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On subgroups of crystallographic Coxeter groups

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A framework is presented based on color symmetry theory that will facilitate the determination of the subgroup structure of a crystallographic Coxeter group. It is shown that the method may be extended to characterize torsion-free subgroups. The approach is to treat these groups as groups of symmetries of tessellations in space by fundamental polyhedra.

1. Introduction

One of the important problems in mathematical crystallography is the characterization of the subgroup structure of crystallographic groups. Crystallographic groups and their subgroups, and relations between these groups, are essential in understanding the fundamental properties of symmetry and periodicity of crystals, topological properties of crystal structures, twins, modular and modulated structures, as well as the symmetry aspects of phase transitions and physical properties of crystals.

In this work, the main focus is to discuss a process to derive the subgroup structure of crystallographic Coxeter groups, one of the largest families of crystallographic groups. The method uses the connection between group theory and color symmetry theory, brought about by representing crystallographic Coxeter groups and their subgroups as isometries acting on tessellations in Euclidean, spherical or hyperbolic space. The approach used allows for the characterization of each subgroup by types of symmetries, made possible by constructing colorings of its corresponding tessellation. This facilitates the discovery of subgroups with interesting symmetrical structures. This is particularly pertinent in exploring groups in hyperbolic space, which have not been as widely discussed compared to the Euclidean and spherical cases, and contain an abundance of hyperbolic symmetries.

Two-dimensional hyperbolic crystallographic groups, for instance, contain five-, eight- and 12-fold rotational symmetries which can be used to describe quasicrystal structures. Moreover, understanding subgroups of crystallographic groups acting as symmetries on tessellations in hyperbolic space provides advantages in establishing connections of these groups to infinite periodic minimal surfaces. These have been used to describe crystals of surfaces or films, such as liquid crystalline structures (Sadoc & Charvolin, 1990). Interest in hyperbolic crystallographic groups and their subgroups also arises in the study of crystal nets (Ramsden *et al.*, 2009) and chemical networks as hyperbolic forms (Nesper & Leoni, 2001). These groups also play a role in the study of emerging new structures, such as for example in the fullerene family (Pisani, 1996; Rasetti, 1996) and in snow crystals (Janner, 1997, 2001).

The role of the subgroup structure of crystallographic Coxeter groups in the construction of color groups associated with tilings has been recognized in previous works (see De Las Peñas *et al.*, 2006; Frettlöh, 2008, and references therein). Knowledge of these subgroups in terms of their symmetries facilitates the use of colorings of tilings to model crystals and sheds light on their symmetrical structures.

Consider, for instance, the *cubic honeycomb* $\{4, 3, 4\}$ shown in Fig. 1(a) defined as the regular space-filling tessellation of the Euclidean space $\mathbb{E}^3$ made up of cubes or *cubic cells*. The symmetry group of the tessellation is the crystallographic Coxeter group

$$\langle P, Q, R, S | P^2 = Q^2 = R^2 = S^2 = (PQ)^4 = (QR)^3 = (RS)^4 = (PR)^2 = (PS)^2 = (QS)^2 = e\rangle.$$

The generators are the reflections P, Q, R, S about the planes m_P, m_Q, m_R, m_S. This group is isomorphic to the space group $Pm\overline{3}m$ (in IUCr notation). A cubic cell presented in Fig. 1(b) from the $\{4, 3, 4\}$ honeycomb in Fig. 1(a) shows the planes of reflections. The plane m_P (yellow) is parallel to the top and bottom faces of the cube and cuts the other faces in half; the plane m_Q (red) is the diagonal plane which cuts the front and back faces of the cube into right triangular regions; similarly, the plane m_R (blue) is also a diagonal plane, this time cutting the top and bottom faces into right triangular regions; finally, the plane m_S (gray) is the plane which is off the center of the cube and contains the front face. These four planes form the walls of a tetrahedron with dihedral angles $\pi/4, \pi/3, \pi/4, \pi/2, \pi/2, \pi/2$, which serves as a fundamental polytope (asymmetric unit) of the tessellation. The group $G = \langle P, Q, R, S\rangle \cong Pm\overline{3}m$ has a translation subgroup generated by the standard orthogonal basis a, b, c of the cubic lattice. A vertex coloring of the $\{4, 3, 4\}$ honeycomb where the elements of the subgroup $H = \langle Q, R, S, PQRPQP\rangle$ of G effect a permutation of the colors (H is the color group) is shown in

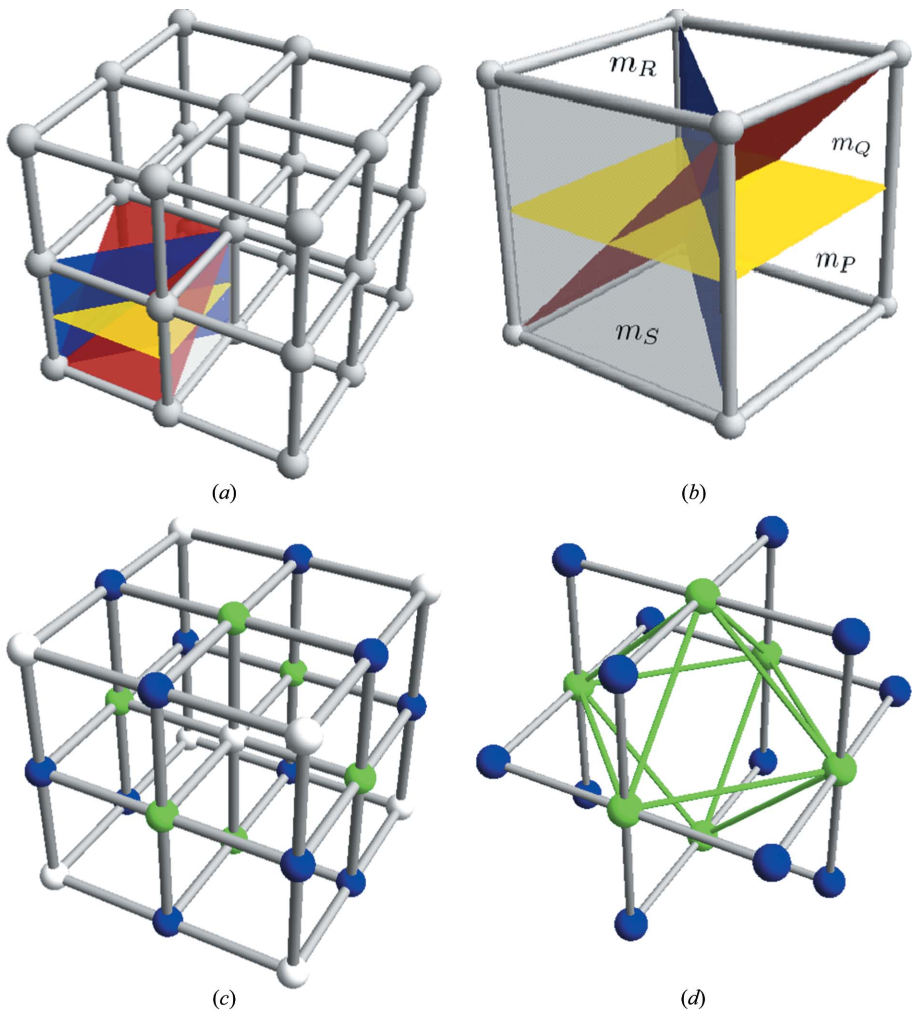

Figure 1
(*a*) Uncolored honeycomb with planes of reflections (generators) for its symmetry group G. (*b*) The planes m_P, m_Q, m_R, m_S of the reflections P, Q, R, S viewed on a cubic cell. (*c*) A vertex-coloring of the cubic honeycomb {4, 3, 4}. (*d*) Unit cell of NbO.

Fig. 1(*c*). The group $H \cong Im\overline{3}m$ has the same point group as G with translation lattice the body-centered lattice generated by $2a, 2b, 2c$ and the centering vector $a+b+c$. This coloring models the crystal niobium monoxide (NbO) with unit cell shown in Fig. 1(*d*). The niobium (Nb) atoms are represented by the green vertices while the oxygen (O) atoms are represented by the dark blue vertices. In this representation, the vertices colored white do not represent a particular type of atom. The white vertices form the orbit of the origin under H, which consists of one quarter of the lattice vertices of the original cubic lattice, since H is a subgroup of index 4 in G. The remaining vertices given by the Nb and O atoms are also invariant under H and form a single orbit. The generators Q, R, S and the twofold rotation $PQRPQP$ of H act as color symmetries on the vertices, and thus H acts as a group of color symmetries. The symmetries in H that fix the colors are the index-2 subgroup K of H, obtained by removing the translation $a+b+c$ (which interchanges the colors). The group K has translation lattice spanned by $2a, 2b, 2c$ and is isomorphic to $Pm\overline{3}m$. K is the symmetry group of NbO. This coloring exhibits geometrically the embedding of the symmetrical structure of NbO in the cubic crystal family.

In this paper, an approach to determine the torsion-free subgroups of crystallographic Coxeter groups will also be presented. By a *torsion-free* subgroup, we mean a subgroup all of whose non-identity elements are of infinite order. The geometrical interest of such a subgroup is that when the points on the plane of the tiling are identified using the elements of the subgroup, the result is a manifold. The role of torsion-free subgroups and their importance in crystallography have been discussed in the literature (*e.g.* Sadoc & Charvolin, 1990).

We apply our methodology to two particular examples involving index-6 subgroups (a Euclidean and a hyperbolic case) including the derivation of torsion-free subgroups.

We begin our discussion by describing the setting of our study on crystallographic Coxeter groups.

2. Crystallographic Coxeter groups

We first consider a *Coxeter polytope D* in $\mathbb{X}^d = \mathbb{E}^d, \mathbb{S}^d$ or $\mathbb{H}^d$, that is, in either Euclidean, spherical or hyperbolic d-space, respectively. In this case, D is a convex polytope of finite volume bounded by hyperplanes H_i, $i \in I$ such that for all $i, j \in I, i \neq j$, the hyperplanes H_i and H_j are disjoint or form a dihedral angle of π/m_{ij} for some integer $m_{ij} \geq 2$. The group of isometries generated by the reflections R_i in the hyperplanes H_i of D is called a *Coxeter group G* with defining relations $R_i^2 = (R_iR_j)^{m_{ij}} = e$. If the two hyperplanes are parallel, the corresponding relation with $m_{ij} = \infty$ is omitted.

The Coxeter group G is discrete and D is a fundamental polytope for G. This means that the polytopes gD, $g \in G$ do not have pairwise common interior points and cover $\mathbb{X}^d$; that is, they form a tessellation $\mathcal{T}$ for $\mathbb{X}^d$. The tessellation $\mathcal{T}$ is the G-orbit of D, that is, $\mathcal{T} = \{gD | g \in G\}$. Moreover, $\mathrm{Stab}_G(D) = \{g \in G | gD = D\}$ is the trivial group $\{e\}$ and G acts transitively on $\mathcal{T}$. We call discrete Coxeter groups with fundamental polytopes of finite volume *crystallographic Coxeter groups* (Vinberg, 1985).

In $\mathbb{X}^2$, an example of a crystallographic Coxeter group is the *triangle group*. A triangle group $*abc$ is generated by the reflections A, B, C about the sides of a triangle Δ (a two-dimensional Coxeter polytope) with interior angles π/a, π/b and π/c. The generators A, B, C satisfy the relations

$$A^2 = B^2 = C^2 = (BA)^c = (CA)^b = (BC)^a = e.$$

Among the well known triangle groups are the three crystallographic Coxeter groups in $\mathbb{E}^2$, namely, *p*4*mm*, *p*6*mm* and *p*3*m*1 (in IUCr notation). In $\mathbb{H}^2$, an example is the extended modular group $*32\infty$. We illustrate in Fig. 2 a tessellation by a hyperbolic triangle Δ with interior angles $\pi/3$, $\pi/2$ and zero. The extended modular group is generated by A, B, C whose axes of reflections are shown.

In $\mathbb{X}^3$, the Coxeter tetrahedron groups, generated by reflections along the faces of a tetrahedron of finite volume, are examples of crystallographic Coxeter groups. A well known example in $\mathbb{E}^3$ is the Coxeter tetrahedron group discussed earlier, isomorphic to the space group $Pm\overline{3}m$. In the hyperbolic case there are 32 Coxeter tetrahedron groups with fundamental tetrahedra of finite volume, nine compact types with no vertices at infinity and 23 non-compact ones with at least one ideal vertex (Johnson *et al.*, 1999).

Some other known examples of crystallographic Coxeter groups include those having Coxeter simplices as fundamental polytopes. In $\mathbb{H}^4$, for instance, there are five compact and nine non-compact Coxeter simplices. There are 12, three, four, five and three Coxeter simplices in $\mathbb{H}^5$, $\mathbb{H}^6$, $\mathbb{H}^7$, $\mathbb{H}^8$ and $\mathbb{H}^9$, respectively, all of which are non-compact (Johnson *et al.*, 1999).

3. Colorings of *n*-dimensional tessellations by Coxeter polytopes

In this section we will discuss the underlying ideas used in determining the subgroups of a crystallographic Coxeter group. The link between group theory and color symmetry theory will be the basis for the derivation of these subgroups.

Let us consider a subgroup H of a Coxeter group G of finite index and $\mathcal{O}_H = HD = \{hD | h \in H\}$, the H-orbit of the corresponding fundamental polytope D of G. Then $\mathrm{Stab}_H(D) = \{e\}$ and H acts transitively on $\mathcal{O}_H$ (Vinberg, 1985). Consequently, there exists a one-to-one correspondence between H and $\mathcal{O}_H$ given by $h \to hD$, $h \in H$ and $h' \in H$ acts on $hD \in \mathcal{O}_H$ by sending it to its image under h'.

In this work, the index-n subgroups of H will be derived using n-colorings of $\mathcal{O}_H$. An *n-coloring* of $\mathcal{O}_H$ refers to an onto function g from $\mathcal{O}_H$ to a set $C = \{c_1, c_2, \ldots, c_n\}$ of n colors, that is, to each $hD \in \mathcal{O}_H$ is assigned a color in C. This coloring determines a partition $\{g^{-1}(c_i) | c_i \in C\}$ where $g^{-1}(c_i)$ is the set of elements of $\mathcal{O}_H$ assigned color c_i. Equivalently, we may think of the coloring as a partition of $\mathcal{O}_H$ (which corresponds to a partition of H). We will consider H-transitive n-colorings of $\mathcal{O}_H$, that is, colorings for which H has a transitive action on the set C of n colors.

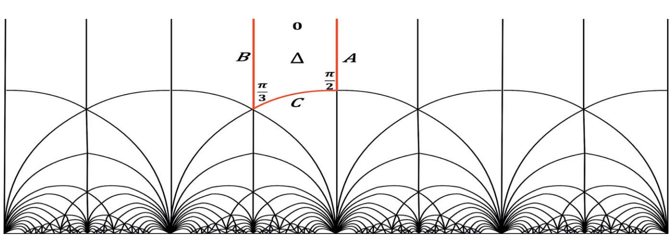

Figure 2
A tessellation of the upper half plane by a hyperbolic triangle Δ with interior angles $\pi/3$, $\pi/2$ and zero. The axes of reflections A, B, C are shown.

The theorem below forms the basis of our methodology. For a proof of the theorem, the reader may refer to De Las Peñas *et al.* (2010).

Theorem 1. Let H be a subgroup of a Coxeter group G and consider $\mathcal{O}_H = \{hD | h \in H\}$ the H-orbit of the corresponding Coxeter polytope D.

(i) Suppose M is a subgroup of H of index n. Let $\{h'_1, h'_2, \ldots, h'_n\}$ be a complete set of left coset representatives of M in H and $\{c_1, c_2, \ldots, c_n\}$ a set of n colors. Then the assignment $h'_i MD \to c_i$ defines an n-coloring of $\mathcal{O}_H$ which is H-transitive.

(ii) In an H-transitive n-coloring of $\mathcal{O}_H$, the elements of H which fix a specific color in the colored set $\mathcal{O}_H$ form an index-n subgroup of H.

If a coloring of $\mathcal{O}_H$ is given by $g: \mathcal{O}_H = HD \to C = \{c_1, c_2, \ldots, c_n\}$ where $g(x) = c_i$ if $x \in h'_i MD$, then $g^{-1}(c_i) = h'_i MD$. The group H acts transitively on $\{h'_1 MD, h'_2 MD, \ldots, h'_n MD\}$ with $h \in H$ sending $h'_i MD$ to $hh'_i MD$. We get a transitive action of H on C by defining for $h \in H$, $hc_i = c_j$ if and only if $hg^{-1}(c_i) = g^{-1}(c_j)$. The n-coloring of $\mathcal{O}_H$ determined by g is H-transitive. This n-coloring corresponds to the action of H on the cosets of M in H.

Given a subgroup M of H of index n and the set C of n colors, there will correspond $(n-1)!$ H-transitive n-colorings of $\mathcal{O}_H$ with M fixing a specific color (say c_1). In a H-transitive n-coloring of $\mathcal{O}_H$ with M fixing c_1, the set of Coxeter polytopes MD is assigned c_1 and the remaining $n-1$ colors are distributed among the $h'_i MD$, $h_i \in H$.

4. Setting in determining subgroups of crystallographic Coxeter groups

If we let $H = \langle h_1, h_2, \ldots, h_l \rangle$ be a subgroup of G, Theorem 1 tells us that there is a one-to-one correspondence between the set of index-n subgroups of H and the set of all H-transitive n-colorings of $\mathcal{O}_H$. To arrive at a subgroup of H, we construct all transitive n-colorings of $\mathcal{O}_H$ using a set $C = \{c_1, c_2, \ldots, c_n\}$ of n-colors with the property that all elements of H effect permutations of C and H acts transitively on C. Now, for each such coloring of $\mathcal{O}_H$, a homomorphism $f: H \to S_n$ is defined where, for each $h \in H$, $f(h)$ is the permutation of the colors in $\mathcal{O}_H$ effected by h. Note that f is completely determined when $f(h_1), f(h_2), \ldots, f(h_l)$ are specified. We call the set $\{f(h_1), f(h_2), \ldots, f(h_l)\}$ a permutation assignment that gives rise to a subgroup M of H of index n. The subgroup M consists of all the elements of H that fix a specific color in the n-coloring.

The goal is to come up with a set $\mathbb{P}$ of permutation assignments $\{f(h_1), f(h_2), \ldots, f(h_l)\}$ corresponding to the H-transitive n-colorings of $\mathcal{O}_H$ that will give rise to the index-n subgroups of H distinct up to conjugacy in H. See Holt *et al.*

Table 1
Colorings corresponding to the index-6 subgroups of the modular group 632.

	$f(632)$	$f(BA)$	$f(CA)$	$f(BC)$	Generators
(*a*)	C_6	(14)(25)(36)	(135)(246)	(123456)	$BACBAC, BCABCA$
(*b*)	$S_3(6)$	(12)(36)(45)	(135)(246)	(16)(25)(34)	$BACBCA, BCABAC$
(*c*)	$A_4(6)$	(25)(36)	(123)(456)	(135)(246)	$BA, CABACBCA, CABCBACBAC$
(*d*)	$F_{18}(6)$	(12)(34)(56)	(246)	(165432)	$CA, BACABACBACAB$
(*e*)	$2A_4(6)$	(36)	(123)(456)	(135462)	$BA, CABC, ACBACABCABCA$

(2005) for a related discussion. To do this, we first consider the set $\mathbb{T} = \{T_1, T_2, \ldots, T_k\}$ of transitive subgroups of S_n. Then for each $T_j \in \mathbb{T}$, $j = 1, 2, \ldots, k$, we put together the set $\mathbb{P}_j$ consisting of permutation assignments such that $f(H) = T_j$. Note that in each set $\mathbb{P}_j$ there corresponds, for each index-n subgroup M of H, $(n-1)!$ H-transitive n-colorings of $\mathcal{O}_H$ with M fixing c_1. That is, $(n-1)!$ permutation assignments in $\mathbb{P}_j$ will yield the subgroup M. To ensure an enumeration of distinct subgroups, if the permutation assignment $\{f(h_1), f(h_2), \ldots, f(h_l)\} \in \mathbb{P}_j$ corresponds to a subgroup M we delete the elements $s\{f(h_1), f(h_2), \ldots, f(h_l)\}s^{-1}$ from $\mathbb{P}_j$ for all non-identity elements s of S_n fixing 1. Furthermore, we also remove from $\mathbb{P}_j$ the permutation assignments that will yield conjugate subgroups of M and the resulting set is then called $\mathbb{P}'_j$. Finally, from the union of the sets $\mathbb{P}'_j$, we form the set $\mathbb{P}$ consisting of the permutation assignments satisfying the divisibility conditions relative to the defining relations of H such as the order of $f(h_i)$ divides the order of h_i.

To illustrate the methodology just described, we derive the index-6 subgroups of the group $H = abc$, an index-2 subgroup of the triangle group $*abc$ consisting of orientation-preserving isometries. The group H has generators BA, CA, BC satisfying the relations $(BA)^c = (CA)^b = (BC)^a = e$. In the tiling obtained by reflecting a triangle Δ with interior angles π/a, π/b and π/c, we consider all transitive 6-colorings of the H-orbit $\mathcal{O}_H$ of Δ using a set $C = \{c_1, c_2, c_3, c_4, c_5, c_6\}$ of 6 colors with the property that all elements of H effect permutations of C and H acts transitively on C. To achieve this goal, we get the set $\mathbb{P}$ of permutation assignments $\{f(BA), f(CA), f(BC)\}$ corresponding to the H-transitive 6-colorings of $\mathcal{O}_H$ that will give rise to the index-6 subgroups of H distinct up to conjugacy in H.

In this case, the set $\mathbb{T}$ consisting of the transitive subgroups of the symmetric group S_6 (Conway *et al.*, 1998; Jones, 2006) consists of 16 groups: S_6, the dihedral group D_6, the alternating group A_6, the two order-6 groups, C_6 and $S_3(6)$ (isomorphic to the cyclic group Z_6 and S_3, respectively), the order-12 group $A_4(6)$ (isomorphic to $A_6 \cap S_4$), the three order-24 groups $2A_4(6)$, $S_4(6d)$ and $S_4(6c)$ [isomorphic to $C_2 wr_3 C_3$, $A_6 \cap (S_2 wr_3 S_3)$ and S_4, respectively], the order-18 group $F_{18}(6)$ (isomorphic to $C_3 wr_2 C_2$), the two order-36 groups $F_{18}(6):2$ and $F_{36}(6)$ [isomorphic to $A_6 \cap (S_3 wr_2 C_2)$], the order-48 group $2S_4(6)$ (isomorphic to $S_2 wr_3 S_3$), the order-60 group $A_5(6)$ [isomorphic to $PSL(2, 5)$, a two-dimensional projective special linear group over a field of order 5], the order-72 group $F_{36}(6):2$ (isomorphic to $S_3 wr_2 S_2$) and the order-120 group $S_5(6)$ [isomorphic to $PGL_2(5)$, a two-dimensional projective general linear group over a field of order 5].

For each transitive subgroup $T_j \in \mathbb{T}$, we form the set $\mathbb{P}_j$ consisting of permutation assignments to $\{f(BA), f(CA), f(BC)\}$ such that $f(H) = T_j$. To arrive at the set $\mathbb{P}'_j$, for each M, we eliminate from $\mathbb{P}_j$ the $(6-1)!$ permutation assignments from $\mathbb{P}_j$ that will yield the same subgroup M and all those elements that will yield the conjugate subgroups of M. Combining the elements of the sets $\mathbb{P}'_j$ altogether yields 624 permutation assignments that will give rise to 624 index-6 subgroups of H distinct up to conjugacy if a, b and c are all divisible by 2, 3, 4, 5 and 6.

To demonstrate the applicability of the above result, we derive the index-6 subgroups of the group 632. For this group, BA, CA, BC satisfy the relations $(BA)^2 = (CA)^3 = (BC)^6 = e$. Thus, from the list of permutation assignments, we consider those where the order of $f(BA)$ divides 2, the order of $f(CA)$ divides 3 and the order of $f(BC)$ divides 6. Of the 624 permutation assignments, we find five such permutation assignments that give rise to index-6 subgroups of 632. The list is presented in Table 1.

For example, the permutation assignment

$$\{f(BA), f(CA), f(BC)\} = \{(14)(25)(36), (135)(246), (123456)\}$$

corresponds to the H-transitive 6-coloring of $\mathcal{O}_H$ in Fig. 3(*a*) which gives rise to the index-6 subgroup $\langle BACBAC, BCABCA\rangle$. The colors yellow, orange, pink, green, blue and violet are assigned the numbers 1, 2, 3, 4, 5, 6, respectively. It can be verified that the group of symmetries fixing the color yellow is generated by the translations $BACBAC = (BACAB)C$ and $BCABCA = [BA(CAC)AB]CAC$.

Similarly, we take the index-6 subgroups of the modular group 32∞, which is an index-2 subgroup of the extended modular group $*32\infty$, consisting of orientation-preserving isometries. It may be generated by CA, BC satisfying the relations $(BC)^3 = (CA)^2 = e$. Consequently, from the list of 624 permutation assignments, we consider only those where the order of $f(BC)$ divides 3 and the order of $f(CA)$ divides 2. The list of eight permutation assignments that give rise to index-6 subgroups of the modular group is presented in Table 2.

5. Torsion-free subgroups of orientation-preserving subgroups

In this part of the paper, we extend the methodology given in the previous sections to determine torsion-free subgroups of the subgroup consisting of orientation-preserving isometries of a given crystallographic Coxeter group.

Table 2
Colorings corresponding to the index-6 subgroups of the modular group 32∞.

	$f(32\infty)$	$f(BA)$	$f(CA)$	$f(BC)$	Generators
(*a*)	C_6	(123456)	(14)(25)(36)	(153)(264)	*BACBCA*, *BCBABA*
(*b*)	$S_3(6)$	(14)(23)(56)	(12)(36)(45)	(153)(264)	*BABA*, *CBABCA*
(*c*)	$A_4(6)$	(123)(456)	(25)(36)	(153)(264)	*CA*, *BABABA*, *BACBABCABA*
(*d*)	$F_{18}(6)$	(123456)	(12)(34)(56)	(246)	*CB*, *ABACBABA*, *ACBABABCBA*
(*e*)	$2A_4(6)$	(123456)	(36)	(126)(345)	*BCAB*, *ABABCABABA*, *ABABABABABAB*, *CA*
(*f*)	$S_4(6c)$	(2356)	(12)(36)(45)	(126)(345)	*BA*, *CBABABABAC*
(*g*)	$S_4(6d)$	(1245)(36)	(23)(56)	(135)(246)	*CA*, *BABABABA*, *BABCBABA*
(*h*)	$A_5(6)$	(12345)	(35)(46)	(125)(364)	*CA*, *BACB*, *ABABABABAB*

We recall that a crystallographic Coxeter group G has as generators the reflections R_i and defining relations $R_i^2 = (R_iR_j)^{m_{ij}} = e$, $m_{ij} \in \mathbb{Z}$, $m_{ij} \geq 2$. One of the important subgroups of G is its index-2 subgroup G^0 consisting of orientation-preserving isometries. We term the product R_iR_j a *relator* of G^0, if it is of finite order. Note that the set of relators generates the group G^0.

As in §4, given a transitive n-coloring of a partition of G^0, let f be the homomorphism from G^0 to S_n, and let α be a permutation assignment which gives rise to an index-n subgroup M of G^0 with M fixing color 1. Suppose y is a relator of G^0. If $f(y)$ fixes a number $i \in \{1, 2, \ldots, n\}$, then $zyz^{-1} \in M$ for some $z \in G^0$. Moreover, if $f(y)$ is of order l, then $y^l \in M$. Note that it is a well known result that an element $w \in G^0$ is of finite order if and only if it is conjugate to a power of a relator of G^0 (Magnus, 1974). We can then say that a permutation assignment α which gives rise to a subgroup M of G^0 is torsion free if, for each relator y, $f(y)$ does not fix any number i and the order of $f(y)$ is equal to the order of y. To satisfy both conditions, if y has order d, $f(y)$ should be a permutation consisting of a product of n/d disjoint d-cycles. Such a permutation assignment α with this property is called a *semi-regular* permutation assignment.

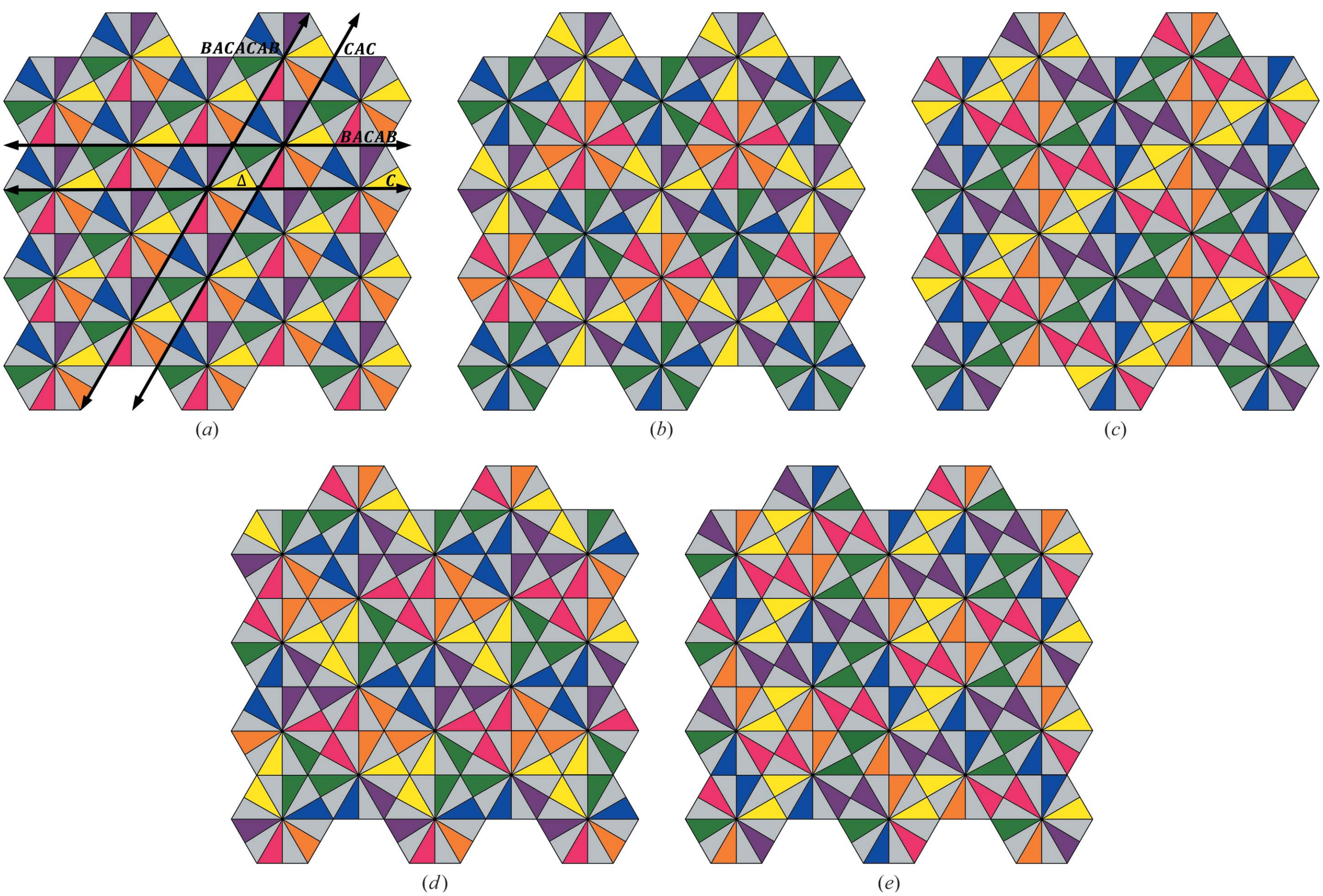

Figure 3
The transitive 6-colorings corresponding to the index-6 subgroups of 632 given in Table 1.

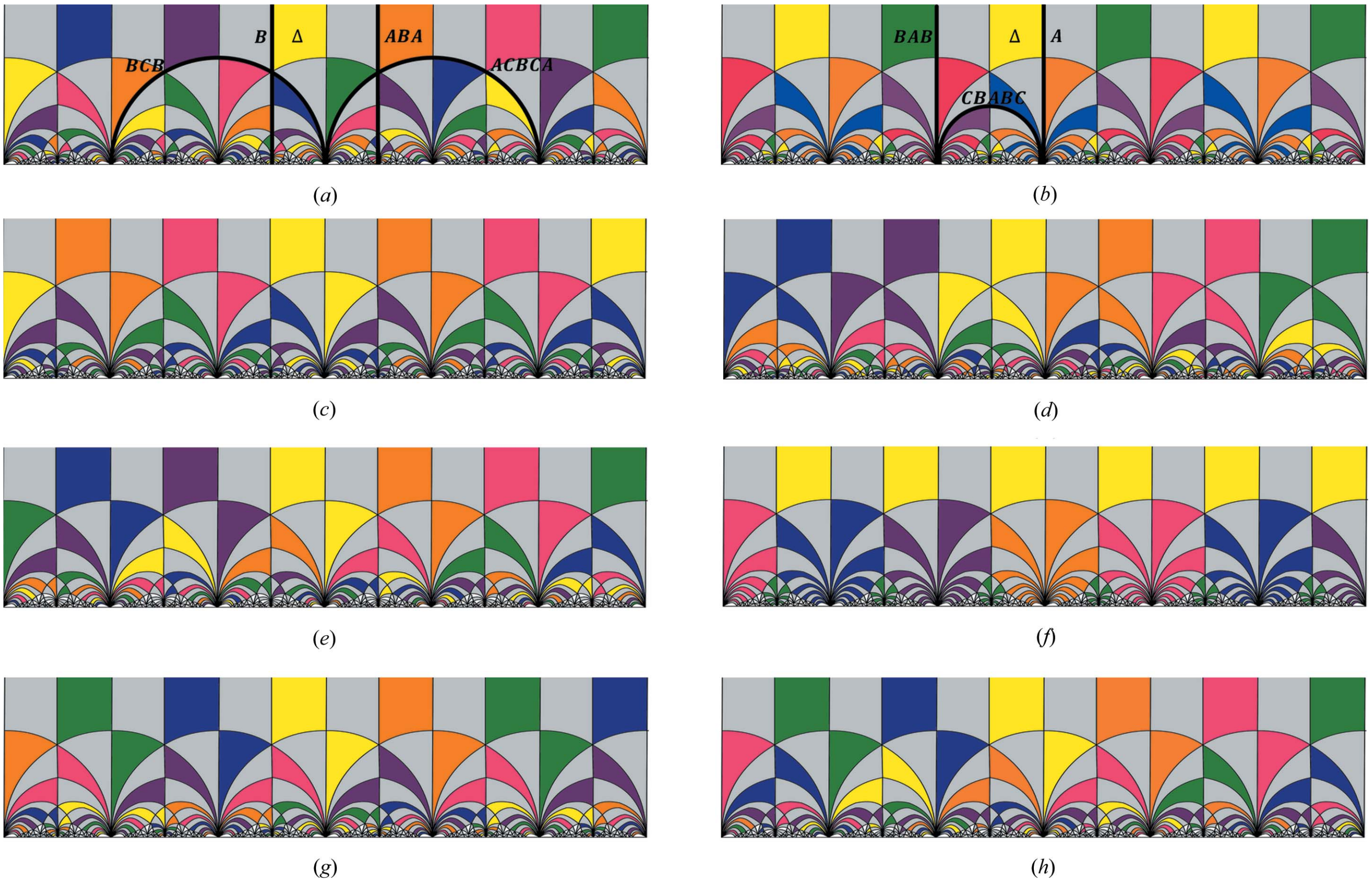

Figure 4
The transitive 6-colorings corresponding to the index-6 subgroups of 32∞ given in Table 2.

Theorem 2. A subgroup M of G^0 is torsion free if and only if the permutation assignment α that gives rise to M is a semi-regular permutation assignment.

Proof. Let M be an index-n subgroup of G^0.

Suppose α is a semi-regular permutation assignment that gives rise to M. Consider z an element of order m in G^0. Then z is a conjugate to a power of a relator of G^0, say, v; that is $z = wvw^{-1}$, for some $w \in G_0$. Since $f(z) = f(wvw^{-1}) = f(w)f(v)f(w)^{-1}$ and $f(v)$ is a permutation having n/m disjoint m-cycles, $f(z)$ is a permutation having n/m disjoint m-cycles which implies that z does not fix 1. Thus every element of finite order in G^0 is not an element of M and, consequently, M is torsion free.

Conversely suppose M is a torsion-free subgroup of G^0. Let g be an element of G^0 of order m. It is easy to see that $g^k \in M$ if and only if m divides k, since M is torsion free. This means that if k is not divisible by m, then $f(g^k)$ does not fix 1, and so $f(g^k)$ also does not fix $2, \ldots, n$ because $f(hg^kh^{-1})$ cannot fix 1 for any $h \in G^0$. Therefore, $f(g)$ is a permutation of order m and no nontrivial power of $f(g)$ fixes any number in $\{1, 2, \ldots, n\}$; that is, $f(g)$ is a permutation having n/m disjoint m-cycles. In particular, $f(y)$ is a permutation having n/d disjoint d-cycles, for every relator y of order d. Hence the permutation assignment α corresponding to the torsion-free subgroup M of G^0 is semi-regular.

As an illustration, we derive the index-6 torsion-free subgroup of the modular group 32∞. From the list of permutation assignments that give rise to index-6 subgroups of the modular group as presented in Table 2, we consider the permutation assignments α, β and γ where

$$\begin{aligned}
\alpha &= \big\{f(BA), f(CA), f(BC)\big\} \\
&= \big\{(1, 2, 3, 4, 5, 6), (14)(25)(36), (153)(264)\big\}, \\
\beta &= \big\{f(BA), f(CA), f(BC)\big\} \\
&= \big\{(14)(23)(56), (12)(36)(45), (153)(264)\big\}, \\
\gamma &= \big\{f(BA), f(CA), f(BC)\big\} \\
&= \big\{(2356), (12)(36)(45), (126)(345)\big\}.
\end{aligned}$$

Note that BA is of infinite order since it is a translation; hence it is not a relator. The relators are CA and BC which are of order 2 and 3, respectively. Now α is a semi-regular permutation assignment since $f(CA) = (14)(25)(36)$ is a product of three disjoint 2-cycles and $f(BC) = (153)(264)$ is a product of two disjoint 3-cycles. Thus, by Theorem 2, the permutation assignment α gives rise to an index-6 torsion-free subgroup of the modular group generated by translations $B(ACBCA)$ and $(BCB)(ABA)$ which are products of reflections across parallel hyperbolic lines as shown in Fig. 4(*a*). Similarly, β and γ are also semi-regular permutation assignments which give rise to two more index-6 torsion-free subgroups of the modular group. The torsion-free subgroup corresponding to β is generated by translations $A(BAB)$ and $(CBABC)A$ that are products of reflections across hyperparallel hyperbolic lines shown in Fig. 4(b), while the one corresponding to γ is generated by translations BA and $C(BABABA)C$ illustrated in Fig. 4(f). In summary, 32∞ has three index-6 torsion-free subgroups, namely $\langle BACBCA, BCBABA\rangle$, $\langle ABAB, CBABCA\rangle$ and $\langle BA, CBABABABAC\rangle$.

Moreover, the group 632 has one index-6 torsion-free subgroup $\langle BACBAC, BCABCA\rangle$ which arises from the semi-regular permutation assignment

$$\{f(BA), f(CA), f(BC)\} = \{(14)(25)(36), (135)(246), (123456)\}.$$

As expected, this subgroup is generated by translations $(BACAB)C$ and $[BA(CAC)AB]CAC$ exhibited in Fig. 3(a).

6. Conclusion and outlook

In this work, we have presented a method for determining the subgroups of a crystallographic Coxeter group G and its subgroups, where G is generated by reflections in the hyperplanes containing the sides of a Coxeter polytope. The approach is geometric, and facilitates the characterization of the groups in terms of symmetries in Euclidean, spherical or hyperbolic space. In this way, it allows for a more systematic and helpful representation of crystal structures. The results given here are also applicable in studying the subgroup structure of other classes of symmetry groups in hyperbolic space and facilitate the derivation of higher-index subgroups.

Having acquired the means to characterize the subgroup structure of crystallographic Coxeter groups and their subgroups in terms of symmetries, it would be interesting to probe further their applications (*e.g.* to crystal networks, infinite periodic minimal surfaces, nanostructures) and to study next the usage of these groups to represent other crystalline materials.

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