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EXCESSIVE INDEX OF CERTAIN CHEMICAL STRUCTURES

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Abstract: The structural formulae of chemical compounds are molecular graphs where vertices represent atoms and edges represent chemical bonds. A kekule structure in a molecular graph is nothing but a perfect matching in the graph. The minimum number of kekule structures that cover the edge set of a molecular graph G is known as the excessive index of G. In this paper we determine the excessive index of the unit cell representation of sodium chloride and 3-D mesh networks representing oxides and selenides of certain chemical compounds. Further we determine the excessive index of hexagonal networks.

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1. Introduction

Mathematical chemistry has been formally recognized only during the last few decades, with a strong influence involving graph theoretic work. This special influence is perhaps quite appropriate in view of its relevance in the classical core of chemistry, the characterization of molecular structure, and valence theory [18]. Chemical graph theory models have been extensively used as predictors of the properties of chemical compounds. All structural formulae of chemical compounds are molecular graphs where vertices represent atoms and edges represent chemical bonds.

The study of Kekule structures of chemical compounds have many *hidden treasures* [22] and have for a long time been the focus of interest of scholars working on the theory of benzenoid molecules [14]. A vast amount of theoretical work also has been done on Kekule structures [10, 11, 12, 13]. Carbon compounds without kekule structures are considered in [22].

One major direction of research is finding the number K of Kekule structures [7] and trying to relate K with various physico–chemical properties of the underlying compounds [15]. Another direction is the study of individual Kekule structures and finding relations between them. A famous problem along these lines which has not been satisfactorily solved is the identification of the Kekule structure that provides the most faithful representation of the true bonding in the respective molecule [17].

A kekule structure in a molecular graph is nothing but a perfect matching in the graph. The minimum number of kekule structures (perfect matchings) that cover the edge set of a molecular graph G (or simply a graph G) is known as the excessive index of G [2].

Excessive index has a number of applications particularly in scheduling theory to complete a process in the minimum possible time [5]. Scheduling is important in modern production and chemical industries, where it can have a major impact in the productivity of a process. In this paper we determine the excessive index for hexagonal and 3-D mesh network.

2. Preliminaries

A *matching* in a graph $G = (V, E)$ is a subset M of edges, no two of which have a vertex in common. A matching M is said to *perfect* if every vertex in G is an endpoint of one of the edges in M. Thus a perfect matching in G is a 1-regular spanning subgraph of G. In the literature it is also known as a 1-

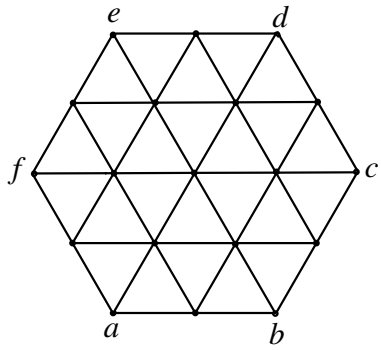

Figure 1: Hexagonal Network of dimension 3

factor of G. A *near-perfect* matching covers all but exactly one vertex. A graph G is 1-*extendable* if every edge of G belongs to at least one 1-factor of G. A 1-*factor cover* of G is a set $\mathcal{F}$ of 1-factors of G such that $\cup_{F\in\mathcal{F}}F = E(G)$. A 1-factor cover of minimum cardinality is called an *excessive factorization* [2]. An excessive near 1-factorization of a graph G is a minimum set of near 1-factors whose union contains all the edges of G [4].

The *excessive index* of G, denoted $\chi_e^{'}(G)$, is the size of an excessive factorization of G. We define $\chi_e^{'}(G) = \infty$ if G is not 1-extendable. A graph G is 1-*factorizable* if its edge set $E(G)$ can be partitioned into edge-disjoint 1-factors. The problem of determining whether a regular graph G is 1-factorizable is NP-complete [16]. Bonisoli et al. [2] observed that the problem of determining the excessive index for regular graphs is NP-hard. Cariolaro et al. [3] determined the excessive index of complete multipartite graphs, which proved to be a challenging task. The excessive index of a bridgeless cubic graph has been studied by Fouquet et al. [9]. Excessive index of certain regular graphs has been determined in [1, 20].

3. Hexagonal Networks

Hexagonal networks are based on regular triangular tessellations, or the partition of a plane into equilateral triangles and are widely studied in [6]. They are applied in chemistry to model benzenoid hydrocarbons [23], in image processing & computer graphics [19], and wireless & interconnection networks. Hexagonal network $HX(n)$ of dimension n has $3n^2-3n+1$ vertices and $9n^2-15n+6$ edges, where n is the number of vertices on one side of the hexagon [6]. See Figure 1. The diameter is $2n-2$. There are six vertices of degree three which we call

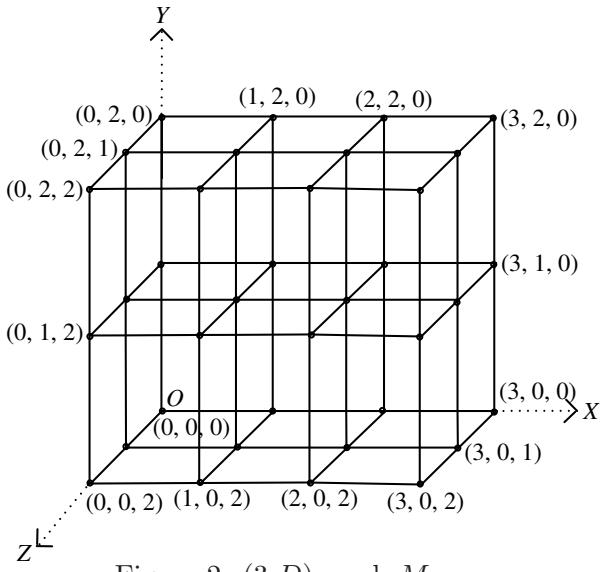

Figure 2: (3-D) mesh $M_{4\times3\times3}$

as *corner vertices*. Name the corner vertices as a, b, c, d, e and f as shown in Figure 1. The performance of hexagonal networks was studied in [6, 8, 21].

Theorem 3.1. *[2] Let G be a graph. Then $\chi_e^{'}(G) \geq \triangle$.*

In view of Theorem 3.1, we have the following theorem.

Theorem 3.2. *Let G be the hexagonal network $HX(n)$ of dimension n. Then $\chi_e^{'}(G) \geq 6$.*

We now give a procedure and its proof of correctness to show that the lower bound obtained in Theorem 3.2 is sharp.

Procedure Excessive Index $\chi_e^{'}(HX(n))$

Input: The hexagonal network $HX(n)$ of dimension n.

Algorithm:

Choose ab as the base line. See Figure 1. We note that a and d are diametrically opposite vertices. We construct a hamiltonian path P_{ad} in $HX(n)$ from a to d as follows:

Traverse the base line starting from a and all lines parallel to the base line with appropriate oblique boundary edges connecting these parallel lines. Let M_1 consist of alternate edges on P_{ad} starting from the edge with one end at a. In M_2 choose edges on P_{ad} which are not in M_1. Let M_3 and M_4 be similarly formed by choosing the hamiltonian path P_{be} with bc as the base line. Further M_5 and M_6 are obtained in a similar manner by choosing the hamiltonian path P_{cf} with cd as the base line.

End Excessive Index $\chi_e^{'}(HX(n))$

Output: $\chi_e^{'}(HX(n)) = 6$.

Proof of Correctness. The edges of hexagonal network are in three different direction and each of the hamiltonian paths P_{ad}, P_{be} and P_{cf} covers those edges. The result follows from the observation thus $P_{ad} = M_1 \cup M_2$, $P_{be} = M_3 \cup M_4$ and $P_{cf} = M_5 \cup M_6$. □

Theorem 3.3. *Let G be the hexagonal network $HX(n)$ of dimension n. Then $\chi_e^{'}(G) = 6$.*

4. Mesh Networks

Let P_n denote a path on n vertices. For m, $n \geq 2$, $P_m \times P_n$ is defined as a two dimensional (2-D) mesh with m rows and n columns. A three dimensional (3-D) mesh $M_{r\times s\times t}$ is nothing but $P_r \times P_s \times P_t$. See Figure 2. In a 3-$D$ mesh there are str number of vertices and $(2rs - r - s)t + (t - 1)sr$ number of edges. In our day-to-day life, the common salt NaCl is used as an important preservative because it retards the growth of micro-organisms. It also improves the flavour of food items. Chlorine products are used in metal cleaners, paper bleach, plastics and water treatment. They are also used in medicines. We find that the unit cell representation of Sodium Chloride (NaCl) is the same as the 3-D mesh $M_{3\times3\times3}$. See Figure 3.

In the 3-D mesh $M_{3\times3\times3}$, in the place of chlorine Cl if we take iron and in the place of sodium if we take oxygen it is nothing but the crystal structure of iron oxide. Similarly sodium replaced by magnesium and chloride replaced by selenide is the crystal structure of magnesium selenide. Further the crystal structure of cobalt oxide, magnesium oxide, europium selenide, lead selenide is the 3-D mesh $M_{3\times3\times3}$. For convenience we shall make use of the cartesian coordinate system for the 3-D mesh. Let the mutually perpendicular lines through O be the X-axis, Y-axis and Z-axis respectively. The vertices of $M_{r\times s\times t}$ are

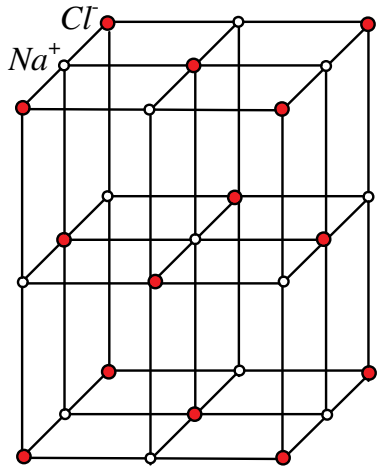

Figure 3: Sodium Chloride (*Nacl*)

denoted by (i, j, k), $0 \leq i \leq r-1$, $0 \leq j \leq s-1$, $0 \leq k \leq t-1$ and the edge joining two vertices (a, b, c) and (d, e, f) is denoted by $((a, b, c), (d, e, f))$. The vertex O is represented as $(0, 0, 0)$ and the remaining vertices are labeled as shown in the Figure 2.

Theorem 4.1. *Let G be the mesh network $M_{r\times s\times t}$. Then $\chi_e^{'}(G) = 6$.*

By Theorem 3.1, $\chi_e^{'}(G) \geq 6$.

Case (i): r even.

In M_1 select the edges $((i, j, k), (i+1, j, k))$, i even, $0 \leq i \leq r-2$, $0 \leq j \leq s-1$, $0 \leq k \leq t-1$. Clearly M_1 is perfect. In M_2 select the edges $((i, j, k), (i+1, j, k))$, i odd, $1 \leq i \leq r-3$, $0 \leq j \leq s-1$, $0 \leq k \leq t-1$. Since r is even, the vertices (i, j, k), $i = 0, r-1$, $0 \leq j \leq s-1$, $0 \leq k \leq t-1$ are unsaturated. To saturate these vertices, select the edges $((i, j, k), (i, j+1, k))$, $i = 0, r-1$ j even, $0 \leq j \leq s-2$, $0 \leq k \leq t-1$.

If s is even then M_2 is perfect. See Figure 4. If s is odd the vertices $(i, s-1, k)$, $i = 0, r-1$, $j = s-1$, $0 \leq k \leq t-1$ are left unsaturated. In order to saturate these vertices, select the edges $((i, s-1, k), (i, s-1, k+1))$, $i = 0, r-1$, k even, $0 \leq k \leq t-2$. If t is even then M_2 becomes perfect. If t is odd the vertices $(0, s-1, t-1)$ and $(r-1, s-1, t-1)$ are left unsaturated. In order to saturate these vertices, consider the vertices $(i, s-1, t-1)$, $0 \leq i \leq r-1$. The edges induced by the vertices $(i, s-1, t-1)$ and $(i+1, s-1, t-1)$, i odd, $1 \leq i \leq r-3$ are already in M_2. Now remove these selected edges from M_2 and include the edges $(i, s-1, t-1)$ and $(i+1, s-1, t-1)$, i even, $0 \leq i \leq r-2$

in M_2. Now M_2 is perfect.

Case (ii): r odd.

In M_1 select the edges $((i,\ j,\ k),\ (i+1,\ j,\ k))$, i even, $0 \leq i \leq r-3$, $0 \leq j \leq s-1$, $0 \leq k \leq t-1$. Since r is odd, the vertices $(r-1,\ j,\ k)$, $0 \leq j \leq s-1$, $0 \leq k \leq t-1$ are unsaturated. To saturate these vertices, select the edges $((r-1,\ j,\ k),\ (r-1,\ j+1,\ k))$, j even, $0 \leq j \leq s-2$, $0 \leq k \leq t-1$. If s is even then M_1 is perfect. If s is odd the vertices $(r-1,\ s-1,\ k)$, $0 \leq k \leq t-1$ are unsaturated. In order to saturate these vertices, select the edges $((r-1,\ s-1,\ k),\ (r-1,\ s-1,\ k+1))$, k even, $0 \leq k \leq t-2$. If t is even then M_1 becomes perfect. If t is odd M_1 becomes near-perfect, since there are odd number of vertices in $M_{r\times s\times t}$ when r, s and t are all odd.

In M_2 select the edges $((i,\ j,\ k),\ (i+1,\ j,\ k))$, i odd, $1 \leq i \leq r-2$, $0 \leq j \leq s-1$, $0 \leq k \leq t-1$. Since r is odd, the vertices $(0,\ j,\ k)$, $0 \leq j \leq s-1$, $0 \leq k \leq t-1$ are left unsaturated. Repeat the procedure as in M_1 when $(r-1,\ j,\ k)$, $0 \leq j \leq s-1$, $0 \leq k \leq t-1$ are unsaturated. Thus in M_1 and M_2 we consider the edges parallel to X-axis and to make them perfect if necessary we consider the edges parallel to Y-axis then Z-axis. We denote this process by $X \longrightarrow Y \longrightarrow Z$. In M_3 and M_4, repeat the procedure with $Y \longrightarrow Z \longrightarrow X$ and in M_5 and M_6 with $Z \longrightarrow X \longrightarrow Y$.

Thus $M_1 \cup M_2$ covers all edges parallel to X-axis except when r is even and s and t are odd. In this case in order to cover $((i,\ s-1,\ t-1),\ (i+1,\ s-1,\ t-1))$, i odd, $1 \leq i \leq r-3$ edges parallel to X-axis, remove the edges parallel to Z-axis as well as edges parallel to X-axis in M_3 and include the edges $((i,\ s-1,\ k),\ (i+1,\ s-1,\ k))$, i odd, $1 \leq i \leq r-3$, $1 \leq k \leq t-1$, $((i,\ s-1,\ k),\ (i,\ s-1,\ k+1))$, $i = 0, r-1$, k odd, $1 \leq k \leq t-2$ and $((i,\ s-1,\ 0),\ (i+1,\ s-1,\ 0))$, i even, $0 \leq i \leq r-2$. □

5. Conclusion

In this paper we have determined the excessive index of hexagonal and 3-D mesh networks yielding the excessive index of sodium chloride, cobalt oxide, magnesium oxide, europium selenide, lead selenide and many more. It would be an interesting line of research to determine the excessive index for other chemical structures since scheduling theory has gained momentum in biotechnology and even in nanotechnology.

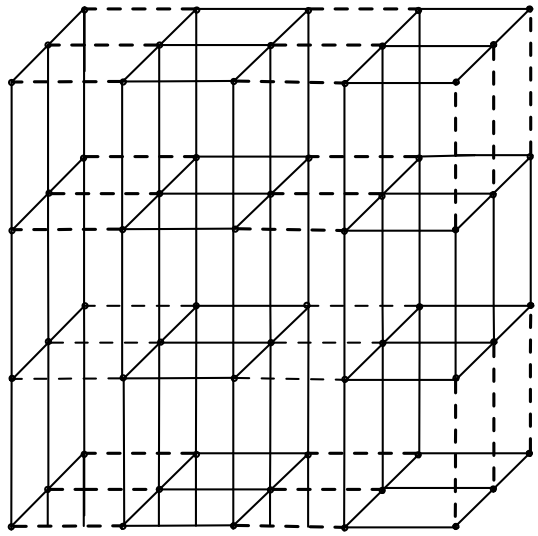

Figure 4: Dotted lines shows the edges selected in M_1 of $M_{5\times4\times3}$

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