Periodic Euclidean Graphs on Integer Points

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Abstract

A uniformly discrete Euclidean graph is a graph embedded in a Euclidean space so that there is a minimum distance between distinct vertices. If such a graph embedded in an $n$-dimensional space is preserved under $n$ linearly independent translations, it is “$n$-periodic” in the sense that the quotient group of its symmetry group divided by the translational subgroup of its symmetry group is finite. We present a refinement of a theorem of Bieberbach: given a $n$-periodic uniformly discrete Euclidean graph embedded in a $n$-dimensional Euclidean space of symmetry group $S$, there is another $n$-periodic uniformly discrete Euclidean graph embedded in the same space whose vertices are integer points (possibly modulo an affine transformation) and whose symmetry group has a (not necessarily proper) subgroup isomorphic to $S$. We conclude with a discussion of an application to the computer generation of “crystal nets”.

Keywords. Crystal nets, crystallographic groups, Euclidean graphs of integer points, periodic graphs, symmetry groups of geometric graphs.

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1 Introduction

Given a Euclidean graph\(^1\) – a graph embedded in a Euclidean space – that is “periodic” with respect to some basis of that space, and assuming that it is “uniformly discrete (i.e., there is a minimum distance between distinct vertices), we will demonstrate the existence of an isomorphic Euclidean graph of at least “comparable” symmetry whose vertices are all points on a geometric lattice. But first, we will define our terms.

We are working with Euclidean graphs.

**Definition 1.1** A Euclidean graph is a graph whose vertices are points in some Euclidean space and whose edges are line segments joining those vertices.

There are several definitions of periodicity. One of the more popular definitions (\(^2\)) requires a prior definition of the graph’s “symmetry group”. Recall that a Euclidean space has an isometry group and that the graph itself has an automorphism group.

**Definition 1.2** Given a Euclidean graph of automorphism group \(A\) embedded in a Euclidean space of isometry group \(I\), the symmetry group of that graph is the group of isometries in \(I\) that induce automorphisms in \(A\).

There is a tendency to treat the symmetry group and the corresponding group of automorphisms interchangeably.

Returning to periodicity, for the graphs we will be considering in this paper, the popular definition may be boiled down to:

**Definition 1.3** A Euclidean graph in an \(n\)-dimensional Euclidean space of translation group \(T\) is \(n\)-periodic if its symmetry group \(S\) admits a subgroup \(S \cap T\) generated by \(n\) linearly independent translations so that \(S/(S \cap T)\) is finite.

Notice that an \(n\)-periodic Euclidean graph embedded in a \(n\)-dimensional Euclidean space admits \(n\) linearly independent translations that preserve the graph, and thus these translations form a geometric lattice that have the effect of chopping the space in which the graph is embedded into \(n\)-dimensional parallelopipeds, “unit cells”, all of which contain congruent portions of the graph.

We now state the main theorem of this article.

**Theorem 1.1** Suppose that a uniformly discrete Euclidean graph \(N\) is embedded in a Euclidean space of dimension \(n\). Suppose that it is \(n\)-periodic and has a symmetry group \(S\).

Then there is a Euclidean graph \(N'\) embedded in the same space such that:

- \(N'\) is isomorphic to \(N\).

\(^1\)Also known as a geometric graph or an embedded graph or even an embedded net.
• If $V'$ is the vertex set of $\mathcal{N}'$, then $V'$ is a subset of some geometric lattice. Viz., there exists an affine transformation $f$ such that $f[V']$ consists of integer points.

• The symmetry group $S'$ for $\mathcal{N}'$ admits a subgroup isomorphic to $S$.

We will gild the lily somewhat by showing that no if no two edges of $\mathcal{N}$ (taking the edges here as line segments) intersect, then the same is true of the edges of $\mathcal{N}'$.

Our goal is to set up a description of the given Euclidean graph $\mathcal{N}$ based on cyclic paths across labeled vertices, and then using the language of words consisting of these labels to compose a system of simultaneous equations; the solutions to these systems will define a class of Euclidean graphs – including graphs $\mathcal{N}'$ with the desired properties. Here is an outline of this paper.

• In Section 2, we will set up a labeling system that will look familiar to group theorists, although this article is self-contained.

• In Section 3, we will use the labels developed in Section 2 to set up the systems of simultaneous equations, and then we will demonstrate that solutions to those systems exist, and hence that the desired Euclidean graphs exist.

In Section 4, we will conclude with a discussion of the relationship between Theorem 1.1 and the “Third Bieberbach Theorem” (of mathematical crystallography), and a discussion of an application to computational crystallography. This paper is a companion of [25], which goes into properties of the labeling system.

Since this paper lies in the intersection of several quite different fields, there is a variety of extant notations and nomenclatures. (See, e.g., [14] for a “dictionary” for translating back and forth between the nomenclatures of crystallography and graph theory.) We fix the conventions of this note as follows.

• Given groups $G, H$, let “$G \leq H$” mean that $G$ is a subgroup of $H$. If $X$ is a set, let $\text{Perm}(X)$ be the permutation group on $X$; if $G \leq \text{Perm}(X)$, then $G$ is a group of permutations of $X$.

  – If $G$ is a group of permutations of $X$, and if $f, g \in G$, denote the composition of $f$ and $g$ by $fg$ so that $(fg)(x) = f(g(x))$ for each $x \in X$. Given $f, g \in G$, the left conjugate of $g$ under $f$ is $fg = fgf^{-1}$; for a subgroup $H \leq G$, let $fH$ be the subgroup \( \{fh : h \in H\} \).

  – If $G$ is a group of permutations of $X$, and if $Y \subseteq X$ and $g \in G$, let $g_Y$ be the restriction of $g$ to $Y$; let $g[Y] = \{g(y) : y \in Y\}$. We will restrict $G$ to $Y \subseteq X$ to get a group acting on $Y$ as follows:

\[
G_Y = \{g_Y : g \in G \& g[Y] = Y\};
\]

note that $G_Y$ is indeed a group of permutations of $Y$. 

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• For sets $S$, $T$, let $S - T$ be the set difference $\{s \in S \colon s \notin T\}$.

• If $\mathcal{N} = \langle V, E \rangle$ is a graph of vertices $V$ and edges $E$, and if $v \in V$, let $\text{nhbd}(v) = \{v\} \cup \{w \in V \colon \{v, w\} \in E\}$ and if $S \subseteq V$, let

$$\partial S = \left( \bigcup_{v \in S} \text{nhbd}(v) \right) - S$$

be the boundary of $S$, so that $\text{nhbd}(v) = \partial\{v\} \cup \{v\}$.

• In this article we will presume $n$ to be some fixed finite dimension. Let $\mathbb{R}$ be the set of real numbers, so that $\mathbb{R}^n$ is an $n$-dimensional space, which we will (sloppily) treat both as Euclidean $n$-space and as a vector space.

• Recall (from, say, [38]) that an isometry on $\mathbb{R}^n$ is a map $g \in \text{Perm}(\mathbb{R}^n)$ such that for all $x, y \in \mathbb{R}^n$, $\|x - y\| = \|g(x) - g(y)\|$, where $\| \cdot \|$ is the usual Euclidean metric. Let $I_n$ be the group of isometries on $\mathbb{R}^n$, and let $T_n$ be the group of translations on $\mathbb{R}^n$; recall (from, say, [38] again) that $T_n$ is a normal subgroup of $I_n$.

• A set $S \subseteq \mathbb{R}^n$ is uniformly discrete if there exists $\varepsilon > 0$ such that for all $x, y \in S$,

$$x \neq y \implies \|x - y\| \geq \varepsilon.$$
We compose isometries so:

\[
[b, M][a, N] = [b + Ma, MN],
\]

and hence \([b, M]^{-1} = [-M^{-1}b, M^{-1}]\).

Given a group \(G \leq I_n\), the point group of \(G\) is the quotient group

\[
G/(G \cap T \mathbb{Z}^n) \cong \{[0, M] : \text{for some } a \in \mathbb{R}^n, [a, M] \in G\}
\]

\[
\cong \{M \in \mathbb{R}^n : \text{for some } a \in \mathbb{R}^n, [a, M] \in G\}.
\]

where 0 is the zero vector. In this article, we will follow the chemists and treat a point group as the corresponding group of matrices.

- Let \(Z\) be the integers. A (geometric) lattice in \(\mathbb{R}^n\) is a set \(L \subseteq \mathbb{R}^n\) such that for some basis \(l_1, \ldots, l_n\) of \(\mathbb{R}^n\),

\[
L = \{c_1 l_1 + \cdots + c_n l_n : c_1, \ldots, c_n \in \mathbb{Z}\},
\]

and we say that this lattice is generated by a group \(G\) of translations if \(L = G(0)\).

## 2 Touring Crystal Graphs

To prove Theorem 1.1, we will employ a procedure for encoding cycles in Euclidean nets, similar to the algorithm described in [25]. We are interested in uniformly discrete \(n\)-periodic Euclidean graphs in a Euclidean space of dimension \(n\); for the rest of this paper, call such a graph a crystal graph.

### 2.1 The Symmetry Group of a Crystal Graph

We review some basic points of mathematical crystallography (see, e.g., [8], [38], and [34]). We also employ a bit of topology: given a set \(S \subseteq \mathbb{R}^n\), let \(\text{int}(S)\) be the interior of \(S\) and let \(\text{cl}(S)\) be the topological closure of \(S\).

- A group \(G \leq \mathbb{I}_n\) is crystallographic if its elements map an \(n\)-dimensional lattice \(L \subseteq \mathbb{R}^n\) of points to itself, and if there is a (topological) neighborhood of \(0\) whose intersection with the orbit \(G(0)\) is \(\{0\}\).

- If \(G\) is crystallographic, then it admits a fundamental region \(\Omega \subseteq \mathbb{R}^n\) such that for some complex polytope \(P\), \(\text{int}(P) \subseteq \Omega \subseteq P\). Furthermore, the points in the interior of this fundamental region are free in the sense that they are not fixed points of any symmetry of \(G\) besides the identity.

\[\text{This Dirichlet domain of a free point is described in [34].}\]
• Suppose that $G$ is crystallographic. If $T_n$ is the group of translations on $\mathbb{R}^n$, then then $G \cap T_n$ admits a fundamental region $U \subseteq \mathbb{R}^n$ such that for some closed $n$-dimensional parallelopiped $P$, $\text{int}(P) \subsetneq U \subsetneq P$. We call $U$ a unit cell of $G$.

We can articulate these two fundamental regions (of the symmetry group and of its subgroup of translations) as follows. Suppose that $G$ is crystallographic.

• If $\Omega$ is a polytopic fundamental region of $G$ and $x \in \text{int}(\Omega)$, then for any $g, h \in G$, $g(x) = h(x) \implies g = h$. (We usually say that $x$ is free in $G$.)

• $G$ admits an $n$-dimensional parallelopiped $U$ with edges parallel to the lattice vectors of some geometric lattice of $G$ such that for some finite subgroup $H \subseteq G$,

$$\bigcup_{g \in G} \text{cl}(g[\Omega]) = \text{cl}(U).$$

This parallelopiped is called a unit cell of $G$.

Given a crystal graph $\mathcal{N}$, we obtain its group of symmetries:

**Definition 2.1** Given a Euclidean graph $\mathcal{N}$ embedded in a Euclidean space $\mathbb{R}^n$, a symmetry of $\mathcal{N}$ is an isometry of $\mathbb{R}^n$ whose restriction to the vertex set of $\mathcal{N}$ is an automorphism of $\mathcal{N}$. The group of symmetries is the symmetry group of $\mathcal{N}$.

We will build a scaffolding of free and lattice points about the crystal graph. Note that a crystal graph in $\mathbb{R}^n$ must have a symmetry group whose translation subgroup is generated by $n$ linearly independent translations, whose vector components generate a geometric lattice. We want to associate a crystal graph with a lattice of points. We do this as follows.

**Convention 2.1** Let $\mathcal{N}$ be a crystal graph whose symmetry group $S$ has a translation subgroup $S \cap T_n$ generated by translations of vector components $l_1, \ldots, l_n$. We can call $\{l_1, \ldots, l_n\}$ a lattice basis for the geometric lattice

$$\{c_1 l_1 + \cdots + c_n l_n : c_1, \ldots, c_n \in \mathbb{Z}\}.$$  

In addition, choose any point $a$ that is not a fixed point of any symmetry besides the identity, and the corresponding lattice of points for $\mathcal{N}$ is the set of points

$$\{b + c_1 l_1 + \cdots + c_n l_n : c_1, \ldots, c_n \in \mathbb{Z}\},$$

and we say that this lattice of points is centered at $b$. Let $\Omega$ be a (polytopic) fundamental region of $S$ containing $a$ in its interior.
We can require that $\Omega \subseteq U$, and in fact, that for a set $G \subseteq S$, $U = \bigcup_{g \in G} g[\Omega]$. Let’s augment our scaffold of lattice points with the orbit $S(a)$, which we call the set of scaffolding points. Call two scaffolding points $g_1(a), g_2(a) \in S(a)$ adjacent if their fundamental regions are adjacent, i.e., if $\text{cl}(g_1[\Omega]) \cap \text{cl}(g_2[\Omega])$ is a polytope of dimension $n - 1$, where again $\Omega$ is the (closure of the) fundamental region containing $a$. Notice that if $g_1(a)$ is adjacent to $g_2(a)$, then there exists exactly one symmetry of $S$, namely $g_2g_1^{-1}$, that sends $g_1(a)$ to $g_2(a)$ and hence $g_1[\Omega]$ to $g_2[\Omega]$. So this is our image of the scaffolding: a trellis of points, anchored on a lattice, where for any two free scaffolding points, there is exactly one symmetry of $S$ that maps the first point to the second (and this symmetry also is a symmetry of the entire scaffolding). It’s ready for the graph itself to grow on the trellis.

Let’s formalize this. Suppose that one is given a crystal graph $\mathcal{N} = \langle V, E \rangle$ and a free point $a$. If $a \not\in V$, choose $v \in V$ such that if $\Omega$ is a (polytopic) fundamental region containing $a$, then $v \in \text{cl}(\Omega)$.

**Convention 2.2** Suppose that one is given a crystal graph $\mathcal{N} = \langle V, E \rangle$ of symmetry group $S$, with a unit cell $U$ consisting of a union of images of a fundamental region $\Omega$, a free point $a \in \Omega$, and if necessary a vertex $v \in V$ such that $v \in \text{cl}(\Omega)$. Then the scaffolded graph of $\mathcal{N}$ is

$$\mathcal{N}^\dagger = \langle V \cup S(a), E \cup S(\{a, v\}) \cup D \rangle,$$

where

$$D = \{\{g_1(a), g_2(a)\} : g_1(a) \text{ is adjacent to } g_2(a); g_1, g_2 \in \text{Sym}(\mathcal{N})\}.$$

**2.2 Traveling Through the Graph**

Our goal is a system of linear equations, each representing a cycle in the crystal graph. We will imagine that each vertex of the graph is a sort of train station, each edge is a track, and that the isometries of the underlying Euclidean space are potential trains that can transport travelers down tracks from one vertex to an adjacent vertex. We do not require that these train isometries be symmetries of the Euclidean graph, in fact, in general, they are not, for we can use such an isometry to transport a traveler from a vertex to an adjacent vertex of a different orbit (under the symmetry group).

But we want to be very particular about which isometries we use as trains: in fact, we will choose a fragment of the graph, select as train isometries the translations between vertices in this fragment, and then use conjugates of these isometries for touring the rest of the graph. We first need to identify this fragment of the graph.

**Definition 2.2** Given a crystal graph $\mathcal{N} = \langle V, E \rangle$ on $\mathbb{R}^n$ with a symmetry group $S$, a fundamental transversal is a set $S \subseteq V$ such that $S$ intercepts each orbit of $S$ in $V$ at exactly one vertex, and $\mathcal{N}[S]$ is connected.

If $S$ is a fundamental transversal, call the tuple $\langle S, \partial S, E^*[S] \rangle$ the transversal subgraph of $S$. If $S = \langle S, \partial S, E^*[S] \rangle$ is a transversal subgraph of $S$, let $\kappa_S : V \rightarrow S$ be the function
which, given any \( v \in S \) and \( w \in S(v) \), gives us \( \kappa_S(w) = v \). If \( S \) is understood, we will just write \( \kappa \).

Before we go any further, we should observe that every Euclidean graph actually admits a fundamental transversal.

**Proposition 2.1 (Proposition 2.6 of [15])** Each Euclidean graph \( N \) in \( \mathbb{R}^n \) admits a fundamental transversal.

We continue, but now with scaffolding from the previous subsection. We assign “train isometries” as follows.

**Definition 2.3** Suppose that we are given a Euclidean graph \( N = (V, E) \) centered at \( a \), with symmetry group \( S \) and fundamental transversal \( S \). Define \( \kappa : V \to S \) so that for each \( v \in V \), \( \kappa(v) \in S \cap S(v) \); notice that as \( S \) is a fundamental transversal, this defines \( \kappa \) precisely. A transversal system is a tuple \( S = (S, \partial S, A, B) \), where

\[
A = \{ (u, v) \in S \times (S \cup \partial S) : \{u, v\} \in E \},
\]

where \( B \) satisfies the following. First, for each \( (x, y) \in A \), fix a symmetry \([m_{x,y}, M_{x,y}] \in S \) so that \([m_{x,y}, M_{x,y}](\kappa(y)) = y \) (if \( \kappa(y) = y \), let \([m_{x,y}, M_{x,y}] = [0, I] \)). Then:

- If \( (x, y) \in (S \times S) \cap A \), then the train isometry from \( x \) to \( y \) is the translation \( g_{x,y} = [y - x, I] \).
- If \( (x, y) \in (S \times \partial S) \cap A \), then the train isometry from \( x \) to \( y \) is

\[
g_{x,y} = [m_{x,y}, M_{x,y}] [\kappa(y) - x, I] = [m_{x,y} + M_{x,y}(\kappa(y) - x), M_{x,y}].
\]

Let

\[
B = \{ [m_{x,y}, M_{x,y}] : (x, y) \in (S \times \partial S) \cap A \}.
\]

Once we have these symmetries, we can walk from the fundamental transversal through the graph as follows. Assume that the traveler started at the free point \( a \in S \).

- We start with the first fundamental transversal \( S \), with the traveler moving around within \( S \) using the train isometries \( g_{x,y} \) (which, within \( S \), are all translations).

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3 Their proof was composed for graphs alone, but it works for Euclidean graphs as well. Start with any vertex \( v_0 \in V \) and let \( S_0 = \{v_0\} \). For any \( n \), if there are any vertices in \( V \) not in an orbit intersecting \( S_n \), choose a vertex \( v \) in an unrepresented orbit and a path from a vertex in \( S_n \) to \( v \), and let \( v' \) be the first vertex on that path in an orbit unrepresented in \( S_n \). There must be a vertex \( v_{n+1} \in \partial S_n \) such that \( v_{n+1} \sim v' \), so let \( S_{n+1} = S_n \cup \{v_{n+1}\} \). Continue until all orbits are represented. See [9].
Reaching a vertex \( y \in \partial S \), the traveler uses the train isometries \( g_{x,y} \) to move from \( x \) to \( y \). Once the traveler has departed from \( S \cup \partial S \), the traveler will employ conjugates of these train isometries.

We first observe that if the traveler is at \( x \not\in S \cup \partial S \) and desires to move to an adjacent \( y \), and if the composition of the train isometries employed thus far is \([m, M](a) = x\), we have

\[
x = [m, M][a - \kappa(x), I] = [m + a - \kappa(x), M](\kappa(x)).
\]

Let \( m' = m + a - \kappa(x) \). We will define the subsequent train isometries so that \([m', M]\) above is always a symmetry of the Euclidean graph. We first define the subsequent train isometries, and then demonstrate that \([m', M]\) is a symmetry. Let \( y' = [m', M]^{-1}(y) \), and observe that if \([m', M]\) is a symmetry of the Euclidean graph, then either \( y' = \kappa(y) \) or \( y' \in \partial S \). Either way, the traveler may employ as a train isometry

\[
[m', M]g_{\kappa(x), y'}
\]

to go from \( x \) to \( y \).

**Claim 2.1** \([m', M]\) as defined above is a symmetry of the Euclidean graph.

**Proof.** This is true by definition when \( x \in S \), so we prove it by induction on the composition.

If \( x \in \partial S \), where the preceding move was the first one out of the fundamental transversal, where the position prior to \( x \) was \( z \in S \), then

\[
[m', M] = g_{z,x}[z - a, I][a - \kappa(x), I] = [m_{z,x} + M_{z,x}(\kappa(x) - z), M_{z,x}][z - \kappa(x), I] = [m_{z,x}, M_{z,x}] \in S
\]

as desired.

The remaining case is when \( x \not\in S \cup \partial S \). Suppose that again, \( z \) preceded \( x \), and that the previous step was \([m, M]\) where, by induction,

\[
[m, M][a - \kappa(z), I] \in S.
\]

Compute, for \( x' = [m, M]^{-1}(x) \in S \cup \partial S \),

\[
[m', M] = [m, M]g_{\kappa(x), x'}[m, M][a - \kappa(x), I] = [m, M]g_{\kappa(x), x'}[a - \kappa(x), I].
\]

There are two cases.
1. \( x' = \kappa(x) \). Then \( g_{\kappa(z),x'} = [\kappa(x) - \kappa(z)] \), and we have
   \[
   [m', M] = [m, M][\kappa(x) - \kappa(z)][a - \kappa(x), I] \\
   = [m, M][a - \kappa(z)] \in S.
   \]

2. \( x' \in \partial S \). Then \( g_{\kappa(z),x'} = [m_{\kappa(z),x'} + M_{\kappa(z),x'}(\kappa(x') - \kappa(z)), M_{\kappa(z),x'}] \), and we have (as \( \kappa(x') = \kappa(x) \)):
   \[
   [m', M] = [m, M][m_{\kappa(z),x'} + M_{\kappa(z),x'}(\kappa(x') - \kappa(z)), M_{\kappa(z),x'}][a - \kappa(x), I] \\
   = [m, M][m_{\kappa(z),x'}, M_{\kappa(z),x'}][a - \kappa(z), I],
   \]
   which is a product of two symmetries.

2.3 Encoding Walks

We will now set up a labeling system to represent these walks through crystal graphs. To minimize misunderstandings, we will emphasize the distinction between syntax (names of things) versus semantics (things named).

The first discrete structure will be a syntactic representation of the transversal subgraph of Definition 2.2. It will assign names to vertices and to each ordered pair of names of adjacent vertices (i.e., to each oriented edge), and it will assign a matrix representing the linear (point) component of an isometry sending the first vertex to the second.

If a traveller is to walk through the graph, there should be an itinerary, so we first turn to the question of how to generate this itinerary, and the decoding scheme for translating itineraries into (compositions of) isometries. This itinerary will be a purely syntactic object, i.e., a list of instructions of the form, “assuming that you are in the initial orientation within the initial fundamental transversal on a vertex \( x \in S \), take the isometry \( g_{x,y} \) to vertex \( y \in S \cup \partial S \).”

The placement of the traveller, as well as the exact point the traveller is at, is critical. Imagine a train station with gates at all four points of the compass. Suppose that the itinerary says, “take the train at the gate to your left.” What departing train the traveler takes depends on where the traveler was facing when the traveler read that instruction. Following literary convention, let us refer to this placement as point of view (POV), and observe:

**Observation 2.1** The point of view of the traveller is determined by the matrix component of the isometry that placed the traveller.
POV is thus determined by the point group.

Suppose that the traveler has employed \( g[x - a, I] \) to travel from \( a \) to \( g(x) \), with \( x \) an element of the transversal domain \( S \) and \( g \) a symmetry of the Euclidean graph \( N \). If the traveler’s next trip is to go to the adjacent vertex \( g(y) \) — where \( y \in S \cup \partial S \) is adjacent to \( x \) — then the traveler will employ \( g_{x,y} \) to travel from \( g(x) \) to \( g(y) \). So the traveler should be instructed to go from \( x \) to \( y \) by taking a train isometry that looks like \( g_{x,y} \) — i.e., that is the appropriate conjugate of \( g_{x,y} \) and thus has the same label. We set up the labels as follows (the construction should be familiar to extant navigations of Cayley digraphs; see, e.g., [27].)

We first devise the itineraries, and then the mechanism for assigning itineraries to (compositions of) isometries. To do this, we need a purely syntactic representation of the transversal subgraph. Since this is the diagram from which itineraries are generated, let’s extend the railroad metaphor and call this a “chart,” and we will use it to “schedule” isometries.

**Definition 2.4** Let \( \mathcal{T} = \langle T, \partial T, \Sigma, \kappa^* \rangle \) be a tuple such that:

- \( T \) and \( \partial T \) are mutually disjoint sets. \( T \) can be considered as a set of names of vertices in \( S \), and \( \partial T \) can be considered as a set of names of vertices in \( \partial S \).
- \( \langle T \cup \partial T, \Sigma \rangle \) is a digraph such that the restriction \( \Sigma[T] \) is a symmetric relation, with no arcs running out of \( \partial T \) while every \( t \in \partial T \) is a target of an arc in \( \Sigma \), and with no two vertices of \( \partial T \) joined by an arc in \( \Sigma[T] \).
- \( \kappa^* : (T \cup \partial T) \to T \) is a function such that for any \( t \in T \), \( \kappa^*(t) = t \).

Call \( \mathcal{T} \) a transversal chart.

Then given a transversal subgraph \( S \) of a net \( N \), say that \( \mathcal{T} \) is a chart of \( S \) if there exists a bijection \( \pi : (T \cup \partial T) \to (S \cup \partial S) \) such that:

- \( \pi[T] = S \) and \( \pi[\partial T] = \partial S \), and
- \( \pi \) is an isomorphism from \( \langle T \cup \partial T, \{\{t, t\}' : (t, t') \in \Sigma \} \rangle \) onto \( \langle S \cup \partial S, E^*[S] \rangle \).
- For each \( t \in \partial T \), \( \pi(\kappa^*(t)) = \kappa(\pi(t)) \). (In other words, \( \kappa^* \) encodes \( \kappa \) on the transversal subgraph.)

Call \( \pi \) a scheduling function for the transversal system.

Following the travellers on trains analogy, given a scheduling function \( \pi \) for a chart \( \mathcal{T} \) of a transversal system \( S \) of a net \( N \), say that the **schedule** is the function \( \sigma \) defined by:

\[
\sigma(t, t') = g_{\pi(t), \pi(t')} , \quad t \in T \land (t, t') \in \Sigma.
\]

Thus an itinerary will be a sequence of pairs \((t, t')\) telling the traveller which isometry to take next. We will follow standard practice in automata theory and read itineraries from left to right.
Definition 2.5 Fix a transversal chart $\mathcal{T} = \langle T, \partial T, \Sigma, \kappa^* \rangle$. An itinerary is a string $(t_1, t'_1)(t_2, t'_2) \cdots (t_n, t'_n)$ in $\Sigma^*$ such that for each $i < n$, $\kappa^*(t'_1) = t_{i+1}$.

Let $\square$ be the empty string, and suppose that it, too, is an itinerary. From this we extend the schedule $\sigma^*$ by recursion on itineraries:

$$\sigma^*(\square) = [0, I],$$

and

$$\sigma^*((t_1, t'_1) \cdots (t_n, t'_n)(t_{n+1}, t'_{n+1})) = \sigma^*((t_1, t'_1) \cdots (t_n, t'_n)) \sigma^*((t_{n+1}, t'_{n+1}))$$

$$= \sigma^*((t_1, t'_1) \cdots (t_n, t'_n)) \sigma(t_{n+1}, t'_{n+1}).$$

A little computation then gives us, for any $n$,

$$\sigma^*((t_1, t'_1) \cdots (t_n, t'_n)) = \sigma(t_1, t'_1) \cdots \sigma(t_n, t'_n)$$

$$= g_{\pi(t_1), \pi(t'_1)} \cdots g_{\pi(t_n), \pi(t'_n)}.$$

Thus $\sigma^*$ is a homomorphism from itineraries to compositions of isometries that the traveller employs to follow those itineraries.

Definition 2.6 Fix a positive integer $n$. Given a transversal chart $\mathcal{T}$, a matrix assignment is a map $\mu: \Sigma \to \mathbb{R}^{n \times n}$. An $n$-periodic Euclidean graph $\mathcal{N}$ in $\mathbb{R}^n$ is represented by the ordered pair $(\mathcal{T}, \mu)$ if there exists a transversal subgraph $\mathcal{S}$ of $\mathcal{N}$ admitting a schedule function $\sigma$ such that for each $(t, t')$, the linear component of $\sigma(t, t') = g_{\pi(t), \pi(t')}$ is $M_{\pi(t), \pi(t')} = \mu((t, t'))$.

In effect, what we fix in advance is this syntactic object, the transversal chart, and the linear components of the isometries to be listed in the schedule. Note that these itineraries will carry a traveller far beyond the fundamental transversal, so we will need:

Definition 2.7 Given an itinerary $(t_1, t'_1)(t_2, t'_2) \cdots (t_n, t'_n)$, it’s matrix component is the product of matrices $\prod_{i=1}^n \mu((t_i, t'_i))$.

Notice that these matrix components are all from symmetries of the graph. Recall from the Introduction that the set of matrix components is a matrix group under multiplication, and is isomorphic to the point group of the symmetry group of the graph.

3 Net Generation

Now that we have our itineraries for transversing the net $\mathcal{N}$ (or the scaffolded net $\mathcal{N}^\dagger$), we use these itineraries to generate ensembles of isomorphic nets. We will show that among these ensembles will be nets of vertices of integer points (modulo affine transformations, if necessary), completing the proof of Theorem [4]. We will proceed as follows.
• First, we will use the transversal charts to set up systems of simultaneous equations whose solution spaces define Euclidean graphs (and some symmetries of those nets). We will do this by generating syntactic representations of some paths in the net, and reduce each of these representations to simultaneous systems of homogeneous linear equations whose solutions represent nets. In order to do this, we will need to represent not only the steps \((t, t')\) but also lattice vectors.

• Second, we need to eliminate those solutions whose corresponding nets would have two distinct vertices at the same place, or two different (non-scaffolding!) edges intersecting. We will eliminate these solutions by representing the solutions as ensembles of vector spaces, and then delete these “bad” vector spaces from the solution space, leaving only “good” vector spaces of solutions for nets with no such collisions or intersections.

We will then confirm that if such an adjusted solution space is nonempty, then it has integer point solutions, and we will be done.

We have two agenda in dealing explicitly with the lattice that we generate with the net:

• Notice that when we construct the transversal charts, we got fixed matrices for the linear components of the isometries, and thus the resulting systems of equations are linear.

• Each path in the net that we use to generate equations will be a path from a (path representing a) vertex within the original fundamental transversal out to a (path representing a) different vertex of the same orbit in the translational subgroup of the symmetry group, so that the displacement between the two vertices will be a lattice vector. (We will use the matrix components of the itineraries to determine when we have a lattice vector below.) We construct a syntactical representation of a cycle composed of a path from the first vertex to the second using a traveller’s itinerary as in the previous section, and then an integral linear combination of lattice basis vectors to traverse back to the first vertex.

Notice that we need the matrix components in the second agenda, for we recognize that an itinerary goes from a vertex to a lattice-equivalent vertex by looking at the itineraries and checking that the product of the matrices is the identity matrix.

And now for a useful fact about point groups.

Theorem 3.1 (From Bieberbach’s Third Theorem, see, e.g., [32, p. 29], [6, Theorem 7.1] or [36, Theorem 3.2.2].) For each \(n\), there are finitely many isomorphism classes of crystallographic space groups for lattices on \(\mathbb{R}^n\), and any two isomorphic crystallographic space groups are actually affine conjugates. Thus for each \(n\), there are finitely many isomorphism classes of crystallographic point groups (treated as groups of matrices), with any two isomorphic crystallographic space groups being linear conjugates.
Thus there exist finitely many maximal point groups. In fact, for $n = 3$, there are two maximal point groups, one of which we can call the cubic point group (which is the symmetry group of the cube, denoted $O_h$ in the Schönflies notation, $m3m$ in the Hermann-Mauguin notation, and $*432$ in orbifold notation) and the other being the hexagonal point group (which is the symmetry group of the hexagonal prism, denoted $D_{6h}$ in in the Schönflies notation, $6/mmm$ in the Hermann-Mauguin notation, and $*622$ in orbifold notation).

**Remark 3.1** For each $n$, one of the maximal point groups is the point group of the integer lattice $\mathbb{Z}^n$, which consists of integer matrices (in fact, of $n \times n$ matrices whose entries are $-1, 0,$ and $1$). Every other maximal point group is a linear conjugate of a group of matrices for a linear group on $\mathbb{Z}^n$, i.e., a linear conjugate of a group of integer matrices (these integer matrices need not be orthonormal, although the matrices of the maximal point group itself are). For the rest of this article, we fix a maximal crystallographic point group $H$, which is a linear conjugate of a group $H^*$ of integer matrices. Let’s fix this linear equivalence: for the rest of this article, let $F$ be the matrix such that $H = FHF^{-1} = \{FMF^{-1} : M \in H^*\}$. Thus $H = H^*$ iff $H$ is a point group of the integer lattice (i.e., the symmetry group of the $n$-cube) iff $F$ is the identity matrix.

### 3.1 Naive Net Generation

In order to proceed, we fix the dimension $n$ of the lattice, and then choose which of the finitely many maximal point groups of $n$-dimensional lattices to use (again, calling this maximal point group $H$), find the conjugacy matrix $F$ and the corresponding conjugacy group $H^*$ of integer matrices, and then we go on to describe the walks. In the process, we develop a copy of a repeating connected subgraph of the Euclidean graph $N$; we will call this repeating subgraph a “quotient graph” after [5] and [22] (which are, by the way, quite different from the “quotient graphs” of [15]). However, we will be constructing a “quotient graph” from a scaffolded graph, which will thus be distinct from the “quotient graphs” of after [5] and [22].

Fix a crystal graph $N = \langle V, E \rangle$ whose symmetry group’s matrix components is a subgroup of $H$. Fix a lattice $L = \{c_1l_1 + \cdots + c_nl_n : c_1, \ldots, c_n \in \mathbb{Z}\}$ of $N$ and central standard unit cell $U$ and fundamental region $\Omega$. Given a free point $a \in \partial(\Omega)$, we obtain the “scaffolded graph” $N$ of Convention 2.2. Notice that the addition of the free points corresponding to $a$ to each fundamental region, with scaffolding edges from the point corresponding to $a$ to the vertex corresponding to $v$, is preserved under $S$:

**Observation 3.1** The symmetry group of a crystal graph $N$ is the symmetry group of a scaffolded graph of $N$.

And from this scaffolded graph, we obtain a “quotient graph” from the itineraries as follows.
Construction 3.1 Given the scaffolded graph \( \mathcal{N}^\dagger \) of a crystal graph \( \mathcal{N} \), we construct a quotient graph of \( \mathcal{N}^\dagger \) as follows.

Construction. We first develop the vertices of the quotient graph. In the following procedure, we obtain vertices by developing itineraries to reach them, and the sequence of sets of itineraries \( Q_0 \subseteq Q_1 \subseteq \cdots \) has as its limit a set of itineraries for the vertex set of a quotient graph, while the sets \( \partial Q_0 \subseteq \partial Q_1 \subseteq \cdots \) has as its limit a set of itineraries for the vertices of the boundary of that quotient graph. Let \( a \) be the free (scaffolding) point used to develop \( \mathcal{N}^\dagger \), and let \( v \) be the vertex of \( \mathcal{N} \) connected by a scaffolding edge to \( a \).

- Let \( S \) be a fundamental transversal of \( \mathcal{N} \), including the presumed free vertex of name \( t_0 \) so that \( \pi(t_0) = a \). Let \( \pi(t_1) = v \) and \( Q_0 = \{(t_0, t_1)\} \) and install a copy of the lattice \( L \) by adding a symbol \( t_i \) for each \( i = 1, \ldots, n \) with \( \pi(t_i) = 1 \), and \( u((t_0, t_i)) = I \), to get \( \partial Q_0 = \{(t_0, t_i); i = 1, \ldots, n\} \), which will start the process of adding scaffolding edges up the lattice starting from \( a \).

- A set of strings \( Z \) is closed under prefixes if \( st \in Z \implies s \in Z \). Given a set of itineraries \( Q_m \supseteq Q_{m-1} \supseteq \cdots \supseteq Q_0 \) that is closed under prefixes, we construct \( Q_{m+1} \supseteq Q_m \) as follows. For each itinerary \( t \) in \( Q_m \) and for each \( (t, t') \in \Sigma \) such that \( t(t, t') \) is an itinerary, proceed as follows:
  - If every \( t'(t'', t''') \in Q_m \) satisfies \( \kappa^*(t') = \kappa^*(t''') \implies \mu(t(t, t')) \neq \mu(t'(t'', t''')) \) – i.e., if every path in \( Q_m \) that terminates at a vertex of the type \( \kappa^*(t') \) terminates in a POV different from that of \( t(t, t') \) – then place \( t(t, t') \) in \( Q_{m+1} \).
  - Otherwise, if the terminal POV of \( t(t, t') \) has already been encountered, place \( t(t, t') \) in \( \partial Q_{m+1} \).

Since all matrices \( \mu(t) \) are elements of the finite group \( \mathbb{H} \), this recursion eventually halts. Collapse this set into equivalence classes:

\[
    t \simeq t' \quad \text{iff} \quad \sigma^*(t)(a) = \sigma^*(t')(a)
\]

and let \( Q = \{[t]_\sim; t \in \bigcup_m Q_m\} \) and \( \partial Q = \{[t]_\sim; t \in \bigcup_m \partial Q_m\} \). Thus \( Q \) is the set of classes of itineraries to vertices in a connected subnet, with exactly one vertex from each orbit of \( \mathcal{N} \) in the translation subgroup \( \text{Sym}(\mathcal{N}) \cap \mathbb{T}_n \), while \( \partial Q \) consists of the itineraries to adjacent vertices.

Thus a particular vertex in \( \mathcal{N} \) can be assigned a matrix from a collection of possible orientation matrices, but not necessarily a unique one. Let

\[
    E_Q = \{([t]_\sim, [t']_\sim); \{\sigma^*(t), \sigma^*(t')\} \in E\}.
\]

We now have a quotient graph \( Q = \langle Q, E_Q \rangle \) of equivalence classes of itineraries. 🔗

From this quotient graph, we will generate a system of simultaneous linear equations whose solutions will represent nets isomorphic to \( \mathcal{N} \) (and degenerate nets that we will
delete in the next subsection). Let’s construct these linear equations. First, we need to construct linear forms from itineraries.

**Construction 3.2** Given a Euclidean net, each itinerary is assigned corresponding linear form as follows.

**Construction.** Before we start the construction, we first remark that we will use the matrix components of isometries represented by itineraries. Recall the linear change of basis matrix $F$ from Remark 3.1 so that the matrices represented in the linear forms are integral — and hence the linear forms themselves have integer coefficients. (After we have used the linear forms to generate the systems of equations which we then solve, we will have to reverse the change of basis to obtain the desired nets, by returning from subgroups of the group of integer matrices $\mathbb{H}^*$ to the point group $\mathbb{H} = F\mathbb{H}^*$.) Notice also that $\mathbb{H}^* = F^{-1}\mathbb{H}$.

Here is the recursive construction.

- Here is the basis of the recursion. If $(t, t') \in \Sigma$ and $M = \mu((t, t'))$, let
  \[
  x_{(t,t')} = \begin{pmatrix}
  x_{1(t,t')} \\
  \vdots \\
  x_{n(t,t')}
  \end{pmatrix},
  \]
  where $x_{1(t,t')}, \ldots, x_{n(t,t')}$ are real-valued variables, and let the form of $(t, t')$ be the expression
  \[
  [(x_{1(t,t')}, \ldots, x_{n(t,t')}), F^{-1}M].
  \]
  Notice that this form is a syntactic object set up to represent an affine map with an integral linear component.

- Here is the recursive step. If an itinerary $t$ has form $[(x, F^{-1}M]$ and $(t, t')$ has form $[x', F^{-1}M']$, then the form of $t(t, t')$ will be $[x + F^{-1}Mx', F^{-1}(MM')]$, where addition and multiplication of variable vectors is performed in the usual way. Notice that the vector component of a form of an itinerary will be an $n$-dimensional vector whose components will be linear combinations involving a potentially large number of variables.

Continue the recursion. ■

It will turn out that we only need forms from itineraries of the quotient graph. Now that we have these linear forms, we can use them to build homogeneous linear equations as follows.
Construction 3.3 Given a scaffolded graph \( N^\dagger \) of a crystal graph \( N \) with itineraries and linear forms as above, and with a symmetry group \( S \), construct a system of linear equations from the itineraries of the quotient graph as whose solutions will be lattice vectors and positions of vertices of scaffolded graphs isomorphic to \( N^\dagger \), including \( N^\dagger \) itself, possibly with vertex collisions (i.e., two or more vertices assigned to the same point).

Construction. Let \( u_1, \ldots, u_n \) be vectors of variables \( u_i = \langle u_{i,1}, \ldots, u_{i,n} \rangle \), where each \( u_{i,j} \) is real-valued. The motivation is that these variable vectors will range over lattice vectors. We will use \( x \) to represent variable vectors \( x(t,t') \) ranging over positions of transversal vertices, or to represent sums of products of integer matrices with variable vectors. Recall that \( Q \) is a set of equivalence classes of itineraries, two itineraries being equivalent if they start at \( t_0 \) and terminate at the same vertex. As before, \( a \) is a free points used to construct \( N^\dagger \).

- For each \( q \in Q \) and each \( t, t' \in q \), of forms \([x, F^{-1}M] \) and \([x', F^{-1}M'] \), the equation witnessing the equivalence of \( t \) and \( t' \) is
  \[ E_{t \rightarrow t'} = "x - x' = 0". \]

- For each \( t \) and \( t' \) such that \( \sigma^*(t)(a) - \sigma^*(t')(a) \in L \), let \( t \) have form \([x, F^{-1}M] \) and let \( t' \) have form \([x', F^{-1}M'] \). Suppose that \( \sigma^*(t)(a) - \sigma^*(t')(a) = a_1l_1 + \cdots + a_nl_n \) (and notice that \( a_1, \ldots, a_n \in \mathbb{Z} \)). Then the equation witnessing the lattice displacement of \( t \) to \( t' \) by \( \sigma^*(t')(a) - \sigma^*(t)(a) \) is
  \[ E_{t \rightarrow t', \sigma^*(t) - \sigma^*(t')} = "x - x' - \sum_{i=1}^{n} a_iu_i = 0". \]
  where \( u_1, \ldots, u_n \) are \( n \)-tuples of real variables.

- In particular, recalling that we are dealing with a scaffolded net, in which \( a \) is the initial scaffolding point, for any itinerary \( t \) for a path from \( a \) to another scaffolding point \( \sigma^*(t)(a) \) in a(nother) unit cell, we have an equation
  \[ E_{a \rightarrow t, \sigma^*(t) - \sigma^*(\Box)} = "x - \sum_{i=1}^{n} a_iu_i = x_0", \]
  where \([x, F^{-1}M] \) is the form of \( t \), \([x_0, I] \) is the form for \( \Box \) (where \( I \) is the identity matrix) and where the integer coefficients \( a_1, \ldots, a_n \) are computed from the original scaffolded net \( N^\dagger \).

We now add some equations to build in the symmetries of \( N \). But first, recall from Subsection 2.1 that if \( U = \{g_0, g_1, \ldots, g_p \} \), where \( g_0 \) is the identity, then \( \Omega_i = g_i[\Omega] \) for each \( i \), where \( \Omega \) is the fundamental region that we started with, \( a \in \text{int}(\Omega) \), and our initial unit cell is \( U = \bigcup_i \Omega_i \). Thus every symmetry of \( N \) can be expressed as a composition \( t_1t_0g \), where \( g \in U \) and \( t_0 \) and \( t_1 \) are translations by lattice vectors in \( L \).
We would also like to identify each point of \( \mathbb{R}^n \) with corresponding points in the initial unit cell \( U \) in the same orbit under the lattice group \( S \cap T_n \). Let
\[
\mathbf{r} \mod L = \{ \mathbf{r}' \in U : \mathbf{r} - \mathbf{r}' \in L \}
\]
and
\[
\mathbf{r} \rem L = \{ (d_1, \ldots, d_n) \in \mathbb{Z}^n : \mathbf{r} - \sum_{i=1}^{n} d_i \mathbf{l}_i \in \mathbf{r} \mod L \}.
\]
We use these tuples \( \mathbf{d} = (d_1, \ldots, d_n) \) to encode the lattice translations necessary to map a given point of \( \mathbb{R}^n \) to \( U \).

Without loss of generality, suppose that the center of \( U \) (i.e., the centroid of its corners) is the origin. Now for more equations for our system.

- We integrate the symmetries of \( \mathcal{N} \) with the lattice \( L \), and hence \( \mathcal{N}' \) with \( L' \), as follows. For any \( \mathcal{N}' \) whose vertex points and lattice vectors form a solution to this system, we will want the following. For each \( g \in \mathbb{U} \), we have an \( n \)-tuple \( y_g \) of real-valued variables to represent the vector component of what will be the symmetry \( g' \) of \( \mathcal{N}' \) corresponding to \( g \) of \( \mathcal{N} \). If \( M_g \) is the linear part of the matrix of \( g \), it will also be the linear part of \( g' \). As \( g \) can be fixed in \( \mathbb{U} \) by its permutation of the corners
\[
\text{corner}(\mathbf{u}) = \frac{1}{2} \sum_{i=1}^{n} (-1)^{\iota_i} \mathbf{l}_i, \quad \mathbf{u} = (\iota_1, \ldots, \iota_n) \in \{0, 1\}^n
\]
of \( U \), we use the correspondence \( g : \text{corner}(\mathbf{u}) \mapsto \text{corner}(\mathbf{u}') \), represented by an equation
\[
[\mathbf{y}_g, F^{-1}M_g] \left( \frac{1}{2} \sum_{i=1}^{n} (-1)^{\iota_i} \mathbf{u}_i \right) = \frac{1}{2} \sum_{i=1}^{n} (-1)^{\iota_i'} \mathbf{u}_i,
\]
or, more precisely, by
\[
\mathcal{E}_{g, \mathbf{u} \rightarrow \mathbf{u}'} = 2\mathcal{E}_g + \sum_{i=1}^{n} \left( (-1)^{\iota_i} \left( F^{-1}M_g \right) - (-1)^{\iota_i'} I \right) \mathbf{u}_i = 0',
\]
where again \( I \) is the identity matrix.

- We integrate the initial unit cell permutations of the free scaffolding points as follows. Notice that the scaffolding points represented in the quotient graph \( Q \cup \partial Q \) need not be in \( U \), so for each \( \mathbf{t} \) terminating in a code for a free scaffolding point, let \( \text{displace}(\mathbf{t}) \) be the unique \( n \)-tuple \( \mathbf{d} \in \mathbb{Z}^n \) such that \( \mathbf{d} = (d_1, \ldots, d_n) \in \sigma^*(\mathbf{t})(\mathbf{a}) \rem L \).

\[\text{Unique as } \sigma^*(\mathbf{t})(\mathbf{a}) \text{ is free in } S.\]
For $t_0, \ldots, t_p$ being the itineraries for travelling to the free points in the quotient graph that are in the orbit of $\sigma^*(t)(a)$ so that

$$g_i(\sigma^*((t_0, t_1))(a)) = \sigma^*(t_i)(a) - \sum_{j=1}^{n} d_j l_j \in \Omega_i, i = 1, \ldots, p,$$

we can fix this assignment by the equation

$$[y_g, F^{-1} M_g](x_0) = x_i - \sum_{j=1}^{n} d_j u_j,$$

for $[x_i, F^{-1} M_g]$ being the form for $t_i, i = 0, \ldots, n$. More precisely, we have the linear equations

$$E_t = "y_g + F^{-1} M_g x_0 - x_i + \sum_{j=1}^{n} d_j u_j = 0".$$

We also have the corresponding equations for all classes of itineraries in $Q \cup \partial Q$ in order to fix $U$ as the group of symmetries of the vertices and edges of $N$ within or incident to $U$.

• Finally, in a mathematically superfluous but psychologically reassuring step, we encode the multiplication table of $U$ itself: for each $i, j, k$ such that $g_i g_j = g_k$, we have the equation

$$[y_{g_i}, F^{-1} M_{g_i}][y_{g_j}, F^{-1} M_{g_j}] = [y_{g_k}, F^{-1} M_{g_k}],$$

or, more precisely,

$$E_{i,j;k} = "y_{g_i} + F^{-1} M_{g_i} y_{g_j} - y_{g_k} = 0,$$

which suffices since we already have, by construction, $M_{g_i} M_{g_j} = M_{g_k}$.

The result is a system $E$ of homogeneous linear equations with integer coefficients.

Since the displacements of $N^+$ itself gives a solution to this system, this system is soluble. The solution represents the central standard unit cell of a crystal net, using the unit defined by the solutions to $u_1, \ldots, u_n$ as the lattice basis. This gives us some of what we want. We now posit a solution to this system of simultaneous equations.

**Definition 3.1** Let the assignments

$$x_i \rightarrow v'_i, \quad i = 0, \ldots, m,$$

$$y_{g_j} \rightarrow b'_j, \quad j = 0, \ldots, p$$

$$u_k \rightarrow l'_k, \quad k = 0, \ldots, n$$

be a solution to the simultaneous system of equations $E$ so that:
• \(v'_0\) is free, and \(v'_0, \ldots, v'_m\) are the positions of the vertices of the interior of the quotient graph, while \(v'_{m+1}, \ldots, v'_m\) are positions of vertices on the boundary, and

• \(l'_1, \ldots, l'_n\) are lattice vectors, and let

\[
L' = \{a_1l'_1 + \cdots + a_nl'_n: a_1, \ldots, a_n \in \mathbb{Z}\},
\]

and let \(U'\) be the convex hull of the corners

\[
\frac{1}{2} \sum_{i=1}^{n} (-1)^{-a_i}l'_i, \quad i = 1, \ldots, n,
\]

which is preserved by the subgroup \(U' = \{g'_0, \ldots, g'_p\}\), where \(g'_j = \left[ b'_j, M_{g'_j} \right] \), and

• letting

\[
V' = \{v' + l': v' \in V'_0 \land l' \in L'\}
\]

be the vertices of the resulting net, and letting

\[
E' = \{\{v' + l', v'' + l'\}: \{v', v''\} \in E'_0 \land l' \in L'\}.
\]

then the net \(N' = \langle V', E' \rangle\) is a solution to the system \(\mathcal{E}\).

We have a nuisance to watch for. Given points \(b, c\) in a Euclidean space, let \([b, c]\) be the line segment

\[
\{b + sc: s \in [0, 1]\}.
\]

Recall from Definition 1.1 that the edges of a Eulerian graph are the line segments joining adjacent pairs of vertices.

**Definition 3.2** A Euclidean graph \(N'\) is degenerate if it admits four distinct vertices \(v_{11}, v_{12}, v_{21}, v_{22}\) and edges \([v_{11}, v_{12}]\) and \([v_{21}, v_{22}]\) such that \([v_{11}, v_{12}] \cap [v_{21}, v_{22}] \neq \emptyset\).

Recall that \(\mathcal{S}\) is the symmetry group of \(N'\), and we get:

**Proposition 3.1** Suppose that \(N'\) is not degenerate. Then \(N'\) is a graph homomorphic image of \(N'\) (of symmetry group \(\mathcal{S}\)), from the homomorphism induced by the (equivalence of paths of) the itineraries. Further, the lattice translation of \(N'\) and the symmetries in \(\mathcal{U}\) correspond to lattice translations of \(N'\) and symmetries of \(\mathcal{S}'\) of the central unit cell of the lattice of \(N'\). Thus the symmetry group \(\mathcal{S}\) is isomorphic to a (not necessarily proper) subgroup of \(\mathcal{S}'\).

**Proof.** For the first sentence, we claim three things:

1. The homomorphism induced by the itineraries preserves the edges.
2. All edges of $\mathcal{N}'$ are derived from edges of $\mathcal{N}$ via the homomorphism.

3. The homomorphism is onto.

First, note that by the definition, the homomorphism preserves vertices and edges in the standard unit cell (with respect to the given bases). Given itineraries $t_1, t_2$, where $[\sigma^*(t_1)(a), \sigma^*(t_2)(a)] \in E$, for each $i = 1, 2$, there exist $(d_{i,1}, \ldots, d_{i,n}) \in \sigma^*(t_i)(a) \text{ rem } L$ such that applying $\sigma^*$ to $\mathcal{N}'$

$$v_i = \sigma^*(t_i)(v_0) + \sum_{j=1}^{n} d_{i,j} l_j$$

is in the central unit cell. As $\mathcal{N}$ is periodic with periodicity witnessed by the lattice $L$, $[v_1, v_2] \in E$. Let $t'_1$ and $t'_2$ be itineraries such that $\sigma^*(t'_i)(v_0) = v_i$ for $i = 1, 2$, and these itineraries on $\mathcal{N}'$ produce $v'_i$ for $i = 1, 2$. As $\{v_1, v_2\} \in E$, $[v'_1, v'_2] \in E'$. But then, for $i = 1, 2$, the vertices

$$w_i = v'_i + \sum_{j=1}^{n} d_{i,j} l'_j$$

satisfies $\{w_1, w_2\} \in E'$ by the periodicity of $\mathcal{N}'$, so the homomorphism

$$\sigma^*(t)(a) \mapsto \sigma^*(t)(v_0)$$

preserves edges.

The second claim is a sort of converse of the first. Suppose that $[w_1, w_2] \in E'$; by periodicity, we get a corresponding $[v'_1, v'_2] \in E'$ within the standard unit cell of $\mathcal{N}'$. But the edge of $[v_1, v_2] \in E$ is induced by the corresponding edge of $\mathcal{N}$ within $\mathcal{N}'$’s initial unit cell, and the periodicity of $\mathcal{N}$ does the rest.

The third is straightforward.

Finally, suppose $\mathcal{N}^\dagger$ is defined from a unit cell of vertex positions $v_i$, unit cell symmetries of vector components $b_j$, and lattice vectors $l_k$. Let’s formalize a mapping $\nu$ by: $v_i \mapsto v'_i$, $b_j \mapsto b'_j$, and $l_k \mapsto l'_k$ for all $i, j, k$. We can extend this mapping to $\nu(g_j) = \nu([b_j, M_{g_j}]) = [b'_j, M_{g_j}]$, and we find that as we have encoded both the multiplication table of $\mathbb{U}$ and the preservation of $U$ by $\mathbb{U}$ into $\mathbb{E}$, that $\nu$ can be extended to all maps $[l_s, I] [l^{s}, M]_{g_j} \in \mathbb{S}$ for $l_s, l^{s} \in L$ so that

$$\nu: [l_s, I] [l^{s}, M]_{g_j} \mapsto [l'_s, I] [l'^{s}, M]_{\nu(g_j)}$$

is a homomorphism from the symmetry group $\mathbb{S}$ of $\mathcal{N}$ into the symmetry group $\mathbb{S}'$ of $\mathcal{N}'$. ■

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3.2 Deleting the Bad Nets

Following Definition 3.2, a solution would be “degenerate” if two edges of the original net $N$ intersected. Notice that degeneracy can be captured by systems of linear equations, as follows. Formally, the edge $\{x, y\}$ would intersect the edge $\{z, w\}$ if there existed $p, q \in [0, 1]$ such that

$$x + p(y - x) = z + q(w - z),$$

i.e., if

$$(1 - p)x + py - (1 - q)z - qw = 0.$$  

(Notice that if $p, q \in \{0, 1\}$, then this would characterize a collision of two vertices.) For each $p, q \in [0, 1]$, this gives us a vector space to avoid, the result being that we want to take the nets generated in Subsection 3.1 and delete these vector subspaces.

More generally, notice that $\bigcup Q$ is a prefix-closed set of itineraries, and consider the following. For each itinerary $t \in \bigcup Q$ that is not maximal in $\bigcup Q$, and for each $(t, t')$ such that $t(t, t') \in \bigcup Q$, the last symbol $(t, t')$ represents an edge for the traveller to traverse. Represent that edge $e$ with $n$-tuples of real variables $x_e$ and $y_e$, respectively — representing the endpoints of $e$. Then, for each pair of distinct edges $e_1, e_2$ so represented in $\bigcup Q$, and for each pair of constants $p_{e_1}, p_{e_2} \in [0, 1]$, we have the equation

$$(1 - p_{e_1})x_{e_1} + p_{e_1}y_{e_1} - (1 - p_{e_2})x_{e_2} - p_{e_2}y_{e_2} = 0.$$  

That includes, as special cases, for $t_1, t_2 \in \bigcup Q$ with $|t_1|_\sim \neq |t_2|_\sim$, the equation

$$x_{t_1} - x_{t_2} = 0.$$  

Let $\mathcal{E}^*$ be the set of all these equations generated from intersections of edges or collisions of vertices.

**Proposition 3.2** If $N'$ is a solution of $\mathcal{E}$ but not a solution of any of the equations of $\mathcal{E}^*$, then $N' \cong N$.

**Proof.** By Proposition 3.1, it suffices to observe that the failure to satisfy any of the Equations 3.2 forces the homomorphism induced by the (equivalence classes of) itineraries to be one-to-one. ■

We would prefer that the edges don’t intersect, which is guaranteed by the failure to satisfy any of the equations of the Equations 3.1.

There are uncountably many vector subspaces to delete, so we should be a little careful. We will use a straightforward observation from analysis.

*Scaffolding edges, i.e., edges incident to one or two scaffolding points, don’t matter as they don’t occur in $N$ — and wouldn’t represent edges in any crystal graph represented by $N$.}
Proposition 3.3 Let $C \subseteq \mathbb{R}^n$ be compact and $f : \mathbb{R}^m \times \mathbb{R}^n \to \mathbb{R}$ be continuous. For each $c \in \mathbb{R}^n$, let $W_c = \{x : f(x, c) = 0\}$. Then $W = \bigcup_{c \in C} W_c$ is closed.

Proof. It suffices to verify that $\mathbb{R}^m - W$ is open. Suppose that $x \notin W$; we claim that $\inf\{\|f(x, c)\| : c \in C\} > 0$. Towards contradiction, suppose that there exists a sequence $c_j, j \to +\infty$, with $\|f(x, c_j)\| \to 0$. By the compactness of $C$, there is in $C$ an accumulation point $c_\infty$ of the sequence $c_j, j \to +\infty$, so by the continuity of $f$ we get $f(x, c_\infty) = 0$ and $x \in W$ after all.

So if $x \notin W$ and we set $\varepsilon = \inf\{\|f(x, c)\| : c \in C\} > 0$, by the continuity of $f$ we can choose $\delta > 0$ so that for all $y \in \mathbb{R}^m$,

$$\|x - y\| < \delta \implies \|f(x, c) - f(y, c)\| < \varepsilon.$$ 

Thus for all such $y, y \notin W$. So all points $x$ in $\mathbb{R}^m - W$ are interior points, so $\mathbb{R}^m - W$ is open, so $W$ is closed. ■

We pull all this together.

Theorem 3.2 For each periodic net, there is an isomorphic periodic net whose vertices are integer points (modulo an appropriate affine transform). Thus $\nu$ maps the symmetry group $\mathbb{S}$ of $\mathcal{N}$ to a subgroup of the symmetry group $\mathbb{S}'$ of $\mathcal{N}'$, and hence every orbit of $\mathcal{N}$ is a (not necessarily proper) suborbit of an orbit of $\mathcal{N}'$.

Thus the symmetry group $\mathbb{S}$ of $\mathcal{N}^\dagger$ is isomorphic to a (not necessarily proper) subgroup of $\mathbb{S}'$ of $\mathcal{N}'$, so in particular the point group of $\mathcal{N}^\dagger$ is a (not necessarily proper) subgroup of the point group of $\mathcal{N}'$.

Proof. Let $\mathcal{N}^\dagger$ be a scaffolded net obtained from a periodic net $\mathcal{N}$, and let its point group be a subgroup of the maximal point group $\mathbb{H}$, conjugate to the integer matrix group $\mathbb{F}^{-1}\mathbb{H}^*$. By Proposition 2.1, $\mathcal{N}$ admits a fundamental transversal and using it and matrices from $\mathbb{H}^*$, we can generate a quotient graph $Q$ as in Subsection 3.1.

From the quotient graph $\mathcal{N}^\dagger$, we get a system of equations $\mathcal{E}$ whose solutions give the positions of vertices and edges within, on, or adjacent to the standard unit cell of nets that are homomorphic images of $\mathcal{N}^\dagger$; this set of solutions forms a vector space $\mathbb{E}$. Meanwhile, we also get a system of equations $\mathcal{E}^*$ such that any solution of $\mathcal{E}$ represented by a tuple of vertices in $\mathbb{E}$ is a (not necessarily proper) suborbit of an orbit of $\mathcal{N}'$.

Let $\mathbb{E}^*$ be the set of all tuples of $\mathbb{E}$ that satisfy some equation of $\mathcal{E}^*$, and notice that $\mathcal{E}^*$ consists of homogeneous linear equations that are of one of two forms.

One form is

$$\sum_i c_i x_i + \sum_j c'_j y_j = 0$$
where the set of all tuples \( c = (c_1, \ldots, c_1', \ldots) \) satisfies \( c_i, c_j' \geq 0 \) for all \( i, j \), and there exist \( i_1, i_2, j_1, j_2 \) such that
\[
i \not\in \{i_1, i_2\} \implies c_i = 0 \quad \& \quad j \not\in \{j_1, j_2\} \implies c_j = 0
\]
and \( c_{i_1} + c_{i_2} = c_{j_1} + c_{j_2} = 1 \). This set of tuples \( c \) is compact, so by Proposition 3.3, the union \( \mathbb{W} \) of all the solution spaces \( \mathbb{W}_c \) of equations of the first form is closed.

The kind of equation of \( \mathcal{E}' \), corresponding to vertex collisions, is
\[
x_i - x_j = 0,
\]
and there are only finitely many of these, and each of their solution spaces \( \mathbb{W}_{i,j} \) is a vector space, hence closed. It follows that the finite union
\[
\mathbb{W}' = \mathbb{W} \cup \bigcup_{i,j: \text{"}x_i - x_j = 0\text{"}} \mathbb{W}_{i,j}
\]
is closed. Thus the space \( \mathbb{E} - \mathbb{W}' \) of solutions representing nets isomorphic to \( \mathcal{N} \) is open.

As the tuple of vertices of \( \mathcal{N}' \)'s standard unit cell is an element of \( \mathbb{E} - \mathbb{W}' \), \( \mathbb{E} - \mathbb{W}' \neq \emptyset \). As \( \mathbb{E} - \mathbb{W}' \) is open, there exists a neighborhood \( \mathcal{N} \) around \( \mathcal{N}' \)'s tuple wholly within \( \mathbb{E} - \mathbb{W}' \). As all the coefficients of equations of \( \mathcal{E} \) are integers, \( \mathbb{E} \) is spanned by integer vectors, and hence the set of tuples of tuples of rationals is dense in \( \mathbb{E} \). Thus there is a tuple of tuples of rationals in \( \mathcal{N} \), i.e., there exists a net \( \mathcal{N}' \) whose vertices in its standard unit cell, and making up its lattice, are all rational; thus by periodicity, all the vertices of \( \mathcal{N}' \) are rational. Expressing all coordinates of vertices and lattice vectors of \( \mathcal{N}' \) as reduced fractions, there are finitely many integers appearing in the denominators, so we can choose the least common multiple \( m \) of all denominators appearing in these fractions, and multiply every vertex vector by \( m \) to get a net \( m\mathcal{N}' \) isomorphic to \( \mathcal{N} \) and whose vertices are all at integer points.

Now we make the final change of basis back to get the desired scaffolded net \( \mathcal{N}' \). □

Having obtained the net \( \mathcal{N}' \) of integer points, isomorphic to \( \mathcal{N} \) and whose symmetry group admits a subgroup isomorphic to \( \text{Sym}(\mathcal{N}) \), we have completed the proof of Theorem 1.1.

4 Conclusion

The original motivation for this paper was the development of a “Crystal Turtlebug” algorithm that enumerates crystal graphs with vertices on a geometric lattice. The question was whether this algorithm eventually enumerates representatives (of maximal symmetry) of all isomorphism classes of crystal graphs. One consequence of Theorem 1.1 is that it does.
The Crystal Turtlebug is a project in a growing field of mathematical and computational crystallography. Although graphical representations of molecules and solids go back to the Nineteenth century, it is only in the last few decades that a systematic attempt has been made to design, organize, catalogue and apply graphical representations of specific crystals. The thread of research arising from [35] through [29] to recent works for chemists like [28] and [24] is motivated by a desire to design crystals in advance prior to synthesis, rather than relying on combinatorial chemistry to physically search through thousands of initial conditions in the hope of finding one that it interesting ([16], [37]).

Recently, several groups have composed computer programs that generate crystal nets in the hope that they may prove to be viable blueprints. Some groups have developed algorithms based on fundamentally geometric principles, e.g., by enumerating tilings of 3-space ([11]), by reflecting a fundamental region around ([33]), or by attaching polyhedra together one at a time ([23]). (There are groups employing more distant algorithms, e.g., [18] and [10]; see [12] and [19] for more.) And many of the catalogues (e.g., the library attached to SYSTRE (of the Generation, Analysis and Visualization of Reticular Ornaments using GAVROC [13]), the Reticular Chemistry Structure Resource ([30]), and TOPOS (see, e.g., [4] or go to http://www.topos.ssu.samara.ru/) use crystal net isomorphism as a principle standard of identification, the issue of whether a crystal net is novel depends on whether it is isomorphic to any extant crystal nets.

For crystal design, then, the message of this paper is that if all one desires is to generate isomorphism classes of crystal nets, it suffices to generate (representative) nets with integer points as vertices. In addition, because we are usually interested in the symmetry groups of these nets (i.e., isometry groups that induce automorphisms on these nets), for a given isomorphism class of crystal nets, we can generate such a representative net so that its point group is maximal among the point groups of nets within this isomorphism class.

This result is not surprising, considering Bieberbach’s “Second” Theorem ([3], see [6]) that every crystallographic group is an affine conjugate of a group whose orbit of the origin consists of integer points. Indeed, the main result of this paper is a generalization of the Second Theorem:

- Given any crystallographic group \( G \) whose subgroup of translations is generated by translation of vectors \( \mathbf{l}_1, \ldots, \mathbf{l}_n \), start with the transversal consisting of a vertex at the origin and edges from the origin to adjacent vertices (of the same orbit) at \( \mathbf{l}_1, \ldots, \mathbf{l}_n \).

- By Theorem 1.1, there is another Euclidean graph isomorphic to the one just constructed, whose symmetry group is represented by matrices of integers (possibly modulo an affine transformation) and having a subgroup \( G' \) isomorphic to \( G \).

Then \( G' \) is the desired conjugate.

The intended application of this theorem was to verify that if a computer program will generate a (unit cell of) any crystal net whose vertices are integer points (modulo the
This project started with a computing project proposed by the author to W. E. Clark in 2007, who composed a sequence of programs in MAPLE, one of which was generating novel uninodal nets by early 2008, and whose underlying rationale is explained in [7], resting on the results on vertex transitivity in [31]. The author modified this algorithm to obtain a program for binodal edge transitive nets, and conceptually for any net ([26], the latter program being under development).

The author is grateful in particular to W. E. Clark for his assistance and advice, and to the University of South Florida for providing a sabbatical during the spring of 2008, during which the author composed the first versions of the program that is now generating nets for chemists to try to realize in the lab.

References

[1] H. Abelson & A. A. deSessa, Turtle Geometry: The Computer as a Medium for Exploring Mathematics (MIT Pr., 1980).

[2] L. Bieberbach, Uber die Bewegungsgruppen der Euklidischen Raüme mit einem endlichen Fundamentalbereich, Gött. Nachr. (1910), 75 – 84.

[3] L. Bieberbach, Uber die Bewegungsgruppen der Euklidischen Raüme, Math. Ann. 70 (1910), 297 – 336 & 72 (1912), 400 – 412.

[4] V. A. Blatov & D. M. Proserpio, Periodic-Graph Approaches in Crystal Structure Prediction, in: A. R. Oganov, Modern Methods of Crystal Structure Prediction (Wiley, 2010), 1 – 28.

[5] S. J. Chung, T. Hahn & W. E. Klee, Nomenclature and Generation of Three-Periodic Nets: the Vector Method, Acta Cryst. A40 (1984), 42 – 50.

[6] L. S. Charlap, Bieberbach groups and flat manifolds (Springer-Verlag, 1986).

[7] W. E. Clark, Notes on Uninodal Nets, http://shell.cas.usf.edu/~eclark/ UninodalNetNotes.doc, unpublished.

[8] H. S. M. Coxeter, Regular Polytopes (Dover, 1973).

[9] J. D’Andrea, Fundamental Transversals on the Complexes of Polyhedra (Master’s Thesis, University of South Florida, 2011).

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6For physical crystallography, the transformations are either the identity (if the crystal’s point group is a subgroup of m\(3\m)\)) or the map generated by the assignment of basis elements \(\langle1,0,0\rangle \mapsto \langle1,0,0\rangle, \langle0,1,0\rangle \mapsto \langle1/2,\sqrt{3}/2,0\rangle, \langle0,0,1\rangle \mapsto \langle0,0,1\rangle\) (if the crystal’s point group is a subgroup of 6/m\(3\m)\)).
[10] M. W. Deem, R. Pophale, P. A. Cheeseman & D. J. Earl, Computational Discovery of New Zeolite-Like Materials, J. Phys. Chem. C 113

[11] O. Delgado-Friedrichs, A. W. M. Dress, D. H. Huson, J. Klowski & A. L. MacKay, Systematic enumeration of crystalline networks, Nature 400 (12 Aug. 1999), 644 - 647.

[12] O. Delgado-Friedrichs, M. Foster, M. O'Keeffe, D. Proserpio, M. M. J. Treacy & O. M. Yaghi, What do we know about three-periodic nets? J. Solid State Chem. 178:8 (2005), 2533 - 2554.

[13] O. Delgado-Friedrichs & M. O'Keeffe, Identification of and symmetry computation for crystal nets, Acta Cryst. A59 (2003), 351 – 360; see [http://gavrog.sourceforge.net/](http://gavrog.sourceforge.net/).

[14] O. Delgado-Friedrichs & M. O'Keeffe, Crystal nets as graphs: Terminology and definitions, J. Solid State Chemistry 178 (2005), 2480 - 2485.

[15] W. Dicks & M. J. Dunwoody, Groups acting on graphs (Cambridge U. Pr., 1989).

[16] C. M. Draznieks & G. Férey, Simulations of inorganic crystal structures: Recent advances in structure elucidation, Current Opinion in Solid State and Materials Science 7 (2003), 13 - 19.

[17] M. Eddaoudi, G. L. McColm, L. Wojtas & M. Zaworotko, A de novo approach to the design of metal-organic frameworks and other crystal nets, in preparation.

[18] S. T. Hyde, O. Delgado-Friedrichs, S. J. Ramadam, V. Rabins, Towards enumeration of crystalline frameworks: the 2D hyperbolic approach, Solid State Sciences 8 (2006), 740 – 752.

[19] S. T. Hyde, M. O'Keeffe, and D. M. Proserpio, A Short History of an Elusive Yet Ubiquitous Structure in Chemistry, Materials, and Mathematics, Angew. Chem. Int. Ed. 47 (2008), 7996 – 8000.

[20] N. Jonoska & G. McColm, Flexible versus Rigid Tile Assembly, in: Cristian S. Calude et al, eds., 5th International Conference on Unconventional Computation (Proc. LNCS 4135, 2006), 139 - 151.

[21] N. Jonoska & G. McColm, Describing Self-assembly of Nanostructures, in: Villiam Geffert, Juhani Karhumki, Alberto Bertoni, et al, eds., SOFSEM 2008: Theory and Practice of Computer Science (Proc. LNCS 4910, Nový Smokovec, Slovakia, 2008), 66 - 73.
[22] W. E. Klee, Crystallographic nets and their quotient graphs, Cryst. Res. Technol. 39:11 (2004), 959 – 968.

[23] A. Le Bail, Inorganic structure prediction with GRINSP, J. Appl. Cryst. 38 (2005), 389 - 395.

[24] E. A. Lord, A. L. Mackay & S. Ranganathan, New Geometries for New Materials (Cambridge U. Pr., 2006).

[25] G. L. McColm, Generating Graphs Using Automorphisms, submitted for publication.

[26] G. L. McColm, W. E. Clark, M. Eddaoudi, L. Wojtas & M. Zaworotko, Crystal Engineering using a “Turtlebug” algorithm, a de novo approach to the design of binodal metal-organic frameworks, submitted for publication.

[27] J. Meier, Groups, Graphs and Trees: An Introduction to the Geometry of Infinite Groups (Cambridge U. Pr., 2008).

[28] L. Öhrström & K. Larsson, Molecule-Based Materials: The Structural Network Approach (Elsevier, 2005).

[29] M. O’Keeffe & B. G. Hyde, Crystal Symmetry I: Patterns and Symmetry (Mineralogical Society of America, 1996).

[30] M. O’Keeffe, M. A. Peskov, S. J. Ramsden, O. M. Yaghi, The Reticular Chemistry Structure Resource (RCSR) Database of, and Symbols for, Crystal Nets, Accts. Chem. Res. 41:12 (2008), 1782 – 1789; see [http://rcsr.anu.edu.au/]

[31] G. Sabidussi, Vertex-transitive graphs, Monatsh. Math. 68 (1964), 426 – 438.

[32] R. E. L. Schwarzenberger, N-dimensional crystallography (Pitman, 1980).

[33] M. M. J. Treacy, I. Rivin, E. Balkovsky, K. H. Randall & M. D. Foster, Enumeration of periodic tetrahedral frameworks. II. Polynodal graphs, Microporous and Mesoporous Materials 74:1-3 (2004), 121 - 132.

[34] E. B. Vinberg & O. V. Shvartsman, Discrete Groups of Motions of Spaces of Constant Curvature, in: E. B. Vinberg, ed., Geometry II: Spaces of Constant Curvature (Springer-Verlag, 1993), 139 – 248.

[35] A. Wells, Three dimensional nets and polyhedra (Wiley, 1977).

[36] J. A. Wolf, Spaces of Constant Curvature (McGraw-Hill, 1967).
[37] O. M. Yaghi, M. O’Keeffe, N. W. Ockwig, H. K. Chae, M. Eddaoudi, J. Kim, J. (2003), Reticular synthesis and the design of new materials, Nature 423:12 (2003) 705714.

[38] P. B. Yale, Geometry and Symmetry (Holden-Day, 1968).