Symmetry groups and reticulations of the hexagonal $H$ surface

Vanessa Robins*, S.J. Ramsden, Stephen T. Hyde

Department of Applied Mathematics, Research School of Physical Sciences, The Australian National University, Canberra ACT 0200, Australia

Abstract

We describe a systematic approach to generate nets that arise from decorations of periodic minimal surfaces. Such surfaces are covered by the hyperbolic plane, in the same way that the euclidean plane covers a cylinder. Thus, a symmetric hyperbolic network can be wrapped onto an appropriate minimal surface to obtain a 3D periodic net. This requires symmetries of the hyperbolic net to match the symmetries of the minimal surface. Here, we tabulate all such symmetry groups that are compatible with the $H$ minimal surface.

PACS: 61.50.Ah; 89.75.Hc; 02.20.−a; 02.40.−k

Keywords: Hyperbolic tilings; Minimal surfaces; Networks; Frameworks; Reticular chemistry; Symmetry groups

Network, or reticular, models are widely used descriptions of three-dimensional (3D) structure in chemistry [1]. Nature provides a rich set of examples for us to study, e.g. the covalent bonding structure of crystalline minerals, the alumino-silicate backbone of zeolites, and metal-organic frameworks. Chemists interested in synthesizing materials with particular properties need to know what structures are possible, and which are the most likely to form. Statistical physicists are also becoming increasingly interested in networks as models for complex systems, and allowed graph embeddings in 3D euclidean space are of some interest [2]. Systematic techniques for generating 3D periodic networks are still being developed and are yet to provide a complete enumeration
of possible network structures [3,4]. Our approach generates 3D euclidean networks by wrapping 2D hyperbolic nets onto triply periodic minimal surfaces (TPMS). Formally, this is done by constructing a covering map from the hyperbolic plane onto the minimal surface. Periodic 3D nets are obtained only when the symmetries of the hyperbolic net and the covering map are commensurate with the symmetries of the surface.

This work follows a number of earlier explorations of the route to 3D structure from 2D curved space [5–7]. The goal here is to enumerate all allowed symmetries of tilings or reticulations on a particular TPMS that retain the translational symmetries of the oriented surface. This relies on identifying the full group structure of the TPMS (its “hyperbolic crystallography”), derived previously for the primitive (P), diamond (D), and gyroid (G) surfaces by Sadoc and Charvolin [8]. A complete enumeration of symmetries compatible with these simplest cubic genus-three TPMS is given in Ref. [9]. In this paper, we present similar results for the hexagonal H surface. The approach is generic and can be extended to arbitrarily complex TPMS, once their hyperbolic crystallography is known.

The fundamental tool in our generation of 3D nets is a map that wraps the hyperbolic plane onto the periodic minimal surface, \( \phi : \mathbb{H}^2 \rightarrow M \). The pairing of the hyperbolic plane with this map is called a cover. (The existence of this map is guaranteed by fundamental results from topology [10].) A more familiar example is the map from the euclidean plane onto the cylinder defined by taking the fractional part of the \( x \)-coordinate. A cover is a useful tool for many reasons—the covering space, \( \mathbb{H}^2 \), has simpler topology than the original surface, \( M \), and properties of \( M \) can be determined from the action of the covering map, \( \phi \). Specifically, it is much simpler to study symmetry groups and generate nets in the hyperbolic plane than in 3D euclidean space. The complexity is shifted to finding an appropriate covering map. We describe a covering map for the \( H \) surface below; see [9] for further examples.

There are many possible ways to define the covering map \( \phi : \mathbb{H}^2 \rightarrow H \). We require that the cover respect the symmetries of the hexagonal minimal surface. The \( H \) surface (illustrated in Fig. 1) has intrinsic surface symmetry related to the \(*2226\) hyperbolic reflection group [7].\(^1\) This group is generated by four reflections, \( R_1, R_2, R_3, \) and \( R_4 \) whose mirror lines bound a quadrilateral in \( \mathbb{H}^2 \) with one vertex angle of \( \pi/6 \), and three others of \( \pi/2 \). By applying these operations in all possible combinations, images of the initial tile cover the entire hyperbolic plane. Of course, not every word over \( \{ R_1, R_2, R_3, R_4 \} \) gives a unique image, there is a set of relations for the group generated by the following identities: \( R_1^6 = R_2^2 = R_3^2 = R_4^2 = I \) (the identity) and \( (R_1 R_2)^6 = (R_1 R_4)^2 = (R_2 R_3)^2 = (R_3 R_4)^2 = I \).

A disc-like euclidean translational unit cell for the \( H \) surface was described in Ref. [6], and is illustrated here in Fig. 1 together with the corresponding hyperbolic polygon. With initial domain as defined by the figure, the hyperbolic translations that map

\(^1\) Throughout this paper, we refer to groups by their orbifold symbol. This symbol is analogous to the standard 2D crystallographic notation, but it encompasses all discrete 2D symmetry groups of the sphere, euclidean, and hyperbolic planes. Details of this notation are given in Ref. [11].

Fig. 1. Left: An 18-sided translational patch in the hyperbolic plane (drawn in the Poincaré disc model). The grey and white quadrilaterals are fundamental tiles of *2226. Edges that are identified by translation are labelled by the same letter. Vertices are numbered consecutively in an anti-clockwise direction. Some labels are omitted for clarity of illustration. Right: corresponding translational unit cell for the H minimal surface. The numbers refer to the vertices of the hyperbolic domain. We thank C. Oguey for the figure on the left, and G. Schröder for generating the surface on the right.

this domain so as to pair edges labelled by the same letter are:

\begin{align*}
t_a &= (R_1 R_2)^2 R_1 R_3, & t_f &= R_2 R_1 R_2 t_d^{-1} R_2 R_1 R_2, \\
t_b &= (R_2 R_1)^2 R_3 R_1, & t_g &= (R_1 R_2)^2 R_1 t_d^{-1} R_1 (R_2 R_1)^2, \\
t_c &= R_2 R_1 R_3 R_1 R_2 R_1, & t_h &= (R_2 R_1)^2 t_d (R_1 R_2)^2, \\
t_d &= R_4 R_2 R_4 R_2, & t_i &= R_2 R_1 t_d R_1 R_2, \\
t_e &= R_1 t_d^{-1} R_1.
\end{align*}

These translations define a normal subgroup, \( T \), of *2226, and they satisfy the following relations:

\begin{align*}
t_a^{-1} t_g t_a t_d &= I, & t_b^{-1} t_h t_b t_e &= I, & t_c^{-1} t_i t_c t_f &= I, & t_d t_h t_g t_f t_c t_d &= I.
\end{align*}

We now define the covering map \( \phi \) by specifying how the hyperbolic isometries map to transformations in \( \mathbb{E}^3 \). The hyperbolic reflections \( R_1, R_3, R_4 \) map to euclidean reflections in mirror planes, while \( R_2 \) maps to a rotation by \( \pi \) about an axis lying in the surface and perpendicular to the \( R_3 \) mirror plane. The translations commute in \( \mathbb{E}^3 \), so

\[ \phi(t_x t_y) = \phi(t_y t_x) \quad \text{for } x \neq y \in \{a, b, \ldots, i\}. \]

Finally, there are only three independent translations in \( \mathbb{E}^3 \) so the covering map induces dependencies between \( \{t_a, \ldots, t_i\} \). For this choice of unit cell for the \( H \) surface we have

\begin{align*}
\phi(t_a) &= X, & \phi(t_b) &= X + Y, & \phi(t_c) &= Y, & \phi(t_d) &= Z, \\
\phi(t_e) &= -Z, & \phi(t_f) &= Z, & \phi(t_g) &= -Z, & \phi(t_h) &= Z, & \phi(t_i) &= -Z.
\end{align*}

The next step is to find all sub-symmetries, \( G \), that are commensurate with the intrinsic symmetry, \( S \), of a given minimal surface. Algebraically, \( G \) must be a subgroup
of $S$, and a supergroup of the translation subgroup, $T$. An elementary result from group theory [12] tells us that such groups $G$ satisfying $T \subset G \subset S$ are in one-to-one correspondence with subgroups of the quotient group: $\overline{G} \subset S/T$. The covering maps defined above allow us to work with hyperbolic groups rather than the more complex surface groups. For the $H$ surface, we must enumerate all subgroups of $*2226$ / [$t_a = \cdots = t_l = I$]. Although the hyperbolic group $*2226$ is infinite, the quotient group is finite, so enumerating these subgroups is a simple matter for the computational discrete algebra package, Groups, Algorithms and Programming (GAP) [13]. The result from GAP is a list of finitely presented groups, with generators in the quotient group. Adding back in the hyperbolic translation subgroup generators, $\{t_a, \ldots, t_l\}$ and using GAP’s group isomorphism tools, gives us a list of finitely presented subgroups of $*2226$. We compute orbifold symbols for each subgroup using various tools from computational group and tiling theory including word reduction and enumeration from the KBMAG extension to GAP [14], and a re-implementation of Delgado-Friedrichs’ combinatorial tiling algorithms [15]. Further details are given in Ref. [9]. The results of this process are presented in Table 1, and the subgroup lattice is illustrated in Fig. 2.

Once we know the subgroup domains and their adjacency pattern it is straightforward to generate a vertex-transitive net with the symmetry of the subgroup. This is achieved by putting a single vertex in each subgroup domain, then joining vertices by an edge if the two domains are adjacent. The result is a periodic net in the hyperbolic plane. Careful use of word reduction with respect to the translation subgroup $T$ gives us explicit knowledge of the translational unit for the hyperbolic net and the connections between nodes in successive translational cells. For example, the following hyperbolic net comes from the $22222222$ ($2^8$) orbifold, with vertex 1 in the identity domain, $I$, and vertex 2 in $R_2R_3$

\[
\begin{align*}
1 & 1 t_a, & 1 & 1 t_d, & 1 & 1 t_e, & 1 & 2 I, \\
1 & 2 t_a, & 1 & 2 t_h^{-1} t_a, & 1 & 2 t_f^{-1} t_a, & 1 & 2 t_l t_a, \\
2 & 2 t_d, & 2 & 2 t_a^{-1} t_c t_a, & 2 & 2 t_a^{-1} t_b t_a.
\end{align*}
\]

Each triple above represents an edge: the first entry denotes one vertex in the initial unit cell and the other two entries denote the second vertex type and its cell location. To map this net onto the $H$ surface we set $\phi(t_a)$ to the $E^3$-translations given above. The euclidean net topology is then

\[
\begin{align*}
1 & 1 (0, 1, 0), & 1 & 1 (0, 0, 1), & 1 & 2 (0, 0, 0), & 1 & 2 (1, 0, 0), \\
1 & 2 (0, -1, 0), & 1 & 2 (1, 0, -1), & 2 & 2 (0, 1, 0), & 2 & 2 (0, 0, 1).
\end{align*}
\]

Note that some of the hyperbolic edges or vertices are mapped onto the same edge or vertex in $E^3$, lowering the network connectivity from that in $H^2$. Now we have the net topology, we need to assign coordinates to the vertices. This can be done in a number of ways including (i) a direct map from the hyperbolic plane onto the periodic minimal surface [5], (ii) equilibrium (or barycentric) placements [16], or (iii) relaxation according to an energy potential that is minimized by equal edge-lengths and angles [7].
Table 1
Subgroups of *2226 commensurate with the H surface

<table>
<thead>
<tr>
<th>Orbifold symbol</th>
<th>Index</th>
<th>Conjugacy class size</th>
<th>Subgroup generators in *2226/T</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 ooo</td>
<td>24</td>
<td>1</td>
<td>I</td>
</tr>
<tr>
<td>2 2222222222</td>
<td>12</td>
<td>1</td>
<td>R1R2R1R2R1R2</td>
</tr>
<tr>
<td>3 o**</td>
<td>12</td>
<td>1</td>
<td>R4</td>
</tr>
<tr>
<td>4 xxxx</td>
<td>12</td>
<td>1</td>
<td>R1R2R1R2R1R2R4</td>
</tr>
<tr>
<td>5 **xx</td>
<td>12</td>
<td>3</td>
<td>R1</td>
</tr>
<tr>
<td>6 oo</td>
<td>12</td>
<td>3</td>
<td>R2R4</td>
</tr>
<tr>
<td>7 o2222</td>
<td>12</td>
<td>3</td>
<td>R1R4</td>
</tr>
<tr>
<td>8 **xx</td>
<td>12</td>
<td>3</td>
<td>R2</td>
</tr>
<tr>
<td>9 o33</td>
<td>8</td>
<td>1</td>
<td>R2R1R2R1</td>
</tr>
<tr>
<td>10 2222*</td>
<td>6</td>
<td>1</td>
<td>R3R2, R4</td>
</tr>
<tr>
<td>11 22*2222</td>
<td>6</td>
<td>3</td>
<td>R1, R3R2R3R4</td>
</tr>
<tr>
<td>12 **x</td>
<td>6</td>
<td>3</td>
<td>R2, R3R4</td>
</tr>
<tr>
<td>13 **x</td>
<td>6</td>
<td>3</td>
<td>R2, R4</td>
</tr>
<tr>
<td>14 *2222x</td>
<td>6</td>
<td>3</td>
<td>R1, R4</td>
</tr>
<tr>
<td>15 222222</td>
<td>6</td>
<td>3</td>
<td>R3R2, R4R1</td>
</tr>
<tr>
<td>16 22*x</td>
<td>6</td>
<td>3</td>
<td>R2, R4R3</td>
</tr>
<tr>
<td>17 <em>3</em>3</td>
<td>4</td>
<td>1</td>
<td>R2, R3, R1</td>
</tr>
<tr>
<td>18 3**</td>
<td>4</td>
<td>1</td>
<td>R3R1, R4</td>
</tr>
<tr>
<td>19 <em>33</em></td>
<td>4</td>
<td>1</td>
<td>R1, R3</td>
</tr>
<tr>
<td>20 o3</td>
<td>4</td>
<td>1</td>
<td>R3R1, R4R2</td>
</tr>
<tr>
<td>21 3xx</td>
<td>4</td>
<td>1</td>
<td>R3R1, R4R2R4</td>
</tr>
<tr>
<td>22 23222</td>
<td>4</td>
<td>1</td>
<td>R3R1, R4R4</td>
</tr>
<tr>
<td>23 6262</td>
<td>4</td>
<td>1</td>
<td>R3R1</td>
</tr>
<tr>
<td>24 2*2222</td>
<td>3</td>
<td>3</td>
<td>R1, R3R2, R4</td>
</tr>
<tr>
<td>25 *6226</td>
<td>2</td>
<td>1</td>
<td>R1, R2</td>
</tr>
<tr>
<td>26 *32222</td>
<td>2</td>
<td>1</td>
<td>R1, R3, R4</td>
</tr>
<tr>
<td>27 <em>3</em></td>
<td>2</td>
<td>1</td>
<td>R1, R3, R4R2</td>
</tr>
<tr>
<td>28 <em>3</em></td>
<td>2</td>
<td>1</td>
<td>R2, R3R1, R4</td>
</tr>
<tr>
<td>29 22*3</td>
<td>2</td>
<td>1</td>
<td>R2, R3R1, R4R1</td>
</tr>
<tr>
<td>30 62*</td>
<td>2</td>
<td>1</td>
<td>R2R1, R4</td>
</tr>
<tr>
<td>31 2622</td>
<td>2</td>
<td>1</td>
<td>R2R1, R4R4</td>
</tr>
<tr>
<td>32 *6222</td>
<td>1</td>
<td>1</td>
<td>R1, R2, R3, R4</td>
</tr>
</tbody>
</table>

We generate one vertex-transitive net for each subgroup listed in Table 1; the results can be viewed in supplementary material online.\(^2\) The coordination numbers for these nets take the values 4, 5, 6, 7, 8, 10, and 12. Some subgroups induce nets with the same topology because they have the same domain geometry, resulting in seventeen distinct nets. Of these seventeen, five are simple laminar stacks of 2D euclidean archimedean nets with vertex symbols 6\(^3\) (hexagonal), 4\(^4\) (square), 6.3.6.3 (Kagomé), 4\(^2\).3\(^3\) (see Fig. 3, net 10) and 3\(^6\) (triangular). Vertices in each layer connect to identical vertices in the layers above and below; for example, the laminar square net is the familiar simple cubic net. The net generated from the translation subgroup (1 in Table 1) has a single vertex per unit cell, coordination 12, and is readily identified as \(ccp\), the

network of adjacencies in a cubic close packing of spheres. The remaining eleven nets are less simply described; they are illustrated in Fig. 3. The two four-coordinated nets (25 and 32) model the \( T \)-atom adjacencies in the zeolites \textit{cancrinite} and \textit{gmelinite}, respectively. Net 28 is five-coordinated, has a channel structure of 6.4.3.4 rings, and transverse rings of orders 4.4.4.6. Net 17 has the same channel structure as net 28, but it is six-coordinated and has a transverse channel structure consisting of rows of alternating kites and diamonds. A distinct six-coordinated net arises from subgroup 16, containing puckered layers of the archimedean net with vertex symbol 3.3.4.3.4, plus a single transverse edge at each vertex connecting to a layer above or below. Nets 20 and 21 are complex eight-coordinated structures with 3- and 4-rings. Nets 2 and 8 are also eight-coordinated but have regular structure. Net 8 has hexagonal channels with triangular facets, while net 2 is built from layers of triangular prisms sharing square faces arranged in alternating orientations. Lastly, there are two 10-coordinated nets: net 4 has approximately square channels with triangular facets; net 6 is self-catenating and includes two transverse four-rings forming a Hopf link. Such self-linked “catenated”
networks are found in dense chemical frameworks, such as the silicate mineral, coesite [4].

The examples presented in this paper are a small sample of a complete enumeration of nets embedded in the $H$ surface. They reveal the wealth of patterns that can be generated by our projection technique, including networks with many distinct coordinations and ring-sizes as well as self-catenated examples. Further examples can be generated from the symmetry groups derived here by using more sophisticated combinatorial tiling algorithms in the hyperbolic plane.
References