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# AUTOMORPHISM GROUPS AND SPECTRA OF HIGHLY SYMMETRICAL GRAPHS GENERATING POSSIBLE CARBON AND BORON NITRIDE STRUCTURES BY LEAPFROG TRANSFORMATIONS: THE KLEIN AND DYCK GRAPHS*

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**Abstract.** Symmetrical structures for carbon and the isoelectronic boron nitride, $(BN)_x$, can be generated from trivalent graphs constructed from non-hexagons using a leapfrog transformation, which consists of omnicapping (stellation) followed by dualization, which triples the number of vertices with the following effects: (a) The automorphism group of the original graph is preserved; (b) The minimum number of new hexagons is provided to dilute the non-hexagons so that no pair of non-hexagons have a common edge. Such a process can be used to construct the truncated icosahedron graph of the $C_{60}$ fullerene from the regular dodecahedron. The most symmetrical trivalent graphs containing heptagons or octagons do not lead to analogous finite polyhedral structures but instead can be embedded into infinite periodic minimal surfaces based on unit cells with a genus 3 surface. A graph described by Klein in the 19th century consisting of 24 heptagons can be used to generate possible but not yet experimentally realized carbon structures through such a leapfrog transformation. The automorphism group of the Klein graph is the simple PSL(2,7) group of order 168, which can be generated from $2 \times 2$ matrices in a seven-element finite field $F_7$ analogous to the generation of the icosahedral group of order 60 by a similar procedure using $F_5$. Similarly a graph described by Walther Dyck, also in the 19th century, consisting of 12 octagons on a genus 3 surface can generate possible carbon or boron nitride structures consisting of hexagons and octagons through a leapfrog transformation. The automorphism group of the Dyck graph is a solvable group of order 96 but does not contain the octahedral group as a normal subgroup and is not a normal subgroup of the automorphism group of the four-dimensional analogue of the octahedron. The spectra of the Klein and Dyck graphs and their duals exhibit many features similar to the spectra of the dodecahedron/icosahedron and cube/octahedron dual pairs, respectively.

*This paper is dedicated to Prof. Alexandru Balaban in recognition of his pioneering contributions to mathematical chemistry.

## INTRODUCTION

Many interesting possible structures for allotropes of carbon and the isoelectronic boron nitride, $(BN)_n$, can be constructed from polygonal networks of trigonal ($sp^2$-hybridized) atoms and thus can be described by trivalent graphs. The flat graphite and corresponding boron nitride structures arise if all of the polygons are hexagons and correspond to the well-known {6,3} tessellation (Figure 1). Positive curvature arises if some of the polygons have less than six edges and the resulting structures are closed polyhedral cages. In the most favorable structures no pair of non-hexagons shares any edges. Such structures are said to satisfy the *isolated non-hexagon rule* (INHR). Of particular interest is the truncated icosahedral structure (Figure 1) exhibited by the experimentally observed $C_{60}$ fullerene, which has 12 pentagonal faces and 20 hexagonal faces [1]. This structure can be generated by a so-called *leapfrog transformation* of the regular dodecahedron, which consists of omnicapping (stellation) followed by dualization to triple the number of vertices from 20 to 60 (Figure 2a) [2]. Such leapfrog transformations on trivalent graphs containing polygons other than hexagons triple the number of vertices while preserving the automorphism group of the original graph and provide the minimum number of new hexagons to "dilute" the non-hexagons in the original graph so that the INHR rule is satisfied. A similar leapfrog transformation on the cube (Figure 2b) generates the truncated octahedron, which is a promising candidate for a boron nitride structure since it is a bipartite graph, which allows construction of a structure having an equal number of boron and nitrogen atoms and only boron-nitrogen chemical bonds (i.e., all edges connect a boron vertex with a nitrogen vertex).

If the only non-hexagons in the INHR carbon or boron nitride structure have more than six edges, then negative curvature structures are required. Favorable structures of this type exhibiting the highest possible symmetries are based on infinite periodic minimal surfaces (IPMS) having genus 3 unit cells [3], where a unit cell refers to the unit that repeats to form the infinite three-dimensional lattice.

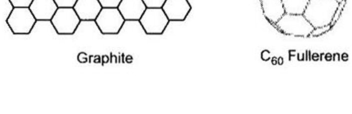

FIGURE 1 Carbon allotropes constructed from $sp^2$ (trigonal) carbon atoms and thus based on trivalent graphs.

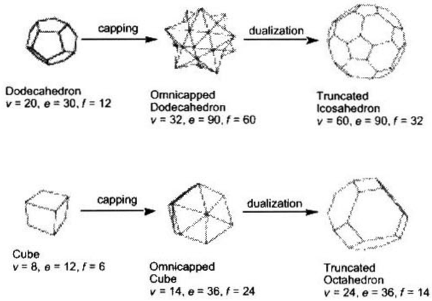


FIGURE 2. Applications of the leapfrog transformation to the cube and regular dodecahedron.

A suitable carbon structure containing only hexagons and heptagons with the minimum number of hexagons required to satisfy the INHR (the D168 structure) can be generated by a leapfrog transformation on a genus 3 surface containing 24 heptagons based on a graph (Figure 3) described in the 19th century by Felix Klein [4] (the D56 structure). Similar a suitable carbon or alternant boron nitride structure containing only hexagons and octagons with the minimum number of hexagons to satisfy the INHR (the D96 structure) can be generated by a leapfrog transformation on a genus 3 surface containing 12 octagons based on a graph (Figure 3) described by Walther Dyck, also in the 19th century [5] (the D32 structure).

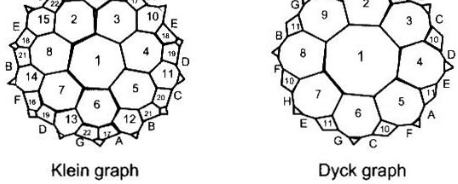


FIGURE 3. The Klein graph of 24 heptagons and the Dyck graph of 12 octagons. In both graphs the pairs of outer arcs indicated by the same letters (A through G or H) are joined to form a genus 3 surface.

The highest symmetry unit cells of the genus 3 IPMS's in which the Klein or Dyck graphs can be embedded have cubic symmetry and thus can be divided into eight equivalent octants. Each such octant contains three heptagons for the Klein graph or 1 $^1/_2$ octagons for the Dyck graph. The effect of leapfrog transformations on individual octants of the Klein and Dyck graphs is depicted in Figure 4. The properties of the leapfrog transformations relevant to this paper are summarized in Table 1.

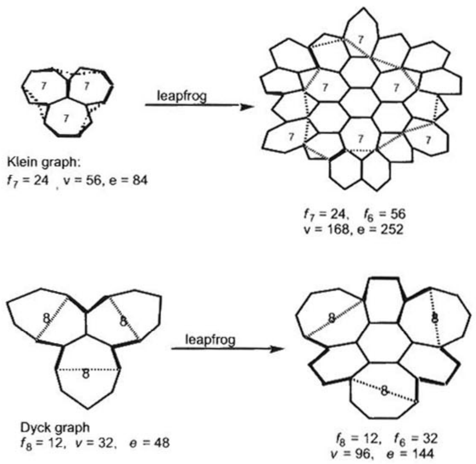


FIGURE 4: Leapfrog transformations on octants of the Klein and Dyck graphs. The boundaries of the octants are indicated by dashed lines.

TABLE 1. Comparison of Several Leapfrog Transformations

| Polygon combination | Squares + Hexagons | | Pentagons + Hexagons | | Heptagons + Hexagons | | Octagons + Hexagons | |
|---|---|---|---|---|---|---|---|---|
| leapfrog process | $(BN)_4 \xrightarrow{\text{leapfrog}} (BN)_{12}$ | | $C_{20} \xrightarrow{\text{leapfrog}} C_{60}$ | | $D56 \xrightarrow{\text{leapfrog}} D168$ | | $D32 \xrightarrow{\text{leapfrog}} D96$ | |
| original figure | $O_h$ cube | | $I_h$ dodecahedron | | Klein graph | | Dyck graph | |
| vertices | 8 | 24 | 20 | 60 | 56 | 168 | 32 | 96 |
| edges | 12 | 36 | 30 | 90 | 84 | 252 | 48 | 144 |
| faces | 6 | 14 | 12 | 32 | 24 | 80 | 12 | 44 |
| $f_{\neq 6}$ | 6 | 6 | 12 | 12 | 24 | 24 | 12 | 12 |
| $f_6$ | 0 | 8 | 0 | 20 | 0 | 56 | 0 | 32 |
| $f_{\neq 6}$–$f_{\neq 6}$ edges | 12 | 0 | 30 | 0 | 84 | 0 | 48 | 0 |
| $f_{\neq 6}$–$f_6$ edges | 0 | 24 | 0 | 60 | 0 | 168 | 0 | 96 |
| $f_6$–$f_6$ edges | 0 | 12 | 0 | 30 | 0 | 84 | 0 | 48 |

The Klein and Dyck graphs have some interesting properties. Thus their automorphism groups and graph spectra bear some resemblances to those of the regular polyhedra. In particular, the automorphism group of the Klein graph of order 168 has some of the properties of the icosahedral rotation group of order 60. In addition, the automorphism group of the Dyck graph of order 96 bears some relationship to that of the octahedral rotation group of order 24. Furthermore, the spectra of the Klein graph and the Dyck graph can be compared with those of the regular dodecahedron and cube, respectively. This paper summarizes some of these observations.

## AUTOMORPHISM GROUPS OF THE KLEIN AND DYCK GRAPHS

### Generalization of Symmetry Point Groups to Graph Automorphism Groups and Permutation Groups

The most familiar applications of group theory in chemistry use symmetry point groups, which describe the symmetry of molecules [6]. The elements of symmetry point groups can include only the standard symmetry operations in three-dimensional space, namely the identity ($E$), proper rotations ($C_n$), reflections ($\sigma$), inversion ($i$), and improper rotations ($S_n$). However, the concepts of group theory can also be applied to more abstract sets such as the permutations of a set $X$ of $n$ objects. A set of permutations of $n$ objects (including the identity "permutation") with the structure of a group is called a *permutation group* of *degree n* and the number of permutations in the set is called the *order* of the group [7]. The standard symmetry operations in symmetry point groups (e.g., $E$, $C_n$, $\sigma$, $i$, $S_n$) can be considered to be special types of permutations when applied to discrete sets of points or lines such as the vertices or edges of polyhedra [8]. In such situations, symmetry point groups can be regarded as special cases of permutation groups. Furthermore, the concept of symmetry groups can also be extended to the automorphism groups of graphs, which are analogous to symmetry groups except that they may also include permutations that are not recognizable as the standard symmetry operations in three-dimensional space.

Let $G$ be a permutation group acting on the set $X$ and let $g$ be any operation in $G$ and $x$ be any object in set $X$. The subset of $X$ obtained by the action of all operations in $G$ on $x$ is called the *orbit* of $x$. A *transitive* permutation group has only one orbit containing all objects of the set $X$. Sites permuted by a transitive permutation group are thus equivalent. Transitive permutation groups represent permutation groups of the "highest symmetry" and thus play a special role in permutation group theory.

Let $A$ and $X$ be two elements in a group. Then $X^{-1}AX = B$ is equal to some element in the group. The element $B$ is called the *similarity transform* of $A$ by $X$ and $A$ and $B$ are said to be *conjugate*. A complete set of elements of a group which are conjugate to one another is called a *class* (or more specifically a *conjugacy class*) of the group. The number of elements in a conjugacy class is called its *order*; the orders of all conjugacy classes must be integral factors of the order of the group.

A group $G$ in which every element commutes with every other element (i.e., $xy = yx$ for all $x$, $y$ in $G$) is called a *commutative* group or an *Abelian* group. In an Abelian group every element is in a conjugacy class by itself, i.e., all conjugacy classes are of order one. A *normal subgroup* $N$ of $G$, written $N \lhd G$, is a subgroup which consists only of *entire* conjugacy classes of $G$ [9]. A *normal chain* of a group $G$ is a sequence of normal subgroups $C_1 \lhd N_{a_1} \lhd N_{a_2} \lhd N_{a_3} \lhd \cdots \lhd N_{a_s} \lhd G$, in which $s$ is the number of normal subgroups (besides $C_1$ and $G$) in the normal chain (i.e., the length of the chain). A *simple* group is a group having no *normal* subgroups other than the identity group $C_1$. Simple groups correspond to the transitive groups of "highest symmetry" and are particularly important in the theory of finite groups [10,11]. The only non-trivial simple group found as a symmetry point group is the icosahedral pure rotation group, $I$, of order 60.

The permutation groups involved in the structures of carbon and boron nitride allotropes based on finite polyhedra necessarily correspond to familiar polyhedral point groups. Thus the truncated icosahedral structure of the fullerene $C_{60}$ is derived from the leapfrog transformation of the regular dodecahedron (Figure 2a). During this transformation the icosahedral symmetry $I_h$ is preserved. Similarly the truncated octahedral structure of the boron nitride $B_{12}N_{12}$ is derived from the leapfrog transformation of the cube during which the octahedral symmetry $O_h$ is preserved (Figure 2b).

**The Automorphism Group of the Klein Graph: Analogy with the Icosahedral Group**

Now let us consider the automorphism group of the Klein graph. First consider an alternative definition of the icosahedral pure rotation group, which can be extended to larger simple permutation groups which do not occur as symmetry point groups [12]. In this connection consider a prime number $p$ and let $\mathsf{F}_p$ denote the finite field of $p$ elements which can be represented by the $p$ integers $0,\ldots,p-1$; larger integers can be converted to an element in this finite field by dividing by $p$ and taking the remainder (i.e., the number is taken "mod $p$"). For example, the finite field $\mathsf{F}_5$ contains the five elements represented by the integers 0, 1, 2, 3, and 4 and other integers are converted to one of these five integers by dividing by 5 and taking the remainder, e.g., $7 \to 2$ in $\mathsf{F}_5$ (written frequently as "$7 \equiv 2 \bmod 5$"). The group SL(2,$p$) is defined to be the group of all $2 \times 2$ matrices with entries in $\mathsf{F}_p$ having determinant 1 and its subgroup PSL(2,$p$) for odd $p$ is defined to be the quotient group of SL(2,$p$) modulo its center, where the center of a group is the largest normal subgroup that is Abelian. In the case of the groups SL(2,*p*) where $p \geq 5$, the center has only two elements and the quotient group PSL(2,*p*) is a simple group. The group PSL(2,5) contains 60 elements and is isomorphic to the icosahedral pure rotation group *I*.

An important property of the PSL(2,*p*) permutation groups for $p = 5$, 7, and 11 (Table 2) is that they can function as *transitive* permutation groups on sets of either *p* or *p*+1 objects. In the case of the group PSL(2,5), these transitive permutation groups on 5 and 6 objects can be visualized as permutations of parts of an icosahedron since PSL(2,5) is isomorphic to the icosahedral pure rotation group. Thus the PSL(2,5) group acts as a transitive permutation group on the six diameters of a regular icosahedron, where a diameter of an icosahedron is defined as a line drawn between a pair of antipodal vertices. In order to obtain in an icosahedron a set of *five* objects that is permuted transitively by the PSL(2,5) group, the 30 edges of an icosahedron are partitioned into five sets of six edges each by the following method [13]:

(1) A straight line is drawn from the midpoint of each edge through the center of the icosahedron to the midpoint of the opposite edge.

(2) The resulting 15 straight lines are divided into five sets of three mutually perpendicular straight lines.

Each of these five sets of three mutually perpendicular straight lines resembles a set of Cartesian coordinates and defines a regular octahedron. The PSL(2,5) permutation group as manifested in its isomorphic *I* symmetry point group functions as a transitive permutation group on these five sets of three mutually perpendicular straight lines. In fact the PSL(2,5) permutation group is also isomorphic with the so-called *alternating permutation group* on five objects [14], namely $A_5$, where an alternating permutation group on *n* objects is the set of all possible *even* permutations and is of order $n!/2$.

The PSL(2,*p*) ($p = 5, 7, 11$) groups are simple groups and thus have no non-trivial *normal* subgroups. However, they contain two different sets of *n* smaller non-normal subgroups corresponding to pure rotation groups of regular polyhedra; these regular polyhedral rotation groups are subgroups of index *p* of the groups PSL(2,*p*). However, the PSL(2,11) group has been proven to the largest group of the general type PSL(2,*p*) with *p* a prime which has a subgroup of index *p* [15]. A corollary derived from this theorem is that if $p > 11$, the PSL(2,*p*) group cannot be a transitive permutation group for a set with fewer than *p*+1 elements in contrast to the PSL(2,*p*) ($p = 5, 7, 11$) groups which can be transitive permutation groups for sets of *p* elements, namely 5, 7, and 11 respectively (Table 2). Since the PSL(2,*p*) ($p = 5, 7, 11$) groups contain polyhedral point groups as subgroups they are conveniently designated as pollakispolyhedral groups [16]. Thus the PSL(2,5), PSL(2,7) and

PSL(2,11) groups can be called the pentakistetrahedral, heptakisoctahedral, and undecakisicosahedral groups, respectively, and designated as ${}^{5}T$, ${}^{7}O$, and ${}^{11}I$, respectively.

TABLE 2: Properties of the Pollakispolyhedral Groups Derived from the PSL(2,$p$) Groups ($p$ = 5, 7, 11)

| Group | Order | Conjugacy Classes | Polyhedral Subgroup |
|---|---|---|---|
| ${}^{5}T \approx$ PSL(2,5) | 60 | $E+12C_5+12C_5^2+20C_3+15C_2$ | $T$ |
| ${}^{7}O \approx$ PSL(2,7) | 168 | $E+24C_7+24C_7^3+56C_3+21C_2+42C_4$ | $O$ |
| ${}^{11}I \approx$ PSL(2,11) | 660 | $E+60C_{11}+60C_{11}^2+110C_3+55C_2+$ $132C_5+132C_5^2+110C_4$ | $I$ |

The simplest example of the polyhedral subgroups of index $p$ in the pollakispolyhedral groups occurs in the pentakistetrahedral group, ${}^{5}T$, which is equivalent to the icosahedral rotation group. Thus, ${}^{5}T$ can be decomposed into two different sets of five tetrahedra corresponding to the conjugacy classes $12C_5$ and $12C_5^2$. This is related to the partitioning of the 20 vertices of a regular dodecahedron into five sets of four vertices each corresponding to a regular tetrahedron. The permutations of the group PSL(2,5) act as the icosahedral pure rotation group $I$ on the regular dodecahedron partitioned in this manner and correspondingly as the alternating group $A_5$ on the five subtetrahedra.

The next higher pollakispolyhedral group, namely the heptakisoctahedral group ${}^{7}O$ of order 168, corresponds to the automorphism group of the Klein graph. This group can be decomposed into two sets of seven octahedral subgroups [16,17]. This relates to the embedding of the Klein graph into a cubic unit cell of an IPMS [3] of genus 3. The symmetry group of the pure rotations of the cubic unit cell is the octahedral rotation group $O$, which, as noted above, is a subgroup of index 7 in ${}^{7}O$, so that this embedding of the Klein graph can be seen to have seven-fold ($C_7$) *hidden symmetry*.

Another question of interest is the relationship of the operations of the heptakisoctahedral group to permutations in the Klein graph (Figure 3) [16]. In this connection the 168 operations of ${}^{7}O$ can be divided into the following conjugacy classes:

(1) The identity operation $E$.

(2) Permutations of period 7 ($C_7$), each of which leave three heptagons invariant so that the cycle index on the set of 24 hexagons is $x_1^3x_7^3$. There are eight distinct "$C_7$ axes," each of which passes through the midpoints of three heptagons. The resulting 48 operations can be partitioned into two conjugacy classes of 24 operations each, corresponding to $C_7$ and $C_7^3$ rotations.

(3) Permutations of period 3 ($C_3$), each of which leave two vertices invariant so that the 56 vertices of the Klein graph are partitioned into 28 "$C_3$ axes." There are 56 operations in the $C_3$ class.

(4) Permutations of period 2 ($C_2$), each of which leave four edges invariant so that the 84 edges of the Klein graph are partitioned into 21 "$C_2$ axes." There are thus a total of 21 operations in the $C_2$ class. The $C_2$ operations can be generated by combination of a $C_7$ and $C_3$ operation, i.e., $C_2 = C_7 \times C_3$.

(5) Permutations of period 4 ($C_4$), which partition the 24 heptagons into six groups of 4. The $C_4$ operations are related to the other operations by the relationships $C_4 = C_7{}^4 \times C_3$ and $(C_4)^2 = C_2$. Because of the latter relationship there are a total of $21 \times 2 = 42$ operations in the $C_4$ class realizing that "$C_4$" and "$C_4{}^3$" belong to the same conjugacy class.

Thus permutations of these five types can be seen to lead to all 168 permutations and the six conjugacy classes of the heptakisoctahedral group listed in Table 2.

**The Automorphism Group of the Dyck Graph: Analogy with the Octahedral Group**

The permutational symmetry of the Dyck graph was already recognized by Dyck [5] to be described by an automorphism group consisting of the following 96 permutations:

(1) The identity permutation.

(2) Permutations of period 4, each of which leaves four octagons invariant. There are thus three distinct "$C_4$ axes," each of which passes through the midpoints of four octagons. Since "$C_4$," and "$C_4{}^3$" are in the same conjugacy class, there are a total of $3 \times 2 = 6$ permutations in this class and these may be regarded as analogues of proper rotations $C_4$.

(3) Permutations of period 2, using the same three "$C_4$ axes" as the $C_4$ permutations mentioned above and thus corresponding to $C_4{}^2$. There are obviously three of these permutations.

(4) Permutations of period 8, each of which leave two octagons invariant. These operations are analogous to an improper rotation $S_8$ rather than a proper rotation $C_8$ since although $S_8$ leaves only two octagons invariant, $S_8{}^2 = C_4$ leaves four octagons invariant. Furthermore, the number of "$S_8$ axes" is double the number of "$C_4$ axes" since for each of the three "$C_4$ axes" passing through the midpoints of four octagons, there are two ways of choosing the pair of octagons that is permuted and the pair of octagons that remains fixed when an $S_8$ operation is applied. Since "$S_8$," "$S_8{}^3$," "$S_8{}^5$," and "$S_8{}^7$," are in the same conjugacy class, there are a total of $6 \times 4 = 24$ operations in this class.

(5) Permutations of period 3, each of which pass through 2 of the 32 vertices of the Dyck graph. Since there are 16 distinct pairs of such vertices and since "$C_3$" and "$C_3{}^2$" are in the same conjugacy class, there are a total of $16 \times 2 = 32$ operations in this class.

(6) Permutations of period 2 ($C_2$), each of which pass through the midpoints of 4 of the 48 edges so that there are 12 operations in this class.

(7) Permutations of period 4, which are not derived by squaring permutations of period 8. These may be regarded as analogues of improper rotations $S_4$ and there are 18 operations in this class.

These seven classes add up to the 96 operations in the automorphism group of the Dyck graph as $E + 24S_8 + 6C_4 + 3C_4^2 + 32C_3 + 12\,C_2 + 18S_4$. Dyck [5] designates this group as G[2,3,8] relating to the description of the Dyck graph as a tessellation (see below).

The automorphism group of the Dyck graph, namely G[2,3,8], has some interesting properties. The pure octahedral rotation group, $O$, is a subgroup of index 4 in G[2,3,8] so that G[2,3,8] can also be described as the tetrakisoctahedral group and designated as ${}^4O$ to emphasize its pollakispolyhedral origin. However, the octahedral rotation group $O$ is not a *normal* subgroup of the tetrakisoctahedral group since it cannot be constructed from entire conjugacy classes of ${}^4O$. Nevertheless, the tetrakisoctahedral group is not a simple group since other subgroups of ${}^4O$, albeit ones unfamiliar in chemistry or as symmetry point groups, can be constructed from entire classes of ${}^4O$. Thus ${}^4O$ has a normal subgroup of order 48 and index 2 that can be obtained by deleting the entire classes of permutations of periods 8 and 4 leaving only the permutations with periods 2 and 3 to give $E + 3C_4^2 + 32C_3 + 12C_2$ designated as $G[3,3,4]$ by adapting terminology already used by Dyck [5]. The group $G[3,3,4]$ is clearly different from the full octahedral group $O_h$, which has elements of periods 4 and 6 and the very different conjugacy class structure $E + 8C_3 + 6C_2 + 6C_4 + 3C_4^2 + i + 6S_4 + 8S_6 + 3\sigma_h + 6\sigma_d$.

The group $G[3,3,4]$ is also not a simple group since deletions of its entire class of permutations of period 3 gives a subgroup of order 16 and index 3 with only the identity and 15 permutations of period 2, namely $E + 3\,C_4^2 + 12\,C_2$, which can be designated as $G[4,4,4]$, again adapting terminology used by Dyck [5]. This leads to the following normal subgroup chain for the tetrakisoctahedral group ${}^4O$:

$$
\begin{array}{ccccccc}
{}^4O & \xrightarrow{\div 2} G[3,3,4] & \xrightarrow{\div 3} G[4.4,4] & \xrightarrow{\div 2} D_{2h} & \xrightarrow{\div 2} D_2 & \xrightarrow{\div 2} C_2 & \xrightarrow{\div 2} C_1 \\
\text{Order:} & & & & & & \\
96 & 48 & 16 & 8 & 4 & 2 & 1
\end{array}
$$

The normal subgroup chain of the tetrakisoctahedral group ${}^4O$ can be depicted by representing ${}^4O$ and its normal subgroups as tessellations (Figure 5), where a tessellation of a surface is an embedding of a network of polygons into a surface.[18] Such tessellations can be described in terms of their *flags*, where a *flag* is a triple ($V,E,F$) consisting of a vertex $V$, and edge $E$, and a face $F$ which are mutually incident. A tessellation $T$ is considered to be *regular* if its symmetry group $G(T)$ is transitive on the flags of $T$. A permutation group can be depicted as a regular tessellation on whose flags it acts transitively.

The tetrakisoctahedral group, ${}^4O$, of the Dyck figure can be described by a tessellation with 96 white triangles and 96 black triangles so that the 96 operations of ${}^4O$ act transitively on the triangles of a given color (Figure 5). Such a tessellation can be described as {2,3,8} indicating that two white (or black) triangles meet at the midpoints of each edge of an octagon of the Dyck figure, three triangles of the same color meet at each vertex of such an octagon, and eight triangles of the same color meet at the center of each such octagon. Halving the number of triangles in this tessellation by combining adjacent triangles in a symmetrical manner gives a figure with 48 triangles of each color corresponding to the normal subgroup $G$[3,3,4] of order 48 and index 2 in ${}^4O$ (Figure 8). The designation {3,3,4} for this tessellation relates to the points at the vertices of the original octagons where three triangles of a given color meet and the points at the centers of the original octagons where four triangles of a given color meet. Taking the 96 triangles of both colors in the tessellation {3,3,4} and recoloring them in alternate colors so that six triangles in the original {2,3,8} tessellation have a single color leads to a regular tessellation with only 16 triangles of each color corresponding to the normal subgroup $G$[4,4,4] of index 3 in $G$[3,3,4]. The designation {4,4,4} for this tessellation relates to the fact that exactly four triangles of a given color meet at each vertex. Note that in order to show the relationship of the {4,4,4} tessellation to its "parent" {2,3,8} some of the so-called edges of its "triangles" are actually bent rather than straight lines in Figure 5.

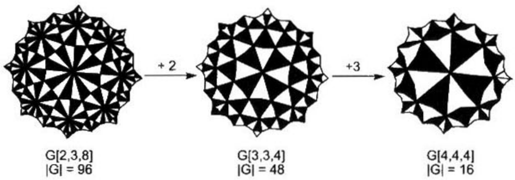


FIGURE 5. Tessellations showing the normal subgroup structure of the group G[2,3,8] ( = ${}^4O$) of the Dyck graph.

## SPECTRA OF THE KLEIN AND DYCK GRAPHS AND THEIR DUALS

### Dualization of a Graph Corresponding to a Network of Polygons

A given polyhedron $P$ can be converted into its dual $P^*$ by locating the centers of the faces of $P^*$ at the vertices of $P$ and the vertices of $P^*$ above the centers of the faces of $P$. Two vertices in the dual $P^*$ are connected by an edge if and only if the corresponding faces in $P$ share an edge. The duals of the cube and regular dodecahedron are the regular octahedron and regular icosahedron, respectively (Figure 6).

The process of dualization has the following properties:

(1) The numbers of vertices and edges in a pair of dual polyhedra $P$ and $P^*$ satisfy the relationships $v^* = f$, $e^* = e$, $f^* = v$;

(2) Dual polyhedra have the same symmetry elements and thus belong to the same symmetry point group;

(3) Dualization of the dual of a polyhedron leads to the original polyhedron, i.e., $(P^*)^* \approx P$.

(4) The degrees of the vertices of a polyhedron correspond to the number of edges in the corresponding face polygons in its dual.

Since the cube and regular dodecahedron have only degree 3 vertices, the corresponding dual polyhedra have only triangular faces, which are all equivalent equilateral triangles because of the symmetry of the regular polyhedra.

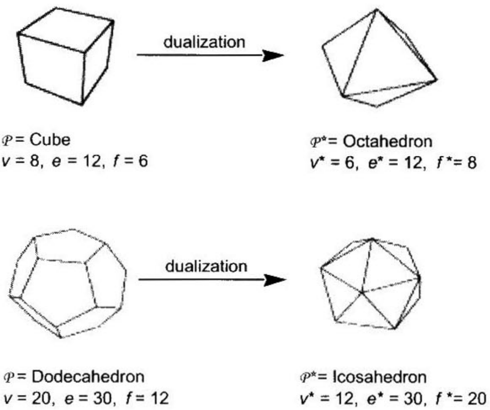


FIGURE 6: Dualization of the cube and regular dodecahedron to give the octahedron and icosahedron, respectively.

The concept of dualization can readily be extended to networks of polygons on genus 3 surfaces such as the Klein and Dyck graphs. Since both of these graphs, like the cube and regular dodecahedron, have only degree 3 vertices, the corresponding duals are networks of triangles, which have the same automorphism groups and all vertices of degrees 7 and 8 for the duals of the Klein and Dyck graphs, respectively. The dual of the Dyck graph looks like the tessellation corresponding to the G[3,3,4] group in Figure 5.

**Spectra of the Klein and Dyck Graphs**

Graph spectra are well-known to correspond to molecular orbital energy levels and are thus very useful for the study of delocalization in chemical bonding [19,20]. The spectra of the Klein and Dyck graphs and their duals have been determined using Mathematica [16]. The spectrum of the Klein graph dual bears an interesting resemblance to that of the icosahedron with the required non-degenerate $p$ eigenvalue, a $p$-fold degenerate $-1$ eigenvalue, and matching degenerate $\pm\sqrt{p}$ eigenvalues where $p = 5$ for the icosahedron and 7 for the Klein graph dual (Figure 7).

The spectra of the Dyck graph and its dual bear interesting resemblances to the spectra of the cube and octahedron, respectively. The Dyck graph is a bipartite trivalent graph like the cube and thus has the non-degenerate $\pm 3$ and degenerate $\pm 1$ values of the cube as well as the unexpected set of $\pm\sqrt{5}$ eigenvalues of degeneracy 6. The Dyck graph dual, like the octahedron, has only three distinct eigenvalues, namely a

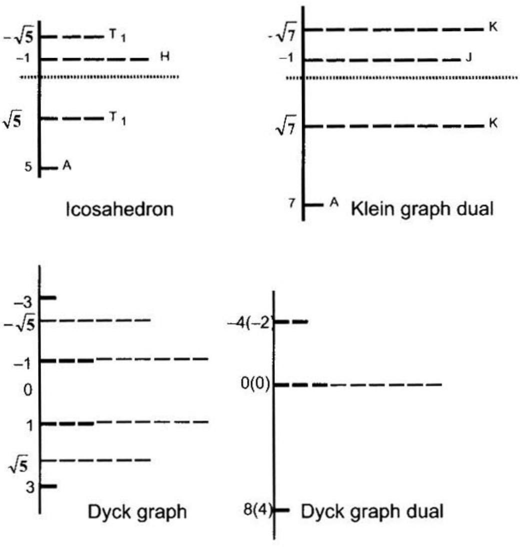


FIGURE 8. Comparison of the spectra of the Dyck graph and its dual with the spectra of the cube and octahedron, respectively. The eigenvalues of the cube and octahedron are indicated by bold lines and, in the case of the octahedron, the figures in parentheses.

non-degenerate $+d$ eigenvalue, a doubly degenerate $-2d$ eigenvalue, and a multiply degenerate 0 eigenvalue, where $d$ is the degree of the equivalent vertices of the graph, namely 4 for the octahedron and 8 for the Dyck graph dual.

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