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# Independent Sets of $m, n$-gonal Graphs

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**Abstract :** An $m$,$n$-gonal system $\pi = (V, E, F)$, where $V$ is a vertex set, $E$ is an edge set and $F$ is a face set, is a graph of cyclic hydrocarbon molecules: each vertex represents a carbon atom and each edge represents a chemical bond. A Kekule structure, $K \subseteq E$ is a perfect matching and the edges of the matching correspond to double bonds. We count a number of perfect matchings (Kekule structures) in $m$,$n$-gonal systems where $m, n \equiv 2(mod\ 4)$. Our result is shown that the number of perfect matchings is $\phi(\pi) = |detA(\pi)|$, where $A(\pi)$ is a biadjacency matrix for each system. Moreover, we study the interesting properties of vertex and face independence sets of $m$,$n$-gonal systems.

**Keywords :** Kekule structure; perfect matching; m,n-gonal system; cyclic hydrocarbon; independent set.
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## 1 Introduction

The $m$,$n$-gonal graph is a graph $H = (V, E, F)$ that it consists of only $M$ and $N$ cycles, such that is special classes of graphs corresponded to some chemical structure, it is called cyclic hydrocarbon molecule. The $m$,$n$-gonal system $\pi$ is

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obtained by removing the edges representing carbon-hydrogen bonds and letting the remaining edges of $\pi$ represent either single or double carbon-carbon bonds. A vertex independent set correspond to independent set of carbon atom and an edge independent set correspond to double bonds. Therefore, chemical properties of cyclic hydrocarbon molecule such as stability and energy levels depend on maximumlity of vertex independent set and the number of edge independent sets (denoted by $\phi(\pi)$) in its corresponding $m$,$n$-gonal system, so chemists seek efficient methods to calculate them [1,2]. In Figure 1, we show an example of $m$,$n$-gonal systems associated with cyclic hydrocarbon molecules.

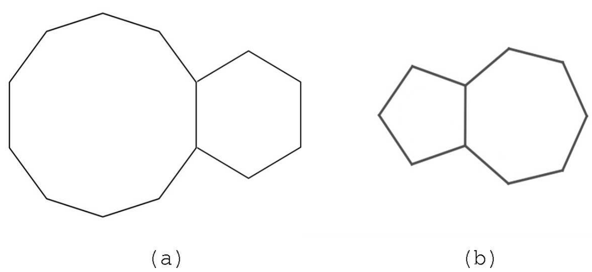


Figure 1: (a)The 10,6-gonal system (b)The 5,7-gonal system.

Graph theory is the study of vertices and edges. In this study, the authors are not only interested in the general graph, but also the hydrocarbon system, which is one of chemical graphs. Chemical graphs are just graph-based descriptions of molecules, with vertices representing the atoms, each one of them labeled by the type (name of the corresponding element), and edges representing the bonds [3]. Therefore the hydrocarbon molecule will be transformed to a graph of vertices and edges by removing the edges representing carbon-hydrogen bonds and letting the remaining edges of this graph represent either single or double carbon-carbon bonds. Then the graph of $\pi = (V, E, F)$ of hydrocarbon molecules are presented and called hydrocarbon systems in the rest of this work. The more information related to this study, i.e. their chemical meaning as representations of hydrocarbons, is reported by manuscript [4,5,6].

In this paper, we will research about $m$,$n$-gonal hydrocarbon systems, which is a 2-connected plane graph with a plane embedding such that every interior face is bounded by a regular $m$-gon and $n$-gon. For example, naphthalene is the benzenoid whose hexagonal (6-gonal) system is the linear chain. It is used to help derive the antibiotic aureomycin. Chrysene the benzenoid whose hexagonal system is the chain with 4 hexagons(6-gons), present in coal heated at high temperatures. For further discussion about some chemical properties of $m$,$n$-gonal system and connections between chemistry and $m$,$n$-gonal systems, see [7,8,9,10,11].

For previous research of $m$,$n$-gonal systems, the researchers studied Kekule structures of hexagonal systems [1,12]. They counted a maximum number of edge independent sets in hexagonal systems. Their result show the maximum number

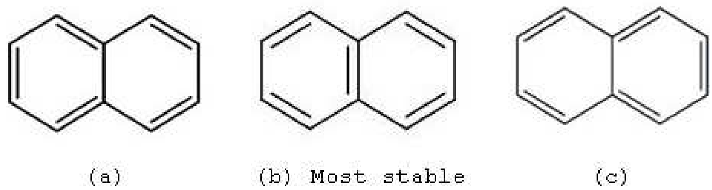


Figure 2: The three edge independence sets of naphthalene (a) Only left ring corresponds to edge independence set of benzene (b) Both ring corresponds to edge independence set of benzene (c) Only right ring corresponds to edge independence set of benzene

of edge independent sets is $\phi(\pi) = |detA(\pi)|$ when $A(\pi)$ is a biadjacency matrix for each system. In 2006 and 2007, Jack E. Graver [13,14] explores the structure of independent sets in fullerenes, which were plane trivalent graphs with pentagonal and hexagonal faces. They proved that the construction of a maximum vertex independent set in a benzenoid was similar to the dual paths between pentagonal faces replaced by dual circuits through the outside face. In this research, we will study all properties of independent sets in $m$,$n$-gonal system $\pi = (V, E, F)$, a graph of chemical system called cyclic hydrocarbons, because properties of independent sets in $m$,$n$-gonal system $\pi = (V, E, F)$ correspond with chemical properties of cyclic hydrocarbons. For example, the most stable structure formula for a cyclic hydrocarbon is an edge independent set which has the greatest number of rings that correspond to an edge independent set of benzene. Naphthalene is a fairly typical example; referred to Figure 2. Of the three edge independent sets ($\phi(\pi) = 3$) shown, the most stable one is the one in which both rings correspond to edge independent set of benzene [2].

## 2 Vertex Independent Set

Let $\pi = (V, E, F)$ be $m$,$n$-gonal system, that is a trivalent plane graph with $m$-gonal and $n$-gonal faces. A vertex independent set of a graph $\pi$ is a subset of the vertices such that no two vertices in the subset represent an edge of $\pi$. Given a vertex cover of a graph, all vertices not in the cover define a vertex independent set. Given $\alpha(\pi)$ denote the vertex independent number of $\pi$, which is a maximum vertex independent set is a vertex independent set containing the largest possible number of vertices for a given graph [6]. We wish to compute $\alpha(\pi)$. Next, we assume that $W$ be a maximum vertex independent set of $\pi$, $B$ be a maximum vertex independent set of $\pi$ in $V - W$ and let $G = V - B - W$. We color the vertices in $W$ white, the vertices in $B$ black, and the vertices in $G$ gray. A gray vertex with only black and gray neighbors could be recolored white, and a gray vertex with only white and gray neighbors could be recolored black. Hence, by the maximality of $W$ and $B$, we obtain the following.

**Theorem 2.1.** *In m,n-gonal system with the vertex coloring defined above, each gray vertex is adjacent to a black vertex and to a white vertex.*

Now if $g \in G$ is adjacent to two black vertices, let $w$ be the white vertex adjacent to $g$ and assign $(g, w)$ to the edge set $E_W$; referred to Figure 3(a). If $g \in G$ is adjacent to two white vertices, let $b$ be the black vertex adjacent to $g$ and assign $(g, b)$ to $E_B$, Figure 3(b). Referring to Figure 3(c), there are two adjacent gray vertices, arbitrarily labeled $g_1$ and $g_2$; then let $b_1$ be the black vertex adjacent to $g_1$ and let $w_2$ be the white vertex adjacent to $g_2$. Assign $(g_1, b_1)$ to $E_B$, $(g_2, w_2)$ to $E_W$ and assign $(g_1, g_2)$ to the edge set $E_G$. Finally, if $\pi$ is an $m$,$n$-gonal and admits a gray degree 2 vertex, that vertex must be adjacent to one black and one white vertex. Hence we may interchange its color with that of either of its neighbors without altering $|W|$, $|B|$ and $|G|$. Repeat this operation as often as necessary, we may move each degree 2 gray vertex into a degree 3 gray vertex. Hence, without loss of generality, we may assume that an $m$,$n$-gonal has no degree 2 gray vertices.

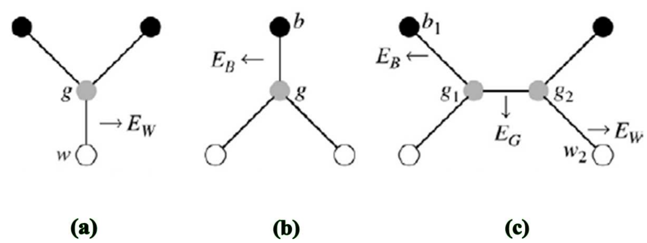


Figure 3: The set of $E_W$, $E_B$ and $E_G$.[14]

**Theorem 2.2.** *Let $\pi = (V, E, F)$ be an m,n-gonal system with the vertex coloring and edge partition defined above. Then $|G| = |E_B| + |E_W|$ and no two edges in $E_B \cup E_W$ have a common endpoint.*

*Proof.* By definition, each gray vertex is the endpoint of exactly one edge in $E_B \cup E_W$ and each edge in $E_B \cup E_W$ has exactly one gray endpoint. Hence, $|G| = |E_B \cup E_W| = |E_B| + |E_W|$; the last equality holds since $E_W$ and $E_B$ are disjoint.

Now suppose $e, e^{'} \in E_B \cup E_W$ have a common endpoint $x$. Since each gray vertex is incident with exactly one edge in $E_B \cup E_W$, $x \notin G$. Suppose $x \in B$ and let $y$ and $y^{'}$ be the other endpoints of $e$ and $e^{'}$, respectively. Clearly, $y$, $y^{'} \in G$. If $y$

were adjacent to another black vertex, we would have Figure 3(a) and $(x, y)$ would not belong to $E_B$. Thus, neither $y$ nor $y^{'}$ is adjacent to another black vertex. But, then we may recolor $x$ gray and both $y$ and $y^{'}$ black, contradicting the maximality of $B$. Similarly, $x \notin W$ and we conclude that no such $x$ exists. □

**Theorem 2.3.** *Let $\pi = (V, E, F)$ be an m,n-gonal system with the vertex coloring and edge partition defined above. Then:*

$$|W| = \frac{|E|+|W_2|}{3} - \frac{2|E_W|+|E_B|}{3} \text{ and } |B| = \frac{|E|+|B_2|}{3} - \frac{2|E_B|+|E_W|}{3}.$$

*where $|W_2|$ and $|B_2|$ are the set of degree 2 white and black vertices, respectively.*

*Proof.* Let $c_i$ denote the number of type $i = a, b, c$ configurations from Figure 3 in $\pi$ and let $e_{bw}$, $e_{gw}$, $e_{gb}$ and $e_{gg}$ denote the number of blackwhite edges, graywhite edges, grayblack edges and graygray edges, respectively. These parameters are related by the following equations:

$e_{gb} = 2c_a + c_b + 2c_c$
$e_{gw} = c_a + 2c_b + 2c_c$
$e_{gg} = c_c$
2 $e_{bw} = |E| - e_{gg} - e_{gb} - e_{gw}$.

We also have:

$|E_B| = c_b + c_c$
$|E_W| = c_a + c_c$
$|E_G| = c_c$.

Eliminating the $c_i$, we get:

$e_{gb} = 2\,|E_W| + |E_B| - |E_G|$
$e_{gw} = 2\,|E_B| + |E_W| - |E_G|$
$e_{gg} = |E_G|$
$e_{bw} = |E| - 3\,|E_B| - 3\,|E_W| + |E_G|$.

Then:

$$3\,|W| - |W_2| = e_{bw} + e_{gw} = |E| - (2\,|E_W| + |E_B|).$$

Next, moving $|W_2|\,|$ to the right-hand side and dividing by 3 gives the required formula for $|W|$. A similar derivation gives the formula for $|B|$. □

# 3 Edge Independent Set

An edge independent set (matching) $M$ in a graph $\pi$ is a set of edges of $\pi$ such that no two edges from $M$ have a vertex in common. The number of edges in a matching $M$ is called the size of $M$. A vertex $v \in V(\pi)$ incident to some edge $e \in M$, is covered by the matching $M$. Matching $M$ is perfect if it covers every vertex of $\pi$. Perfect matchings are known in chemistry as Kekule structures. As the number of Kekule structures of a chemical compound is often correlated with its stability, it may be of interest to find the number of different perfect matchings in the corresponding graph [2,10,11]. Given $\phi(\pi)$ denote the number of perfect matchings (maximum edge independent sets) of $\pi$. In this section, we wish to compute $\phi(\pi)$. An $m$,$n$-gonal system may be represented by a matrix, defined as follows [5]. Let $\pi$ be an $m$,$n$-gonal system and let $E$ denote the set of edges in $\pi$. Let $U \cup W$ be the set of vertices of $\pi$, where $U = \{u_1, u_2, ...u_m\}, W = \{w_1, w_2, ...w_n\}$ and all edges in $\pi$ join vertices in $U$ to vertices in $W$. The biadjacency matrix, written $A(\pi) = [a_{ij}]$ , is defined by $a_{ij} = 1$ if the edge $\{u_i, w_j\} \in E$ , and $a_{ij} = 0$ if $\{u_i, w_j\} \notin E$.

We will assume that $U$ and $W$ contain the same number of vertices since this is a necessary condition for the existence of perfect matching (maximum edge independent set). Thus the biadjacency matrix is square. In this paper, we will use following definition of determinant:

**Definition 3.1.** *Let $A(\pi) = [a_{ij}]_{n\times n}$. The determinant of $A(\pi)$ which is denoted by $det(A(\pi))$ is*

$$det(A(\pi)) = \sum(\pm)a_{1j_1}a_{2j_2}...a_{nj_n}$$

*when $\sigma = j_1j_2j_3...j_n$ is a pernutation of $\{1, 2, 3, ..., n\}$, we define the sign$(\pm)$ to be $+1$ if $\sigma$ is an even permutation and $-1$ if $\sigma$ is odd.*

**Remark 3.1.** *Let $\pi$ be an $m$,$n$-gonal system such that $m, n \equiv 2(mod\ 4)$ and $C$ be a cycle in each union of two perfect matchings (maximum edge independent sets), then the number of vertices inside $C$ is even.*

*Proof.* Let $M$ and $M^*$ be perfect matchings (maximum edge independent sets) in $\pi$ and $C$ be a cycle in $M \cup M^*$. Given $v_{int}$ be the number of vertices inside $C$. Since the edges in $C$ come alternately from $M$ and $M^*$, no vertex on $C$ can be matched to any vertex in the interior of $C$ by an edge in $M$. Since $\pi$ is a planar graph and $M$ is a perfect matching (maximum edge independent set), each vertex $b$ in the interior of $C$ lies in a unique edge $\{u, w\}$ in $M$, with also in the interior of $C$. Thus $v_{int}$ is even.

□

**Theorem 3.2.** *If $m, n \equiv 2(mod\ 4)$, then $m$,$n$-gonal system $\pi$ has $\phi(\pi) = |detA(\pi)|$.*

*Proof.* Let $m, n \equiv 2$ (mod 4) and $M$, $M^*$ be perfect matchings (maximum edge independent sets) in $m$,$n$-gonal system $\pi$. Give $C$ be a cycle in $M \cup M^*$. Let $v_{int}$ be the number of vertices inside $C$, $e_{int}$ be the number of edges inside $C$, $r_m$ be the number of $m$-gons inside $C$ and $r_n$ be the number of $n$-gons inside $C$. Applying Euler's formula to $C$ and its interior gives

$$(v_{int} + |C|) - (e_{int} + |C|) + (r_m + r_n + 1) = 2$$

Thus

$$e_{int} = v_{int} + r_m + r_n - 1 \tag{3.1}$$

Since every $m$-gon ($n$-gon) has $m$ ($n$) edges and every edge in the interior of $C$ is in exactly two $m$-gons ($n$-gons), the number of edges in $C$ and its interior is

$$e_{int} + |C| = mr_m + nr_n - e_{int}$$

By equation (3.1),

$$|C| = mr_m + nr_n - 2e_{int} = mr_m + nr_n - 2(v_{int} + r_m + r_n - 1) = \\ (m-2)r_m + (n-2)r_n - 2v_{int} + 2$$

Since $m, n \equiv 2(mod\ 4)$ and $v_{int}$ is even (lemma 3.2),

$$|C| \equiv 2\ (mod\ 4) \tag{3.2}$$

Next, we will show that all perfect matchings (maximum edge independent sets) of $\pi$ have the same sign. Consider $M$ and $M^*$ in $\pi$, without loss of generality, we may label the vertices in $\pi$ so that $M$ corresponds to identity permutation, say $\sigma$. Then $M^*$ corresponds to a permutation we denoted by $\sigma^*$. Now $M \cup M^*$ is a union of disjoint cycles and isolated edges. Let $C_1, C_2, C_3, ..., C_k$ denote the cycles in $M \cup M^*$. Since $|C_i| \equiv 2(mod\ 4)$ for all $i$, $C_i$ corresponds to a cyclic permutation, say $\sigma_i$. Moreover, the length of each cyclic permutation $\sigma_i$ is $\frac{|C_i|}{2}$, which is odd. Therefore $\forall \sigma_i$ can be factored into an even number of transpositions. Since $\sigma^* = \sigma\sigma_1\sigma_2...\sigma_k$, both $\sigma$ and $\sigma^*$ have the same sign.

Next we consider $A(\pi)$. We have $a_{ij}$ in $A(\pi)$ is either 0 or 1 for all $i, j$, then nonzero terms in the expansion of $detA(\pi)$ are all either 1 or -1. Since all the nonzero summands in $detA(\pi)$ have the same sign, $\phi(\pi) = |detA(\pi)|$.

□

# 4 Face independent set

A face independent set of a graph $\pi$ is a subset of the faces such that no two faces in the subset are adjacent in $\pi$. Let $K \subseteq E$ be a Kekule structure of $\pi$. It is convenient to use the Kekule number, $k = |K|$, as a basic parameter for the $m$,$n$-gonal system $\pi$. Then we have $|V| = 2k - b$,where $b$ is the number of edges in $K$ such that be boundary of $\pi$. We denote the face independent number of $\pi$ by $\alpha^* = \alpha^*(\pi) = \alpha(\pi^*)$.

**Theorem 4.1.** *Let $m$ and $n$ be odd then $m$,$n$-gonal system $\pi = (V, E, F)$ have not perfect face independent set.*

*Proof.* Let $m$ and $n$ be odd number and $\pi = (V, E, F)$ be an $m$,$n$-gonal system. Support that $\pi$ have a perfect face independent set $R$, thus each vertex of $\pi$ is incident with a face in $R$. Then for all odd face necessary belong in $R$. Since for all face of $\pi$ are odd, all face belong in $R$. It contradics with perfect independent set property, then $\pi$ have not perfect independent set. □

For $K \subseteq E$ be a Kekule structure for the $m$,$n$-gonal system $\pi = (V, E, F)$. An $m$-gonal face of $\pi$ may have $0, 1, 2, 3, ..., \lfloor \frac{m}{2} \rfloor$ of its bounding edges in $K$ and an $n$-gonal face of $\pi$ may have $0, 1, 2, 3, ..., \lfloor \frac{n}{2} \rfloor$ of its bounding edges in $K$. We denote by $B_i(K)$ the set of faces that have exactly $i$ of their bounding edges in $K$. The faces in $B_0(K)$ are called the *void faces* of $K$ and (for even $n$) the faces in $B_{\lfloor \frac{n}{2} \rfloor}(K)$ of $n$-gonal face and (for even $n$) $B_{\lfloor \frac{m}{2} \rfloor}(K)$ of $m$-gonal face are called the *full faces* of $K$. We define $\beta = \beta(\pi)$, the Fries number or Kekule parameter of $\pi$, to be the maximum of the number of full faces over all Kekule structures for $\pi$. Closely related to both of the parameters $\alpha^*(\pi)$ and $\beta(\pi)$ is the Clar number [13] of the $m$,$n$-gonal system $\pi$. A set of full faces such that any two are pairwise disjoint is said to be *resonant*. The Clar number of $\pi$, $\gamma(\pi)$, is the size of the largest resonant set of full faces over all Kekule structures for $\pi$ or, equivalently, the largest independent set of full faces over all Kekule structures for $\pi$.

**Theorem 4.2.** *Let $R \subseteq F$ be a face independent set of the $m$,$n$-gonal system $\pi = (V, E, F)$, where $m$ is an odd and $n$ is even. Let $p^*(R)$ be the number of $m$-gonal faces NOT in $R$ and let $v^*(R)$ be the number of vertices NOT incident with a face in $R$. Then:*

*(i)* $|R| = \frac{2k}{n} + \frac{(m-n)M}{n} - \frac{(m-n)p^*(R)+v^*(R)}{n}$*;*

*(ii)* $\alpha^*(\pi) \leq \frac{2k}{n} + \frac{(m-n)M}{n}$ *with equality if and only if $\pi$ admits a perfect face independent set;*

*(iii) $R$ is a perfect face independent set if and only if $p^*(R) = v^*(R) = 0$.*

*Proof.* Given $M$ denote the number of $m$-gonal faces in $\pi$. Let $R$, $v^*(R)$ and $p^*(R)$ be as above and $p(R)$ denote the number of $m$-gonal faces in $R$, then $p^*(R) + p(R) = M$. Since $\pi$ is trivalent, each vertex is incident with at most 1 face in $R$. The number of vertices incident with some face in $R$ is then

$$\begin{aligned} n|R| - (n-m)p(R) &= n|R| - (n-m)(M - p^*(R)) \\ &= n|R| - (n-m)M + (n-m)p^*(R). \end{aligned}$$

So, $n|R| - (n-m)M + (n-m)p^*(R) = |V| - v^*(R)$

$n|R| - (n-m)M + (n-m)p^*(R) = 2k - v^*(R)$,

thus $n|R| = 2k - v^*(R) + (n-m)M - (n-m)p^*(R)$

giving $|R| = \frac{2k}{n} + \frac{(n-m)M}{n} - \frac{v^*(R)+(n-m)p^*(R)}{n}$.

Parts (ii) and (iii) follow at once. □

In next theorem we will prove about $\beta(\pi)$. Define $b$ is the number of edges in $K$ which are boundary of $\pi$.

**Theorem 4.3.** *Let $K \subseteq E$ be a Kekule structure for the $m$,$n$-gonal system $\pi = (V, E, F)$, where $m$,$n$ are even and $m < n$. For $i = 0, 1, 2, 3, ..., \frac{n}{2}$, let $B_i(K)$ denote the set of faces of $\pi$ that have exactly $i$ of their bounding edges in $K$. Then:*

*(i)* $mB_{\frac{m}{2}}(K) + nB_{\frac{n}{2}}(K) = 4k - 2b - 2(|B_1(K)|) + 2|B_2(K)| + ... + \left(\frac{m}{2} - 1\right)\left|B_{\left(\frac{m}{2}-1\right)}(K)\right| + ... + \left(\frac{n}{2} - 1\right)\left|B_{\frac{n}{2}-1}(K)\right|$*;*

*(ii)* $\beta(H) = B_{\frac{m}{2}}(K) + B_{\frac{n}{2}}(K)$ *and* $mB_{\frac{m}{2}}(K) + nB_{\frac{n}{2}}(K) \leq 4k - 2b$ *with equality*

*if and only if $\pi$ admits a perfect Kekule structure;*

*(iii) $K$ is a perfect Kekule structure if and only if $|B_i(K)| = 0 \ \forall i \notin \left\{\frac{m}{2}, \frac{n}{2}\right\}$.*

*Proof.* Let $b$ be the number of edges in $K$ such that be boundary of $\pi$. Adding up the number of edges of $K$ in the boundary of each face, we get $|B_1(K)| + 2|B_2(K)| + ... + \left(\frac{m}{2}\right)\left|B_{\frac{m}{2}}(K)\right| + ... + \left(\frac{n}{2}\right)\left|B_{\frac{n}{2}}(K)\right| = 2k - b$. Solving for $B_{\frac{m}{2}}(K)$ and $B_{\frac{n}{2}}(K)$ gives (i). Parts (ii) and (iii) follow at once from (i). □

**Theorem 4.4.** *Let $K \subseteq E$ be a Kekule structure for the m,n-gonal system $\pi = (V, E, F)$,where $m$ is odd and $n$ is even. For $i = 0, 1, 2, 3, ...,$ $z = max\left\{\lfloor\frac{m}{2}\rfloor, \frac{n}{2}\right\}$, let $B_i(K)$ denote the set of faces of $\pi$ that have exactly $i$ of their bounding edges in $K$. Then:*

*(i)* $$B_{\frac{n}{2}}(K) = \frac{4k-2b}{n} - \frac{2}{n}\left(|B_1(K)|\right) + 2|B_2(K)| + ... + \left(\frac{n}{2} - 1\right)\left|B_{\left(\frac{n}{2}-1\right)}(K)\right| + \left(\frac{n}{2} + 1\right)\left|B_{\left(\frac{n}{2}+1\right)}(K)\right| + ... + (z)|B_z(K)|;$$

*(ii) $\beta(H) \leq \frac{4k-2b}{n}$ with equality if and only if $\pi$ admits a perfect Kekule structure;*

*(iii) $K$ is a perfect Kekule structure if and only if $|B_i(K)| = 0 \ \forall i \neq \frac{n}{2}$.*

*Proof.* Let $b$ be the number of edges in $K$ such that be boundary of $\pi$. Adding up the number of edges of $K$ in the boundary of each face, we get $|B_1(K)| + 2|B_2(K)| + ... + (z)|B_z(K)| = 2k - b$. Solving for $B_{\frac{n}{2}}(K)$ gives (i). Parts (ii) and (iii) follow at once from (i). □

**Theorem 4.5.** *Let $K \subseteq E$ be a Kekule structure for the m,n-gonal system $\pi = (V, E, F)$. If m,n are both odd integers. Then $\pi$ does not admit a perfect Kekule structure.*

*Proof.* It is obvious that if $m$,$n$ are both odd integers then it has not full face in $\pi$. □

What can we say about the Clar number? First of all, since a resonant set is an independent set, $\gamma(\pi) \leq \alpha^*(\pi)$ [13]. Hence, we do not expect equality here. The best that we can say at this time is stated in the next theorem.

**Theorem 4.6.** *Let $C \subseteq F$ be a resonant face set of the m,n-gonal system $\pi = (V, E, F)$, where $m$ is an odd and $n$ is even. Let $p^*(C)$ be the number of m-gonal faces NOT in $C$ and let $v^*(C)$ be the number of vertices NOT incident with a face in $C$. Then:*

*(i) $|C| = \frac{2k}{n} + \frac{(m-n)M}{n} - \frac{(m-n)p^*(C)+v^*(C)}{n}$;*

*(ii) $\gamma(\pi) \leq \frac{2k}{n} + \frac{(m-n)M}{n}$.*

*Proof.* Since $C$ is an independent face set $|C| = \frac{2k}{n} + \frac{(m-n)M}{n} - \frac{(m-n)p^*(C)+v^*(C)}{n}$, giving the result. □

Next theorem, we will talk about the relationship between perfect face independent sets and perfect Kekule structure.

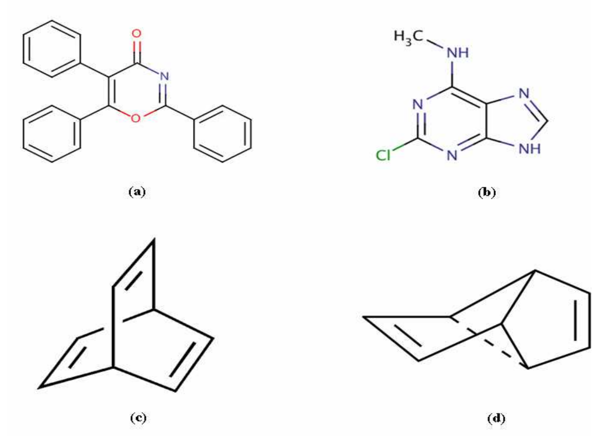


Figure 4: The structure of some chemical componds (a) 4H-1,3-Oxazin-4-one, 2,5,6-triphenyl-($C_{22}H_{15}NO_2$) (b) 2-Chloro-6(methylamino)purine($C_6H_6ClN_5$) (c) Barrelene($C_8H_8$) (d) Tricyclo[3,3,0,0$^{2,6}$]octa-3,8-diene

**Theorem 4.7.** *Let the m,n-gonal system $\pi = (V, E, F)$ be given. Then*

*(i) The collection of void faces of a Kekule structure for $\pi$ is a face independent set of $\pi$.*

*(ii) The collection of void faces of a perfect Kekule structure for $\pi$ is a perfect face independent set of $\pi$(Only in case $m$ is odd and $n$ is even).*

*Proof.* (i) Let $K$ be a Kekule structure for $\pi = (V, E, F)$ and let $F$ be a void face. Note that all of the edges that share exactly one vertex with $F$ must belong to $K$. Hence, all of the faces that share a common boundary edge with $F$ belong to $B_i(K)$ for some $i = 0, 1, 2, 3, ...,$ $\max\{\lfloor \frac{m}{2} \rfloor, \frac{n}{2}\}$ and no two void faces are adjacent.

(ii) Assume $K$ is a perfect Kekule structure and we have $m$ is odd and $n$ is even. Then $|B_i\,(K)| = 0\ \forall i \neq \frac{n}{2}$. Let $R$ be the independent collection of void faces for $K$. Since $m$-gons cannot be full, they must be void. Hence, $p^*\,(R) = 0$. Next we note that, at each vertex, we have 2 full and one void face. Hence $v^*\,(R) = 0$. By Theorem 4.2., we conclude that $R$ is a perfect face independent set. □

# 5 Comments

The authors can develop this study to another cyclic hydrocarbon's derivatives or three dimension structures in order to understand about some mathematical properties of chemical componds, which correspond to chemical properties of it. For example, see Figure 4.

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