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Graph-theoretical characterization of periodicity in crystallographic nets and other infinite graphs

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Local automorphisms in infinite graphs are defined as those automorphisms for which the distance (in the graph-theoretical sense) between any vertex and its image possesses an upper bound. Abelian subgroups of direction-preserving local automorphisms without fixed point, so-called shift groups, are used to determine the quotient graph of infinite graphs. It is shown that the shift group, the closest topological analogue to a translation group in crystal structures, is isomorphic to the quotient group $\mathbf{C}/\mathbf{C}_0$ of the cycle space $\mathbf{C}$ of the quotient graph by some subgroup $\mathbf{C}_0$, its kernel. As a main consequence, the isomorphism class of nets can be determined directly from their labeled quotient graph, without having recourse to any embedding. A general method is formulated and illustrated in the case of cristobalite and moganite structures. Application to carbon and other kinds of nanotubes is also described.

1. Introduction

Nets or crystallographic nets have been defined as simple 3-connected periodic graphs. Periodicity, however, is a metric property in the Euclidean space and cannot hold directly for a graph. Early workers such as Chung *et al.* (1984) defined the periodicity of a net as that of an embedding of higher translational symmetry. Conversely, nets can be attached to crystal structures viewed as 1-complexes in order to represent their topological properties. In parallel, a quotient graph can be attributed to a net *via* an embedding. As a finite graph, it is easier to handle than the net. But relationships between nets and quotient graphs, both derived from the same crystal structure, are not always clear. It frequently happens that related structures have the same underlying net but different quotient graphs, as in the case of diamond and α-cristobalite. This difference naturally reflects distortions of the structures, with breaking of some translational symmetry. For this reason, it is expected that infinitely many representations of the same net may be found when quotient graphs are systematically generated and labeled in order to predict new crystal structures. Polyknotting is another phenomenon where a self-penetrated network admits both the same net and the same quotient graph as a simpler non-penetrated network (see Carlucci *et al.*, 2003). In all these cases, it is of fundamental importance to attribute the isomorphism class of the net from the labeled quotient graph.

Delgado-Friedrichs & O'Keeffe (2003) proposed an algorithm to determine the true translational symmetry of a net from its quotient graph, but the method, which was applied to the moganite structure, is based on the use of the so-called barycentric embedding. This paper was born from the observation that some automorphism of the labeled quotient graph is associated with the lost translation of the moganite net. More exactly, a new translation can be associated with that automorphism that leaves invariant the sum of the vector labels along the cycles of the quotient graph (see §4.5 for a complete description). But is this the rule? Is it possible to argue about the translational symmetry of a net in the absence of any knowledge other than a labeled quotient graph? It appears that an answer to this question demands some topological characterization of periodicity in infinite graphs.

Recently, Delgado-Friedrichs (2004) proposed to define a periodic graph as a graph on which the group of integers $\mathbf{Z}^n$ acts freely as a subgroup of the group of automorphisms. In addition, the number of vertex orbits under the translation subgroup must be finite. Klee (2004) adopted a similar viewpoint by defining a crystallographic net as a net whose automorphism group is isomorphic to a crystallographic space group. Both definitions are based on formal group-theoretical properties and have been applied with success to special classes of 3-connected graphs. Their extension to arbitrary graphs, however, is generally not possible.

The infinite 3-connected graph on the left of Fig. 1, for instance, admits the automorphisms $\tau = (\ldots, M_i, M_{i+1}, \ldots)$ for $M \in \{A \ldots I\}$, $\rho = (A_i, C_i, E_i)\,(B_i, D_i, F_i)\,(G_i, H_i, I_i)$ and $\phi = \rho\tau$. In the embedding of Fig. 1, τ is realized by a translation and ϕ by a screw axis. Their roles, however, can be exchanged if the embedding is regularly twisted along its axis. Each automorphism, τ or ϕ, determines individually a maximal subgroup of automorphisms isomorphic to $\mathbf{Z}$, each with nine vertex orbits. This way, we can say that the graph of the infinite prism is 1-periodic following Delgado-Friedrichs (2004). But non-isomorphic labeled quotient graphs, shown on the right of Fig. 1, are obtained whether τ or ϕ is used to define the periodic structure. On the other hand, the whole automorphism group is not isomorphic to any crystallographic space group. Following the definition proposed by Klee (2004), the prism is not a crystallographic net and we cannot attribute any periodic structure to the infinite graph.

Let us take now the reverse point of view: assume that in some systematic analysis of possible structures by the vector method (Chung *et al.*, 1984) we generated the two labeled graphs shown in Fig. 1. Could we tell without prior knowledge whether they must be rejected or are the labeled quotient graphs of some periodic structure and, in this case, what is its isomorphism class?

The aim of this study is to propose a graph-theoretical characterization of periodicity that is equivalent to the previously reported group-theoretical definitions where they apply, but can be helpful in other cases. The concept of local automorphism is introduced to this end and allows a partial answer to the above questions. We shall see that the analysis of the automorphisms of the labeled quotient graph enables one to determine the isomorphism class of the crystallographic nets associated with crystal structures.

Since much confusion arises from sometimes incompatible notations used in the graph literature, we begin with a review of the most important definitions in §2. In fact, objects such as a walk in a graph are generally given an empirical definition; we have found it convenient to insert the walk into the adequate algebraic structure, which is the free group on the edge set of the graph. In §3, the topological essence of the translation operation in Euclidean spaces is extracted in the notion of local automorphism, and new definitions of a periodic graph and of a net are derived. Different applications are analyzed in §4, from the description of nanotubes to the systematic determination of the isomorphism class of periodic graphs.

2. An incursion into graph theory

2.1. Graphs and subgraphs

Most of the following is in accordance with Harary (1972). A graph $G(V, E, m)$ is defined as an ordered pair of sets (V, E), together with a function m from E to V^2. The members of the sets V and E are called respectively the vertices and edges of the graph; the function m is called the incidence function. If, for some edge $e \in E$, $m(e) = (u, v)$, we say that e links the vertices u and v, which are called the ends of the edge e. Also, e is incident with u and v. The shorthand notation $e = uv$ will also be used. It is possible that the two ends are identical; in this case, the edge is called a loop. As the function m need not be 1–1, several edges might have the same ends; the graph is then said to have multiple edges. A graph without loops and multiple edges is called a simple graph.

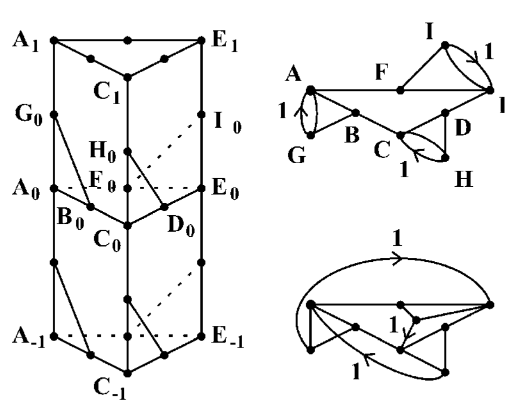

Figure 1
An infinite trigonal prism and two possible quotient graphs.

Observe that the given definition shows the edge as an ordered pair of vertices. The edges are then naturally oriented, which can be formally stated by using the projection functions p_1 and p_2 from V^2 to V defined as follows:

$$p_1(u, v) = u, \quad p_1 \circ m = \alpha$$
$$p_2(u, v) = v, \quad p_2 \circ m = \omega.$$

We say that the edge e runs from $u = \alpha(e)$ to $v = \omega(e)$.

A graph $G'(V', E', m')$ is a subgraph of the graph $G(V, E, m)$ if V' and E' are subsets of V and E, respectively, and m' is a restriction of m to E'. Conversely, if E' is any subset of the edge set of a graph G, the induced subgraph has for vertex set the union of the images of E' by the functions α and ω. The incidence function is clearly the restriction of m to E'.

2.2. Paths and cycles of a graph

We define 0-words and 1-words of a graph $G(V, E, m)$ as elements of the free groups $F[V]$ and $F[E]$ on the alphabets V and E, respectively. In the sequel, words will be noted multiplicatively and only the reduced form of the words is considered. The length $|g|$ of a word $g = \prod a_i^{n_i}$ is the sum $\sum |n_i|$ of the absolute values of the exponents of all its letters, a_i. A 1-word g is said to decompose into a set of words g_i if the following conditions hold:

$$g = \prod g_i \quad \text{and} \quad |g| = \sum |g_i|.$$

Decompositions of a 1-word into itself and possibly the empty word are called trivial decompositions. The boundary morphism ∂ is the homomorphism from the free group $F[E]$ to the free group $F[V]$ defined by $\partial e = u^{-1}v$ for the edge $e = uv$. We have then

$$\partial e^{-1} = (\partial e)^{-1} = v^{-1}u,$$

suggesting that e^{-1} can be interpreted as the complementary edge to e, that is the same edge considered with the reverse orientation (see also Klein, 1996). Although this observation is meaningless for a loop e, the complementary loop is also defined by analogy to be its inverse e^{-1} in $F[E]$.

We call closed a 1-word belonging to the kernel of ∂, and two-ended a 1-word g with a boundary $\partial g = u^{-1}v$ of length 2. The vertices u and v will be referred to as the end-points of the two-ended word. A walk is a two-ended 1-word w that can only decompose into a set of closed or two-ended 1-words. The 1-word $\gamma = abcdefgh$ of the graph drawn in Fig. 2, for example, is two-ended since it satisfies $\partial\gamma = A^{-1}D$ but it is not a walk since it admits the decomposition $\gamma = \alpha\beta$ with $\alpha = abcd$ and $\beta = efgh$ verifying $|\partial\alpha| = |A^{-1}DE^{-1}F| = 4$. A circuit is a closed walk; in the same graph of Fig. 2, the 1-word $\gamma' = bjdefghi$ is an example of a circuit.

A path is then defined as a walk that cannot contain circuits in any decomposition. Intuitively, the edges of a path are traversed continuously between its two ends without passing more than once through each vertex. Analogously, a cycle is a closed path and can be defined rigorously as a circuit that cannot be decomposed further into smaller circuits, *i.e.* non-trivial decompositions of a cycle only contain a set of paths. The two-ended word γ of the above example decomposes into the path *abc* and the cycle *defgh*, while the circuit γ' decomposes into the two paths *bj* and *i* and the cycle *defgh*.

A graph G is said to be connected if, for any pair of distinct vertices u and v, there is at least one walk w of G for which $\partial w = u^{-1}v$. A tree is a connected graph without cycle.

A geodesic g is a shortest path between two given vertices u and v ($\partial g = u^{-1}v$). We define the distance d between the two vertices in V by $d(u, v) = |g|$. It is easy to check that (V, d) is a metric space. The diameter $d(G)$ of a finite graph G is the length of its longest geodesic.

2.3. Morphisms of graphs

A morphism of the graph $G(V, E, m)$ to the graph $G'(V', E', m')$ is a pair of functions (f_V, f_E) between the two vertex and edge sets that preserve the incidence relationships. This can be schematized with the following commutative diagram.

$$\begin{array}{llcl} f_E: & e \in E & \longrightarrow & e' \in E' \\ & \big\downarrow m & & \big\downarrow m \\ f_V \times f_V: & (u, v) \in V \times V & \longrightarrow & (u', v') \in V' \times V' \end{array}$$

In practice, however, we shall use the same symbol f for both the edge and vertex functions. The morphism f of G to G' can be extended to a morphism between the corresponding free groups by setting $f(\prod a_i^{n_i}) = \prod f(a_i)^{n_i}$. It is clear that a morphism of graphs commutes with the boundary morphism (for which we use the same symbol ∂ in the two graphs):

$$\partial[f(e)] = u'^{-1}v' = f(u^{-1}v) = f[\partial(e)], \quad \text{that is: } \partial \circ f = f \circ \partial.$$

An isomorphism of graphs is a morphism that is also a bijective function. As usual, an automorphism of a graph G is an isomorphism of G on itself. It clearly preserves the distances in the vertex set. In fact, if g is a geodesic between two vertices u and v, it is clear that $f(g)$ is a geodesic between $f(u)$ and $f(v)$:

$$d\{f(u), f(v)\} = d\{u, v\}.$$

2.4. Chain modules on Z

The 0-chains and 1-chains on $\mathbf{Z}$ of a graph $G(V, E, m)$ are generally defined as formal linear combinations of the vertices and edges of G with integer coefficients. They are thus isomorphic to the free abelian groups on the bases V and E. Although additive notations are normally used, we shall stick here to the multiplicative notation to keep the continuity in passing from words to chains. The boundary operator is defined in the same fashion as in the word groups; the kernel of the boundary operator will be called the cycle space and its elements the cycle vectors. It is known that the maximum number of independent cycle vectors is given by the cyclomatic number $\upsilon = \#E - \#V + 1$, where $\#E$ and $\#V$ represent the cardinality (the number of elements) of the edge and vertex sets, respectively.

3. Automorphisms in infinite graphs

3.1. Local automorphisms

We start from the observation that the translation in the Euclidean space $\mathbf{E}^n$ is the only bonded isometry, in the sense that the distance between any point and its image has an upper bound. This metrical property can be transported to infinite graphs; we say that f is a local automorphism of an infinite graph G if there exists an upper bound b such that, for all vertices v, $d\{v, f(v)\} \leq b$.

We check now that local automorphisms constitute a normal subgroup of the graph group Aut(G). It is clear that the inverse f^{-1} has the same upper bound b as f since

$$d\{v, f^{-1}(v)\} = d\{f(v), f(f^{-1}(v))\} = d\{v, f(v)\}.$$

Let f and g be two local automorphisms with upper bounds b and c, respectively. Their product $f \circ g$ is a local automorphism since

$$\begin{aligned} d\{v, f(g(v))\} &\leq d\{v, f(v)\} + d\{f(v), f(g(v))\} \\ &\leq b + d\{v, g(v)\} \\ &\leq b + c. \end{aligned}$$

Thus, the local automorphisms of G form a subgroup H of Aut(G). Let f be any automorphism of G and h a local automorphism with upper bound b. We have

$$d\{v, f^{-1}[h(f(v))]\} = d\{f(v), h(f(v))\} \leq b.$$

Thus, $f^{-1} \circ h \circ f$ is also a local automorphism so that H is a normal subgroup of Aut(G).

3.2. Shift groups, periodic graphs and nets

There is no reason, in general, why every automorphism of an infinite graph should be associated with an isometry in

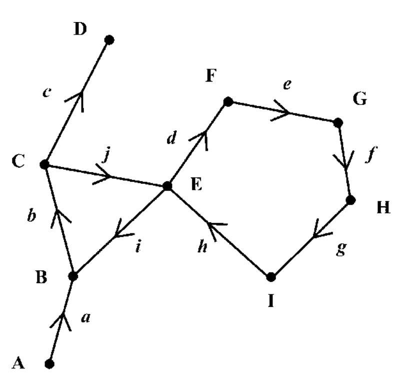

Figure 2
Circuits, paths and cycles (see text).

some embedding. Fig. 3(*a*), for example, shows a graph that we would like to call periodic but has local automorphisms that exchange only two of its vertices. To avoid these cases, we introduce the following:

Definition. A shift group of an infinite graph G is an abelian subgroup of the group of local automorphisms of G which have the properties that

(i) the only automorphism f with a fixed vertex, *i.e.* satisfying $f(v) = v$ for some vertex v of G, is the identity I of $\mathrm{Aut}(G)$;

(ii) no two complementary edges belong to the same orbit (the shift group is orientation preserving).

Observe that the term orientation preserving has no geometrical meaning. We shall call shifts the elements of a shift group. Note that being a shift is not, in general, an intrinsic property of the automorphism but a simple reference to the group it belongs to. In a shift group, there is at most one shift that carries some vertex u to another pre-defined vertex v; suppose there were two such shifts, say f and g, then the product $g^{-1} \circ f$ would have u as a fixed vertex, so that $g^{-1} \circ f = I$, or $f = g$. A group K is said to be admissible if the number of orbits of G (vertex and edge orbits) under K is finite. Shift groups are the closest topological analogs to translation groups. At first sight, it might seem interesting to restrict to shifts of infinite order but, as we shall see later, this extension opens new perspectives in the field of descriptive chemistry.

We define now a periodic graph as an infinite graph with an admissible shift group and a net as a simple, connected, periodic graph, the group of local automorphisms of which is a shift group. For example, the infinite graph in Fig. 3(*a*) admits three kinds of automorphisms such as $(A_i, A_{-i})(B_i, B_{-i})(C_i, C_{-i})$, (B_0, C_0) and $(\ldots, A_i, A_{i+1}, \ldots)(\ldots, B_i, B_{i+1}, \ldots)(\ldots, C_i, C_{i+1}, \ldots)$. The first one is not a local automorphism since the distance $d\{A_i, A_{-i}\} = 2i$ has no upper bound. The second is a local automorphism but has infinitely many fixed points; it cannot belong to a shift group. The third generates a free abelian group that is clearly an admissible shift group; the graph is thus periodic but it is not a net. The group of automorphisms of the graph displayed in Fig. 3(*b*) admits the three generators $(A_i, A_{-i})(B_i, B_{-i})$, (A_i, B_i) and $(\ldots, A_i, A_{i+1}, \ldots)(\ldots, B_i, B_{i+1}, \ldots)$. The second and third generators are local automorphisms without a fixed point. But the second generator, (A_i, B_i), transforms the edge A_iB_i into the complementary edge B_iA_i. On the other hand, the subgroup generated by $(\ldots, A_i, A_{i+1} \ldots)(\ldots, B_i, B_{i+1} \ldots)$ is clearly an admissible shift group, for which the graph is periodic. The graph of the prism shown in Fig. 1 is an example of a net.

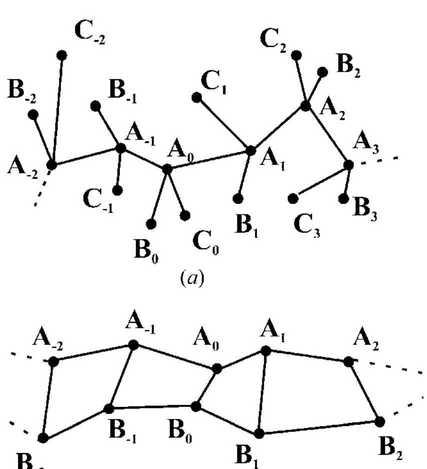

Figure 3
Two 1-periodic graphs.

Finally, we define a crystallographic net as a net with no local automorphism of finite order; *i.e.* the group of local automorphisms of a crystallographic net is a free admissible shift group. As shown in Appendix *A*, this implies that the group of automorphisms of the graph is isomorphic to a space group, so that this definition practically meets that given by Klee (2004). Indeed, the only difference is that 3-connectivity has not been required. We can even say (see Appendix *B*) that a crystallographic net is a connected graph with a free abelian admissible group of local automorphisms.

3.3. Quotient graphs of a periodic graph

Let $\mathbf{N}(V, E, m)$ be a periodic graph and K an admissible shift group (K need not be the whole group of local automorphisms). We define the quotient graph $\mathbf{N}/K$ as the graph whose vertices and edges are respectively the orbits V/K and E/K of the vertices and edges of $\mathbf{N}$ under the action of K; clearly $\mathbf{N}/K$ is a finite graph. An edge and a vertex of $\mathbf{N}/K$ are incident if they have representatives in $\mathbf{N}$ that are themselves incident. The quotient function, q, which is the function mapping the periodic graph on its quotient graph is thus a morphism of graphs; as in the usual case, we use the same notation for the function on the vertex and edge sets and extend the quotient function to a morphism from the free groups of $\mathbf{N}$ to the free groups of $\mathbf{N}/K$:[1]

$$q\big(\prod e_i^{n_i}\big) = \prod q(e_i)^{n_i}.$$

The quotient function also induces a linear function between the corresponding chain modules on $\mathbf{Z}$. The same notation, q, will be used since no confusion is generally possible.

Our next step is to provide a representation of the periodic graph from its quotient graph. We choose for this an arbitrary vertex o of $\mathbf{N}$ and its image $O = q(o)$ in $\mathbf{N}/K$ as the origin of the periodic graph and of its quotient graph, respectively. The infinite graph and its quotient graph are said to be based. We observe then that the quotient map carries a walk w from o to some vertex v of $\mathbf{N}$ to a walk $q(w)$ in $\mathbf{N}/K$ from $q(o)$ to $q(v)$. If, moreover, v belongs to the orbit of o under K, then $q(w)$ is a circuit of $\mathbf{N}/K$. Let us call a walk starting at the origin a based walk. Conversely, any based walk W of $\mathbf{N}/K$ determines a unique vertex in the based periodic graph $\mathbf{N}$. To prove this, we need to lift W to a unique walk w in $\mathbf{N}$ starting at the origin of

[1] Here, the full meaning of the orientation-preserving condition can be made clear. Assume that an edge e and its complementary e^{-1} belong to the same orbit, *i.e.* $q(e) = q(e^{-1})$. Then: $q(ee^{-1}) = q(1) = 1 = q(e)q(e^{-1}) = q(e)^2$, from which it appears that the map q would not be a morphism between free groups.

the graph. We shall define $v = o\partial w$, so that $o^{-1}v = \partial w$ with $q(w) = W$. The proof is by induction on the length of the walk in $\mathbf{N}/K$. Consider first a based walk of length 1 and call e the unique edge of W starting at O; its inverse image $q^{-1}(e)$ is the orbit of the edges mapped on e and originating from the vertices of the orbit $q^{-1}(O)$ to which o belongs. But there is just one edge of $q^{-1}(e)$ starting at o; if there were two such edges (from the same orbit), there would exist a shift exchanging them ($\neq I$) so that their initial vertex o would be a fixed point, which is impossible; let us call this edge $q_o^{-1}(e)$. Then $o\partial q_o^{-1}(e)$ is the ending vertex of this edge in the periodic graph. The same argument can be carried out in the induction step if the walk is decomposed as $W = eW'$, and the induction hypothesis is applied to W' with $|W'| = |W| - 1$. If we call $q_o^{-1}(W)$ the lifted walk, we find $v = o\partial q_o^{-1}(W)$. If the infinite graph is connected, the set of all based walks in $\mathbf{N}/K$ gives a complete representation of $\mathbf{N}$. In particular, the set of all based circuits in $\mathbf{N}/K$ provides a complete representation of the orbit of the origin under the shift group K. This representation is onto but it is not 1–1; many different based circuits of the quotient graph may generate the same vertex in the periodic graph.

3.4. Representation of the shift group

Consider an element f of the shift group K; the image $f\{q_o^{-1}(W)\}$ of the lift $q_o^{-1}(W)$ is an equivalent walk in $\mathbf{N}$, which means that it is mapped on the same walk W in $\mathbf{N}/K$ by the quotient morphism. Moreover, this walk starts at $f(o)$, from which we deduce

$$f\{q_o^{-1}(W)\} = q_{f(o)}^{-1}(W).$$

On the other hand, the image of the origin can be represented by $f(o) = o\partial q_o^{-1}(C)$ for some based circuit C of $\mathbf{N}/K$, since this vertex belongs to the orbit of o. Take now an arbitrary vertex v of $\mathbf{N}$ represented by the walk $q_o^{-1}(W)$ starting at the origin. We can construct a walk to the image of this vertex by concatenation of the two walks $q_o^{-1}(C)$, running from the origin to its image $f(o)$ and the image walk $f\{q_o^{-1}(W)\}$. This observation allows representation of the shift as the function that carries the vertex

$$v = o\partial q_o^{-1}(W) \quad \text{to}$$
$$f(v) = o\partial q_o^{-1}(C)\partial q_{f(o)}^{-1}(W) = o\partial q_o^{-1}(CW). \qquad (1)$$

Conversely, given any based circuit C of $\mathbf{N}/K$, its lift $q_o^{-1}(C)$ defines a vertex $o\partial q_o^{-1}(C)$ belonging to the orbit of the origin. We can thus associate with C the unique shift f_C of K that sends the origin to this vertex through the above formula (1); this defines a function φ: $C \to f_C \in K$, which is clearly onto.

Consider now a new origin $o' = o\partial q_o^{-1}(C')$ of the same orbit $q^{-1}(O)$ and the shift $g = \varphi(C')$ sending o to o'. We get successively [by applying formula (1) for f and g, and by commutativity of shifts]:

$$f(o') = o\partial q_o^{-1}(CC') = f \circ g(o) = g \circ f(o) = o\partial q_o^{-1}(C'C)$$
$$= o'\partial q_{o'}^{-1}(C). \qquad (2)$$

This last expression for $f(o')$ is formally similar to that for $f(o)$, which shows that the given representation of the shift by the circuit C is independent of the vertex chosen as origin of the periodic graph in the same orbit. This conclusion allows the formal reading of equations (2) as $\varphi(CC') = \varphi(C) \circ \varphi(C') = \varphi(C') \circ \varphi(C) = \varphi(C'C)$, which holds for any pair of based circuits C and C'.

Moreover, the set of based circuits of the quotient graph $\mathbf{N}/K$ forms a subgroup Ω of the corresponding free group $F[E]$. It comes then that φ is a group homomorphism; the kernel Ω_0 of φ is the subgroup of the based circuits C of $\mathbf{N}/K$ that the inverse quotient function sends to circuits in $\mathbf{N}$: $\partial q_o^{-1}(C) = 0$. The shift group K is then isomorphic to the quotient group Ω/Ω_0.

3.5. Change of base point

Consider a circuit C based on a vertex A of the quotient graph $\mathbf{N}/K$ (see Fig. 4*a*), and some vertex $B \neq A$ on C. More exactly, consider the decomposition $C = uv$ with $\partial u = A^{-1}B$ and $\partial v = B^{-1}A$ and note:

$$C_A = uv$$
$$C_B = vu,$$

where the subscript indicates the base point for the corresponding circuit.

Let us calculate the image of some vertex b of the orbit $q^{-1}(B)$, with $a \in q^{-1}(A)$ and $b = a\partial q_a^{-1}(u)$ as the origins of the periodic graph when A and B are used as the base points of the quotient graph, respectively.

Take A as the base point; the image of b by the shift $f = \varphi(C_A)$ is given by

$$f(b) = a\partial q_a^{-1}(C_A u) = a\partial q_a^{-1}(uvu) = a\partial q_a^{-1}(u)\partial q_b^{-1}(vu)$$
$$= b\partial q_b^{-1}(vu) = b\partial q_b^{-1}(C_B).$$

The last result is the same as would have been obtained by using B as the base point with origin b and the shift $g = \varphi(C_B)$. This means that we can perform a circular permutation on the

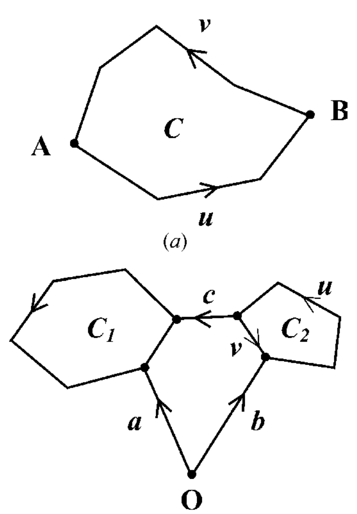

Figure 4
Change of base point (see text).

walks in any decomposition of the circuit C without affecting the result. We can write this as $\varphi(C_A) = \varphi(C_B) = \varphi(C)$, where reference to the base point can be dropped.

We can now announce the fundamental result that each circuit of Ω in the representation of any shift can be substituted by the product of the cycles it maps in the 1-chain space of the quotient graph. A complete demonstration can easily be done by induction on the total number of repeated vertices along the circuit but, instead, we shall deal with the example given in Fig. 4(*b*).

Take O as the base point and a circuit C, decomposed as follows:

$$C = aC_1a^{-1}bucC_1c^{-1}vb^{-1}.$$

A first change of base point equivalent to the permutation of the initial walk, a, with the sequel is performed.

$$\begin{aligned}\varphi(C) &= \varphi(C_1a^{-1}bucC_1c^{-1}vb^{-1}a)\\ &= \varphi(C_1)\varphi(a^{-1}bucC_1c^{-1}vb^{-1}a),\end{aligned}$$

where the factorization of C_1 is by homomorphism of φ. Applying two permutations on a and b and reducing the new word, we get

$$\varphi(C) = \varphi(C_1)\varphi(ucC_1c^{-1}v).$$

Permutation on the product uc and factorization of C_1 gives

$$\varphi(C) = \varphi(C_1)\varphi(C_1c^{-1}vuc) = \varphi(C_1)^2\varphi(c^{-1}vuc).$$

Permutation of the walk c and formation of the cycle C_2 finally gives:

$$\varphi(C) = \varphi(C_1)^2\varphi(C_2).$$

As a consequence, the homomorphism φ can be factorized through the cycle space $\mathbf{C}$ of the quotient graph. The shift group K is then isomorphic to the quotient group $\mathbf{C}/\mathbf{C}_0$ of the cycle space by some subgroup $\mathbf{C}_0$. The highest possible shift group associated with some quotient graph is obtained when the kernel $\mathbf{C}_0$ is reduced to the identity. In this case, the shift group is isomorphic to the abelian free group generated by an independent set of cycles of the quotient graph $\mathbf{N}/K$. This is the same maximum property that led Beukemann & Klee (1992) to the definition of the minimal net associated with the quotient graph.

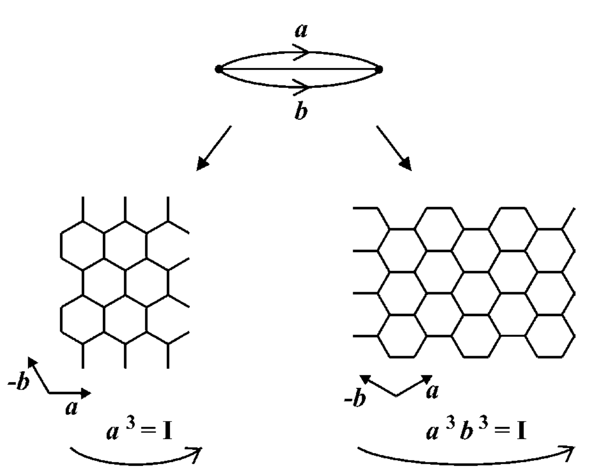

Figure 5
The labeled quotient graph K_2^3 (top) and two carbon nanotube structures described by the relators a^3 (left) and a^3b^3 (right), with their axis running parallel to the height of the figure.

3.6. Labeled quotient graphs

Periodic graphs with non-trivial kernels can be better described by labeled quotient graphs. The same procedure as used by Chung *et al.* (1984) to describe three-dimensional crystallographic nets can be followed. One needs to choose a spanning tree; the edges that do not belong to the spanning tree represent independent cycles of the quotient graph and receive different labels c_i of a set $\mathbf{c}$ symbolizing the free basis of the cycle space. Now, if $\mathbf{C}_0$ is not reduced to the identity of $\mathbf{C}$, one can find a presentation $[\mathbf{c}:\mathbf{r}]$ of the quotient group $\mathbf{C}/\mathbf{C}_0$ with a set of relators $\mathbf{r}$ written as combinations of the elements of the basis $\mathbf{c}$. If possible, the set of labels is simplified in order to take into account the relators. That is: a set of independent generators is chosen to express the elements of the basis set $\mathbf{c}$. Otherwise, the relators are directly reported on the quotient graph. It is known that such groups $[\mathbf{c}:\mathbf{r}]$ are isomorphic to direct products of cyclic groups (these groups are abelian by definition): we say that the graph is n-periodic if the subgroup of infinite cyclic groups of the quotient group $\mathbf{C}/\mathbf{C}_0$ is isomorphic to $\mathbf{Z}^n$.

4. Applications

4.1. Planar graphs and nanotubes

Consider the graph K_2^3 shown in Fig. 5 with cyclomatic number 2. The cycle space is generated by the two cycles denoted a and b. The minimal net corresponding to the graphite structure is obtained for $\mathbf{C}_0 = \{1\}$, *i.e.* generated by the free basis $\{a, b\}$. Two examples of periodic graphs corresponding to non-trivial kernels are described in Fig. 5, with relators a^n and a^nb^non the left and on the right, respectively (with $n = 3$). Both describe different possible structures for carbon nanotubes, where the exponent n indicates the dimension of the perimeter of the tube and the cycle vector, a or ab, refers to the orientation of the carbon 6-ring in relation to the axis of the tube. In both cases, it is easy to verify that the complete group of local automorphisms is not an admissible shift group. The topology of carbon nanotubes is thus described by 1-periodic graphs.

Another example is provided by the graph K_4, shown in Fig. 6. The minimal net is known to be the three-dimensional *srs* net generated by the free basis $\{a, b, c\}$. Using c as the single relator, the planar net $(3.9^2, 9^3)$ is generated. In the same way, with bc as single relator, the planar net 4.8^2 is obtained; but adding the relator a^n generates a 1-periodic tube. The relator bc introduces the 4-ring in the planar net, while a^n folds it in the a direction. The axis of the tube is along the b (or c) direction and, as in the previous case, n indicates the perimeter of the tube.

4.2. Extension of the shift group

Suppose the quotient graph $\mathbf{N}/K$ of a periodic graph $\mathbf{N}$ has been obtained for a subgroup K of a higher admissible shift group H and let f be a shift of H that is not in K. By hypothesis, f commutes with any shift s of K. Consider two vertices (or edges, respectively) x and y of $\mathbf{N}$ in the same orbit under K, and a shift s sending x to y: $s(x) = y$. Then, we have

$$f(y) = f \circ s(x) = s[f(x)],$$

so that $f(x)$ and $f(y)$ also belong to the same orbit under K. This shows that f induces a function ϕ in $\mathbf{N}/K$, which is clearly an automorphism of the quotient graph since it preserves incidence relations.

Consider now a cycle C of $\mathbf{N}/K$ and its image $\phi(C)$ (see the schema in Fig. 7); both cycles define the shifts $\varphi(C)$ and $\varphi[\phi(C)]$ of K. Let $a = o\partial q_o^{-1}[C] = \varphi(C)\{o\}$ be the image of the origin o [with $q(o) \in C$ for simplicity] by $\varphi(C)$; then, the image of a by f is given by

$$f(a) = f(o)\partial q_{f(o)}^{-1}[\phi(C)] = \varphi[\phi(C)]\{f(o)\}.$$

But we can write

$$o = [\varphi(C)]^{-1}\{a\} = \varphi(C^{-1})\{a\}$$
$$f(a) = \varphi[\phi(C)]\{f(o)\} = \varphi[\phi(C)] \circ f \circ [\varphi(C^{-1})]\{a\}.$$

Since f commutes with the shift $\varphi(C^{-1})$, we find that $f(a)$ is a fixed point of the product shift $\varphi[\phi(C)] \circ [\varphi(C^{-1})] = \varphi[\phi(C)C^{-1}]$, which is then the identity I, so that the product $\phi(C)C^{-1}$ is a cycle vector of the kernel $\mathbf{C}_0$. Thus, the automorphism ϕ of the quotient graph $\mathbf{N}/K$ induces the automorphism identity on the quotient group $\mathbf{C}/\mathbf{C}_0$. In other words, ϕ exchanges cycles of the same label in the labeled quotient graph.

Conversely, let $\phi \neq I$ be an automorphism of $\mathbf{N}/K$ that leaves identically invariant the quotient group $\mathbf{C}/\mathbf{C}_0$. Define a function f in $\mathbf{N}$ by:

$$f(o\partial q_o^{-1}[W]) = o\partial q_o^{-1}[\delta\phi(W)],$$

where δ is some fixed walk from the origin O of the quotient graph to its image $\phi(O)$ and the walk W of $\mathbf{N}/K$ describes any vertex of the periodic graph. Clearly, the image only depends on the vertex and not on the particular walk used to describe it since, for another equivalent walk $W' = CW$ with $C \in \mathbf{C}_0$, we have $\phi(W') = \phi(C)\phi(W)$, with $\phi(C) \in \mathbf{C}_0$, so that the walks $\phi(W')$ and $\phi(W)$ describe the same vertex after lifting.

It is useful to observe the following relations:

$$f(o) = o\partial q_o^{-1}[\delta],$$
$$f(o\partial q_o^{-1}[W]) = f(o)\partial q_{f(o)}^{-1}[\phi(W)].$$

The function f is onto and 1–1. Indeed, it is easy to check that it has an inverse f^{-1} defined by:

$$f^{-1}(o\partial q_o^{-1}[W]) = o\partial q_o^{-1}[\phi^{-1}(\delta^{-1})\phi^{-1}(W)].$$

It is shown in Appendix C that f is a local automorphism. We shall check here that f commutes with any shift $s = \varphi(C)$ of the group K. Consider some vertex $a = o\partial q_o^{-1}[W]$ of the periodic graph and its image by the product $f^{-1} \circ s \circ f$:

$$\begin{aligned} f^{-1} \circ s \circ f(a) &= f^{-1} \circ s(o\partial q_o^{-1}[\delta\phi(W)]) \\ &= f^{-1}(o\partial q_o^{-1}[C\delta\phi(W)]) \\ &= o\partial q_o^{-1}[\phi^{-1}(\delta^{-1})\phi^{-1}(C\delta\phi(W))]. \end{aligned}$$

Since ϕ^{-1} is an automorphism of $\mathbf{N}/K$, the walk inside the square brackets can be re-written as $\phi^{-1}(\delta^{-1}C\delta)W$. But then $(\delta^{-1}C\delta)$ and consequently $\phi^{-1}(\delta^{-1}C\delta)$ are circuits of $\mathbf{N}/K$ so that we get

$$f^{-1} \circ s \circ f(a) = o\partial q_o^{-1}[\phi^{-1}(\delta^{-1}C\delta)W] = \varphi(\phi^{-1}(C))\{a\}.$$

Remembering that ϕ (and thus its inverse) leaves the quotient group $\mathbf{C}/\mathbf{C}_0$ invariant, we have $\varphi[\phi^{-1}(C)] = \varphi(C)$, and finally

$$f^{-1} \circ s \circ f(a) = \varphi(\phi^{-1}(C))\{a\} = \varphi(C)\{a\} = s(a).$$

That is: $f^{-1} \circ s \circ f = s$, or $s \circ f = f \circ s$.

If ϕ (or its powers $\phi^n \neq I$) has a fixed point in $\mathbf{N}/K$, then, by combining ϕ with some shift of K, we obtain a local automorphism of $\mathbf{N}$ with a fixed vertex, so that ϕ cannot be used to extend the shift group. The same argument applies if ϕ (or its powers $\phi^n \neq I$) transforms some edge to the complementary edge in $\mathbf{N}/K$; otherwise it is possible to extend K by f to get a larger shift group. In particular, if $\mathbf{N}$ is a crystallographic net,

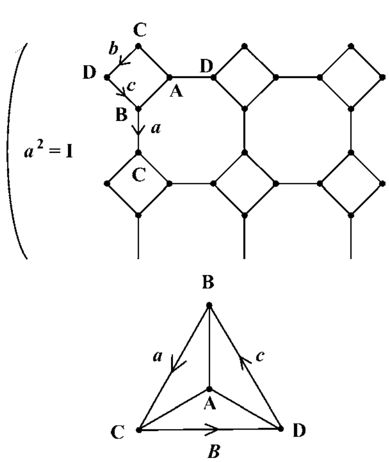

Figure 6
The labeled quotient graph K_4 (bottom) and an *srs* nanotube described by the relators *bc* and a^2 (top), with axis running parallel to the width of the figure.

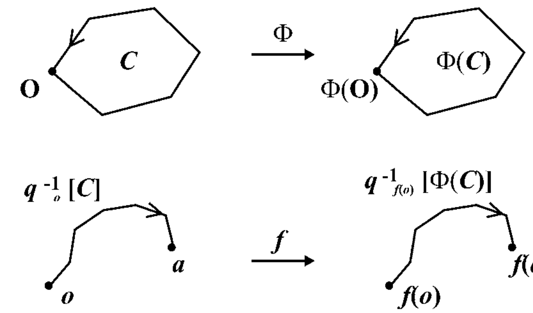

Figure 7
Schema of a based cycle and its image by an automorphism of the quotient graph (top) with the respective lifted walk and its image in the infinite graph (bottom).

any automorphism of its quotient graph that exchanges cycles of the same label in the labeled quotient graph can be used to extend the shift group. This conclusion allows the formal determination of the isomorphism class of the crystallographic net underlying some crystal structure by analysis of the automorphisms of its labeled quotient graph.

4.3. Illustrations

Consider the graph shown in Fig. 8(*a*); it is the quotient of the 1-periodic graph of Fig. 3(*a*) under the action of the shift group described in §3.2. The edges have all been numbered arbitrarily and labeled in accordance with a presentation of the quotient group $\mathbf{C}/\mathbf{C}_0$, as described in §3.6. The automorphism (e_2, e_3), referring to the exchange of the 'dangling' edges numbered 2 and 3 on the figure, leaves the cycle space invariant, as well as the vertex A. It cannot extend the shift group; worse, it evidences the existence of local automorphisms of the 1-periodic group that do not respect the orbits under the shift group.

The graph displayed in Fig. 8(*b*) is the quotient graph of the 1-periodic graph of Fig. 3(*b*), where the periodic structure is defined by the third generator mentioned in §3.2. The automorphism $(e_1, e_2)(e_3, e_3^{-1})$ leaves the quotient group $\mathbf{C}/\mathbf{C}_0$ invariant but it changes the orientation of edge e_3: it cannot be used to extend the shift group.

The graph in Fig. 8(*c*) is the quotient graph of a 2-periodic graph with free basis $\{a, b\}$. The automorphism $\phi = (e_1, e_2)(e_3, e_4)$ leaves the quotient group $\mathbf{C}/\mathbf{C}_0$ invariant and has no fixed vertex nor inverted edge: the automorphism induced in the 2-periodic graph can be used to extend the shift group. Define it as above by $f(o) = o\partial q_o^{-1}[e_3]$, where the origin o belongs to the orbit $q^{-1}(A)$. Since $\phi^2 = I$, the induced automorphism f^2 is just a shift, but we have

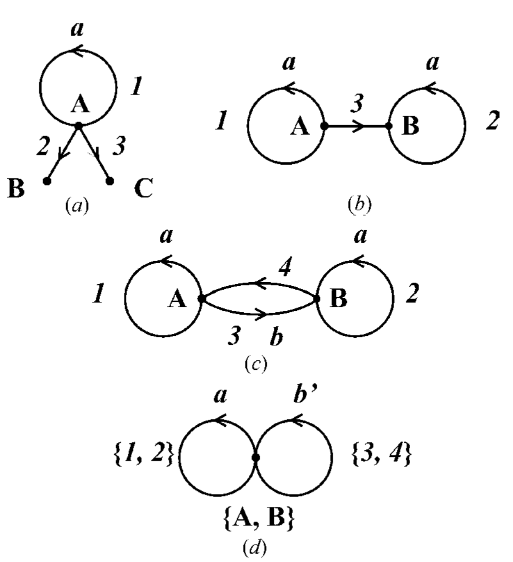

Figure 8
Labeled quotient graphs of the 1-periodic graphs in Fig. 3 (*a* and *b*, respectively), labeled quotient graphs of the square net using a double cell (*c*) and a primitive cell (*d*).

$$\begin{aligned} f^2(o) &= f(o\partial q_o^{-1}[e_3]) = o\partial q_o^{-1}[e_3\phi(e_3)] = o\partial q_o^{-1}[e_3e_4] \\ &= \varphi\{b\}(o). \end{aligned}$$

This result indicates that f^2 is the same automorphism as $\varphi\{b\}$. If we now extend the shift group by the 'half' shift, a reduced quotient graph can be obtained. This has only one vertex, the class $\{A, B\}$ since both vertices are equivalent by ϕ, and two edges formed by the classes $\{1, 2\}$ and $\{3, 4\}$, as shown in Fig. 8(*d*). Labeling of the reduced quotient graph is obtained by lifting the two independent cycles in the quotient graph of Fig. 8(*c*): $\{1, 2\}$ is lifted to e_1 or e_2 with label a, while $\{3, 4\}$ is lifted to e_3, which is now associated with the new half shift denoted b'. This new quotient graph is clearly that of the square net; the labeled graph of Fig. 8(*c*) is thus a quotient of the square net under a subgroup of index two of the full shift (translation) group of the 2-periodic net.

Let us go back to the example of the prism analyzed in the *Introduction*. Both labeled quotient graphs shown on the right of Fig. 1 possess an automorphism of order three leaving the quotient group $\mathbf{C}/\mathbf{C}_0$ invariant. In the graph on the top right, for example, it is given by the permutation of the vertices $(A, C, E)(B, D, F)(G, H, I)$. These automorphisms have neither fixed point nor inverted edge, so they can be used to extend the shift group. The same labeled quotient graph is obtained after factorization in both cases and is shown in Fig. 9. In particular, the shift associated with the third power of the new shift is given by a cycle of the kernel $\mathbf{C}_0$ of the quotient graph, so that it satisfies the relation $a^3 = I$, as indicated in the figure. It is then clear that both labeled quotient graphs of Fig. 1 represent the same net (there is no non-trivial automorphism leaving the final quotient group $\mathbf{C}/\mathbf{C}_0$ invariant), which is not a crystallographic net since there is a shift of finite order.

4.4. Low and high cristobalite

Consider the labeled quotient graph of Fig. 10(*a*), which is isomorphic to that of the low-temperature form of cristobalite. The automorphism $\phi = (e_1, e_8)(e_2, e_7)(e_3, e_6)(e_4, e_5)$ leaves the quotient group $\mathbf{C}/\mathbf{C}_0$ invariant and has neither fixed vertex nor inverted edge: the automorphism induced in the 3-periodic graph can be used to extend the shift group. Define it by $f(o) = o\partial q_o^{-1}[e_1e_5^{-1}]$, where the origin o belongs to the orbit $q^{-1}(A)$.

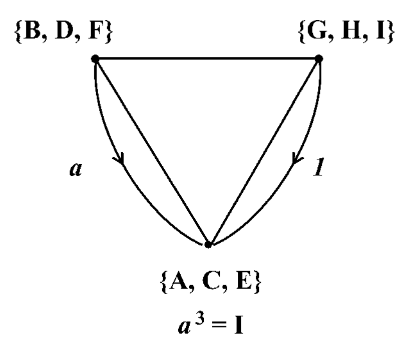

Figure 9
Labeled quotient graph of the infinite prism pictured in Fig. 1.

Since $\phi^2 = I$, the induced automorphism f^2 is just a shift, but we have

$$f^2(o) = f(o\partial q_o^{-1}[e_1 e_5^{-1}]) = o\partial q_o^{-1}[e_1 e_5^{-1}\phi(e_1 e_5^{-1})]$$
$$= o\partial q_o^{-1}[e_1 e_5^{-1} e_8 e_4^{-1}] = \varphi\{c\}(o),$$

so that f^2 is equal to $\varphi\{c\}$. Writing c' the new generator, we obtain the labeled quotient graph of Fig. 10(*b*) as follows. The edge $\{1, 8\}$ is chosen as the unique edge of the spanning tree. To obtain the label of edge $\{2, 7\}$, we lift the cycle $\{2, 7\}\{1, 8\}^{-1}$ in the quotient of Fig. 10(*a*) from the vertex A, for example. There is just one way to get a walk starting at A using the edges of these two classes, which is $e_2 e_1^{-1}$: this in turn is labeled by the generator a, which is then the label of edge $\{2, 7\}$. In the same way, the cycle $\{1, 8\}\{4, 5\}^{-1}$ is lifted to $e_1 e_5^{-1}$, from which we attribute the label c'^{-1} to the new edge $\{4, 5\}$. Now, we use the cycle $\{3, 6\}\{4, 5\}^{-1}$ to obtain the last label; this is lifted from A to $e_3 e_4^{-1}$ with label b. But we already know the label of $\{4, 5\}$ to be c'^{-1} so that the remaining edge $\{3, 6\}$ must be labeled bc'^{-1}.

With all the edges labeled by independent generators, the net is isomorphic to the diamond net or the high-temperature form of cristobalite. We deduce that both the low- and high-temperature forms of cristobalite are described by the same net and are correlated by a periodic distortion along the c axis of the low-temperature form.

4.5. Moganite revisited

Fig. 11 displays the quotient graph of the moganite form of SiO_2. The graph was labeled by applying the program *TOPOLAN* to the data of Heaney & Post (2001). With 12 edges (numbered from 1 to 12) and six vertices (from A to F), the quotient graph has cyclomatic number 7; since it has a planar embedding, the seven independent cycles (C_1 to C_7) of the cycle space have been chosen from the regions delimited on the plane of the drawing and marked on the quotient graph. The orientation of all independent cycles is counter-clockwise. For example, cycle C_3 is defined by the sequence $e_6 e_5 e_{10}^{-1}$ and corresponds to the translation vector b of the moganite cell. It is easy to check that the other two basis vectors of the primitive cell are given by the cycle vectors $C_1^{-1}(a)$ and $C_1C_2(c)$. The kernel $\mathbf{C}_0$ is generated by the four cycle vectors $C_1C_7^{-1}$, $C_2C_6^{-1}$, $C_3C_5^{-1}$ and $C_1C_2C_3C_4$. Now, the automorphism $\phi = (e_1, e_8^{-1})(e_2, e_7^{-1})(e_3, e_6)(e_4, e_5)(e_9, e_{12})(e_{10}, e_{11})$ leaves the quotient group $\mathbf{C}/\mathbf{C}_0$ invariant and has no fixed vertex nor inverted edge: the automorphism induced in the 3-periodic graph can be used to extend the shift group. Define it by $f(o) = o\partial q_o^{-1}[e_2e_6]$, where the origin o belongs to the orbit $q^{-1}(A)$. Once again, $\phi^2 = I$ and the induced automorphism f^2 is just a translation:

$$f^2(o) = f(o\partial q_o^{-1}[e_2 e_6]) = o\partial q_o^{-1}[e_2 e_6\phi(e_2 e_6)]$$
$$= o\partial q_o^{-1}[e_2 e_6 e_7^{-1} e_3] = \varphi\{bc\}(o),$$

so that f^2 is equal to $\varphi\{bc\}$. Writing u for the new generator and using the same method as explained above, we obtain the labeled quotient graph shown in Fig. 12. The labeled quotient graphs of Figs. 11 and 12 represent the same net. This is a crystallographic net since there is no non-trivial automorphism leaving the quotient group $\mathbf{C}/\mathbf{C}_0$ invariant. The new shift describes a true automorphism of the moganite net that is not necessarily associated with a translation of the structure in the Euclidean space. On the contrary, it permits a description of moganite as reported by Heaney & Post (2001), as a

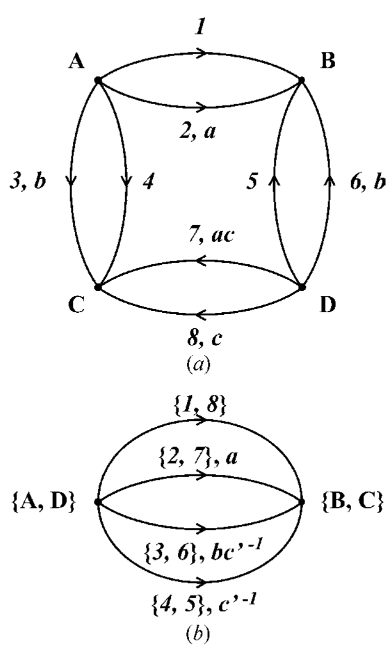

Figure 10
Labeled quotient graphs of the low-temperature form of cristobalite (*a*) and of the associated net (*b*).

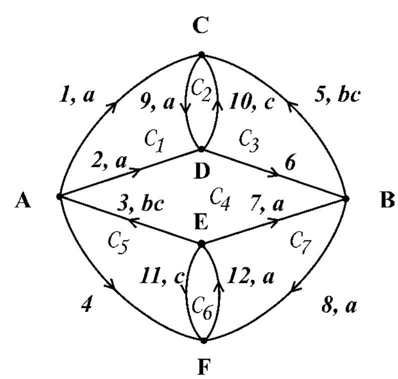

Figure 11
Labeled quotient graph of moganite.

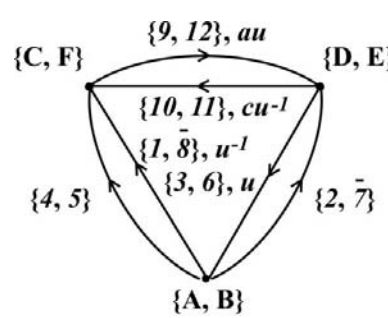

Figure 12
Labeled quotient graph of the net associated with moganite.

modulation of a simpler idealized structure along the 011 (*bc*) axis of the actual form.

5. Concluding remarks

The concept of local automorphism in infinite graphs underlying crystal structures has been introduced to allow a topological characterization of those automorphisms associated with translation symmetries in the crystal. A crystallographic net was defined as a connected graph whose local automorphisms form a free abelian admissible group. It has been shown that this definition is equivalent to that of Klee (2004), *i.e* the group of automorphisms of a crystallographic net is isomorphic to a space group.

It was then shown that the translation group of crystal structures is isomorphic to the quotient group $\mathbf{C}/\mathbf{C}_0$ of the cycle space $\mathbf{C}$ of the quotient graph by some subgroup $\mathbf{C}_0$, its kernel. It is thus equivalent to describe the net by a labeled quotient graph or by its bare quotient graph together with an independent family of circuits defining the kernel $\mathbf{C}_0$ of the cycle space. The isomorphism class of the crystallographic net underlying the structure can be completely determined by the labeled quotient graph obtained under any translation subgroup. The method can be summed up in the following steps.

1. List all automorphisms of the labeled quotient graph that preserve its kernel $\mathbf{C}_0$ (the rings of the crystal structure).

2. Choose the automorphisms that map the cycles of the quotient graph to cycles of the same label. The existence, among these, of automorphisms with fixed points or inverted edges show that the graph is not the quotient graph of a crystallographic net.

3. Automorphisms without fixed vertices or inverted edges and leaving the quotient group $\mathbf{C}/\mathbf{C}_0$ invariant can be used to factor the quotient graph. This step must be repeated until factorization is no longer possible.

4. The final quotient graph must be labeled by lifting its cycles to paths or cycles of the starting quotient graph. The resulting labeled quotient graph provides the isomorphism class of the crystal structure.

APPENDIX *A*

Following a theorem from Schwarzenberger (1980), an abstract group with a normal free abelian subgroup which is maximum abelian and has finite index is isomorphic to a space group.

Consider then an infinite graph $\mathbf{N}$ whose group of local automorphisms $L(\mathbf{N})$ is a free admissible shift group. We already know that $L(\mathbf{N})$ is normal. Let f be an automorphism that commutes with every local automorphism s. Then

$$d\{s(u), f[s(u)]\} = d\{s(u), s[f(u)]\} = d\{u, f(u)\}$$

so that the distance between a vertex and its image by f is constant over the whole orbit. From the admissibility condition, the number of orbits of $L(\mathbf{N})$ is finite and so there is a maximum value over the distances by f. Thus, f is a local automorphism and $L(\mathbf{N})$ is maximum abelian.

It is clear that an automorphism of the infinite graph respects the orbits under the normal subgroup $L(\mathbf{N})$ and thus induces an automorphism of the quotient graph $\mathbf{G}$. In fact, the factor group $\mathrm{Aut}(\mathbf{N})/L(\mathbf{N})$ is isomorphic to the subgroup of $\mathrm{Aut}(\mathbf{G})$ that leaves the kernel invariant. Since $\mathbf{G}$ is a finite graph, the factor group is obviously finite, which completes the proof that $\mathrm{Aut}(\mathbf{N})$ is isomorphic to a crystallographic space group.

APPENDIX *B*

This Appendix proves that the group of local automorphisms $L(\mathbf{N})$ of an infinite graph $\mathbf{N}$ is a shift group if it is a free abelian admissible group. It is sufficient to verify that a local automorphism with a fixed point would have finite order, since the square of an automorphism that exchanges two complementary edges has at least two fixed vertices.

Suppose there exist a local automorphism f and a vertex u satisfying $f(u) = u$. Then, for all local automorphisms s,

$$f[s(u)] = s[f(u)] = s(u),$$

meaning that the whole orbit of u under $L(\mathbf{N})$ is fixed by f. Choose a vertex v from another orbit; since f is an automorphism of $\mathbf{N}$, we have, for any integer value n,

$$d\{u, f^n(v)\} = d\{u, v\}.$$

But the number of vertices at this same distance from u is finite (it is implicitly assumed that the graph has finite degree). There is thus a smallest integer m verifying $f^m(v) = v$. As above, then, the whole orbit of v is fixed by f^m. Now, since the number of orbits under $L(\mathbf{N})$ is finite, we can take the least common multiple p of the m values over all orbits: clearly, $f^p = I$.

APPENDIX *C*

This Appendix shows that the function f defined in §4.1 is a local automorphism.

(*a*) *Preservation of incidence relationships*

Let a and b be two vertices of the periodic graph linked by the edge e, so that $b = a\partial e$, and let W be a walk in $\mathbf{N}/K$ describing the vertex a: $a = o\partial q_o^{-1}[W]$. It is easily verified that $W' = Wq(e)$ is a walk in $\mathbf{N}/K$ describing b, so that

$$\begin{aligned} f(b) &= f(o\partial q_o^{-1}[W']) \\ &= f(o)\partial q_{f(o)}^{-1}[\phi(W)\phi(q(e))] \\ &= f(a)\partial q_{f(a)}^{-1}[\phi(q(e))], \end{aligned}$$

which shows that $f(a)$ and $f(b)$ are linked by an edge of the orbit $q^{-1}\{\phi[q(e)]\}$.

(*b*) *Existence of an upper bound*

Let A be the ending vertex of the walk W in the quotient graph defining some point a of the periodic graph, so that $A = O\partial W$ and $a = o\partial q_o^{-1}[W]$. Let g_A be a geodesic from O to A in

$\mathbf{N}/K$; note that the length $|g_A|$ is smaller than the diameter of the quotient graph $d(G)$. Then, the product Wg_A^{-1} is a circuit of $\mathbf{N}/K$ (with origin at O) and can be decomposed into a product C of cycles C_i, $Wg_A^{-1} = \prod C_i = C$. If we choose the equivalent walk $W' = Wg_A^{-1}g_A = Cg_A$ to describe the vertex a, then we have $\phi(W') = \phi(C)\phi(g_A)$.

The cycle vectors C and $\phi(C)$ of $\mathbf{N}/K$ can now be used to construct a lift from the vertex a to its image $f(a)$. We obtain this lift by concatenating the walk $q_a^{-1}[g_A^{-1}C^{-1}]$ running from a to o and the walk $q_o^{-1}[\delta\phi(W')] = q_o^{-1}[\delta\phi(C)\phi(g_A)]$ running from o to $f(a)$:

$$f(a) = a\partial q_a^{-1}[g_A^{-1}C^{-1}\delta\phi(C)\phi(g_A)].$$

Before going on, we shall show that the lifted walk can be reduced if we take into account the invariance of the quotient group $\mathbf{C}/\mathbf{C}_0$ by the automorphism ϕ. Consider the lift of the simpler circuit $C^{-1}\delta\phi(C)\delta^{-1}$ from the origin:

$$\begin{aligned} oq_o^{-1}[C^{-1}\delta\phi(C)\delta^{-1}] &= \varphi\{C^{-1}\delta\phi(C)\delta^{-1}\}(o) \\ &= \varphi\{C^{-1}\phi(C)\}(o) \\ &= 1(o) = o. \end{aligned}$$

Set $x = oq_o^{-1}[C^{-1}\delta\phi(C)]$, then

$$oq_o^{-1}[C^{-1}\delta\phi(C)\delta^{-1}] = xq_x^{-1}[\delta^{-1}] = o.$$

This last result is equivalent to $x = oq_o^{-1}[\delta]$, which allows the conclusion

$$x = oq_o^{-1}[C^{-1}\delta\phi(C)] = oq_o^{-1}[\delta].$$

The expression for $f(a)$ can thus be reduced:

$$f(a) = a\partial q_a^{-1}[g_A^{-1}C^{-1}\delta\phi(C)\phi(g_A)] = a\partial q_a^{-1}[g_A^{-1}\delta\phi(g_A)].$$

And we get finally $d\{a, f(a)\} \leq |g_A^{-1}\delta\phi(g_A)| \leq |\delta| + 2d(G)$.

The author is much indebted to Professor W. E. Klee for fruitful comments regarding the group-theoretical equivalence of the two definitions of crystallographic nets discussed here. The author thanks CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico of Brazil) for support during this work.

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