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COMPUTING THE ANTI-KEKULÉ NUMBER OF CERTAIN NANOTUBES AND NANOCONES

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ABSTRACT. Let *G(V,E)* be a connected graph. A set *M* subset of *E* is called a *matching* if no two edges in *M* have a common end-vertex. A matching *M* in *G* is *perfect* if every vertex of *G* is incident with an edge in *M*. The perfect matchings correspond to Kekulé structures which play an important role in the analysis of resonance energy and stability of hydrocarbons. The anti-Kekulé number of a graph *G*, denoted as *ak(G)*, is the smallest number of edges which must be removed from a connected graph *G* with a perfect matching, such that the remaining graph stay connected and contains no perfect matching.

In this paper, we calculate the anti-Kekulé number of $TUC_4C_8(S)[p,q]$ nanotube, $TUC_4C_8(S)[p,q]$ nanotori for all positive integers *p, q* and $CNC_{2k-1}[n]$ nanocones for all positive integers *k* and *n*.

Keywords: *Perfect matching, Anti-Kekulé number, Nanotubes, Nanocones*

INTRODUCTION

Mathematical chemistry is a branch of theoretical chemistry in which we discuss and predict the chemical structure by using mathematical tools and does not necessarily refer to the quantum mechanics. *Chemical graph theory* is a branch of mathematical chemistry in which we apply tools of graph theory to model the chemical phenomenon mathematically. This theory plays a prominent role in the fields of chemical sciences. A *moleculer / chemical graph* is a simple finite graph in which vertices denote the atoms and edges denote the chemical bonds between these atoms in the underlying chemical structure. It is important to mention that the hydrogen atoms are often omitted in a molecular graph.

A *nanostructure* is an object of intermediate size between microscopic and molecular structures. It is a product derived through engineering at molecular scale. This is something that has a physical dimension smaller than 100 nanometers, ranging from clusters of atoms to dimensional layers. *Carbon nanotubes* (CNTs)

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are types of nanostructure which are allotropes of carbon and have a cylindrical shape. Carbon nanotubes, a type of fullerene, have potential in fields such as nanotechnology, electronics, optics, materials science, and architecture. Carbon nanotubes provide a certain potential for metal-free catalysis of inorganic and organic reactions. Nanotube-based field emitters have applications as nanoprobes in metrology and biological and chemical investigations and as templates for the creation of other nanostructures. *Carbon nanocones* are conical structures which are allotropes of carbon having at least one dimension of the order one micrometer or smaller.

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 moleculer graphs, perfect matchings correspond to Kekulé structures, playing an important role in analysis of the resonance energy and stability of hydrocarbon compounds [1]. For example, it is well known that carbon compounds without Kekule structures are unstable. The study of Kekule structures of chemical compounds is very important, because they have many “hidden treasures” that may explain their physical and chemical properties [2]. The notations used in this paper are mostly taken from [3].

The *anti-Kekulé number* of a connected graph G is the smallest number of edges that must be removed from the graph G such that the remaining graph is still connected but has no Kekulé structures. For benzenoids, Vukičević and Trinajstić proved in [4] that the anti-Kekulé number of parallelograms with at least three rows and at least three columns is equal to 2, they also showed in [5] that cata-condensed benzenoids have anti-Kekulé number either 2 or 3 and both classes are characterized. Later on, Veljan and Vukičević showed that the anti-Kekulé numbers of the infinite triangular, rectangular and hexagonal grids are 9, 6 and 4, respectively [6]. For fullerene graphs, Vukičević showed that the anti-Kekulé number of the icosahedron C_{60} (buckminister fullerene) is 4. In general, Kutnar et al. proved in [7] that the anti-Kekulé number of all leapfrog fullerene graphs is either 3 or 4 and afterwards Yang et al proved that the anti-Kekulé number of all fullerene graphs is 4 [8]. For further study on anti-Kekulé number of different graphs please consult [9, 10, 11].

Let $G(V,E)$ be a connected graph with vertex set V and edge set E and let G has at least one perfect matching (i.e., Kekulé 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-Kekulé set if $G-S$ is connected but has no perfect matching. The anti-Kekulé set of minimum cardinality in G is called the anti-Kekulé number, and denoted by $ak(G)$.

MAIN RESULTS

In this paper, we calculate the anti-Kekulé number of $TUC_4C_8(S)[p,q]$ nanotube and $TUC_4C_8(S)[p,q]$ nanotori. The anti-Kekulé number of $CNC_{2k}[n]$ nanocones $\forall k \in \mathbb{N}$, was discussed by the present authors in [12]. Now we discuss the anti-Kekulé number of $CNC_{2k-1}[n]$ nanocones $\forall k \in \mathbb{N}$.

RESULTS FOR NANOTUBES

In this section, we compute the anti-Kekulé number for $TUC_4C_8(S)[p,q]$ nanotube. This nanotube is a net of C_4 and C_8, and it can be constructed by alternating C_4 and C_8 following a trivalent decoration as shown in Fig. 2. This type of tiling can cover a cylinder and a torus nanotube. In a 2-dimensional lattice of the $TUC_4C_8(S)[p,q]$ nanotube, p is the number of octagons in one row and q is the number of periods in the whole lattice. A period consist of two rows of edges as shown in Fig. 1. Further detail on the construction of $TUC_4C_8(S)[p,q]$ nanotubes can be found in [13].

Carbon nanotubes are molecular-scale tubes of graphitic carbon with outstanding properties. They are among the stiffest and strongest fibres known, and have remarkable electronic properties and many other unique characteristics. For these reasons they have attracted huge academic and industrial interest, with thousands of papers on nanotubes being published every year. Commercial applications have been rather slow to develop, however, primarily because of the high production costs of the best quality nanotubes.

For our purpose, we call the vertices of degree 2 as the *boundary* vertices of a nanotube. One can observe that the boundary vertices lie on the first and the last layer of the nanotube.

Theorem 2.1 *Let $G = TUC_4C_8(S)[p,q]$ nanotube, then $ak(G) = 3$.*

Proof. Consider the set $S = \{e_1, e_2, e_3\} \subseteq E(G)$, then the graph $G - S$ contains a vertex v such that v is adjacent to two vertices of degree 1, say u and w (see Fig. 1). Since the vertices u and w cannot be matched simultaneously, the graph $G - S$ is connected but contains no perfect matching. This implies that $ak(G) \leq 3$.

Conversely, let $U = \{e, e'\} \subseteq E(G)$. We will show that the graph $G - U$ is connected and it contains a perfect matching. Clearly, the graph $G - U$ will be connected if and only if e and e' are not adjacent to the same boundary vertex.

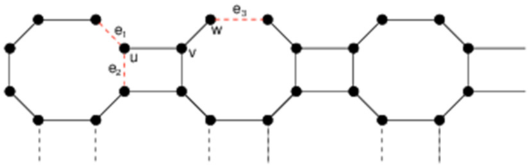

Figure 1. One period of the graph of $TUC_4C_8(S)[p,q]$ with Anti-Kekulé set $S = \{e_1, e_2, e_3\}$ shown by the red edges.

The graph G is tiled with the cycles of lengths 4 and 8, such that each period contain p octagons and there are q such periods. Then the order of G is $|V(G)| = 8pq$ and the number of cycles of length 4 (and length 8 as well) in G is $p(2q-1)$. Let us label all the cycles of length 4 and 8 in G by $C^4_{k,l}$ and $C^8_{k,l}$ (respectively), where $1 \le k \le q$ and $1 \le l \le p$ (see Fig. 2). Let $E(C^4_{k,l})$ (and $E(C^8_{k,l})$) denote the edge set of the cycle $C^4_{k,l}$ (resp. $C^8_{k,l}$) and let $E(C^4_{k,l}) = E^1(C^4_{k,l}) \cup E^2(C^4_{k,l})$, where $E^1(C^4_{k,l})$ and $E^2(C^4_{k,l})$ be the sets containing alternatively the edges of the cycle $C^4_{k,l}$, for each k and l.

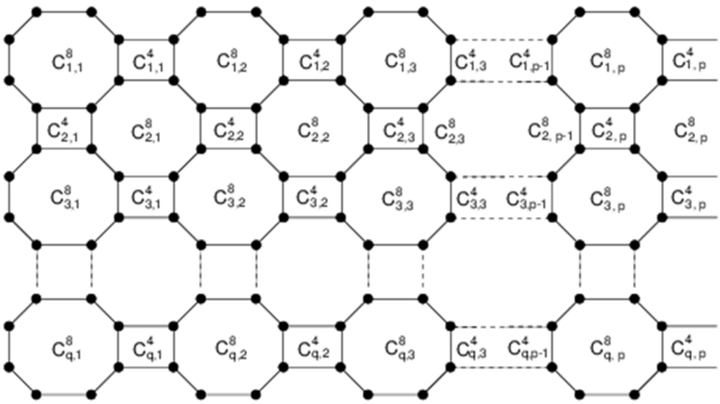

Figure 2. The cycles of length 4 and 8 in $TUC_4C_8(S)[p, \frac{q+1}{2}]$ nanotube

Similarly, let $E(C_{k,l}^8)=E^1(C_{k,l}^8)\cup E^2(C_{k,l}^8)$, where $E^1(C_{k,l}^8)$ and $E^2(C_{k,l}^8)$ be the sets containing alternatively the edges of the cycle $C_{k,l}^8$, for each k and l.

It can be observed that $|E^1(C_{k,l}^4)|=|E^2(C_{k,l}^4)|=2$. Clearly, either $E^1(C_{k,l}^8)$ or $E^2(C_{k,l}^8)$ contains some edges of the cycles of length 4. Without loss of generality, we assume that

$$\begin{cases} E^2(C_{k,l}^8)\cap\{E(C_{k+i,l}^4)\cup E(C_{k,l-j}^4)\}=\varnothing, & for \quad k=odd; \\ E^2(C_{k,l}^8)\cap\{E(C_{k+i,l}^4)\cup E(C_{k,l+j}^4)\}=\varnothing, & for \quad k=even, \end{cases} \quad (1)$$

$where\ i\in\{-1,1\}, j\in\{0,1\}$. We can define two disjoint perfect matchings in G as follows.

$$M_1=\bigcup_{k,l}E^1(C_{k,l}^8) \quad and \quad M_2=\bigcup_{k,l}E^2(C_{k,l}^8). \quad (2)$$

Clearly, $M_1=\bigcup_{k,l}E(C_{k,l}^4)$ and $M_2=E(G)-M_1$. We consider the following three cases.

Case 1. Let e and e' do not lie on a cycle of length 8. Then we have a perfect matching M_1 (or M_2) in the connected graph $G-U$.

Case 2. Let one of e and e' lie on a cycle of length 8. Suppose on contrary that e lies on $C_{k,l}^8$, then without loss of generality we can assume that $e\in E^1(C_{k,l}^8)$. Then we have a perfect matching M_2 in the connected graph $G-U$.

Case 3. Suppose that both e and e' lie on the cycles $C_{k,l}^8$ and $C_{s,t}^8$ (respectively), for $1\le k,s\le q$ and $1\le l,t\le p$.

When $(k,l)\neq(s,t)$ then if $e\in E^1(C_{k,l}^8)$ and $e'\in E^1(C_{s,t}^8)$, then M_2 is a perfect matching in the connected graph $G-U$. Similarly, when $e\in E^1(C_{k,l}^8)$ and $e'\in E^2(C_{s,t}^8)$, then $M'=M_1-E^1(C_{k,l}^8)+E^2(C_{k,l}^8)$ is the required perfect matching in the connected graph $G-U$.

When $(k,l)=(s,t)$, both edges e and e' lie on the same cycle of length 8, say $C_{k,l}^8$. Then we have the following two subcases.

(1) Let e and e' lie in the same class, say $E^1(C_{k,l}^8)$. Then M_2 will be a perfect matching in the connected graph $G-U$.

(2) Let e and e' lie in different classes, say $e \in E^1(C_{k,l}^8)$ and $e' \in E^2(C_{k,l}^8)$. When e and e' are adjacent, it is clear that the edges e and e' cannot be adjacent to the same boundary vertex, as the graph will be disconnected. Then consider a matching N' in $G-U$ defined in four cases corresponding to the possibilities of the edges e and e', as follows.

$$N' = M_1 - \bigcup_{i,j} E^1(C_{k+i,l+j}^8) \cap \{e\}, \; where \; (i,j) = \begin{cases} (0,0) \; and \; (0,1); \\ (0,0) \; and \; (2,0); \\ (0,0) \; and \; (0,-1); \\ (0,0) \; and \; (-2,0). \end{cases} \tag{3}$$

It can be seen that each pair of octagons in the matching defined in Equ. 3 are joined by the cycle $C_{k+i,l+j}^4$, where

$$(i,j) = \begin{cases} (0,0) \;\; for \;\; k = odd \quad and \quad (0,1) \;\; for \;\; k = even; \\ (1,0); \\ (0,-1) \; for \; k = odd \; and \; (0,0) \; for \; k = even; \\ (-1,0). \end{cases} \tag{4}$$

Since $e \in E^1(C_{k,l}^8)$ therefore $e \in M_1$ and thus lies on a cycle of length 4, whereas e' does not. Let $E(C_{k+i,l+j}^4) = \{c_1, c_2, c_3, c_4\}$, for (i,j) as mentioned in Equ. 4. Clearly, $e \in \{c_1, c_2, c_3, c_4\}$. Then label these edges with $e = c_1$ in the clockwise direction starting from e.

Now, using the matching defined in Equ. 3, we can construct a matching N in the graph $G-U$ as follows.

$$N = N' - \{c_3\} + \{c_2, c_4\}. \tag{5}$$

Then N is a perfect matching in the connected graph $G-U$, which implies that $ak(G) \geq 3$, and completes the proof.

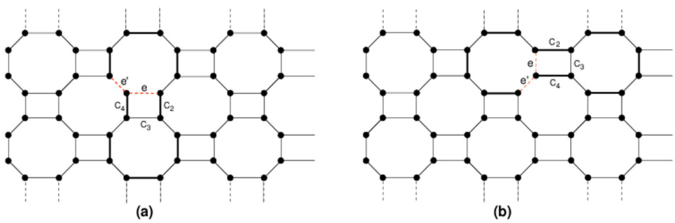

Figure 3. The matching for the pair of octagons corresponding to the first two cases in Equ. (3). The rest of the periods are matched by the matching M_1.

RESULTS FOR $TUC_4C_8(S)[p,q]$ NANOTORI

The $TUC_4C_8(S)[p,q]$ nanotorus (or nanotori) is obtained from the $TUC_4C_8(S)[p,q]$ nanotube by joining the ends of the tube, so giving it the shape of a torus. The spoke type edges in the last layer will be joined to the corresponding vertices in the first layer (see Fig. 4).

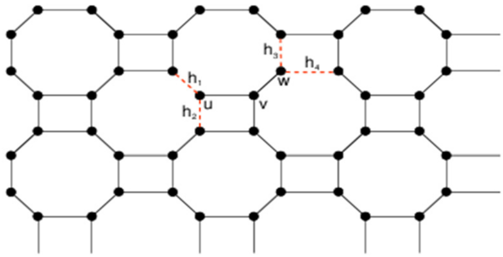

Figure 4. The embedded graph of the $TUC_4C_8(S)[3,2]$ nanotori

Theorem 2.2 *Let $G = TUC_4C_8(S)[p,q]$ nanotori, then $ak(G) = 4$.*

Proof. Consider a period of the 3-regular graph of $TUC_4C_8(S)[p,q]$ nanotori, as shown in Fig. 5. Let E_1, E_2 and E_3 be the edge partitions of $E(G)$ containing all the edges labelled e_1, e_2 and e_3, respectively. It is easy to see that E_1, E_2 and E_3 form three (disjoint) perfect matchings in G.

Let $S = \{h_1, h_2, h_3, h_4\} \subseteq E(G)$, as shown in Fig. 4. Then the graph $G - S$ contains a vertex v such that v has two pendent vertices adjacent to it, which cannot be matched simultaneously. Since no more than two vertices from S are adjacent to a single vertex, the graph G remains connected. Thus, $ak(G) \leq 4$.

Conversely, let $U = \{b_1, b_2, b_3\} \subseteq E(G)$, where all edges of U are not adjacent to a single vertex in G. We have the following three cases to be discussed.

Case 1. When all elements of U belong to same edge class, say E_1. Then we have M_2 (or M_3) as a perfect matching in the graph $G - U$.

Case 2. When two elements of U belong to the same edge class, say E_1. Then the third element of U can be in one of the remaining two edge classes, say E_2. Thus E_3 will be a perfect matching in the connected graph $G - U$.

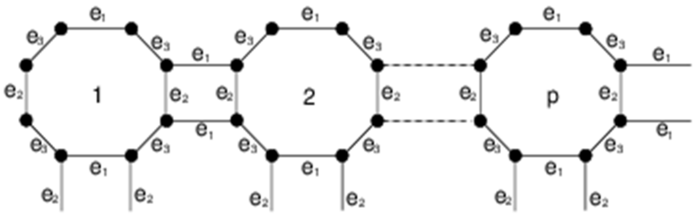

Figure 5. A period of $TUC_4C_8(S)[p,q]$ nanotori

Case 3. When all elements of U belong to different edge classes, say $b_1 \in E_1$, $b_2 \in E_2$ and $b_3 \in E_3$. Consider the labeling of all the cycles of length 4 and 8 in G, as done in Theorem 2.1, respectively by $C_{k,l}^4$ and $C_{k,l}^8$. With one extra row of edges joining the vertices in the last row to corresponding vertices in the first row, and thus $1 \le k \le q+1$ and $1 \le l \le p$. Since $b_1 \in E_1$, which is the class of all horizontal edges, we can assume that $b_1 \in E(C_{k,l}^4)$, for some k and l. Label the edges of $C_{k,l}^4$ with $\{c_1, c_2, c_3, c_4\}$ and let $b_1 = c_1$. Consider a matching M in $G-U$ defined as follows.

$$M = E_1 - \{c_1, c_3\} + \{c_2, c_4\}. \quad (6)$$

Clearly, M is a perfect matching in the connected graph $G-U$. Thus $ak(G) \ge 4$, which completes the proof.

RESULTS FOR $CNC_k[n]$ NANOCONES

Now we determine the anti-Kekulé number of $CNC_k[n]$ nanocones, where $k = 2q-1, q \ge 2, n \ge 1$. This family of nanocones is parameterized in such a manner that k denotes the length of the cycle placed at the core of the nanocone and n is the number of hexagonal layers placed at the conical surface of the nanocone. Now we calculate the anti-Kekulé number of this class of nanocones.

Theorem 2.3 *Let G be the graph of $CNC_k[n]$ nanocone, where $k = 2q-1, q \ge 2, n \ge 1$, then $ak(G) = 2$.*

Proof. First we show that $ak(G) \le 2$. For this purpose, consider a set $S = \{s_1, s_2\} \subseteq E(G)$ and a $\{uvw\}-$path in G as shown in Fig. 6. Then,

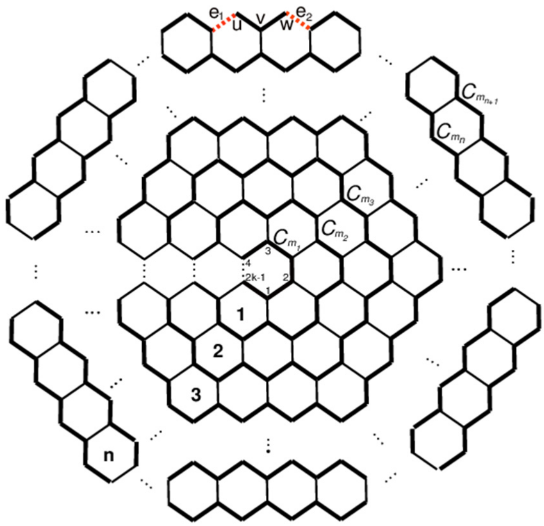

Figure 6. A representation of $CNC_k[n]$ nanocone, with k being an odd integer, with C_{n+1} cycles and a $uvw-$path.

there does not exist any perfect matching in the graph $G-S$. Thus $ak(G)\leq 2$.

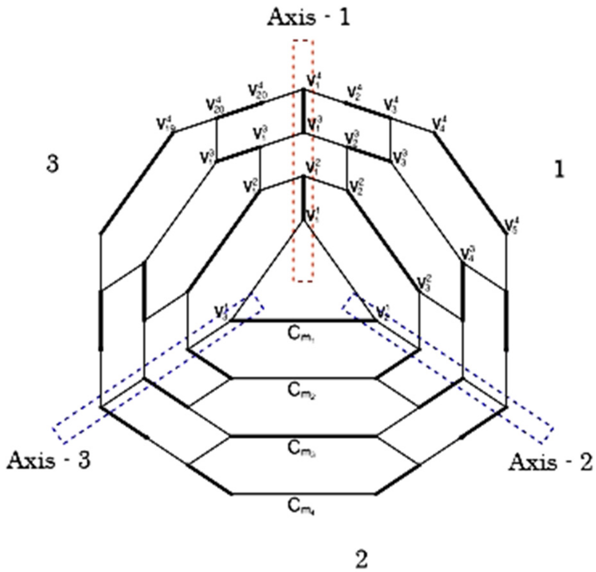

Figure 7. The perfect matching M_1 in $CNC_3[3]$ nanocone obtained by matching the edges on Axis-1. M_2 and M_3 can be obtained by matching other Axis.

Conversely, let $C_{m_i} = \{v_1^i, v_2^i, \ldots, v_{m_i}^i\}$, for $1 \le i \le n+1$, be the cycles as shown in Fig. 7. Then the length of the cycle C_{m_i} is $m_i = k(2i-1)$. Clearly, m_i (for $1 \le i \le n+1$) is always odd.

There are k different perfect matchings of the graph G (as constructed in Fig. 7, for $k=3$), which can be obtained by relabeling the vertices of the graph or just by rotating the graph G. Let $M_1, M_2, \ldots, M_k$ be the perfect matchings in the graph G obtained by selecting the edges of the graph G lying on different axis. The k axis of the $CNC_k[n]$ nanocone (k odd) are shown in Fig. 8.

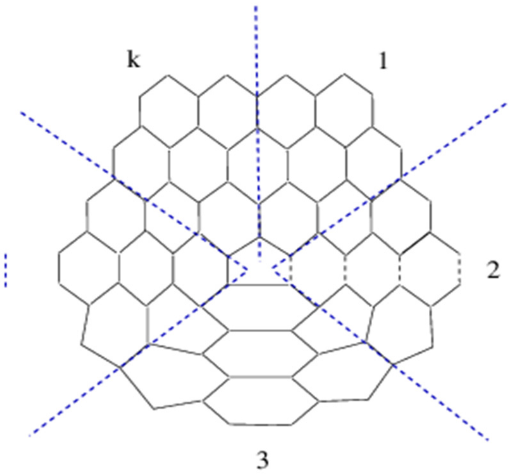

Figure 8. The k axis for the $CNC_k[n]$ nanocone for odd k

The k perfect matchings M_l, for $1 \le l \le k$, are defined as follows.

$$M_l = \{v^i_{l+2(l-1)(i-1)} v^{i+1}_{l+2(l-1)i},\ v^i_{l+2(l-1)(i-1)+s} v^i_{l+2(l-1)(i-1)+s+1},\ v^{i+1}_{l+2(l-1)i+s} v^{i+1}_{l+2(l-1)i+s+1} \mid$$
$$1 \le i \le n+1, \quad s+z \equiv z (\mathrm{mod}\, m_i), \quad where\ i, s\ are\ odd\}.$$

It can be seen that the $(l)-$phase of the matchings M_l and M_{l+1}, for $1 \le l \le k-1$, are same (see Fig. 7, for instance), and the rest of the phases are all different. The edges lying on the axis lines are not included in any phase.

Let $e \in E(G)$, then we have the following two cases.

Case 1. When e lies on an axis line. Since each matching M_l, $1 \le l \le k$, contains a single axis line. There will be $k-1$ perfect matchings in the graph $G-\{e\}$.

Case 2. When e does not lie on an axis line. Then e lies in one of the k phases of the nanocone, say phase$-(l)$. Then if e belongs to the edges of the graph G matched under M_l then we have $k-2$ perfect matchings M_t, $1 \le t \le k$ where $t \ne l$ and $t \ne l+1$, in the connected graph $G-\{e\}$. Thus $ak(G) \ge 2$, which completes the proof.

CONCLUDING REMARKS

The perfect matchings in a graph correspond to Kekulé structures which play an important role in the analysis of resonance energy and stability of hydrocarbons. Nanotubes and nanocones are allotropes of carbon having enormous applications in the field of nanotechnology, electronics, optics, materials science, and architecture. In this study, we proved that the anti-Kekulé number of the finite families of $TUC_4C_8(S)[p,q]$ nanotubes, $TUC_4C_8(S)[p,q]$ nanotubes $\forall p,q \in \mathbb{N}$ and for $CNC_{2k}[n]$ nanocones $\forall k,n \in \mathbb{N}$, is respectively 3, 4 and 2. Calculations showed that the anti-Kekulé number of almost all nanotubes is 2 or 3 in finite case and 4 or 5 if we consider their infinite 2 D lattices. Furthermore, our result of the anti-Kekulé number of a nanotorus agree with the anti-Kekulé number of fulerenes [8].

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