On the number of 5-matchings in boron-nitrogen fullerene graphs *

Yuchao Li, Junfeng Du, Jianhua Tu[†]
School of Science
Beijing University of Chemical Technology, Beijing 100029, China
E-mail: yuchaovivian@sina.cn; djfdjf1990@163.com; tujh81@163.com

Abstract

Given a graph $G = (V, E)$, a matching M of G is a subset of E, such that every vertex of V is incident to at most one edge of M. A k-matching is a matching with k edges. The total number of matchings in G is used in chemoinformatics as a structural descriptor of a molecular graph. Recently, Vesalian and Asgari (MATCH Commun. Math. Comput. Chem. 69 (2013) 33–46.) gave a formula for the number of 5-matchings in triangular-free and 4-cycle-free graphs based on the degrees of vertices and the number of vertices, edges and 5-cycles. But, many chemical graphs are not triangular-free or 4-cycle-free, e.g. boron-nitrogen fullerene graphs (or BN-fullerene graphs). In this paper, we take BN-fullerene graphs in consideration and obtain the formulas for the number of 5-matchings based on the number of hexagons.

Keywords: 5-matching, Boron-nitrogen fullerene, Number of k-matchings

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, k-path denotes the path with k vertices. The number of k-paths in G is denoted by $P_k(G)$. A subset S of V is called an independent set of G if no two vertices of S are adjacent in

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[†]Corresponding author.

G. A k-independent set is an independent set which contains k vertices. The number of k-independent sets in G is denoted by $Ind_k(G)$.

A matching M of a graph $G = (V, E)$ is a subset of E, such that every vertex of V is incident to at most one edge of M. The two endpoints of an edge in M are said to be matched under M. 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. (See [3] for details)

The number of k-matching is closely linked to the coefficients of some graph polynomials, such as the matching polynomial [7], the characteristic polynomial [10], etc. And the total number of matchings in G, the Hosoya index of a graph G, is used in chemoinformatics as a structural descriptor of a molecular graph. Thus many formulas for $M(G, k)$ are given. Constantine et al. [5] gave a formula for $M(G, 3)$ based on the degrees of vertices and the number of vertices, edges and triangles. Behmaram [1] also has calculated $M(G, 4)$ in triangular-free graphs. Klabjan and Mohar [10] calculated $M(G, k)$, $k \leq 5$, in hexagonal systems. Recently, Vesalian and Asgari [13] have given a formula for $M(G, 5)$ in triangular-free and 4-cycle-free graphs based on the degrees of vertices and the number of vertices, edges and 5-cycles. But, many chemical graphs are not triangular-free and 4-cycle-free, e.g. boron-nitrogen fullerene graphs (or BN-fullerene graphs). In this paper, we take BN-fullerene graphs in consideration and obtain explicit formulas for $M(G, 5)$ in them based on the number of hexagons.

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. [11, 12]. 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 this paper we consider boron-nitrogen fullerene graphs, the molecular graphs of boron-nitrogen fullerenes. In fact, a boron-nitrogen fullerene graph (in short BN-fullerene) is a 3-connected cubic planar graph, all of whose faces are squares and hexagons. In Figure 1, a BN-fullerene graph with 24 carbon atoms is depicted. From the very beginning, BN-fullerene graphs have been attracting attention of graph theory researchers. A number of graph-theoretical invariants and some structure properties of BN-fullerene graphs were studied [4, 6, 8, 9]. Recently, Behmaram et al. [2] discussed BN-fullerene graphs and calculated the number of paths of low order and the number of k-matchings and k-independent sets when $k = 2, 3, 4$. In this paper, we will calculate the number of k-matchings when $k = 5$ in BN-fullerene graphs.

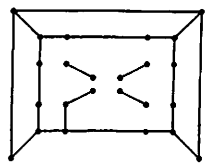

Figure 1: A BN-fullerene with 24 atoms.

2 Preliminaries

As a BN-fullerene graph is a cubic planar graph, all of whose faces are squares and hexagons, by Euler's formula we have:

Lemma 2.1 ([2]). *If F is a BN-fullerene graph, s, h, n and m be the number of squares, hexagons, vertices and edges respectively, then $s = 6$, $n = 2h + 8$ and $m = 3h + 12$.*

Some exact formulas for the number of k-paths, k-matchings and k-independent sets ($k = 2, 3, 4$) in a BN-fullerene graph are presented by the following theorems. These formulas will be used in next section.

Lemma 2.2 ([2]). *If F is a BN-fullerene graph with h hexagons, then*

(i) $P_k(F) = 2^{k-2}(3h + 12), k = 3, 4;$

(ii) $P_5(F) = 24h + 72;$

(iii) $P_6(F) = 48h + 144;$

(iv) $M(F, 3) = \frac{9}{2}h^3 + \frac{63}{2}h^2 + 65h + 44;$

(v) $Ind_3(F) = \frac{4}{3}h^3 + 8h^2 + \frac{38}{3}h + 8.$

Remark. The expressions (iv) and (v) cited in the above lemma are not consistent with the original paper [2]. Behmaram et al. [2] obtained $M(F, 3)$ by using formula $C_m^3 - (m - 2)P_3(F) + P_4(F) + 2n$. This formula is correct, but the calculated result $\frac{9}{2}h^3 + \frac{189}{6}h^2 - 65h + 44$ is incorrect. The correct calculation result is $M(F, 3) = \frac{9}{2}h^3 + \frac{63}{2}h^2 + 65h + 44$.

We have also found that the formula of $Ind_3(F)$ given by Behmaram et al. [2] is incorrect. More details are described below:

The formula of $Ind_3(F)$ can be obtained by subtracting the number of those triples that do not represent 3-independent sets from the number of all triples of vertices. There are two types of induced subgraphs corresponding to those triples that do not represent 3-independent sets. The first type is an edge with a vertex non-incident to the edge and the second is a 3-path. They claimed that the number of the first type of induced subgraphs is $m(n-2)$. This is incorrect. In fact, the number of the first type of induced subgraphs should be $m(n-6)$. Also, they used the wrong number of n which is $2h+8$, not $2h+20$. Thus, the correct formula should be

$$Ind_3(F) = C_n^3 - m(n-6) - P_3(F) = \frac{4}{3}h^3 + 8h^2 + \frac{38}{3}h + 8.$$

3 Main Results

Now, we calculate the number of 5-matchings in BN-fullerene graphs.

Theorem 3.1. *If F is a (4, 6)-fullerene graph with h ($h \geq 2$) hexagons, then*

$$M(F,5) = \frac{81}{40}h^5 + \frac{27}{4}h^4 + \frac{423}{8}h^3 + \frac{579}{4}h^2 - \frac{1722}{5}h - 444.$$

Proof. To calculate $M(F,5)$, we count the number of 5-subsets in F minus the number of those 5-subsets which are not 5-matchings. The cases where 5-subsets do not represent 5-matchings are shown in Figure 2.

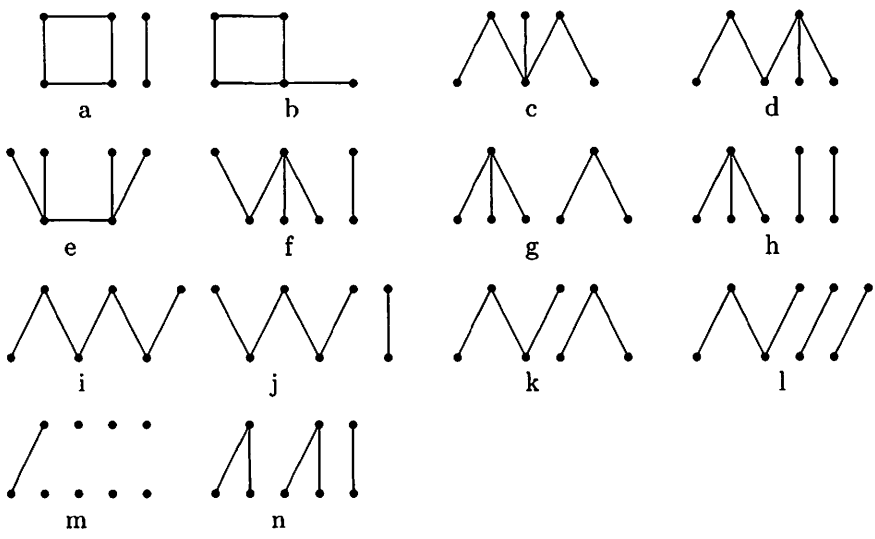

Figure 2. The possible 5-subsets of edges which are not 5-matchings.

Let $N(a)$, $N(b)$, $N(c)$, $N(d)$, $N(e)$, $N(f)$, $N(g)$, $N(h)$, $N(i)$, $N(j)$, $N(k)$, $N(l)$, $N(m)$, $N(n)$ denote the number of subgraphs which are isomorphic to those depicted in Figure 2. Then we calculate as follows:

First, we compute $N(a)$:

$N(a)$: Choose a 4-cycle and an edge which does not have a common neighbor. Thus, we have:

$$N(a) = 6 \times (m - 8) = 18h + 24.$$

Second, we focus on the subgraphs which have at least one vertex of degree 3. These subgraphs are isomorphic to graph (b), (c), (d), (e), (f), (g), (h). To calculate the sum of the numbers of these subgraphs, we choose a vertex and pick all the three edges incident to it. Then we choose two more edges in the remaining edges. But notice that, $N(e)$ is counted twice and $N(e)$ is equal to the number of edges. Thus, we have:

$$N(b) + N(c) + N(d) + N(e) + N(f) + N(g) + N(h)$$

$$= n \times C_{m-3}^{2} - m = 9h^3 + 87h^2 + 273h + 276.$$

In addition, we calculate $N(b)$, $N(c)$ and $N(g)$ for the following calculations.

$N(b)$: Choose a 4-cycle with a pendant edge, then:

$$N(b) = 6 \times 4 = 24.$$

$N(c)$: For computing $N(c)$, we first pick a vertex. Then choose two of its neighbors and for each of them, we pick one more edge from it. But notice that, we may get a subgraph which is isomorphic to graph (b). Therefore,

$$N(c) = n \times C_3^2 \times C_2^1 \times C_2^1 - 6 \times 4 = 24h + 72.$$

$N(g)$: For calculating $N(g)$, we first choose 3-path. Then choose a star with three edges. But when we choose the 3-path, we should consider if it is contained in a square. Then,

$$N(g) = 6 \times 4 \times (n - 7) + h \times 6 \times (n - 8) = 12h^2 + 48h + 24.$$

Then, we calculate the number of the subgraphs which contain no vertices of degree 3.

$N(i)$: By using Lemma 2.2, we have:

$$N(i) = P_6(F) = 48h + 144.$$

$N(j)$: We choose a 5-path and then choose an edge which has no common vertex with it. But when we choose the 5-path, we should consider if three edges of the 5-path are contained in a square. Thus, by using Lemma 2.2, we have:

$$N(j) = 6 \times 4 \times 2 \times (m-10) + (P_5(F) - 6 \times 4 \times 2) \times (m-11)$$
$$= 72h^2 + 240h + 120.$$

To calculate $N(k)$ and $N(l)$, we first consider their sum. We choose a 4-path and two edges that have no common vertices with the path. Like computing $N(j)$, we also consider two circumstances. Then, by using Lemma 2.2, we have:

$$N(k) + N(l) = 6 \times 4 \times C_{m-8}^2 + (P_4(F) - 6 \times 4) \times C_{m-9}^2$$
$$= 54h^3 + 306h^2 + 468h + 216.$$

Now, we calculate $N(k)$ and $N(l)$.

$N(l)$: We choose a 3-matching and pick one of the edges. Then choose one edge from the two vertices of the chosen edge. Notice that, we may have subgraphs isomorphic to graph (a), graph (i) or graph (j). Since graph a is counted forth and graph (j) twice, by using Lemma 2.2, we have:

$$N(l) = M(F,3) \times C_3^2 \times C_2^1 \times C_2^1 - 4N(a) - N(i) - 2N(j)$$
$$= 54h^3 + 234h^2 + 180h + 48.$$

$N(k)$: By doing subtraction, we have:

$$N(k) = 72h^2 + 288h + 168.$$

At last, we compute the sum of $N(m)$ and $N(n)$. We choose a 3-path and pick three edges in the remaining edges which have no common vertex with the path. Notice that, we may have subgraphs isomorphic to graph(n), graph(g) and graph (k). We calculate $N(n)$ firstly.

$N(n)$: We choose a 3-independent sets and pick two of them. For these two picked vertices, we choose two edges from each of them independently. For the third vertex, we choose an edge from it. Notice that, we may have subgraphs isomorphic to graph (a), (b), (c), (i), (j) and (k). Since graph (a) is counted forth, graph (i), (j), (k) are all counted twice, by using Lemma 2.2, we have:

$$N(n) = Ind_3(F)C_3^2C_3^2C_3^2C_3^1 - 4N(a) - N(b) - N(c) - 2N(i) - 2N(j) - 2N(k)$$
$$108h^3 + 360h^2 - 222h - 408.$$

Then,by using Lemma 2.2, we have:

$$N(m) + N(n) = P_3(F) \times C^3_{m-7} - N(n) - N(k) - N(g)$$
$$= 27h^4 + 108h^3 + 129h^2 + 510h + 456.$$

Therefore,

$$M(F,5) = \binom{m}{5} - N(a) - N(b) - N(c) - N(d) - N(e) - N(f) - N(g)$$
$$-N(h) - N(i) - N(j) - N(k) - N(l) - N(m) - N(n)$$
$$= \frac{81}{40}h^5 + \frac{135}{4}h^4 + \frac{1791}{8}h^3 + \frac{2955}{4}h^2 + \frac{6063}{5}h + 792$$
$$-(27h^4 + 171h^3 + 594h^2 + 1557h + 1236)$$
$$= \frac{81}{40}h^5 + \frac{27}{4}h^4 + \frac{423}{8}h^3 + \frac{579}{4}h^2 - \frac{1722}{5}h - 444,$$

which completes the proof. □

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