THE DUAL OF THE DYCK GRAPH AS A REGULAR TRIPARTITE GRAPH: RELEVANCE TO HYPOTHETICAL ZEOLITE-LIKE BORON NITRIDE ALLOTROPES[*]

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The Dyck graph, which consists of 12 octagons on a genus 3 surface, can generate possible zeolite-like carbon or boron nitride allotrope structures by 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. The normal subgroup chain of this automorphism group can be obtained by considering the dual of the Dyck graph as the symmetrical tripartite graph $K_{4,4,4}$ analogous to considering the octahedron as $K_{2,2,2}$. The spectra of the $K_{n,n,n}$ graphs have only three distinct eigenvalues, namely a non-degenerate eigenvalue of $+2n$, a doubly degenerate eigenvalue of $-n$, and a $(3n-3)$-fold degenerate zero eigenvalue.

INTRODUCTION

Symmetrical structures for elemental carbon and the isoelectronic boron nitride, $(BN)_x$, can be generated from trivalent graphs constructed from non-hexagons by using a leapfrog transformation [1]. Such a transformation consists of omnicapping (stellation) followed by dualization, which triples the number of vertices with the following effects: (1) The automorphism group of the original trivalent graph is preserved; (2) The minimum number of new hexagons is provided to dilute the non-hexagon so that no pair of non-hexagons has a common edge. A well-known example of a leapfrog transformation is the conversion of a regular dodecahedron to the truncated icosahedron of C_{60} [1].

The most symmetrical trivalent graphs containing heptagons or octagons do not lead to finite polyhedral structures but instead correspond to genus 3 units which can be repeated indefinitely in all three directions to give an infinite periodic minimal surface (IPMS) [2] exhibiting a zeolite-like structure [3]. Leapfrog transformations are also applicable to such trivalent graphs again tripling the number of vertices of the unit cells while diluting the non-hexagons with the minimum number of hexagons so that no pair of

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[*] This paper is dedicated to Prof. Horst Sachs in recognition of his pioneering contributions to algebraic graph theory including applications in chemistry.

non-hexagons has a common edge. These IPMSs are possible structures for low-density carbon or boron nitride allotropes [4, 5, 6].
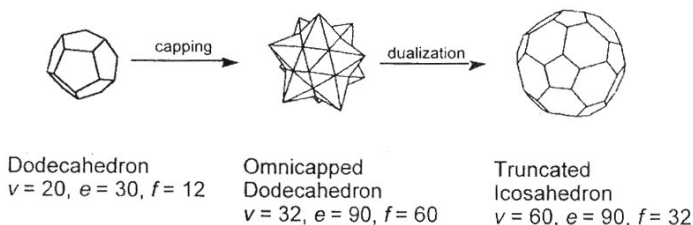

Dodecahedron	Omnicapped	Truncated
$v = 20$, $e = 30$, $f = 12$	Dodecahedron	Icosahedron
	$v = 32$, $e = 90$, $f = 60$	$v = 60$, $e = 90$, $f = 32$

FIGURE 1. The leapfrog transformation converting the regular dodecahedron to the truncated icosahedron of C_{60}.

Of particular interest are two such symmetrical trivalent genus 3 graphs dating back to the 19th century (Figure 2), namely the Klein graph of 24 heptagons [7] and the Dyck graph of 12 octagons [8]. Both of these graphs exhibit interesting automorphism groups, which have more complicated structures than the conventional symmetry point groups [9]. The automorphism group of the Klein graph [7], called the heptakisoctahedral group ^7O [10] or the didodecahedral group D [11] in recent publications, is a simple group of order 168, which can be generated from the prime 7 in a similar way that the icosahedral group (I) of order 60 is generated from the prime 5.

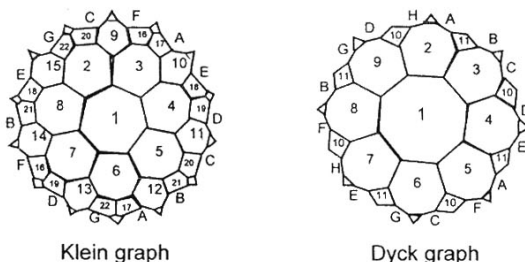Klein graph   Dyck graph

FIGURE 2. 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 automorphism group of the Dyck graph, called the tetrakisoctahedral group ^4O in a recent publication [12], is a solvable group of order 96. However, ^4O does not contain the octahedral group (O or O_h) as a normal subgroup nor is ^4O a normal subgroup of the automorphism group of the four-dimensional analogue of the octahedron [12]. This paper discusses the nature of the tetrakisoctahedral group by considering the group ^4O as the automorphism group of the dual of the Dyck graph, which turns out to be the symmetrical tripartite graph $K_{4,4,4}$.

SYMMETRICAL TRIPARTITE GRAPHS AND THEIR DUALS

A symmetrical tripartite graph, $K_{n,n,n}$, consists of three equivalent sets of n vertices, conveniently designated by the labels $\{1, 2,...,n\}$, $\{1', 2',...,n'\}$, and $\{1'', 2'',...,n''\}$. Edges connect all possible pairs of vertices in different sets. However, no edges connect any pair of vertices within a single set. Each of the $3n$ vertices of $K_{n,n,n}$ is of degree $2n$ leading a total of $(3n)(2n)/2 = 3n^2$ edges. Furthermore, each vertex of $K_{n,n,n}$ is shared by $2n$ triangular faces (i.e., circuits of length 3) leading to a total of $2n^2$ triangular faces. Note that $K_{2,2,2}$ corresponds to the regular octahedron with the three equivalent pairs of vertices $\{1,1'\}$, $\{2,2'\}$, and $\{3,3'\}$ being the pairs of vertices located on the three orthogonal C_4 axes. The numbers of vertices, edges, and faces of the regular octahedron are 6, 12, and 8, respectively, corresponding to $3n$, $3n^2$, and $2n^2$, respectively, for $n = 2$. The symmetrical tripartite graphs of interest in this paper are depicted in Figure 3.

$K_{2,2,2}$ Graph = Octahedron

$K_{3,3,3}$ Graph
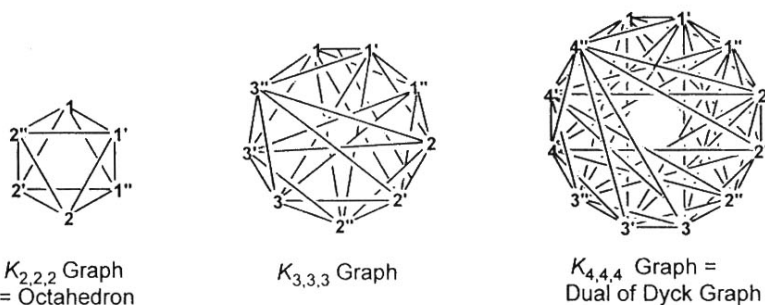
$K_{4,4,4}$ Graph = Dual of Dyck Graph

FIGURE 3. The symmetrical tripartite graphs discussed in this paper.

Now consider the process of forming the dual of a symmetrical tripartite graph, $K_{n,n,n}$, considered as a maximum symmetry embedding in a surface of minimum genus. Such a dual, corresponding to the standard process of dualization of polyhedra, will be designated generically as $K^*_{n,n,n}$. In the dualization process the centers of the faces of $K^*_{n,n,n}$ are located at the vertices of $K_{n,n,n}$ and the vertices of $K^*_{n,n,n}$ are located above the face centers of $K_{n,n,n}$. Two vertices in $K^*_{n,n,n}$ are connected by an edge if and only if the corresponding faces in $K_{n,n,n}$ share an edge. The dualization process has the following properties:

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

(2) Dual graphs have the same symmetry and thus the same automorphism groups;

(3) Dualization of the dual of a graph leads to the original graph;

(4) The degrees of the vertices of a graph correspond to the number of edges in the corresponding faces of the dual and vice versa.

Since each of the vertices of the symmetrical tripartite graph, $K_{n,n,n}$, embedded in a surface of minimum genus, is a part of $2n$ triangular faces, the corresponding dual $K^*_{n,n,n}$ is a trivalent graph in which all of the faces are $2n$-gons. In the simple example of the octahedron as $K_{2,2,2}$ the dual $K^*_{2,2,2}$ is the cube, which has all degree 3 vertices and only square faces (Figure 4). The trivalent nature of the duals $K^*_{n,n,n}$ makes them relevant for the study of possible highly symmetrical structures for carbon and boron nitride allotropes. Furthermore, the preservation of the automorphism group upon dualization means that the automorphism groups for these chemically relevant trivalent graphs $(K^*_{n,n,n})$ is the same as that of their duals $K_{n,n,n}$, which follow a simple pattern because of their symmetrical tripartite nature.
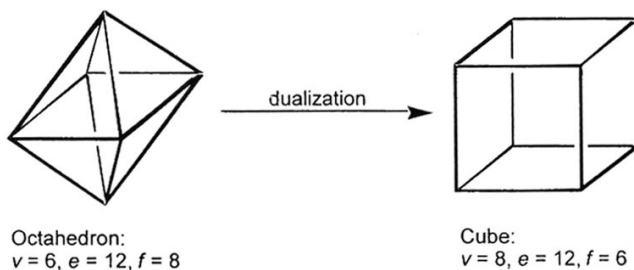

dualization

Octahedron:
$v = 6$, $e = 12$, $f = 8$

Cube:
$v = 8$, $e = 12$, $f = 6$

FIGURE 4. Dualization of the octahedron to give a cube.

AUTOMORPHISM GROUPS OF THE SYMMETRICAL TRIPARTITE GRAPHS

The Octahedron as $K_{2,2,2}$

As noted above the octahedron is the symmetrical tripartite graph $K_{2,2,2}$ (Figure 3). Its automorphism group O has the following normal subgroup chain (using the familiar symmetry point group designations [9]):

$$O \,\hat{\otimes}\, T \,\hat{\otimes}\, D_2 \,\hat{\otimes}\, C_2 \,\hat{\otimes}\, C_1$$

Order: 24   12   4   2   1

This subgroup chain is closely related to the tripartite structure of the octahedron. The process of going from O to its normal subgroup T of index 2 corresponds to removal of the operations of period 2 in the symmetric group S_3 permuting the three sets {1,2}, {1',2'}, and {1",2"}. In terms of the underlying octahedron, going from O to its normal subgroup T removes the operations of period 4. The next part of the subgroup chain from T to D_2 of index 3 corresponds to removing the remaining operations of this symmetric group S_3 (i.e., the operations of period 3). The resulting D_2 normal subgroup represents all possible $2^2 = 4$ permutations within the three individual sets {1,2}, {1',2'}, and {1",2"} without any permutations moving members of one of the three sets to another set.

The Dual of the Dyck Graph as $K_{4,4,4}$

The Dyck graph (Figure 2) has 12 octagonal faces and thus 48 edges and 32 vertices. Its dual is the symmetrical tripartite graph $K_{4,4,4}$, which necessarily has 12 vertices, 48 edges, and 32 triangular faces (Figure 3). Its automorphism group ^4O has the following normal subgroup chain (using a combination of familiar symmetry point group designations and less familiar designations from Dyck's original paper [8]):

$$^4O \,\hat{\otimes}\, G[3,3,4] \,\hat{\otimes}\, G[4,4,4] \,\hat{\otimes}\, D_{2h} \,\hat{\otimes}\, D_2 \,\hat{\otimes}\, C_2 \,\hat{\otimes}\, C_1$$

Order: 96   48   16   8   4   2   1

Again this subgroup chain is closely related to the $K_{4,4,4}$ tripartite structure of the dual of the Dyck graph. The process of going from ^4O to its normal subgroup $G[3,3,4]$ of index 2 corresponds to removal of the operations of period 2 in the symmetric group S_3 permuting the three sets {1,2,3,4}, {1',2',3',4'}, and {1",2",3",4"}. In terms of the underlying dual of the Dyck graph, going from ^4O to its normal subgroup $G[3,3,4]$ removes the operations of periods 8 and 4. The next part of the subgroup chain from

$G[3,3,4]$ to $G[4,4,4]$ of index 3 corresponds to removing the remaining operations of S_3 (i.e., the operations of period 3). The resulting $G[4,4,4]$ normal subgroup represents all possible $4^2 = 16$ permutations within the three individual sets $\{1,2,3,4\}$, $\{1',2',3',4'\}$, and $\{1'',2'',3'',4''\}$ without any permutations moving members of one of the three sets to another set.

The Symmetrical Tripartite Graph $K_{3,3,3}$:

Intermediate between the $K_{2,2,2}$ (octahedron) and $K_{4,4,4}$ (Dyck graph dual) symmetrical tripartite graphs is the $K_{3,3,3}$ tripartite graph consisting of 9 vertices, 27 edges, and 18 faces, all of which are triangles. The Euler characteristic χ ($= v - e + f$) is $9 - 27 + 18 = 0$ corresponding to a genus 1 surface, i.e., a simple torus (Figure 5a). The automorphism group of this graph is a group of order 54, which is one of the groups of genus 1 discussed in a comprehensive 1939 paper by Coxeter [13]. Using the terminology of Coxeter this group can be described as the direct product $3,3|3,3 \times C_2$ and has the following normal subgroup chain:

$$3,3|3,3 \times C_2 \; \overset{2}{\rhd} \; 3,3|3,3 \; \overset{3}{\rhd} \; C_9 \; \overset{3}{\rhd} \; C_3 \; \overset{3}{\rhd} \; C_1$$

Order: 54   27   9   3   1

The group $3,3|3,3$ is a group of order 27 generated by the relationships $R^3 = S^3 = (RS)^3 = (R^{-1}S)^3 = E$ as described by Coxeter [13].
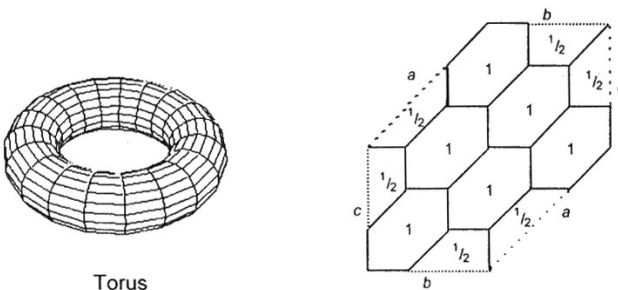

Torus

FIGURE 5. (a) A torus; (b) Embedding the dual of $K_{3,3,3}$ onto a torus. To form the torus the three pairs of edges designed by a, b, and c each are identified. Six of the nine hexagons (designated by 1) are completely within the outer hexagon boundary whereas the other three hexagons (designated by $^1/_2$) are split in half by the boundary.

The dual of $K_{3,3,3}$ is a graph with 18 vertices, 27 edges, and 9 faces, all hexagonal. This graph can be embedded onto a torus as indicated schematically in Figure 5b where the three opposite pairs of edges of the outer hexagon are identified to make the torus, i.e., a to a, b to b, and c to c. This graph can be tripled by the leapfrog transformation to give a graph with 54 vertices, 81 edges, and 9 faces, which in principle could describe a toroidal form of carbon or boron nitride. However, such a toroidal structure is energetically unfavorable because of the need to bend the hexagonal faces to match the curvature of the underlying torus [14]. The experimentally observed forms of toroidal carbon [15, 16, 17] minimize this strain by forming a much larger torus with 2,000 to 30,000 carbon atoms so that the local curvature in individual hexagons is nearly zero. In addition, theoretical work on toroidal graphitic molecules [18, 19] suggests minimization of this strain by replacing pairs of hexagons with pentagon-heptagon pairs so that the pentagons and heptagons are at sites of positive and negative curvature, respectively, of the underlying torus.

The Spectra of the Symmetrical Tripartite Graphs

The high symmetry of the $K_{n,n,n}$ graphs leads to simple spectra with only three distinct eigenvalues, namely a non-degenerate eigenvalue of $+2n$, a doubly degenerate eigenvalue of $-n$, and a $(3n - 3)$-fold degenerate zero eigenvalue. Note that the most positive eigenvalue ($+2n$) corresponds to the vertex degrees of these highly symmetrical graphs. The spectra of the $K_{n,n,n}$ graphs are consistent with the $\{2,-1,-1\}$ spectrum of the triangle C_3, which corresponds also to the complete graph K_3 and is the simplest symmetrical tripartite graph, namely $K_{1,1,1}$. The spectra of the octahedron ($K_{2,2,2}$) and the dual of the Dyck graph ($K_{4,4,4}$) are depicted in Figure 6 as examples.
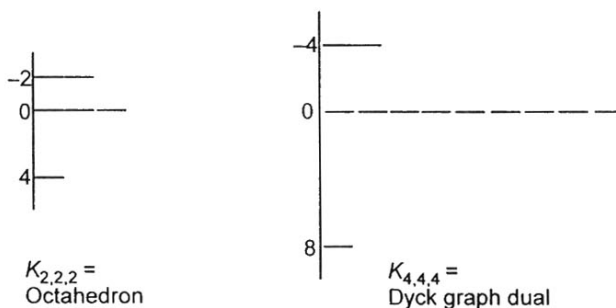

$K_{2,2,2} =$
Octahedron

$K_{4,4,4} =$
Dyck graph dual

FIGURE 6. The spectra of two regular tripartite graphs.

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