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ANTI-KEKULE NUMBER OF CERTAIN CHEMICAL GRAPHS

Antony Xavier[1], A.S. Shanthi[2], Maria Jesu Raja[3]

[1,3]Department of Mathematics
Loyola College
Chennai, 600 034, INDIA

[2]Department of Mathematics
Stella Maris College
Chennai, 600 086, INDIA

Abstract: A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. An edge set M of a graph G is called a matching if no two edges in M have a common end vertex. A matching M of G is perfect if every vertex of G is incident with an edge in M. In organic molecular graphs, perfect matchings correspond to Kekule structures playing an important role in analysis of the resonance energy and stability of hydrocarbon compounds. The anti-Kekule number is the smallest number of edges that must be removed from a connected graph with a perfect matching so that the graph remains connected, but has no perfect matchings. In this paper we find the anti-kekule number for silicate, oxide and honeycomb networks.

AMS Subject Classification: 05C70
Key Words: anti-Kekule number, silicate, oxide and honeycomb networks

1. Introduction

An edge set M of a graph G is called a *matching* if no two edges in M have a common end vertex. A matching M of G is *perfect* if every vertex of G is

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incident with an edge in M. In organic molecular graphs, perfect matchings correspond to Kekule structures, playing an important role in analysis of the resonance energy and stability of hydrocarbon compounds. Cyvin and Gutman systematically gave [1] detailed enumeration formulas for Kekule structures of various types of benzenoids. Kardos et al showed [3] that fullerene graphs have exponentially many Kekule structures.

The anti-Kekule number of a connected graph G is the smallest number of edges such that the remaining graph obtained from G by deleting these edges is still connected but has no Kekule structures. For benzenoids, Vukicevic and Trinajstic showed [9] that the anti-Kekule number of parallelograms with at least three rows and at least three columns is equal to 2, and they also showed [8] that cata-condensed benzenoids have anti-Kekule number as either 2 or 3 and both classes are characterized. Afterwards, Veljan and Vukicevic [7] demonstrated that the anti-Kekule numbers of the infinite triangular, rectangular and hexagonal grids are 9, 6 and 4 respectively.

The anti-kekule number of ladders, cyclic ladders and Mobius ladders are proved to be 3 or 4 by Tang et al [6]. Zhang et al [11] determined the anti-Kekule number of cata-condensed phenylenes as 3. The leapfrog transformation of fullerenes is defined in [2], and the icosahedron C_{60} is the smallest leapfrog fullerene graph. D. Vukicevic showed that the anti-Kekule number of the icosahedron C_{60} is 4.

In general, Kutnar et al [4] proved that the anti-Kekule number of all leapfrog fullerene graphs is either 3 or 4 and for each leapfrog fullerene graph the anti-Kekule number can be established by observing finite number of cases not depending on the size of the fullerene graph. By applying Tutte's theorem on perfect matching of graphs, Yang et al [10] showed that the anti-Kekule number of all fullerene graphs is always equal to 4. In this paper we show that the anti-Kekule number of silicate, oxide, honeycomb networks are all equal to 2.

2. Preliminary

Let $G = (V(G), E(G))$ be a connected graph with at least one perfect matching (i.e. Kekule structure). For $S \subseteq E(G)$, let $G - S$ denote the graph obtained from G by deleting all the edges in S. We call S an anti-Kekule set if $G - S$ is connected but has no perfect matchings. The smallest cardinality of anti-Kekule sets of G is called the anti-Kekule number and denoted by $ak(G)$.

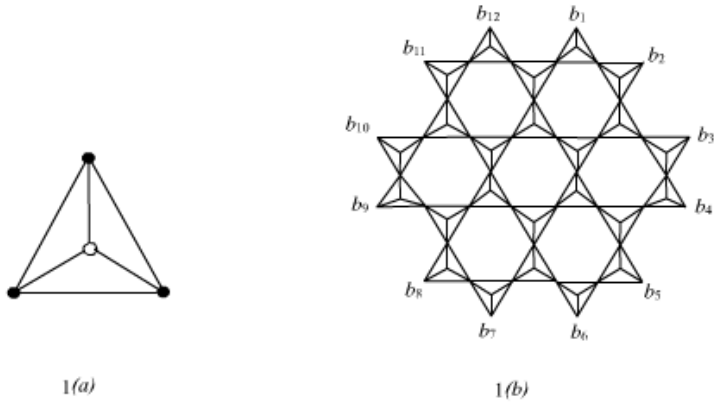

Figure 1: Figure: 1(a) and 1(b)

3. Silicate Network

The silicates are the largest, the most interesting and the most complicated class of minerals by far. The basic chemical unit of silicates is the SiO_4 tetrahedron. A silicate sheet is a ring of tetrahedrons which are linked by shared oxygen nodes to other rings in a two dimensional plane that produces a sheet-like structure. Silicates are obtained by fusing metal oxides or metal carbonates with sand. Essentially all the silicates contain SiO_4 tetrahedra[12]. In chemistry, the corner vertices of SiO_4 tetrahedron represent oxygen ions and the center vertex represents the silicon ion. In graph theory, we call the corner vertices as oxygen nodes and the center vertex as silicon node. See Figure 1(a). The silicate network of dimension n is denoted by $SL(n)$. The graph in Figure 1(b) is a silicate network of dimension two.

The 3-degree oxygen nodes of silicates are called *boundary nodes*. In Figure 1(b), $b_1, b_2...b_{12}$ are boundary nodes of $SL(2)$. The number of nodes in $SL(n)$ is $15n^2 + 3n$. The number of edges in $SL(n)$ is $36n^2$. $SL(n)$ is a bi-regular graph. It has $6n^2 + 6n$ vertices of degree 3 and $9n^2 - 3n$ vertices of degree 6.

Theorem 3.1. *Let G be the silicate network $SL(n)$ of dimension n. Then $ak(G) = 2$.*

Proof. It is easy to see that $ak(G) \geq 2$. Consider the subgraph induced by $N[b_1] \bigcup N[b_n]$ where b_1 and b_2 are the boundary nodes as shown in Figure 2. Now remove the edges (b_n, v) and (b_1, x) from $SL(n)$ then either $\{(b_n, u), (v, w), (b, y)\}$ or $\{(b_n, w), (v, u), (b, y)\}$ has to be in any perfect matching M.

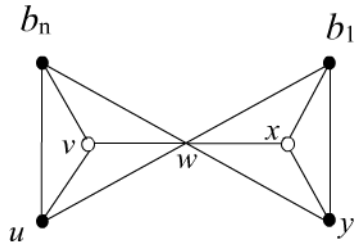

Figure 2: The induced subgraph of $N[b_1] \bigcup N[b_2]$

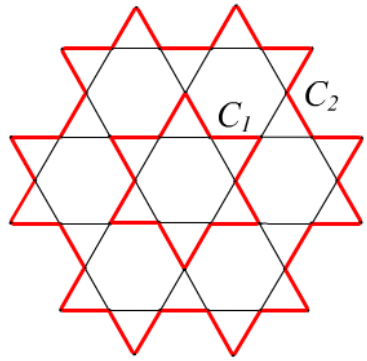

Figure 3: An Oxide Network $OX(2)$

But in both case the vertex x does not belong to M. Therefore $ak(G) = 2$. □

4. Oxide Network

When we delete all the silicon nodes from a silicate network we obtain a new network which we call as an Oxide Network. See Figure 3. An n-dimensional oxide network is denoted by $OX(n)$. Even though $HC(n)$ and $OX(n)$ are subgraphs of $SL(n)$, $OX(n)$ plays more important role in studying the properties of $SL(n)$. The diameter of silicate network $SL(n)$ is equal to the diameter of the oxide network $OX(n)$ [12].

Theorem 4.1. *Let G be the Oxide network $OX(n)$. Then $ak(G) = 2$.*

Proof. Let $C_1C_2.....C_n$ be the cycles of $OX(n)$ as shown in Figure 3. Clearly each C_i is of even length. Let M_1^i consist of alternate edges in C_i and M_2^i consist

of remaining edges in C_i, and $M_1 = \bigcup_{i=1}^{n} M_1^i$, $M_2 = \bigcup_{i=1}^{n} M_2^i$, $1 \leq i \leq n$. Clearly M_1 and M_2 are perfect matchings.

Let $e \in C_i$ then either $e \in M_1^i$ or $e \in M_2^i$. Without loss of generality let $e \in M_1^i$. Then M_2^i is a perfect matching not containing e. Let $E^{'}$ be set of all edges in $E(G) \setminus (M_1 \cup M_2)$. Suppose $e \in E^{'}$ then both M_1 and M_2 are perfect matching not containing e. This implies $ak(G) > 1$ and hence $ak(G) \geq 2$.

We claim that $ak(G) = 2$. Let uvw be the path such that $d(u) = d(w) = 2$ and $d(v) = 4$. Delete the edges with one end incident at u and other the end not incident at v. Similarly delete the edges with one end incident at w and other end not at v. Thus $ak(G) = 2$. □

5. Honeycomb Network

Various surface nanotemplates that are naturally or artificially patterned at the nanometre scale have been used to form periodic nanostructure arrays. The formation mechanism of these nanomesh template is attributed to the self-assembly of accumulated carbon atoms into well-ordered honeycomb structures at the nanometre scale [4]. Built recursively using the hexagon tessellation [12], honeycomb networks are widely used in computer graphics, cellular phone base stations, image processing, and in chemistry as the representation of benzenoid hydrocarbons. Honeycomb network $HC(n)$ is obtained from $HC(n-1)$ by adding a layer of hexagons around the boundary of $HC(n-1)$ [14]. The parameter n of $HC(n)$ is determined as the number of hexagons between the centre and boundary of $HC(n)$. See Figure 5. The number of vertices and edges of $HC(n)$ are $6n^2$ and $9n^2 - 3n$ respectively. The diameter is $4n-1$. The honeycomb cub of dimension 1 and 2 are shown in Figure 4(a) and 4(b).

Theorem 5.1. *Let G be a honeycomb network $HC(n)$, then $ak(G) = 2$.*

Proof. Let $C_1C_2.....C_n$ be the cycles of $HC(n)$ as shown in Figure 5. Clearly each C_i is of even length. Let M_1^i consist of alternate edges in C_i and M_2^i consist of remaining edges in C_i, and $M_1 = \bigcup_{i=1}^{n} M_1^i$, $M_2 = \bigcup_{i=1}^{n} M_2^i$, $1 \leq i \leq n$. Clearly M_1 and M_2 are perfect matchings.

Let $e \in C_i$ then either $e \in M_1^i$ or $e \in M_2^i$. Without loss of generality let $e \in M_1^i$. Then M_2^i is a perfect matching not containing e. Let $E^{'}$ be set of all edges in $E(G) \setminus (M_1 \cup M_2)$. Suppose $e \in E^{'}$ then both M_1 and M_2 are perfect matching not containing e. This implies $ak(G) > 1$ and hence $ak(G) \geq 2$.

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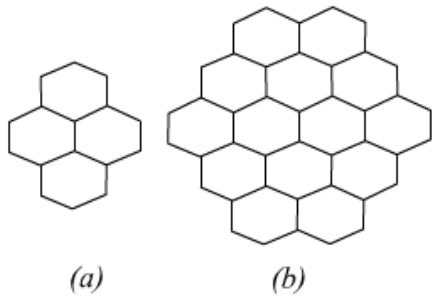

Figure 4: (a) Honeycomb cub Network $HCC(1)$, (b) Honeycomb cub Network $HCC(2)$

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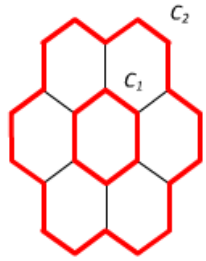

Figure 5: Cycles in Honeycomb Network

not incident at v. Similarly delete the edges with one end incident at w and other end not at v. Thus $ak(G) = 2$. □

By Theorem 5.1 we have the following result.

Corollary 5.2. *Let G be the honeycomb cub network $HCC(n)$. Then $ak(G) = 2$*

6. Conclusion

In this paper we have shown that the anti-Kekule number of silicate, oxide and honeycomb networks are all equal to 2. The Anti-kekule number for other chemical graphs and nanotubes are under investigation.

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