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# On the Number of Paths, Independent Sets, and Matchings of Low Order in $(5, 6)$-Fullerene Graphs*

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**Abstract**

In graph theory, a $(r, s)$-fullerene graph is a 3-regular planar graph whose faces are $r$- or $s$-gons. Recently, Behmaram et al. (*MATCH Commun. Math. Comput. Chem.* **69** (2013) 25–32.) computed the number of paths, matchings and independent sets of low order in (4,6)-fullerene graphs. But, the general form of fullerene graph is (5,6)-fullerene graph. Thus, in this paper, we consider (5,6)-fullerene graphs and calculate the number of paths of low order. Then we apply these numbers to obtain the number of $k$-matchings and $k$-independent sets in (5,6)-fullerene graphs when $k = 2, 3, 4$. By this, we correct some previous results by Behmaram et al. (*Appl. Math. Lett.* **25** (2012) 1721–1724.)

## 1 Introduction

The graphs considered in this paper are finite, loopless and contain no multiple edges. Given a graph $G$, let $V(G)$ and $E(G)$ be the vertex and edge sets of $G$, respectively. As usual, $n$-path denotes the path with $n$ vertices. A subset $M$ of $E$ is called a matching in

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$G$ if it is a set of edges with no shared endpoints. The two endpoints of an edge in $M$ are said to be matched under $M$. (See [3, 6, 9, 10] for details) A $k$-matching is a matching with $k$ edges. We denote $M(G, k)$ the number of $k$-matchings in $G$. It is easy to see that $M(G, 1)$ is equal to the number of edges in $G$. Given a graph $G$, a subset $S$ of $V$ is called an independent set of $G$ if no two vertices of $S$ are adjacent in $G$. The size of independent set is the number of vertices it contains. A $k$-independent set is an independent set of size $k$. The number of $k$-independent sets in $G$ is denoted by $Ind_k(G)$.

A fullerene is any molecule composed entirely of carbon, in the form of a hollow sphere, ellipsoid or tube. The first fullerene was discovered in 1985 by Kroto et al. [19, 20]. The discovery of fullerenes greatly expanded the number of known carbon allotropes, which until recently were limited to graphite, diamond, and amorphous carbon such as soot and charcoal. For the past decade, the chemical and physical properties of fullerenes have been a hot topic in the field of research and development, and are likely to continue to be for a long time.

In graph theory, a $(r, s)$-fullerene graph is a 3-regular planar graph whose faces are $r$- or $s$-gons. From the very beginning, fullerene graphs have been attracting attention of graph theory researchers. A number of graph-theoretical invariants and some structure properties of fullerene graphs were studied [1, 7, 12, 13, 21, 22]. Recently, Behmaram et al. [5] discussed (4,6)-fullerene graphs and computed the number of paths of low order and used these numbers to obtain the number of $k$-matchings and $k$-independent sets when $k = 2, 3, 4$. But, (5,6)-fullerene graphs are more typical in chemistry. In Figure 1, a (5,6)-fullerene graph with 28 carbon atoms is depicted. So, in this paper, we take (5,6)-fullerene graphs in consideration and calculate the number of paths of low order in a fullerene graph. Then we apply these numbers to obtain the number of $k$-matchings and $k$-independent sets when $k = 2, 3, 4$.

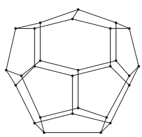


Figure 1: A (5,6)-fullerene with 28 carbon atoms.

Let $F$ be a (5,6)-fullerene graph and $p$, $h$, $n$ and $m$ be the number of pentagons, hexagons, carbon atoms and bonds between them, respectively. We can easily have $3n = 2m$ by using the Handshaking Theorem. Since the number of edges is $m = \frac{(5p+6h)}{2} = \frac{3n}{2}$ and the number of faces is $f = p + h$, we can deduce that $\frac{5p+6h}{3} - \frac{5p+6h}{2} + p + h = 2$ from the Euler's formula. Therefore $p = 12$, $n = 2h + 20$, $m = 3h + 30$. This implies that such molecules made up entirely of $n$ carbon atoms and having 12 pentagons and $\frac{n}{2} - 10$ hexagonal faces [2].

More background material as well as basic computational techniques for matchings and independent sets in a graph can be consulted in [8, 11, 14–17].

## 2 Main Results

Suppose $G$ is a graph. Define $P_k(G)$ and $M(G, k)$ to be the number of $k$-paths and $k$-matchings of $G$, respectively. In this section, exact formulas for the number of $k$-paths ($k \leq 10$), $k$-matchings and $k$-independent sets ($k = 2, 3, 4$), in a (5,6)-fullerene graph are presented by the following theorems.

**Theorem 2.1.** *If $F$ is a (5,6)-fullerene graph with $h$ hexagons, then*

**i)** $P_k(F) = 2^{k-2}(3h + 30), k = 2, 3, 4, 5;$

**ii)** $P_6(F) = 48h + 420;$

**iii)** $P_7(F) = 90h + 840;$

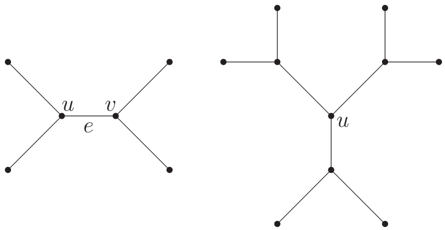
**iv)** $P_8(F) = 180h + 1800;$

**v)** $P_9(F) = 372h + 3720;$

**vi)** $P_{10}(F) = 756h + 7560.$

**Proof.** (i) Since every edge is a 2-path, $P_2(F) = m$ and the number of 3-paths is $P_3(F) = 3n = 2m$ because a fullerene graph is a cubic graph. To count the number of 4-paths, we choose an edge $e = uv$ in $F$. To construct a 4-path in $F$, we have to choose two edges of $F$ such that each of them is incident to exactly one endpoint of $e$, see Figure

2(a). Therefore, we have $P_4(F) = 4m$. To compute the number of 5-paths, we consider a vertex $u$ of $F$. For constructing a 5-path with $u$ as its midpoint, we have twelve choices, see Figure 2(b). Thus $P_5(F) = 12n = 8m$. For $m = 3h + 30$, we have proved (i).




(a) b

Figure 2

(ii) When calculating $P_6(F)$, we first choose an edge $e = uv$ and construct a 6-path with $e$ as its middle edge. To do this, we have four choices to pick a 3-path starting at $u$ and four for $v$, see Figure 3. But there are $5 \times 12 = 60$ cases that we find a pentagon. Thus $P_6(F) = 16m - 60 = 48h + 420$.

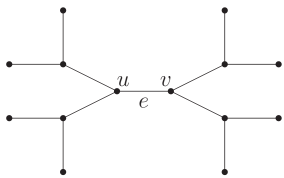



Figure 3

(iii) To calculate $P_7(F)$, we choose a vertex $v$ and then construct a 7-path with $v$ as its midpoint. In a similar way as computing $P_5(F)$, there are 48 ways since there are three edges incident to $v$ and others have exactly two ways to choose. By subtracting the cases that six edges give a pentagon with a hanging edge or a hexagon, we have $P_7(F) = 48n - 6h - 120 = 90h + 840$.

(iv) In this case we apply a similar method as ii. We choose an edge $e = uv$ and count the number of 4-paths start at $u$ and $v$. Then we have to omit the cases where we find one of following subgraphs:

- A subgraph $H_1$ isomorphic to hexagon $T$ with a pendant edge.

- A subgraph $H_2$ constructed from a pentagon and a 3-path by unifying a pendant vertex of the 3-path and a vertex of the pentagon.

By a similar argument as iii, $P_8(F) = 64m - 12h - 120 = 180h + 1800$.

(v) To compute $P_9(F)$, we use a similar method as iii. We choose a vertex $u$ and then paste two 5-paths to $v$. There are $192n$ ways to choose these two paths. By subtracting the cases that eight edges give a subgraph constructed from a pentagon and a 4-path by unifying a pendant vertex of the 4-path with a vertex of the pentagon or a subgraph constructed from a hexagon and a 3-path by unifying a pendant vertex of the 3-path with a vertex of the hexagon, we have $P_9(F) = 192n - 12h - 120 = 372h + 3720$.

(vi) We apply a similar method to that in ii to calculate $P_{10}(F)$. We choose an edge $e = uv$ and count the number of 5-paths starting at $u$ and $v$. Then we have to subtract the cases that we find one of following subgraphs:

- A subgraph $H_1$ constructed from a pentagon and a 5-path by unifying a pendant vertex of the 5-path and a vertex of the pentagon.

- A subgraph $H_2$ constructed from a hexagon and a 4-path by unifying a pendant vertex of the 4-path and a vertex of the pentagon.

Similarly, we have $P_{10}(F) = 256m - 12h - 120 = 756h + 7560$. $\square$

We now apply Theorem 2.1 to count the number of $k$-matchings and $k$-independent sets in a (5,6)-fullerene graph.

**Theorem 2.2.** *Suppose $F$ is a (5,6)-fullerene graph with $h$ hexagons, then*

**i)** $M(F,2) = \frac{9}{2}h^2 + \frac{165}{2}h + 375$;

**ii)** $M(F,3) = \frac{9}{2}h^3 + \frac{225}{2}h^2 + 929h + 2540$;

**iii)** $M(F,4) = \frac{27}{8}h^4 + \frac{405}{4}h^3 + \frac{9021}{8}h^2 + \frac{22167}{4}h + 10155$.

**Proof.** (i) Since for every two edges $e$ and $f$ in graph $G$, either $e$ and $f$ have a common vertex or they constitute a 2-matching, $M(F,2) + P_3(F) = \binom{3h+30}{2}$. By Theorem 2.1(i), $P_3(F) = 2m$, we get $M(F,2) = \frac{9}{2}h^2 + \frac{165}{2}h + 375$.

(ii) We use an argument similar to those given in [18] to calculate $M(F,3)$. It is obtained from the number of all 3-subsets subtracting the number of the 3-subsets which are not 3-matchings. There are three cases that a 3-subset does not represent a 3-matching:

**(1)** A 4-path whose number is $4m$ by Theorem 2.1;

**(2)** A 3-path and an isolated edge and the number $P_3(F)(m-7)$;

**(3)** A star graph with 3 edges and notice that every star graph can be obtained by three 3-paths, thus the number is $\frac{1}{3}P_3(F)$.

Therefore, we have

$$\begin{aligned} M(F,3) &= \binom{m}{3} - P_4(F) - P_3(F)(m-7) - \frac{1}{3}P_3(F) \\ &= \binom{m}{3} - 4m - 2m(m-7) - \frac{2}{3}m \\ &= \frac{9}{2}h^3 + \frac{225}{2}h^2 + 929h + 2540. \end{aligned}$$

(iii) To calculate $M(F,4)$, we count the number of 4-subsets in $F$ minus the number of those 4-subsets which are not 4-matchings. The cases where 4-subsets do not represent 4-matchings are shown in Figure 4.

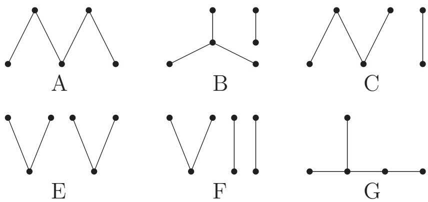



Figure 4. The possible 4-subsets of edges which are not 4-matchings.

Let $N(A), N(B), N(C), N(E), N(F)$ and $N(G)$ are the number of subgraphs which are isomorphic to those are depicted in Figure 4. Then we have:

- $N(A)$: By Theorem 2.1(i), $N(A) = P_5(F) = 24h + 240$.

- $N(B)$: Choose a vertex $v$, three edges incident to $v$ and an edge $e$ which do not have common neighbor. Then we have,

$$N(B) = n(m-9) = 6h^2 + 102h + 420.$$

- $N(C)$: For computing $N(C)$, we choose a 4-path and an edge which is disjoint from this 4-path. Then,

$$N(C) = P_4(F) \times (m-9) = 36h^2 + 612h + 2520.$$

- $N(E)$: To calculate $N(E)$, we have to choose two 3-paths which have no common neighbors. Then we have:

$$N(E) = \frac{1}{2} \times 3n \times [5 + 3(n-8)] = 18h^2 + 303h + 1230.$$

- $N(F)$: We have to choose a 3-path and then pick a 2-matching which do not have common neighbors. Then,

$$N(F) = P_3(F) \times \left\{ \binom{m-7}{2} - [5 + 3(n-8)] \right\} = 27h^3 + 639h^2 + 4962h + 12720.$$

- $N(G)$: In this case, we must count the number of subgraphs of $F$ constructed from a 4-path $T$ and a vertex adjacent to a vertex of degree 2 in $T$. By Theorem 2.1, the number of 4-path is $P_4(F)$ and there are two choices for the added vertex. Therefore,

$$N(G) = \frac{1}{2} \times P_4(F) \times 2 = 12h + 120.$$

Therefore,

$$\begin{aligned} M(F,4) &= \binom{3h+30}{4} - N(A) - N(B) - N(C) - N(E) - N(F) - N(G) \\ &= \frac{27}{8}h^4 + \frac{405}{4}h^3 + \frac{9021}{8}h^2 + \frac{22167}{4}h + 10155, \end{aligned}$$

which completes the proof. □

**Theorem 2.3.** *Suppose $F$ is a (5,6)-fullerene graph with $h$ hexagons, then*

**i)** $Ind_2(F) = 2h^2 + 36h + 160,$

**ii)** $Ind_3(F) = \frac{4}{3}h^3 + 32h^2 + \frac{758}{3}h + 660,$

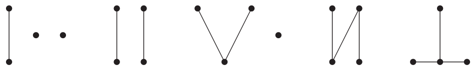
**iii)** $Ind_4(F) = \frac{2}{3}h^4 + \frac{56}{3}h^3 + \frac{580}{3}h^2 + \frac{2689}{3}h + 1630.$

**Proof.** (i) We choose two vertices which are not adjacent. Thus, $Ind_2(F) = \frac{1}{2}n(n-4) = 2h^2 + 36h + 160$.

(ii) This is obtained from the number of all triples of vertices by subtracting the number of those triples that do not represent 3-independent sets. We consider two types of vertices that are not independent. One type is constructed from an edge $f$ and a vertex which is not incident to $f$; the other type is constructed from a 3-path. Clearly, the number of the first type is $m(n-6)$ and the other is $P_3(F)$. Therefore,

$$Ind_3(F) = \binom{n}{3} - m(n-6) - P_3(F) = \frac{4}{3}h^3 + 32h^2 + \frac{758}{3}h + 660.$$

(iii) To count the number of 4-independent sets, we have to count the number of all 4-subsets of vertices and then subtract the number of those 4-subsets that do not represent 4-independent sets. There are exactly five different types of sets of four vertices that are not 4-independent sets, see Figure 5.



(1) (2) (3) (4) (5)

Figure 5. The possible 4-subsets of vertices which are not 4-independent sets.

The first type is 4-subset of vertices constructed from an edge and two components that each of them is a vertex; the second is a 2-matching; the third is a 3-path with a vertex outside the path; the forth is a 4-path and the last one is a 3-star. Notice that, for calculating the number of the first and the second type, we can count the cases that an edge is picked and an edge with two vertices which are not incident to the picked edge is chosen, then add the number of 2-matchings since it is counted twice. Therefore,

$$\begin{aligned} Ind_4(F) &= \binom{n}{4} - \frac{1}{2}m(n-6)(n-7) + M(F,2) - P_3(F)(n-8) - P_4(F) - n \\ &= \frac{2}{3}h^4 + \frac{56}{3}h^3 + \frac{580}{3}h^2 + \frac{2689}{3}h + 1630. \end{aligned}$$

□

**Acknowledgement.** We thank the referees for their helpful comments and suggestions and for pointing out the reference [13].

**Remark.** Recently, Behmaram et al. [4] obtained results almost identical to ours. We didn't know the work done by Behmaram et al. until Professor Gutman mentioned this. In their paper, the numbers $M(F,3)$, $M(F,4)$ and $Ind_4(F)$ are different from ours. We have examined their paper. For the three inconsistent parts, we found that their results were incorrect. More details are in the following:

For computing $M(F,3)$, in the proof of the second formula in Corollary 1, the formula $M(F,3) = \binom{m}{3} - (m-2)P_3(F) + P_4(F) + 2n$ is correct. But the calculated result $\frac{9}{2}h^3 + \frac{225}{2}h^2 + 937h + 2620$ is wrong. By computing this, we have $M(F,3) = \frac{9}{2}h^3 + \frac{225}{2}h^2 + 929h + 2540$ which is as same as ours.

For computing $M(F,4)$, they discussed six cases and calculated the number of these cases which are $N(A)$, $N(B)$, $N(C)$, $N(E)$, $N(F)$ and $N(G)$. When they computed $N(C)$, they did the wrong calculation that $12(h+10)(m-9)$ is $36(h+10)(h+7)$ not $36(h+10)(h-7)$. And $12(h+10)(m-9)$ is $36h^2 + 612h + 2520$ which is as same as ours.

When they calculated $N(E)$, they first chose a 3-path and then picked another 3-path in the remained vertices. Thus they had $9n(n-3)/2$. But when choosing the second 3-path, they may choose a 3-path whose vertices are adjacent to the vertices of the first 3-path. They didn't consider this case. And for computing $N(F)$, they made the same mistake.

For computing $N(G)$, the formula $N(G) = 2P_4(F)$ is wrong. Suppose that $G$ is constructed from a 4-path $abcd$ and a vertex $e$ which is adjacent to $b$. Then $G$ is also constructed from a 4-path $ebcd$ and the vertex $a$ which is adjacent to $b$. Thus each subgraph $G$ is counted twice. So, $N(G) = \frac{1}{2}P_4(F) \times 2 = P_4(F)$.

To sum up, their formula for computing $M(F,4)$ is incorrect.

For computing $Ind_4(F)$, they didn't discussed in details. But from their formula, we can see that they counted the number of 4-subsets of vertices and then subtracted the number of those 4-subsets that do not represent a 4-independent set. According to their method, the 4-paths and 3-stars should be counted thrice, not twice. And a 2-matching is counted twice, a 3-path with a vertex outside the path is counted twice, the two cases were not considered by them. Therefore, their formula is wrong.

Moreover, $\binom{2h+20}{4} - (3h+30)\binom{2h+18}{2} + \binom{3h+30}{2} + 12h^2 + 22h + 1160 \neq \frac{2}{3}h^4 + \frac{74}{3}h^3 + \frac{1075}{3}h^2 - \frac{2675}{3}h - 24610$. Further, if $h$ is a small positive integer, then $\frac{2}{3}h^4 + \frac{74}{3}h^3 + \frac{1075}{3}h^2 - \frac{2675}{3}h - 24610$ is negative.

By correcting their mistakes, we can have the consequence just as the same as ours.

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