}{2} & \frac{a}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{a}{2 \cdot \sqrt{3}} & -\frac{a}{2 \cdot \sqrt{3}} & \frac{a}{\sqrt{3}} & 0 & 0 \\ u & u & u & -u & -u & -u & u + \frac{b}{2} & -u - \frac{b}{2} \end{bmatrix}.$$

In this last matrix, u is an arbitrary parameter. The translation parts of the augmented matrices are more naturally expressed in the cycle vectors basis by choosing the position of vertex I at $x = (e_3 - e_1 - e_2)/2$:

$$u(A) = 0$$

$$u(B) = 0$$

$$u(C) = 0$$

$$u(D) = (-a_1 - a_2 + a_3 + a_4 + a_5)/2.$$

We now examine the nature of the projection by looking at different subgroups of Aut(G). Consider first the subgroup generated by the four matrices $(B \cdot D)^2$, $(A \cdot D)^2$, C, and D. This is matrix representation which is isomorphic to the three-dimensional point group D_{6h}. It is reducible to the sum $E_{1u}+A_{2u}+E_{2u}$. The first irreducible representation in this sum behaves as coordinates (x, y) and the second as coordinate z. The subspace associated with the representation E_{2u} must therefore be the kernel of the projection. Application of the group-theoretical projection operator yields the vectors $\alpha_1-\alpha_3$ and $\alpha_2-\alpha_4$ as a basis for the kernel, and thus as projection vectors. It can be verified that the tridymite net is obtained after projection, with the correct space group.

Consider now the group generated by matrices $B\cdot D\cdot A\cdot D$ and C; it is isomorphic to point group C_{6h}. The reduction of the representation yields $2A_u+B_u+E_{2u}$. Only the former representation behaves as coordinate z; this subgroup cannot generate any three-dimensional net by projection.

Finally, the subgroup generated by matrices B and C is isomorphic to point group S_6, in which the representation is reduced to $3A_u+E_u$. Although the former representation behaves as coordinate z and the latter as the couple (x, y), the projection is not compatible with a three-dimensional embedding because of superposition of the bonds around atoms II and IV.

VI. $N[C_4^{(2)}]$

The labelled quotient graph $C_4^{(2)}$ is shown in Fig. 4a. We list below the generators of its automorphism group Aut(G) and the topological relations.

$$A: (e_1, e_2),$$

$$B: (e_1, e_5)(e_2, e_6)(e_3, e_7)(e_4, e_8),$$

$$C: (e_1, e_3)(e_2, e_4)(e_i, -e_i) \quad i=5, \ldots, 8,$$

$$D: (e_1, e_8, -e_4, -e_5)(e_2, e_7, -e_3, -e_6),$$

$$a_1=e_1-e_2,$$

$$a_2=e_3-e_4,$$

$$a_3=e_5+e_4-e_8-e_2,$$

$$a_4=e_6+e_4-e_8-e_2,$$

$$a_5=e_7-e_8.$$

The transformation matrix P (with cell parameters a and b) giving the coordinates of the basis cycle vectors in the orthonormal basis (α), the matrices of the generators of Aut(G), and finally the matrix giving the coordinates of the line lattices equally in basis (α) are listed below.

$$P=\begin{bmatrix} a & 0 & \frac{a}{2} & \frac{a}{2} & 0 \\ 0 & a & -\frac{a}{2} & -\frac{a}{2} & 0 \\ 0 & 0 & b & b & 0 \\ 0 & 0 & \frac{a}{2} & -\frac{a}{2} & 0 \\ 0 & 0 & \frac{a}{2} & \frac{a}{2} & \frac{a}{2} \end{bmatrix},$$

$$A:=\begin{bmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad B:=\begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix},$$

$$C:=\begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{bmatrix},$$

$$D:=\begin{bmatrix} 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 \end{bmatrix},$$

$$(e_1, \ldots, e_8)=$$

$$\begin{bmatrix} \frac{a}{2} & -\frac{a}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{a}{2} & -\frac{a}{2} & 0 & 0 & 0 & 0 \\ -\frac{b}{4} & -\frac{b}{4} & \frac{b}{4} & \frac{b}{4} & \frac{b}{4} & \frac{b}{4} & -\frac{b}{4} & -\frac{b}{4} \\ 0 & 0 & 0 & 0 & \frac{a}{2} & -\frac{a}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{a}{2} & -\frac{a}{2} \end{bmatrix}.$$

The subgroup of Aut(G) generated by the matrices B and $(C\cdot D)^2$ is a matrix representation which is isomorphic to the three-dimensional point group D_2. This representation is reduced to the sum $\Gamma=2B_1+B_2+2B_3$. The kernel of the projection must contain two vectors behaving as representation B_1+B_3. This may be achieved by choosing the two vectors $\alpha_1-\alpha_2$ and $\alpha_4-\alpha_5$ as projection vectors. The topology obtained after projection of the five-dimensional net is that of $Zn(OH)_2$, or a distortion of the cristobalite structure.

VII. $N[K_2^{(2)}+K_2^{(2)}]$

The labeled quotient graph is shown in Fig. 4b. The generators of the automorphism group Aut(G) and the

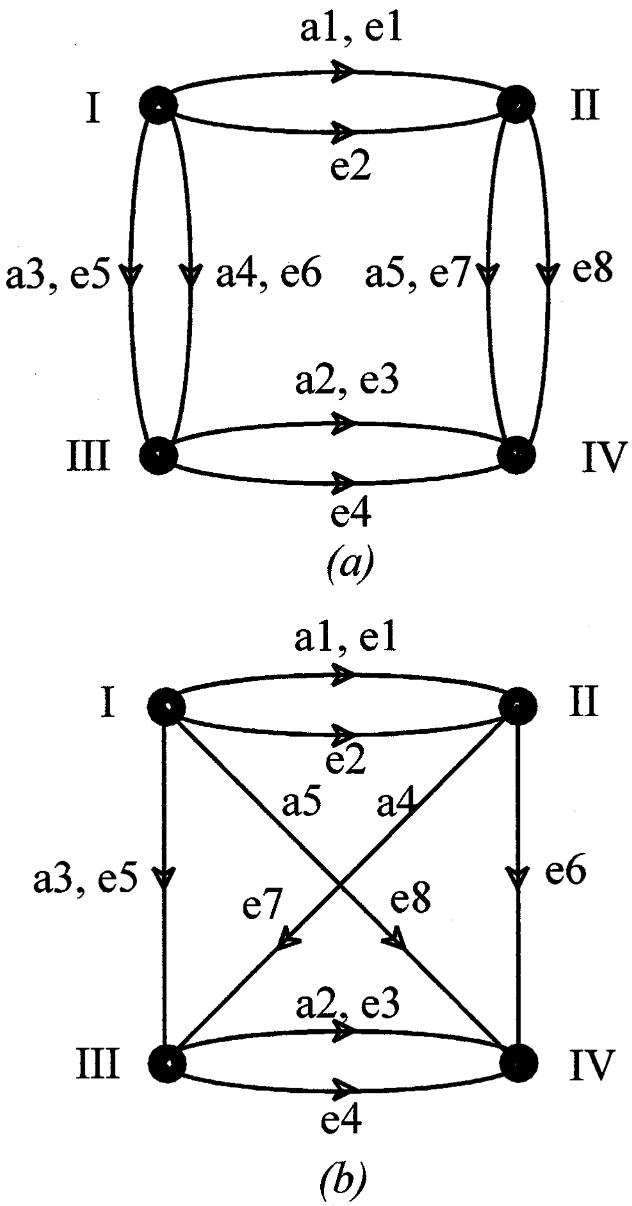

FIG. 4. Labeled quotient graphs: (a) $C_4^{(2)}$; (b) $2K_2^{(2)} + K_2^{(2)}$.

topological relations are given below.

A: (e_1, e_2),

B: $(e_1, e_3)(e_2, e_4)(e_5, -e_5)(e_6, -e_6)(e_7, -e_8)$,

C: $(e_5, e_6)(e_8, e_8)(e_i, -e_i)\ i = 1, \ldots, 4$,

D: $(e_3, -e_3)(e_4, -e_4)(e_5, e_8)(e_6, e_7)$,

$$a_1 = e_1 - e_2,$$

$$a_2 = e_3 - e_4,$$

$$a_3 = e_5 + e_4 - e_6 - e_2,$$

$$a_4 = e_7 + e_4 - e_6,$$

$$a_5 = e_8 + e_6 - e_2.$$

The transformation matrix P (with cell parameters a, b, and c) giving the coordinates of the basis cycle vectors in the orthonormal basis (α), the matrices of the generators of Aut(G), and finally the matrix giving the coordinates of the line lattices equally in basis (α) are listed below.

$$P = \begin{bmatrix} a & 0 & \frac{a}{2} & 0 & \frac{a}{2} \\ 0 & a & -\frac{a}{2} & -\frac{a}{2} & 0 \\ 0 & 0 & b & \frac{b}{2} & \frac{b}{2} \\ 0 & 0 & 0 & \frac{b}{2} & -\frac{b}{2} \\ 0 & 0 & 0 & \frac{c}{2} & \frac{c}{2} \end{bmatrix},$$

$$A := \begin{bmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$B := \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{bmatrix},$$

$$C := \begin{bmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$D := \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{bmatrix},$$

$(e_1, \ldots, e_8) =$

$$\begin{bmatrix} \frac{a}{2} & -\frac{a}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{a}{2} & -\frac{a}{2} & 0 & 0 & 0 & 0 \\ -x & -x & x & x & \frac{b}{2}-x & x-\frac{b}{2} & 0 & 0 \\ x & x & x & x & 0 & 0 & \frac{b}{2}-x & x-\frac{b}{2} \\ 0 & 0 & 0 & 0 & -\frac{c}{4} & -\frac{c}{4} & \frac{c}{4} & \frac{c}{4} \end{bmatrix}.$$

In the line lattices matrix, x is an undefined parameter. Consider now the subgroup of Aut(G) generated by the matrices B, C, and $H = (A \cdot B)^2$. This is a matrix representation which is isomorphic to the three-dimensional point group D_{2h}. Although many isomorphisms map these two groups on each other, only two of them lead to different and realizable projections. The first one is obtained by mapping the inversion on matrix C and the reflections on matrices B, H and $B \cdot C \cdot H$. The representation is then reduced to the sum: $\Gamma = A_u + B_{2g} + B_{1u} + B_{2u} + B_{3u}$. The kernel of the projection consists of the subspace behaving as the sum of the two representations A_u and B_{2g}, whose basis is given by the vectors $\alpha_1 - \alpha_2$ and α_5. The projection is onto the subspace generated by the vectors α_4, $\alpha_1 + \alpha_2$, and α_3. It can be verified that the projection corresponds to the structure of $CaAl_2Si_2O_8$, with space group *Immm*; we may choose the origin so that vertex I is at position $-1/2(e_5 + e_8)$.

The second isomorphism maps the inversion on matrix $B \cdot H$ and the reflections on H, $C \cdot H$, and $B \cdot C \cdot H$. The representation is reduced to $\Gamma = B_{2g} + B_{3g} + B_{1u} + B_{2u} + B_{3u}$. The projection is along the vectors α_4 and $\alpha_1 - \alpha_2$ onto the subspace generated by the vectors α_3, $\alpha_1 + \alpha_2$, and α_5 and defines the structure of $RbAlSiO_4$ with space group *Imma*; we may choose vertex I at position $1/2(e_3 + e_4 - e_6)$.

VIII. RUTILE AND ANATASE: $N[K_{2(6),4(3)}]$

Figure 5 shows the labeled quotient graph. The generators of the automorphism group Aut(G) and the topological relations are given below:

A: (e_1, e_2),

B: $(e_1, e_3)(e_2, e_4)(e_7, e_8)$,

C: $(e_1, e_{12})(e_2, e_{11})(e_3, e_{10})(e_4, e_9)(e_5, e_8)(e_6, e_7)$,

$a_1 = e_1 - e_2$,

$a_2 = e_3 - e_4$,

$a_3 = e_{10} - e_9$,

$a_4 = e_{12} - e_{11}$,

$a_5 = e_5 - e_9 + e_8 - e_4$,

$a_6 = e_6 - e_{11} + e_8 - e_4$,

$a_7 = e_7 - e_2 + e_4 - e_8$.

The transformation matrix P (with cell parameters a, b, and c) giving the coordinates of the basis cycle vectors in the orthonormal basis (α), the matrices of the generators of Aut(G), and finally the matrix giving the coordinates of the line lattices equally in the orthonormal basis (α) are listed below.

$$P = \begin{bmatrix} a & 0 & 0 & 0 & 0 & 0 & \frac{a}{2} \\ 0 & a & 0 & 0 & \frac{a}{2} & \frac{a}{2} & -\frac{a}{2} \\ 0 & 0 & a & 0 & \frac{a}{2} & 0 & 0 \\ 0 & 0 & 0 & a & 0 & \frac{a}{2} & 0 \\ 0 & 0 & 0 & 0 & b & b & 0 \\ 0 & 0 & 0 & 0 & \frac{c}{2} & -\frac{c}{2} & 0 \\ 0 & 0 & 0 & 0 & -\frac{c}{2} & -\frac{c}{2} & c \end{bmatrix},$$

$$A := \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$B := \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix},$$

$$C := \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix},$$

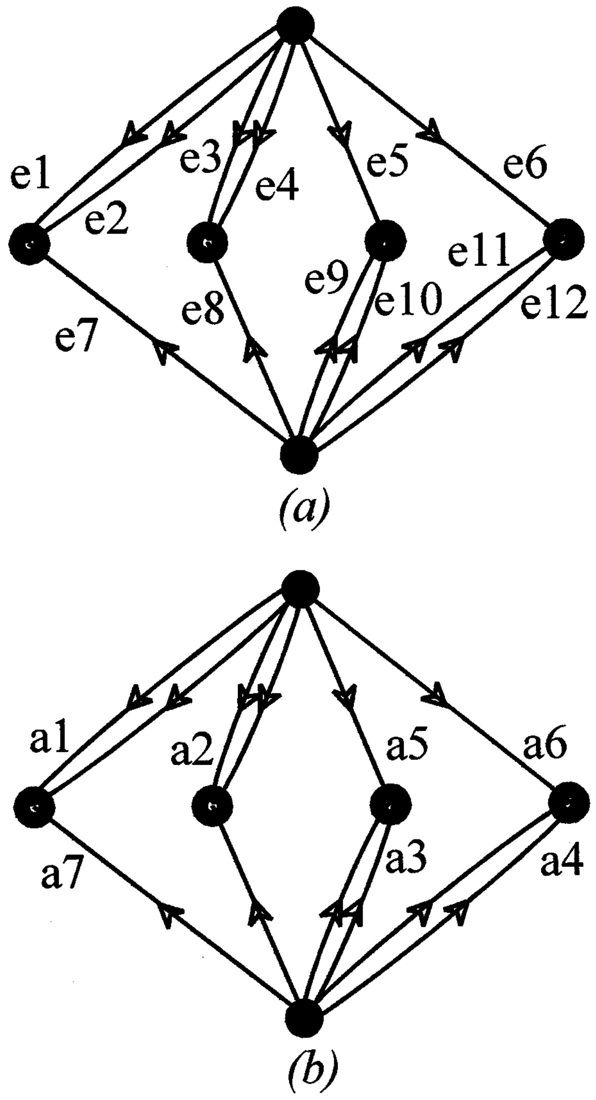

FIG. 5. $K_{2(6),4(3)}$. (a) Line lattices, (b) labeled quotient graph.

$(e_1, \ldots, e_{12}) =$

$$\begin{bmatrix} \frac{a}{2} & -\frac{a}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{a}{2} & -\frac{a}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{a}{2} & \frac{a}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{a}{2} & \frac{a}{2} \\ x & x & x & x & x+\frac{b}{2} & x+\frac{b}{2} & x+\frac{b}{2} & x+\frac{b}{2} & x & x & x & x \\ 0 & 0 & 0 & 0 & y+\frac{c}{2} & -y-\frac{c}{2} & 0 & 0 & y & y & -y & -y \\ y & y & -y & -y & 0 & 0 & y+\frac{c}{2} & -y-\frac{c}{2} & 0 & 0 & 0 & 0 \end{bmatrix}$$

In the line lattices matrix, x and y are arbitrary parameters. Now, we observe that the automorphism group $\mathrm{Aut}(K_{(26),4(3)})$ has two isomorphic subgroups. Both are matrix representations of the three-dimensional point group D_{4h}. The first one is generated by the matrices $(A\cdot C)^2$, C, and $(B\cdot C)^2$, mapping the symmetry operations σ_v, σ_h, and C_2' respectively. This representation is reduced to the sum $\Gamma = A_{1g} + A_{2u} + B_{2g} + E_g + E_u$. There is only one possible projection corresponding to the sum $E_u + A_{2u}$. It is realized in the subspace generated by the vectors $\alpha_1 + \alpha_4$, $\alpha_2 + \alpha_3$, and $\alpha_6 + \alpha_7$. It can be checked that the topology obtained is that of anatase.

The second matrix representation is generated by the matrices B, C, and $((A\cdot C)^2\cdot(B\cdot C)^2)^2$, mapping the symmetry operations σ_v, σ_d, and σ_h respectively. This representation is reduced to the sum $\Gamma = A_{1g} + A_{2u} + B_{2u} + E_g + E_u$. In this case too, there is only one projection in the subspace generated by the vectors $\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4$, α_6, and α_7. This projection gives the rutile topology.

IX. COESITE AND FELDSPAR: N[AP$_4$]

The labeled graph AP_4 is shown in Fig 6. The generators of the automorphism group $\mathrm{Aut}(AP_4)$ and the topological relations are given below.

A: $(e_1, e_2, -e_4, -e_3)(e_6, e_8, -e_7, -e_5)(e_9, e_{11}, e_{13}, e_{15})$
$(e_{10}, e_{12}, e_{14}, e_{16})$

B: $(e_1, e_4)(e_5, -e_7)(e_6, -e_8)(e_{10}, e_{11})(e_{14}, e_{15})(e_9, e_{12})$
$(e_{13}, e_{16})(e_3, -e_3)(e_2, -e_2)$,

C: $(e_1, e_5)(e_2, e_7)(e_3, e_6)(e_4, e_8)(e_9, -e_{15})(e_{10}, -e_{14})$
$(e_{11}, -e_{13})(e_{16}, -e_{16})(e_{12}, -e_{12})$,

$a_1 = e_1 + e_2 - e_3 - e_4,$

$a_2 = e_5 + e_7 - e_6 - e_8,$

$a_3 = e_{10} - e_9 + e_6,$

$a_4 = e_{11} - e_2 - e_9 + e_6,$

$a_5 = e_{12} - e_2 - e_9 + e_6 + e_8,$

$a_6 = e_{13} + e_4 - e_2 - e_9 + e_6 + e_8,$

$a_7 = e_{14} + e_4 - e_2 - e_9 + e_6 + e_8 - e_7,$

$a_8 = e_{15} + e_3 + e_4 - e_2 - e_9 + e_6 + e_8 - e_7,$

$a_9 = e_{16} + e_3 + e_4 - e_2 - e_9.$

In this case, the determination of the transformation matrix P can be done directly by group-theoretical methods because we know the irreducible representations of the automorphism group of the quotient graph, which is isomorphic to point group D_{4d}. We find that the matrices A, B, and C generate a matrix representation that is reduced to the sum $\Gamma = 2A_2 + B_1 + E_1 + E_2 + E_3$. Application of the projection operators associated with each of the representations included in Γ leads to the basis cycle vectors and thus to matrix P with cell parameters a, b, c, d, e, f, and g.

$$
\mathrm{P} = \begin{bmatrix}
\frac{a}{2} & \frac{a}{2} & -\frac{a}{8} & -\frac{a}{4} & -3\cdot\frac{a}{8} & -\frac{a}{2} & -5\cdot\frac{a}{8} & -3\cdot\frac{a}{4} & -3\cdot\frac{a}{8} \\
\frac{b}{2} & -\frac{b}{2} & \frac{c}{4} & 0 & \frac{c}{4} & 0 & \frac{c}{4} & 0 & -\frac{b}{2}+\frac{c}{4} \\
0 & 0 & \frac{d}{4} & 0 & \frac{d}{4} & 0 & \frac{d}{4} & 0 & \frac{d}{4} \\
0 & 0 & 0 & \frac{e}{4} & \frac{e}{4} & 0 & 0 & \frac{e}{4} & \frac{e}{4} \\
0 & 0 & \frac{e}{4} & \frac{e}{4} & 0 & 0 & \frac{e}{4} & \frac{e}{4} & 0 \\
0 & 0 & f\cdot\frac{\sqrt{2}}{8} & f\cdot\frac{\sqrt{2}-1}{8} & f\cdot\frac{\sqrt{2}-1}{8} & f\cdot\frac{\sqrt{2}}{8} & 0 & \frac{f}{8} & \frac{f}{8} \\
0 & 0 & 0 & \frac{f}{8} & f\cdot\frac{\sqrt{2}-1}{8} & f\cdot\frac{\sqrt{2}-2}{8} & f\cdot\frac{\sqrt{2}-2}{8} & f\cdot\frac{\sqrt{2}-1}{8} & -\frac{f}{8} \\
0 & 0 & g\cdot\frac{\sqrt{2}}{8} & g\cdot\frac{\sqrt{2}+1}{8} & g\cdot\frac{\sqrt{2}+1}{8} & g\cdot\frac{\sqrt{2}}{8} & 0 & -\frac{g}{8} & -\frac{g}{8} \\
0 & 0 & 0 & \frac{g}{8} & g\cdot\frac{\sqrt{2}+1}{8} & g\cdot\frac{\sqrt{2}+2}{8} & g\cdot\frac{\sqrt{2}+2}{8} & g\cdot\frac{\sqrt{2}+1}{8} & \frac{g}{8}
\end{bmatrix},
$$

$$
\mathrm{A} := \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0
\end{bmatrix},
$$

$$
\mathrm{B} := \begin{bmatrix}
-1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0
\end{bmatrix},
$$

$$
\mathrm{C} := \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}
\end{bmatrix}.
$$

Finally, we find the line lattices, which are given below in two matrices for convenience. In the first one, we list the coordinates from e_1 to e_8 and in the second one from e_9 to e_{16}; x and y are arbitrary parameters.

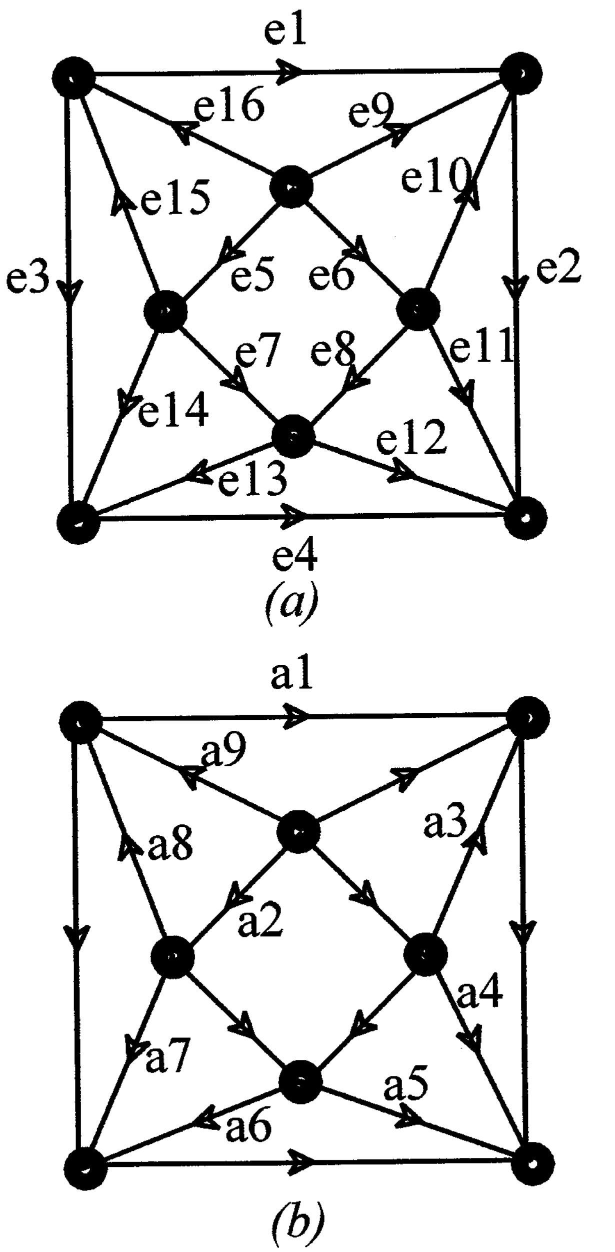

FIG. 6. AP_4. (a) Line lattices, (b) labeled quotient graph.

$$\begin{bmatrix} \frac{a}{8} & \frac{a}{8} & -\frac{a}{8} & -\frac{a}{8} & \frac{a}{8} & -\frac{a}{8} & \frac{a}{8} & -\frac{a}{8} \\ \frac{b}{8} & \frac{b}{8} & -\frac{b}{8} & -\frac{b}{8} & -\frac{b}{8} & \frac{b}{8} & -\frac{b}{8} & \frac{b}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ x & -x & x & -x & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & x & x & -x & -x \\ \frac{f}{8} & \frac{f}{8} & \frac{f}{8} & \frac{f}{8} & 0 & f\cdot\frac{\sqrt{2}}{8} & f\cdot\frac{\sqrt{2}}{8} & 0 \\ -\frac{f}{8} & \frac{f}{8} & \frac{f}{8} & -\frac{f}{8} & f\cdot\frac{\sqrt{2}}{8} & 0 & 0 & f\cdot\frac{\sqrt{2}}{8} \\ y\cdot(\sqrt{2}-2)-\frac{g}{8} & y\cdot(\sqrt{2}-2)-\frac{g}{8} & y\cdot(\sqrt{2}-2)-\frac{g}{8} & y\cdot(\sqrt{2}-2)-\frac{g}{8} & 0 & 2\cdot y\cdot(\sqrt{2}-1)+g\cdot\frac{\sqrt{2}}{8} & 2\cdot y\cdot(\sqrt{2}-1)+g\cdot\frac{\sqrt{2}}{8} & 0 \\ -y\cdot(\sqrt{2}-2)+\frac{g}{8} & y\cdot(\sqrt{2}-2)-\frac{g}{8} & y\cdot(\sqrt{2}-2)-\frac{g}{8} & -y\cdot(\sqrt{2}-2)+\frac{g}{8} & 2\cdot y\cdot(\sqrt{2}-1)+\frac{g}{8} & 0 & 0 & 2\cdot y\cdot(\sqrt{2}-1)+g\cdot\frac{\sqrt{2}}{8} \end{bmatrix}$$

and

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{b}{16}-\frac{c}{8} & -\frac{b}{16}+\frac{c}{8} & \frac{b}{16}-\frac{c}{8} & -\frac{b}{16}+\frac{c}{8} & \frac{b}{16}-\frac{c}{8} & -\frac{b}{16}+\frac{c}{8} & \frac{b}{16}-\frac{c}{8} & -\frac{b}{16}+\frac{c}{8} \\ -\frac{d}{8} & \frac{d}{8} & -\frac{d}{8} & \frac{d}{8} & -\frac{d}{8} & \frac{d}{8} & -\frac{d}{8} & \frac{d}{8} \\ \frac{x}{2}-\frac{e}{8} & \frac{x}{2}-\frac{e}{8} & -\frac{x}{2}+\frac{e}{8} & -\frac{x}{2}+\frac{e}{8} & \frac{x}{2}-\frac{e}{8} & \frac{x}{2}-\frac{e}{8} & -\frac{x}{2}+\frac{e}{8} & -\frac{x}{2}+\frac{e}{8} \\ \frac{x}{2}-\frac{e}{8} & -\frac{x}{2}+\frac{e}{8} & -\frac{x}{2}+\frac{e}{8} & \frac{x}{2}-\frac{e}{8} & \frac{x}{2}-\frac{e}{8} & -\frac{x}{2}+\frac{e}{8} & -\frac{x}{2}+\frac{e}{8} & \frac{x}{2}-\frac{e}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ y\cdot(\sqrt{2}-1) & -y\cdot(\sqrt{2}-1) & -y & -y & -y\cdot(\sqrt{2}-1) & y\cdot(\sqrt{2}-1) & y & y \\ y & y & y\cdot(\sqrt{2}-1) & -y\cdot(\sqrt{2}-1) & -y & -y & -y\cdot(\sqrt{2}-1) & y\cdot(\sqrt{2}-1) \end{bmatrix}.$$

Consider now the subgroup generated by the operations and C and A^2. This is a matrix representation which is isomorphic to the three-dimensional point group C_{2h}. However, there are two possible isomorphisms in which the product $C \cdot A^2$ maps the rotation of order two of C_{2h}. In the first one, the matrix C maps the reflection, whereas in the second it maps the inversion.

In the first case, the representation is reduced to the sum $\Gamma = 2A_g + 3B_g + 2A_u + 2B_u$. The Cartesian coordinates behave as the sum $2B_u + A_u$. The axes for coordinates x and y ($2B_u$) belong to the space generated by the two vectors $\alpha_6 + (\sqrt{2}-1)\alpha_7$ and $(1-\sqrt{2})\alpha_8 + \alpha_9$. The axis corresponding to coordinate z belongs to the space generated by the vectors $(1-\sqrt{2})\alpha_6 + \alpha_7$ and $\alpha_8 + (\sqrt{2}-1)\alpha_9$. If we project onto the vector **k**, defined below, we obtain the topology corresponding to the feldspar structure.

$$\mathbf{k} = [-\alpha_6 + (1+\sqrt{2})\alpha_7]\cdot g/8 + [\alpha_8 + (\sqrt{2}-1)\alpha_9]\cdot f/8$$

In the second case, the representation is reduced to $\Gamma = 2A_g + 2B_g + 2A_u + 3B_u$. The axis associated with coordinate z belongs to the same subspace as before and is also chosen along the vector **k**. The axes for coordinates x and y belong now to the space generated by the three vectors α_2, α_3, and $\alpha_4 - \alpha_5$. By projecting on this space along the vector **v**, the topology of the coesite structure is obtained:

$$\mathbf{v} = (b/2 + c/4)\alpha_2 + d/4\cdot\alpha_3 + 3e/4\cdot(\alpha_4 - \alpha_5).$$

CONCLUSIONS

The archetype associated with some quotient graph has been defined as the net (unique up to isomorphism) of periodicity equal to the cyclomatic number and point group isomorphic to the automorphism group of the graph. The topological features characterizing some simple three-dimensional MA_2 nets have been recovered in the projection of the archetype. However, overly rigorous constraints arising from the higher symmetry of the archetype must be released in order to obtain a geometrically correct description of the structure of the MA_2 compounds.

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