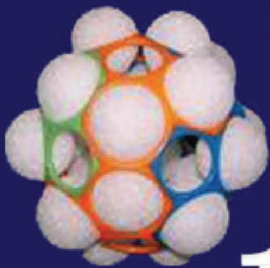

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Stirling Numbers and Generalized Zagreb Indices

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ABSTRACT

We show how generalized Zagreb indices $M_1^k(G)$ can be computed by using a simple graph polynomial and Stirling numbers of the second kind. In that way we explain and clarify the meaning of a triangle of numbers used to establish the same result in an earlier reference.

1. INTRODUCTION AND PRELIMINARIES

The Zagreb indices belong to the oldest and the best researched topological indices.Since their introduction in early seventies [7] they have also given rise to numerous generalizations. (For a survey, see [6].) In this note we show how the information about one of the generalizations, the first general Zagreb index, introduced by Li and Zheng in 2005 [8], can be extracted from a simple, yet neglected, graph polynomial. To the best of our knowledge, the polynomial was introduced and studied in 2008 by two of the present authors and a third one [9], and received no attention afterwards. Crucial to our approach is a family of combinatorial numbers known as the Stirling numbers of the second kind.

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1.1. DEGREE SEQUENCE POLYNOMIAL OF A GRAPH

Let G be a simple connected graph with the degree sequence $\delta = d_1 \le \cdots \le d_m = \Delta$. Its degree sequence polynomial $S_G(x)$ is defined as the generating polynomial of its degree sequence, i.e., as

$$S_G(x) = \sum_{u \in V(G)} x^{d_u} = \sum_{j=\delta}^{\Delta} a_j x^j,$$

where a_j denotes the number of vertices of degree j. The evaluations of the polynomial and its first derivative at 1 give, respectively, the number of vertices and twice the number of edges of G. Hence, $S_G(1) = |V(G)|$ and $S_G'(1) = 2|E(G)|$. Given its simplicity, and proliferation of other graph polynomials, it is surprising that this polynomial attracted no attention of researchers so far. In the following we show that the degree sequence polynomial encodes far more information on G. In order to extract it, we need a family of combinatorial numbers known as Stirling numbers of the second kind.

1.2. STIRLING NUMBERS

The Stirling numbers of the second kind, denoted by $\left\{ n \atop k \right\}$, count the number of partitions of a set of n elements into k non-empty subsets. They form a triangular array whose few beginning rows are shown in Table 1. It can be shown that they satifay a linear recurrence,

$$\left\{ n \atop k \right\} = \left\{ n-1 \atop k \right\} + \left\{ n-1 \atop k-1 \right\}$$

for $n > 0$ with the initial conditions $\left\{ 0 \atop 0 \right\} = 1$ and $\left\{ 0 \atop j \right\} = \left\{ 0 \atop i \right\} = 0$ for all $i, j \neq 0$. We refer the reader to [5] for a thorough discussion of these numbers and their properties. The most important for us is the fact that the Stirling numbers of the second kind are used to convert between powers and falling factorials,

$$x^n = \sum_k \left\{ n \atop k \right\} x^{\underline{k}},$$

where $x^{\underline{k}}$ is the falling factorial defined as $x^{\underline{k}} = x(x-1)\ldots(x-k+1)$. The opposite relationship,

$$x^{\underline{n}} = \sum_k \left[n \atop k \right] (-1)^{n-k} x^k,$$

involves the Stirling numbers of the first kind $\left[\begin{matrix} n \\ k \end{matrix}\right]$ that count the ways to arrange n objects into cycles. In the rest of the paper we will make use of both conversion formulas.

Table 1. Stirling numbers of the second kind $\left\{\begin{matrix} n \\ k \end{matrix}\right\}$.

n/k	0	1	2	3	4	5	6
0	1						
1	0	1					
2	0	1	1				
3	0	1	3	1			
4	0	1	7	6	1		
5	0	1	15	25	10	1	
6	0	1	31	90	65	15	1

1.3. GENERALIZED ZAGREB INDICES

Recall that the first and the second Zagreb indices are defined as

$$M_1(G) = \sum\nolimits_{u\in V(G)} d_u^2 \qquad and \qquad M_2(G) = \sum\nolimits_{uv\in E(G)} d_u d_v,$$

respectively, where d_u denotes the degree of vertex u. The k-th general first Zagreb index $M_1^k(G)$ is defined [8] as the sum of k-th powers of degrees of vertices of G, $M_1^k(G) = \sum\nolimits_{u\in V(G)} d_u^k$. Hence, $M_1^1(G) = 2|E(G)|$ and $M_1^2(G) = M_1(G)$. For $k = 3$ one obtains the forgotten index $F(G)$ [4]. Our main result shows that all information about $M_1^k(G)$ for all k is encoded in the degree sequence polynomial of G.

2. MAIN RESULTS

Theorem 1. Let G be a simple connected graph and $S_G(x)$ its degree sequence polynomial. Then the k–th general Zagreb index of G can be computed as

$$M_1^k(G) = \sum_{j=1}^{k} \left\{\begin{matrix} k \\ j \end{matrix}\right\} S_G^{(j)}(1)$$

for any $k \in \mathbb{N}$.

Proof.

$$M_1^k(G) = \sum_{u\in V(G)} d_u^k = \sum_{u\in V(G)} \sum_j \left\{ {k \atop j} \right\} d_u^{\underline{j}} = \sum_j \left\{ {k \atop j} \right\} \sum_{u\in V(G)} d_u^{\underline{j}} = \sum_j \left\{ {k \atop j} \right\} S_G^{(j)}(1).$$

Corollary 2.

$$S_G^{(k)}(1) = \sum \left[{k \atop j} \right] (-1)^{k-j} M_1^j(G).$$

As an example, we look at the case of tetrameric 1,3–adamantane, considered by Fath–Tabar *et al.* in reference [3]. It is clear by inspection that a chain $TA[n]$ of n such units has $6n$ vertices of degree 2, $2n+2$ vertices of degree 3 and $2n-2$ vertices of degree 4. Hence, its degree sequence polynomial is given by $S_{TA[n]} = 6nx^2 + 2(n+1)x^3 + 2(n-1)x^4$. From there, by using Theorem 1, we immediately obtain $M_1^2(TA[n]) = M_1(TA[n]) = 74n-14$ (as obtained in [3]), $M_1^3(TA[n]) = 230n-74$ and $M_1^4(TA[n]) = 770n-350$.

3. CONCLUDING REMARKS

The same approach we used here could be applied to other topological indices and polynomials. For example, there are variants of eccentricity polynomials that encode the information about sums of powers of vertex eccentricities [2].

A comparable approach to degree–based topological indices was employed by Deutsch and Klavžar [1]. Their M–polynomial is a bivariate generating polynomial encoding the information about the number of edges whose end–vertices have certain degrees. It allows quick finding of any degree–based graph invariant, but it takes more work to compute the polynomial than in the case of degree sequence polynomial.

We conclude by mentioning that our results were anticipated in some earlier papers, but the relationship was never made explicit. For example, in Theorem 3.1 of reference [10] concerned with general Zagreb indices, $M_1^k(G)$ are given as sums of the numbers of (not necessarily induced) star subgraphs of G multiplied by certain coefficients. The coefficients form a triangular array $t_{n,k}$ and it can be easily guessed that $t_{n,k} = k!\left\{ {n \atop k} \right\}$. Our results provide an elegant proof. Similar observation can be made about the triangle of coefficients in Corollary 3.1 of the same reference.

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Relationship between Coefficients of Characteristic Polynomial and Matching Polynomial of Regular Graphs and its Applications

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ABSTRACT

Suppose G is a graph, $A(G)$ its adjacency matrix and $\psi(G,\lambda) = \lambda^n + a_1\lambda_{n-1} + \ldots + a_n$ is the characteristic polynomial of G. The matching polynomial of G is defined as $M(G,x) = m(G,0)x^n - m(G,1)x^{n-2} - m(G,2)x^{n-4} + \ldots$, where $m(G,k)$ is the number of k−matchings in G. In this paper, the relationship between 2k-th coefficient of the characteristic polynomial, a_{2k}, and k-th coefficient of the matching polynomial, $(-1)^k m(G, k)$, $k=0,1,2,\ldots$, in a regular graph is determined. In addition, these relations for finding 5,6-matchings of fullerene graphs are applied.

1. INTRODUCTION

Suppose G is a simple graph with n vertices and m edges, and $A(G)$ is the adjacency matrix of G. The characteristic polynomial of G, denoted by $\psi(G,\lambda)$, is defined as:

$$\psi(G,\lambda) = \det(\lambda I_n - A(G)) = \lambda^n + a_1\lambda^{n-1} + \ldots + a_{n-1}\lambda + a_n .$$

The roots of the characteristic polynomial are the eigenvalues of G. A k–matching in G is a set of k edges without common vertices. Denote the number of k–matchings in G by m(G,k). It is clear that $m(G, 1)=m$ and $m(G, k)=0$ for $k > \lfloor n/2 \rfloor$ or $k < 0$. The matching polynomial of the graph G is defined as:

$$M(G,x) = \sum_{k\geq 0} (-1)^k m(G,k) x^{n-2k} .$$

Go to [9] for details. The girth of G is the length of the shortest cycle contained in G. An edge incident to a vertex of degree one is called a pendant edge.

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Fullerenes are polyhedral cage molecules composed entirely of carbon atoms. The molecular graph of such a molecule is 3–connected and planar with faces all pentagons and hexagons. Suppose p and h are the number of pentagons and hexagons in an n–vertex fullerene F, respectively. Therefore the Euler's theorem implies that $p = 12$ and $h = n/2 - 10$. After the outstanding work of Kroto et al. [14] in discovering the buckminsterfullerene C_{60}, a lot of researchers devoted their time to find mathematical properties of these new materials. The most important book on this topic is the well known book of Fowler and Manolopoulos [12]. There are several different computer programs for working with fullerenes, one of them is developed by Myrvold and her colleagues [16]. Another program is developed by Schwerdtfeger et al. [17].

Fullerenes are also called (5, 6)–fullerenes. An ***IPR*** (5, 6)–fullerene is one for which no two pentagons share an edge. The minimum distance of two vertices of any two nearest pentagons is called the **pentadistance** of fullerene. In this paper, all (5,6)–fullerenes considered are at distance of at least 2. For more information on the fullerenes and additional results you can see [1, 4, 10, 11].

In this section, some operational definitions used in this paper are presented. The symbols P_n and C_n, stand for the path with n vertices and the cycle of size n, respectively, and $\varphi_G(H)$ or $\varphi(H)$ for the number of H–subgraphs of G. Any undefined terminology and notation can be found in [7].

Behmaram in his thesis [2] and in a recent paper [3] extended the notion of fullerene to m–generalized fullerene. By his definition, a 3–connected cubic planar graph G is called m–generalized fullerene if its faces are two m–gons and all other pentagons and hexagons. The concepts of m–generalized (3, 6)–fullerene and m–generalized (4, 6)–fullerene can be defined in a similar way [15]. We refer to Deza and his co–authors for some other generalization of fullerenes [8, 18, 19].

It is easy to see that a (3, 5, 6)–fullerene molecule with n atoms and exactly 2 triangles has 6 pentagons and $n/2-6$ hexagons. A (4, 5, 6)–fullerene molecule with n atoms and exactly 2 squares has 8 pentagons and $n/2-8$ hexagons, see Figure 1. Also a (5, 6, 7)–fullerene molecule with n atoms has exactly 14 pentagons, 2 heptagons and $n/2-14$ hexagons, and a (4, 6, 8)–fullerene molecule with n atoms has exactly 12 squares, 6 octagons and $n/2-16$ hexagons, see Figure 2. The aim of this paper is determination the relationship between $2k$–th coefficient of characteristic polynomial and k–th coefficient of matching polynomial of a regular graph with girth 5. Also in this paper we determine some coefficients of characteristic polynomial of some fullerene graphs. These coefficients are studied in [6].

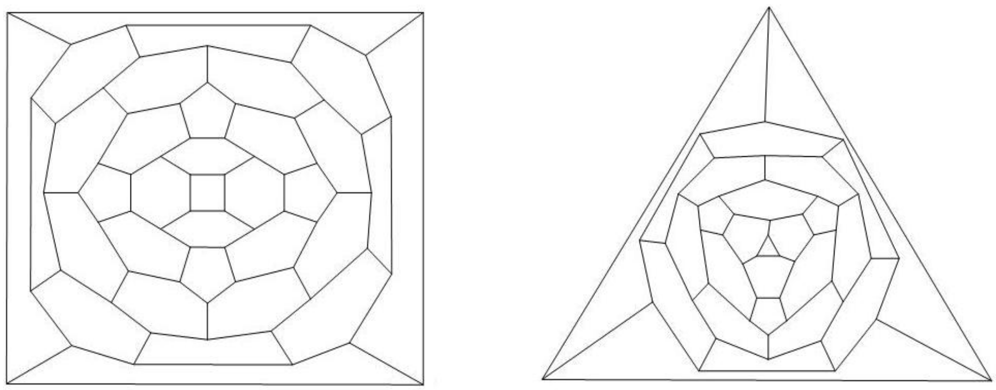


Figure 1. A (4, 5, 6)– (left) and (3, 5, 6)–Fullerene (right).

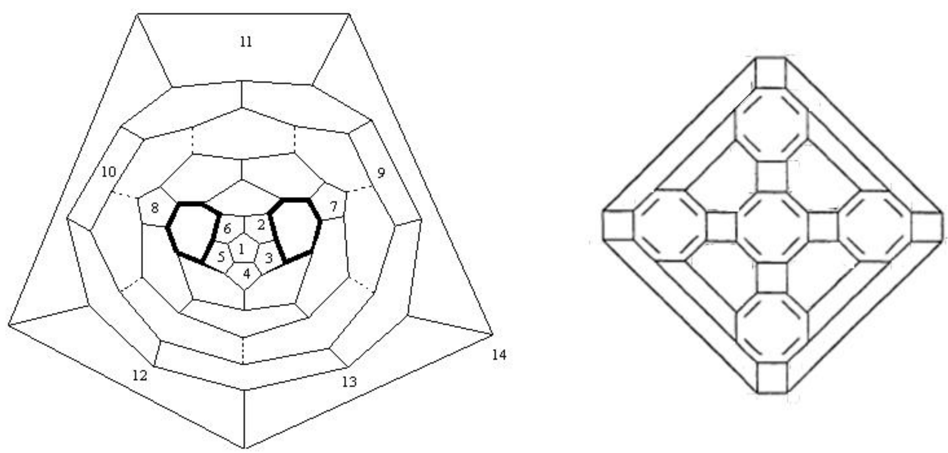


Figure 2. A (5, 6, 7)– (left) and (4, 6, 8)–Fullerene (right).

2. PRELIMINARIES

In this section, we present the definitions and the theorems that are used in the study. Suppose G is a graph with n vertices, m edges and with adjacency matrix $A(G)$. It is easy to see that if G is a regular graph of degree r, then $m=nr/2$. The characteristic polynomial of G, $\psi(G,\lambda)$, is defined as:

$$\psi(G,\lambda) = \lambda^n + a_1\lambda^{n-1} + ... + a_{n-1}\lambda + a_n .$$

An elementary subgraph of G is a subgraph whose connected component is regular and of degree 1 or 2. In other words, the connected components are single edges and/or cycles.

Theorem 1. ([6]) Let G be a graph and $\psi(G,\lambda)$ be the characteristic polynomial of G, then the coefficients of $\psi(G,\lambda)$ are:

$$(-1)^i a_i = \sum (-1)^{r(H)} 2^{s(H)} ,$$

where the summation is over all elementary subgraphs H of G which have i vertices and $r(H)=n-c$ and $s(H)=m-n+c$, where c is the number of connected components of H, and m, n are the number of edges and vertices of H, respectively.

Corollary 2. The relation between $m(G,k)$ and a_{2k} is as the following:

$$a_{2k} - (-1)^k m(G,k) = \sum (-1)^{r(H)} 2^{s(H)},$$

where the summation is over all elementary subgraphs H of G which have $2k$ vertices and at least one cycle.

Proposition 3. ([6]) By the notation given above we have:

(i) $a_1 = 0$,

(ii) $a_2 =$ the number of edges of G,

(iii) $a_3 =$ twice the number of triangles in G.

In the following we consider a walk and the spectral moments in graph G, see [7] for details.

Definition 4. Let G be a graph. A walk of length k in G is an alternating sequence v_1, e_1, v_2, e_2, …, v_k, e_k, v_{k+1} of vertices and edges such that for any i = 1, 2, …, k the vertices v_i and v_{i+1} are distinct end-vertices of the edge e_i. A closed walk is a walk in which the first and the last vertex are the same.

Let $\lambda_1(G), \lambda_2(G), ..., \lambda_n(G)$ be eigenvalues of $A(G)$. The numbers $S_k(G) = \sum_{i=1}^{n} \lambda_i^k$ are said to be the k–th spectral moment of G. It is well–known that $S_0(G) = n$, $S_1(G) = 0$, $S_2(G) = 2m$ and $S_3(G) = 6t$, where n, m and t denote the number of vertices, edges and triangles of the graph, respectively [7].

Lemma 5. ([7]) The k–th spectral moment of G is equal to the number of closed walks of length k.

In [20, 21] the authors calculated the spectral moments of some graphs and they have ordered them with respect to their spectral moments. Also, in [23] the authors studied the signless Laplacian spectral moments of some graphs and then they ordered the graphs with respect to signless Laplacian spectral moments. In [5, 24] the authors computed the number of 4 and 5–matchings in a graph, and in this paper, we consider the relation between the coefficients of characteristic polynomial and the spectral moments are computed, and then by using this relation the relationship between the coefficients of characteristic polynomial and the coefficients of matching polynomial is determined.

Theorem 6.(Newton's identity) Let $\lambda_1(G), \lambda_2(G), ..., \lambda_n(G)$ be the roots of the polynomial $\psi(G,\lambda) = \lambda^n + a_1\lambda^{n-1} + ... + a_{n-1}\lambda + a_n$ with spectral moment S_k. Then

$$a_k = -1/k(S_k + S_{k-1}a_1 + S_{k-2}a_2 + ... + S_1 a_{k-1}).$$

Let F_1, F_2, F_3 and F_4 be a (3, 5, 6)–fullerene, (4, 5, 6)–fullerene, (5, 6, 7)–fullerene and (4, 6, 8)–fullerene, respectively. In [22] the authors computed the spectral moments of this fullerene graphs as in the following:

Theorem 7. The spectral moments of F_1, $S_i(F_1)$, $2 \le i \le 8$, can be computed by the following formulas: $S_2(F_1)=3n$, $S_3(F_1) = 12$, $S_4(F_1) = 15n$, $S_5(F_1) = 180$, $S_6(F_1) = 93n - 60$, $S_7(F_1) = 1932$ and $S_8(F_1) = 639n - 960$.

Theorem 8. The spectral moments of F_2, $S_i(F_2)$, $2 \le i \le 8$, can be computed by the following formulas: $S_2(F_2)=3n$, $S_3(F_2) = 0$, $S_4(F_2) = 15n + 16$, $S_5(F_2) = 80$, $S_6(F_2) = 93n + 96$, $S_7(F_2) = 1120$, $S_8(F_2) = 639n + 400$.

Theorem 9. The spectral moments of F_3, $S_i(F_3)$, $2 \le i \le 8$, can be computed by the following formulas: $S_2(F_3)=3n$, $S_3(F_3) = 0$, $S_4(F_3) = 15n$, $S_5(F_3) = 140$, $S_6(F_3) = 93n - 168$, $S_7(F_3) = 1988$, $S_8(F_3) = 639n - 2464$.

Theorem 10. The spectral moments of F_4, $S_i(F_4)$, $2 \le i \le 8$, can be computed by the following formulas: $S_2(F_4)=3n$, $S_3(F_4) = 0$, $S_4(F_4) = 15n+96$, $S_5(F_4) = 0$, $S_6(F_4) = 93n + 960$, $S_7(F_4) = 0$, $S_8(F_4) = 639n + 8256$.

3. MAIN RESULTS

In this section, we discuss the relationship between the coefficients of characteristic polynomial and the number of 5– and 6– matchings in regular graphs with girth 5 so that every 6–cycle has at most one edge in common with 5–cycles and with other 6–cycles and also any two 5–cycles are at distance at least 2. Then we determine these relations for ***IPR*** (5, 6)–fullerenes, and also we compute the coefficients of the characteristic polynomial of some generalized fullerene graphs.

Theorem 11. Suppose G is an r–regular graph satisfying the above conditions. Then the relation between the tenth coefficient of characteristic polynomial of G and $m(G, 5)$ is the following:

$$\begin{aligned} a_{10} + m(G,5) = {} & -2\varphi(C_{10}) + \varphi(C_8)nr - 16\varphi(C_8)r + 16\varphi(C_8) - 1/4\varphi(C_6)n^2r^2 - 54\varphi(C_6)r^2 \\ & -13/2\varphi(C_6)nr - 54\varphi(C_6) + 108\varphi(C_6)r + 7\varphi(C_6)nr^2 + 2\varphi(C_5)^2 - 2\varphi(C_5). \end{aligned}$$

Proof. By using of Theorem 1, we have:

$$a_{10} = -m(G,5) + \sum_A (-1)^9 2 + \sum_B (-1)^8 2 + \sum_C (-1)^7 2 + \sum_D (-1)^8 4,$$

where A is a 10–cycle, B is a subgraph isomorphic with a 8–cycle and one single edge, C is a subgraph isomorphic with a 6–cycle with two separate edges and D is a subgraph isomorphic with two separate 5–cycles. Now, the values of A, B, C and D are calculated. It is clear that $|A|=\varphi(C_{10})$ and $|B|=\varphi(C_8)(m-8-8(r-2))= \varphi(C_8)(nr/2-8r+8)$. To compute $|C|$ we consider all undesirable cases to have a subgraph isomorphic with C and then subtract these values of all the possible situations. Since all subgraphs isomorphic with C is equal to $\varphi(C_6)$ $(nr/2-6)(nr/2-7)/2$, so if we put $\varphi(C_6)=h$, $\varphi(C_{10})=t$ and $\varphi(C_8)=k$, then $|C|= 1/8hn^2r^2+13/4hnr+27h+27hr^2-54hr-7/2hnr^2$. Also, as it can be observed $|D|= p(p-1)/2$. Therefore

$$a_{10} + m(G,5) = -2t + knr - 16kr + 16k - 1/4hn^2r^2 \\ - 54hr^2 - 13/2hnr - 54h + 108hr + 7hnr^2 + 2p^2 - 2p.$$

In the following section, we consider relationship between the twelfth coefficients of characteristic polynomial of a regular graph with consideration of the above conditions. Before the proof of the main result, we need some technical Lemmas.

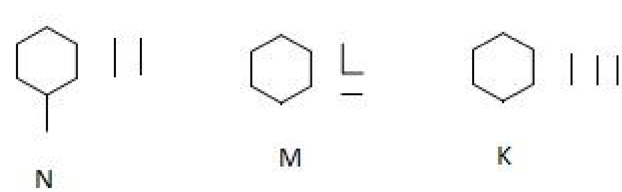


Figure 3. All subgraphs isomorphic with N, M and K.

Lemma 12. Let G be an r–regular graph that above conditions exist for it. Then the number of subgraphs isomorphic with a 6–cycle together with a pendant edge and with two separate edges is equal to:

$$81/2hnr^2 - 33/2hnr^3 - 15hnr - 476h + 160hr^3 - 654hr^2 + 906hr + 3/4hn^2r^3 - 3/2hn^2r^2.$$

Proof. Let N be a subgraph isomorphic with a 6–cycle with a pendant edge and two separate edges, where is depicted in Figure 3. To calculate the number of subgraphs isomorphic with N, first we consider all subgraphs isomorphic with N, that is equal to $6h(r-2)(m-7)(m-8)/2$. Next we consider all of the undesirable cases to have a subgraph isomorphic with N where is shown in Table 1. Therefore, by consideration these values and subtracting all undesirable cases from possible conditions for having a subgraph isomorphic with N we have:

$$|N| = 81/2hnr^2 - 33/2hnr^3 - 15hnr - 476h + 160hr^3 - 654hr^2 + 906hr + 3/4hn^2r^3 - 3/2hn^2r^2.$$

Lemma 13. Let G be an r-regular graph satisfying the above conditions. Then the number of subgraphs isomorphic with a 6–cycles together with a single edge and a path P_3 (where the edge and P_3 are distinct) is equal to:

$$1/4hn^2r^3 + 555hr + 111hr^3 - 420hr^2 + hbr + hbr^3 - 2hbr^2$$
$$-10hnr + 19hnr^2 - 1/4hn^2r^2 - 9hnr^3 - 258h.$$

Proof. Let M be a subgraph isomorphic with a 6–cycle together with a single edge and a path P_3, where is depicted in Figure 3. To calculate $|M|$, the same as previous Lemma, we consider all of the possible cases to have a subgraph isomorphic with M and all adverse conditions that are shown in Table 2. All possible cases is equal to $h(3(r-2)(r-3)+(n-6)r(r-1)/2)(nr/2-8)$, and to obtain adverse conditions, these cases are easily computable and we just compute the cases 8 and 9 in Table 2.

In case 8 (a 6–cycle together with a path P_3 with an edge at the end of this path), first we choose a 6–cycle. Then we consider all the adjacent vertices to 6-cycle, where the number of these vertices is $6(r-2)$. So by a simple check there are $6(r-2)(r-1)(r-2)(2r-2)/2$ ways for selecting the path P_3 with an edge at the end of this path, for the adjacent vertices to 6–cycle. Now we consider all of vertices that are at distance 2 from 6–cycle and we consider the following cases:

Case 1. If this vertex that is at distance 2 from 6–cycle is on a 5–cycle, then we have the following subcases:

Subcase 1.1. If both selected edges to form path P_3 are on 5–cycle, then there are $2(r-2)$ ways for selecting the path P_3 with an edge at the end of this path.

Subcase 1.2. If only an edge of P_3 is on 5–cycle, where the number of these edges are equal to $2(r-2)$, then there are $2(r-2)(2r-3)$ ways for selecting the path P_3 with an edge at the end of this path.

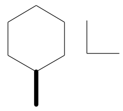
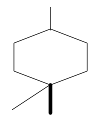
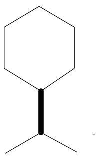
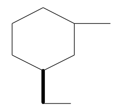
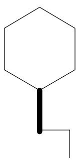
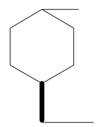
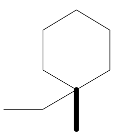
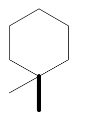
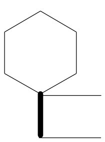
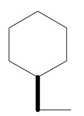
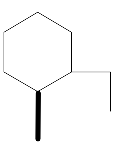
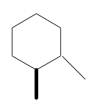
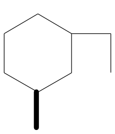
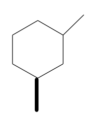
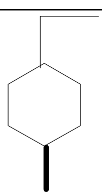
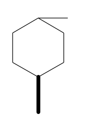
Subcase 1.3. If none of the two edges of path is on 5–cycle, where the number of these edges are equal to $(r-2)(r-3)/2$, then there are $(r-2)(r-3)(2r-2)/2$ ways for selecting the path P_3 with an edge at the end of this path. Finally for the case that the vertex in distance 2 from 6–cycle is on a 5–cycle we have

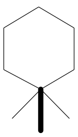
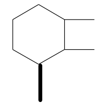
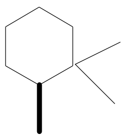
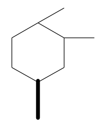
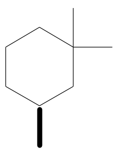
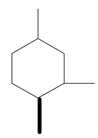
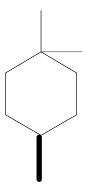
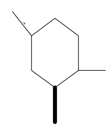
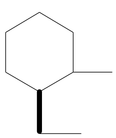
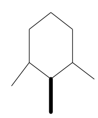
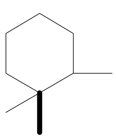
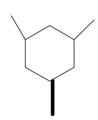
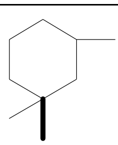
$$b[2r-4+(2r-4)(2r-3)+(r-2)(r-3)(2r-2)/2],$$

where b is the number of edges that are in common with a 6–cycle and a 5–cycle.

Case 2. If the vertex that is at distance 2 from 6–cycle is not on a 5–cycle, where the number of these vertices are equal to $6(r-1)(r-2)-2b$, then there are $(r-1)(2r-3) + (r-1)(r-2)(2r-2)/2$ ways for selecting the path P_3 with an edge at the end of this path.

Table 1. All of the undesirable situations to have a 6–cycle with a pendant edge and with two separate edges and their numbers.

	$3h(r-2)\left(-21r^2+49r-28+nr^2-nr\right)$		$6h(r-2)^2(r-3)$
	$3h(r-2)^2(r-1)$		$6h(r-2)^2(r-1)$
	$6h(r-2)(r-1)^2$		$6h(r-2)^2(r-1)$
	$6h(r-2)(r-1)(r-3)$		$3h(r-2)(r-3)(nr-16r+16)$
	$6h(r-2)(r-1)(r-3)$		$3h(r-2)(r-1)(nr-16r+16)$
	$6h(r-2)^2(r-1)$		$3h(r-2)^2(nr-16r+16)$
	$6h(r-2)^2(r-1)$		$3h(r-2)^2(nr-16r+16)$
	$6h(r-2)^2(r-1)$		$\frac{3}{2}h(r-2)^2(nr-16r+16)$

	$3\,h(r-2)(r-3)(r-4)$		$6\,h\,(r-2)^3$
	$3\,h\,(r-2)^2\,(r-3)$		$6\,h\,(r-2)^3$
	$3\,h\,(r-2)^2\,(r-3)$		$6\,h\,(r-2)^3$
	$3\,h\,(r-2)^2\,(r-3)$		$6\,h\,(r-2)^3$
	$6\,h\,(r-2)^2\,(r-1)$		$6\,h\,(r-2)^3$
	$6\,h\,(r-2)^2\,(r-3)$		$2\,h\,(r-2)^3$
	$6\,h\,(r-2)^2\,(r-3)$		

Finally, for the case that the vertex in distance 2 from 6–cycle is not on a 5–cycle, there are

$$b(2r-4+(2r-4)(2r-3)+(r-2)(r-3)(2r-2)/2)+$$
$$(6(r-1)(r-2)-2b)((r-1)(2r-3)+(r-1)(r-2)(2r-2)/2)$$

ways for selecting the path P_3 with an edge at the end of this path. Therefore, to calculate case 8 in Table 2 we have:

$$\begin{aligned}&h[6(r-2)(r-1)(r-2)(2r-2)/2+b(2r-4+(2r-4)(2r-3)\\&\quad+(r-2)(r-3)(2r-2)/2)+(6(r-1)(r-2)-2b)((r-1)(2r-3)\\&\quad+(r-1)(r-2)(2r-2)/2)+(n-6-6(r-2)-6(r-1)(r-2))r(r-1)(2r-2)/2]\\&\quad=h(nr^3-2nr^2+nr-br^3+2br^2-br+84r^2-24r^3-96r+36).\end{aligned}$$

In case 9 Table 2, (a 6–cycle together with a path P_3 and an edge on middle vertex of P_3), we first select a 6–cycle and then a path P_3 of all the vertices except vertices of 6-cycle. For the vertices that are at distance 1 from 6–cycle, where the number of these vertices are $6(r–2)$, there are $6((r–2)(r–1)(r–2)/2)(r–3)$ ways to choose a path P_3 such that there is an edge on the middle vertex. For other vertices, where the number of these vertices are $n–6–6(r–2)$, there are $(n–6–6(r–2))r(r–1)(r–2)/2)$ ways to choose a path P_3 such that there is an edge on middle vertex. Therefore, there are $h(6(r–2)(r–1)(r–2)/2)(r–3) + (n–6–6(r–2))r(r–1)(r–2)/2)$ ways to choose case 9 of Table 2. Finally, after calculating all adverse conditions in this Table, we have:

$$\begin{aligned}|M|&=1/4hn^2r^3+555hr+111hr^3-420hr^2+hbr+hbr^3-2hbr^2\\&\quad-10hnr+19hnr^2-1/4hn^2r^2-9hnr^3-258h.\end{aligned}$$

Lemma 14. Let G be an r–regular graph with the above conditions. Then the number of subgraphs isomorphic with a 6–cycle together with three separate edges is equal to:

$$\begin{aligned}&-147hr+59/6hnr^3-5/2hnr^2-44/3hnr+2hbr^2-hbr\\&+136h-hbr^3-57hr^3+126hr^2-hn^2r^3+1/48hn^3r^3+7/8hn^2r^2.\end{aligned}$$

P**roof.** Let K be a subgraph isomorphic with a 6–cycle and three separate edges, where is depicted in Figure 3. To calculate $|K|$, we must consider all the undesirable cases for having a subgraph isomorphic with K, that is shown in Table 3 and then we subtract these values of all the possible situations to have a subgraph isomorphic with K. Notice that all subgraphs isomorphic with K is equal to $h(m\text{-}6)(m\text{-}7)(m\text{-}8)/6$, so we must find a formula for all adverse conditions . In this Table all of values in front of figures are easily calculated, and with putting up values of Lemmas 12 and 13 we obtain:

$$\begin{aligned}|K|&=-147hr+59/6hnr^3-5/2hnr^2-44/3hnr+2hbr^2-hbr\\&\quad+136h-hbr^3-57hr^3+126hr^2-hn^2r^3+1/48hn^3r^3+7/8hn^2r^2.\end{aligned}$$

Theorem 15. Suppose G is an r–regular graph satisfying the above conditions. Then the relationship between the twelfth coefficients of characteristic polynomial of G and $m(G, 6)$ is stated in the following:

$$
\begin{aligned}
a_{12}-m(G,6) = {} & -4a-2e-88/3hnr-2hbr+59/3hnr^{3}-5hnr^{2}+7/4hn^{2}r^{2}-72k \\
& +4hbr^{2}-2hbr^{3}-68kr^{2}+20t+1/24hn^{3}r^{3}-20p^{2}-2hn^{2}r^{3}-4kr^{3} \\
& -20tr+9knr^{2}-1/4kn^{2}r^{2}-17/2knr-294hr+pnr+20p^{2}r+270h \\
& +252hr^{2}-114hr^{3}+144kr-20pr+tnr+20p+2h^{2}-p^{2}nr,
\end{aligned}
$$

where $k=\varphi(C_8)$, $e=\varphi(C_{12})$, $t=\varphi(C_{10})$, $p=\varphi(C_5)$, $h=\varphi(C_6)$, a is the number of edges common to two 6-cycles and b is the number of edges that are in common with a 6–cycle and a 5–cycle.

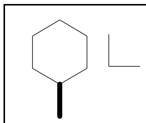
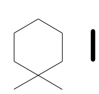
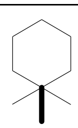
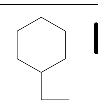
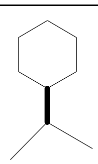
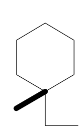
Proof. By Theorem 1 we have:

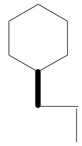
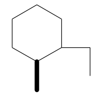
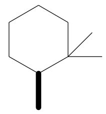
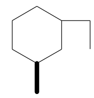
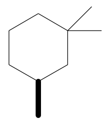
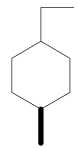
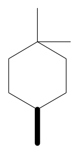
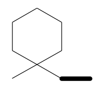
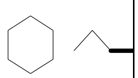
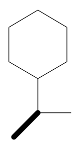
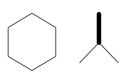
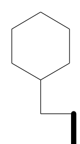
$$a_{12}=m(G,6)+\sum_{A}(-1)^{10}2+\sum_{B}(-1)^{11}2+\sum_{C}(-1)^{9}2+\sum_{D}(-1)^{8}2+\sum_{E}(-1)^{9}4+\sum_{F}(-1)^{10}4,$$

where A is a subgraph isomorphic with a 10–cycle and a single edge, B is a subgraph isomorphic with a 12–cycle, C is a subgraph isomorphic with a 8–cycle and two separate edges, D is a subgraph isomorphic to 6–cycle together with three separate edges, E is a subgraph isomorphic to two separate 5–cycles with one single edge and F is a subgraph isomorphic with two separate 6–cycles. It is easy to see that $|A|=t(nr/2-10r+10)$ and $|B|=e$. To calculate $|C|$, we consider all of the possible cases to have a subgraph isomorphic with a 8–cycle with two separate edges and all of the undesirable situations, and so we obtain:

$$
\begin{aligned}
|C| = {} & k/2(m-8)(m-9)-k(2(r-2)^{2}(r-1)+(n-8r+8)r(r-1)/2) \\
& -4k(r-2)(r-3)-8k(r-2)(r-1)-28k(r-2)^{2}-8k(r-2)(nr/2-9r+9) \\
= {} & 1/8kn^{2}r^{2}+17/4knr+36k+2kr^{3}+34kr^{2}-72kr-9/2knr^{2}.
\end{aligned}
$$

Table 2. All of the undesirable situations to have a 6–cycle with a single edge and a path P_3 and their numbers.

	$3h(r-2)(-21r^{2}+49r-28+nr^{2}-nr)$		$\frac{3}{2}h(r-2)(r-3)(rn-16r+16)$
	$3h(r-2)(r-3)(r-4)$		$3h(r-2)(r-1)(rn-16r+16)$
	$3h(r-2)^{2}(r-1)$		$6h(r-2)(r-1)(r-3)$

	$6h(r-2)(r-1)^2$		$6h(r-2)^2(r-1)$
	$3h(r-2)^2(r-3)$		$6h(r-2)^2(r-1)$
	$3h(r-2)^2(r-3)$		$6h(r-2)^2(r-1)$
	$3h(r-2)^2(r-3)$		$3h(r-2)(r-3)(r-1)$
	$-h\left(-36+96r-nr+2nr^2-nr^3+24r^3-84r^2+br-2br^2+br^3\right)$		$6h(r-2)^2(r-1)$
	$\frac{1}{2}h(r-2)(r-1)(-24r+36+rn)$		$6h(r-2)(r-1)^2$

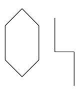
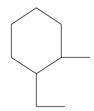
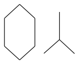
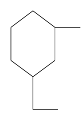
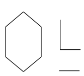
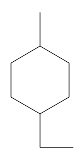
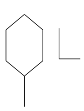
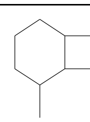
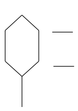
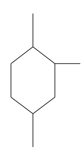
On the other hand, by Lemma 14,

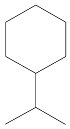
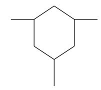
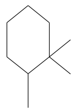
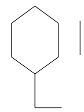
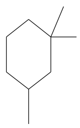
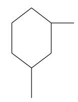
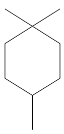
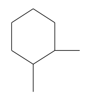
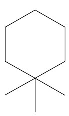
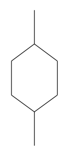
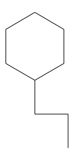
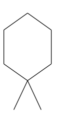
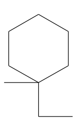
$$|D| = -147hr + 59/6hnr^3 - 5/2hnr^2 - 44/3hnr + 2hbr^2 - hbr + 136h - hbr^3 - 57hr^3 + 126hr^2 - hn^2r^3 + 1/48hn^3r^3 + 7/8hn^2r^2.$$

Let p be the number of 5–cycles that are satisfied in above conditions, i.e. every 6–cycle has at most one edge in common with a 5–cycle and the other 6–cycles and also any two 5–cycles has distance of at least 2. Then, it is clear that $|E|=p(p-1)/2(nr/2-10r+10)$. Now let a be the number of edges common to two 6–cycles, then $|F|=h(h-1)/2-a$. Therefore,

$$
\begin{aligned}
a_{12} - m(G,6) &= 2t(nr/2 - 10r + 10) - 2e - 2(1/8kn^2r^2 + 17knr/4 + 36k + 2kr^3 + 34kr^2 \\
&\quad - 72kr - 9knr^2/2) + 2(-147hr + 59/6hnr^3 - 5/2hnr^2 - 44/3hnr + 2hbr^2 \\
&\quad - hbr + 136h - hbr^3 - 57hr^3 + 126hr^2 - hn^2r^3 + 1/48hn^3r^3 + 7/8hn^2r^2) \\
&\quad - 4(p(p-1)/2(nr/2 - 10r + 10)) + 4(h(h-1)/2 - a) \\
&= -4a - 2e - 88/3hnr - 2hbr + 59/3hnr^3 - 5hnr^2 + 7/4hn^2r^2 - 72k \\
&\quad + 4hbr^2 - 2hbr^3 - 68kr^2 + 20t + 1/24hn^3r^3 - 20p^2 - 2hn^2r^3 - 4kr^3 \\
&\quad - 20tr + 9knr^2 - 1/4kn^2r^2 - 17/2knr - 294hr + pnr + 20p^2r + 270h \\
&\quad + 252hr^2 - 114hr^3 + 144kr - 20pr + tnr + 20p + 2h^2 - p^2nr.
\end{aligned}
$$

Table 3. All of the undesirable situations to have a 6-cycle with three separate edges and their numbers.

	$-12hr^3 + 42hr^2 - 48hr + 18h + \frac{1}{2}hnr^3 - hnr^2 + \frac{1}{2}hnr$		$6h(r-2)^2(r-1)$
	$-4hr^3 + 18hr^2 - 26hr + 12h + \frac{1}{6}hnr^3 - \frac{1}{2}hnr^2 + \frac{1}{3}hnr$		$6h(r-2)^2(r-1)$
	$\frac{1}{4}hn^2r^3 + 555hr + 111hr^3 - 420hr^2 + hbr + hbr^3 - 2hbr^2 - 10hnr + 19hnr^2 - \frac{1}{4}hn^2r^2 - 9hnr^3 - 258h$		$6h(r-2)^2(r-1)$
	$3h(r-2)\left(-21r^2 + 49r - 28 + nr^2 - nr\right)$		$6h(r-2)^3$
	$\frac{81}{2}hnr^2 - \frac{33}{2}hnr^3 - 15hnr - 476h + 160hr^3 - 654hr^2 + 906hr + \frac{3}{4}hn^2r^3 - \frac{3}{2}hn^2r^2$		$6h(r-2)^3$

	$3h(r-1)(r-2)^2$		$2h(r-2)^3$
	$3h(r-3)(r-2)^2$		$3h(r-1)(r-2)(nr-16r+16)$
	$3h(r-3)(r-2)^2$		$3h(r-2)^2(nr-16r+16)$
	$3h(r-3)(r-2)^2$		$3h(r-2)^2(nr-16r+16)$
	$h(r-3)(r-2)(r-4)$		$\frac{3}{2}h(r-2)^2(nr-16r+16)$
	$6h(r-1)^2(r-2)$		$\frac{3}{2}h(r-2)(r-3)(nr-16r+16)$
	$6h(r-3)(r-2)(r-1)$		

In following, suppose G is an ***IPR*** (5, 6)–fullerene such that any two pentagons are at distance at least 2. In [13] the authors calculated some of the coefficients of characteristic polynomial of G. Now, in this paper by using these coefficients and by using of Theorems 11 and 15 we calculate the 5, 6-matchings in G.

Theorem 16. Let G be an ***IPR*** (5, 6)–fullerene such that satisfying the above conditions. Then we have:

$$m(G,5) = 3543/10n - 12 + 1719/64n^3 - 2499/16n^2 - 135/64n^4 + 81/1280n^5.$$

Proof. By using of Theorem 11 we have:

$$a_{10} + m(G,5) = -2t + knr - 16kr + 16k - 1/4hn^2r^2$$
$$- 54hr^2 - 13/2hnr - 54h + 108hr + 7hnr^2 + 2p^2 - 2p.$$

On the other hand by [13] we have:

$$a_{10} = -81/1280n^5 + 135/64n^4 - 1791/64n^3 + 3207/16n^2 - 9003/10n + 2556.$$

Also we have, r=3, $\varphi(C_{10})=a=3n/2$-60, $\varphi(C_8)=0$, $\varphi(C_5)=12$ and $\varphi(C_6)=n/2$-10. Therefore, $m(G,5) = 3543/10n - 12 + 1719/64n^3 - 2499/16n^2 - 135/64n^4 + 81/1280n^5$.

Theorem 17. Let G be an ***IPR*** (5, 6)–fullerene such that satisfies the above conditions. Then we have:

$$m(G,6) = -7607/4n - 10770 + 146177/160n^2 - 21339/128n^3$$
$$+ 4113/256n^4 - 405/512n^5 + 81/5120n^6.$$

Proof. By using of Theorem 15 we have:

$$m(G,6) = a_{12} - (-4a - 2e - 88/3hnr - 2hbr + 59/3hnr^3 - 5hnr^2 + 7/4hn^2r^2 - 72k$$
$$+ 4hbr^2 - 2hbr^3 - 68kr^2 + 20t + 1/24hn^3r^3 - 20p^2 - 2hn^2r^3 - 4kr^3$$
$$- 20tr + 9knr^2 - 1/4kn^2r^2 - 17/2knr - 294hr + pnr + 20p^2r + 270h$$
$$+ 252hr^2 - 114hr^3 + 144kr - 20pr + tnr + 20p + 2h^2 - p^2nr).$$

On the other hand, by [13] and by Newton's identity we have:

$$a_{12} = -31899/4n + 25970 + 240017/160n^2 - 25227/128n^3$$
$$+ 4257/256n^4 - 405/512n^5 + 81/5120n^6.$$

Also, in an IPR (5,6)–fullerene we have, $e = \varphi(C_{12})=0$, $t = \varphi(C_{10})=a=3n/2-60$, $k=\varphi(C_8)=0$, $p=\varphi(C_5)=12$, $h = \varphi(C_6) = n/2-10$ and b = the number of edges are common to 6–cycles and 5–cycles = 60. Therefore,

$$m(G,6) = -7607/4n - 10770 + 146177/160n^2 - 21339/128n^3$$
$$+ 4113/256n^4 - 405/512n^5 + 81/5120n^6.$$

In the following we consider all of the generalized fullerene graphs that were defined in this paper and the coefficients of characteristic polynomial of these graphs are calculated.

Theorem 18. The coefficients of characteristic polynomial of F_1, $a_i(F_1)$, for i =1, 2, 3, …, 8 are: $a_1 = 0$, $a_2 = -3n/2$, $a_3 = -4$, $a_4 = 9/8n^2 - 15n/4$, $a_5 = 6n - 36$, $a_6 = -9n^3/16 + 45n^2/8 - 31/2n + 18$, $a_7 = -9n^2/2 + 69n - 276$, $a_8 = 27n^4/128 - 135n^3/32 + 969n^2/32 - 855n/8 + 264$.

Proof. Apply Theorems 7−10 and Newton's identity.

Theorem 19. The coefficients of characteristic polynomial of F_2 , $a_i(F_2)$, for i =1, 2, 3, …, 8 are: $a_1 = 0$, $a_2 = -3n/2$, $a_3 = 0$, $a_4 = 9n^2/8 - 15n/4 - 4$, $a_5 = -16$, $a_6 = -9n^3/16 + 45n^2/8 - 19n/2 - 16$, $a_7 = 24n - 160$, $a_8 = 27n^4/128 - 135n^3/32 + 825n^2/32 - 327n/8 - 42$.

Theorem 20. The coefficients of characteristic polynomial of F_3, $a_i(F_3)$, for i =1, 2, 3, …, 8 are: $a_1 = 0$, $a_2 = -3n/2$, $a_3 = 0$, $a_4 = 9n^2/8 - 15n/4$, $a_5 = -28$, $a_6 = -9n^3/16 + 45n^2/8 - 31n/2 + 28$, $a_7 = 42n - 284$, $a_8 = 27n^4/128 - 135n^3/32 + 969n^2/32 - 975n/8 + 308$.

Theorem 21. The coefficients of characteristic polynomial of F_4, $a_i(F_4)$, for i =1, 2, 3, …, 8 are: $a_1 = 0$, $a_2 = -3n/2$, $a_3 = 0$, $a_4 = 9n^2/8 - 15n/4 - 24$, $a_5 = 0$, $a_6 = -9n^3/16 + 45n^2/8 + 41n/2 - 160$, $a_7 = 0$ and $a_8 = 27n^4/128 - 135n^3/32 + 105n^2/32 + 2001n/8 - 744$.

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The Topological Indices of some Dendrimer Graphs

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ABSTRACT

In this paper, the Wiener and hyper Wiener indices of two kinds of dendrimer graphs are computed. Using the Wiener index formula, the Szeged, Schultz, PI and Gutman indices of these graphs are also determined.

1. INTRODUCTION

Let $\boldsymbol{G} = (V,E)$ be a simple connected graph with vertex set V and edge set E. A topological index of a simple connected graph G is a graph invariant which is related to the structure of the graph. The Wiener index is one of the best known topological index of a simple connected graph which is studied in both mathematical and chemical literature and it's definition is in terms of distances between arbitrary pairs of vertices, see for example [1, 2, 3, 4]. The Wiener index of G is denoted by $W(G)$ and it is defined by:

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v) = \frac{1}{2}\sum_{u\in V} d(u),$$

where $d(u,v)$ is the distance between vertices u and v and $d(u) = \sum_{v\in V} d(u,v)$.

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The Szeged index [5, 6] is another invariant of a graph which is based on the distribution of the vertices and introduced by Ivan Gutman and it is the same with the Wiener index in the case that G is a tree. The set of vertices of graph G which are closer to u (resp. v) than v (resp. u) is denoted by $N_u(e|G)$ (resp. $N_v(e|G)$). This index is defined as the summation of ($n_u(e|G)\, n_v(e|G)$) where $n_u(e|G)$ (resp. $n_v(e|G)$), is the number of vertices of graph G closer to u (resp. v) than v (resp. u), over all edges $e=uv$ of graph. Now, the Szeged index of G which is denoted by $Sz(G)$ is defined as:

$$Sz(G)=\sum_{e=uv\in E}(n_u(e|G).n_v(e|G)).$$

The Padmaker-Ivan (*PI*) index [7, 8] is another topological index of a simple connected graph that takes into account the distribution of edges so is closely related to Szeged index. The *PI* index of G is defined by

$$PI(G)=\sum_{e=uv\in E}(n_{eu}(e|G)+n_{ev}(e|G)),$$

where $(n_{eu}(e|G)$ (resp. $(n_{ev}(e|G)$) is the number of edges of the subgraph of G which has the vertex set $N_u(e|G)$ (resp. $N_v(e|G)$).

The molecular topological index (Schultz index) was introduced by Schultz and Schultz [9, 10]. In addition to the chemical applications, the Schultz index attracted some attention that in the case of a tree it is related to the Wiener index [11]. It is denoted by $S(G)$ and defined as follows:

$$S(G)=\sum_{\{u,v\}\subseteq V}(\rho(u)+\rho(v)),$$

where $\rho(u)$ (resp. $\rho(v)$) is the degree of vertex u (resp. v).

The Gutman index which attracts more attention recently is defined by Klavžar and Gutman in [11, 12]. This index is also known as the Schultz index of the second kind but in this paper the first name is used. Gutman [11] has proved that if G is a tree then there is a relation between Wiener and Gutman indices of G that we will mention this in Section 2. The Gutman index of G is denoted by $Gut(G)$ and is defined as follows:

$$Gut(G)=\Sigma_{\{u,v\}\subseteq V}(\rho(u)\rho(v))$$

The hyper–Wiener index is one of the graph invariants, used as a structure descriptor related to physicochemical properties of compounds. This index was introduced by Randić in 1993 as extension of Wiener index [13] and it has come to be known as the hyper–Wiener index by Klein [14]. The hyper–Wiener index of G is denoted by $WW(G)$ and is defined as follows:

$$WW(G)=\frac{1}{2}(W(G)+\sum_{\{u,v\}\subseteq V}d^2(u,v)).$$

Here we mainly try to determine the Wiener, hyper Wiener and PI indices of two kinds of dendrimer graphs (explained in Section 2), then the Schultz, Szeged and Gutman indices are obtained as results of the relation between the Wiener index with both the Schultz and Gutman indices.

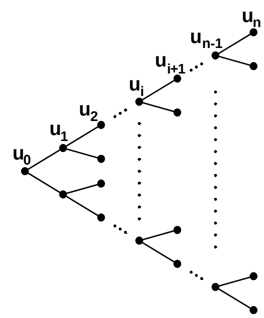

Figure 1. The first dendrimer graph G_n .

2. CALCULATING THE WIENER, HYPER-WIENER AND PI INDICES OF THE FIRST DENDRIMER GRAPH G_n

Let $G = (V,E)$ be the graph with vertex set V and edge set E as in Figure 1. This graph begins with one vertex u_0 which connects to two other vertices such that each one of these two vertices connects to two other vertices and so on. The vertices which have the same distance from u_0 are located on a branch. Let G have $(n+1)$ branches so there are 2^i vertices in the i'-th branch ($0 \le i \le n$). We denote this graph by G_n .

Proposition 2.1. Let $G_n = (V, E)$ be the dendrimer graph in Figure 1, then:

$$W(G_n) = 4^{(n+1)}\ (n - 2) + 2^{(n+1)}\ (n + 4).$$

Proof. From definitions we have:

$$W(G_n) = \sum_{\{u,v\}\subseteq V(G)} d(u,v) = \frac{1}{2}\sum_{u\in V} d(u).$$

This graph has $n+1$ branches and there are 2^i vertices in the i'–th branch, so we denote the vertex set of this branch by V_i, hence we have: $V = \bigcup_{i=0}^{n} V_i$. Because of the symmetric structure of the graph G_n (Figure l), for every vertex u in the n'th branch, $d(u)$ is constant and doesn't depend on u . So we choose u_i as representative of the i'–th branch ($0 \le i \le n$).

$$d(u_n) = \sum_{v \in V_n} d(u_n, v) + \sum_{v \in V - V_n} d(u_n, v). \quad (1)$$

2^{n-1} vertices which are in lower branch of Figure l, are of the same distance from u_n and this value equals to:

$$2d(u_n, u_0) = 2n.$$

Also 2^{n-2} vertices are of the same distance from u_n and this value equals to:

$$2d(u_n, u_1) = 2(n-1).$$

Finally continuing in this way the distance between u_n to the last vertex in the n'–th branch is equals to:

$$2d(u_n, u_{n-1}) = 2\,.$$

So we have:

$$\begin{aligned}
\sum_{v \in V_n} d(u_n, v) &= 2^{n-1} \times 2n + 2^{n-2} \times 2(n-1) + \ldots + 2^{(1-1)}2 \\
= \sum_{v \in V_n} d(u_n, v) &= n2^n \times (n-1)2^{(n-1)} + \ldots + 1.2 \\
= \sum_{i=1}^{n} i2^i &= 2(1 + (n-1)2^n).
\end{aligned} \quad (2)$$

For computing the second part of the summation in (1), note that because the graph G_n is a tree, for every vertex $v \in \bigcup_{i=0}^{n} V_i$ we have:

$$d(u_n, v) = 1 + d(u_{n-1}, v)$$

$$\sum_{v \in \bigcup_{i=0}^{n-1} V_i} d(u_n, v) - \sum_{v \in \bigcup_{i=0}^{n-1} V_i} d(u_{(n-1)}, v) = \sum_{i=0}^{n-1} 2^i. \quad (3)$$

Considering (2) and (3):

$$d(u_n) - d(u_{n-1}) = \sum_{i=0}^{n-1} 2^i + 2(1 + (n-1)2^n) = 2n2^n - 2^n + 1\,.$$

Because, $d(u_o) = 0.$ Hence :

$$d(u_n) = \sum_{i=1}^{n} (d(u_i) - d(u_{i-1})) = \sum_{i=1}^{n} 2i2^i - 2^i + 1 = (2n-3)2^{n+1} + n + 6. \quad (4)$$

By multiplying 2^n in $d(u_n)$ the distance between vertices in the n'–th branch is considered twice, so if the Wiener index of G_n with n (resp. $n+1$) branch is denoted by $W(n+1)$ (resp. $W(n)$) we have:

$$\begin{aligned}
W(n) - W(n-1) &= 2^n((2n-3)2^{n+1} + (n+6)) - \sum_{\{u,v\} \subseteq V_n} d\ (u, v) \\
&= 2^n(2n-3)2^{(n+1)} + 2^n(n+6) - 2^n(1 + (n-1)2^n) \\
&= (3n-5)2^{2n} + (n+5)2^n.
\end{aligned}$$

So,

$$W(n) = \sum_{i=1}^{n} (3k-5)2^{2k} + (k+5)2^{k} = 4^{(n+1)}\,(n-2) + 2^{(n+1)}\,(n+4). \qquad \blacksquare$$

Corollary 2.2. $Sz(G_n) = 4^{(n+1)}\,(n-2) + 2^{(n+1)}\,(n+4).$

Proof. The graph G_n is a tree, so by [11] the result is obtained. ■

Corollary 2.3. $S(G_n) = 4^{(n+1)}\,(4n-9) + 2^{(n+1)}\,(4n+19) - 2.$

Proof. Because G_n is a tree by [11] we have: $S(G_n) = 4W(G_n) - n(n-1)$, where n is the number of vertices of G_n. Now by replacing the closed form of $W(G_n)$ which was obtained from proposition 2.1, the proof is completed. ■

Corollary 2.4. $Gut(G_n) = 4^{(n+1)}\,(4n-10) + 2^{(n+1)}\,(4n+19) + 10.$
Proof. Because G_n is a tree, by [11] we have, $Gut(G_n) = 4W(G_n) - (2n-1)(n-1)$ where n is the number of vertices of G_n and by proposition 2.1 it is done. ■

Corollary 2.5. $PI(G_n) = (2^{(n+1)} - 3)(2^{(n+1)} - 2).$
Proof. Because G_n is a tree so for every edge $e = uv$ of G_n we have:

$$n_u(e\,|\,G_n) + n_v(e\,|\,G_n) = |V| = 2^{n+1} - 1.$$

Subgraphs of G_n with vertex sets $N_u(e\,|\,G_n)$ and $N_v(e\,|\,G_n)$ both are trees and whose number of edges are $n_u(e\,|\,G_n) - 1$ and $n_v(e\,|\,G_n) - 1$ respectively. Then we have:

$$\begin{aligned}
n_{eu}(e\,|\,G_n) + n_{ev}(e\,|\,G_n) &= n_u(e\,|\,G_n) + n_v(e\,|\,G_n) - 2 = 2^{n+1} - 3 \\
|E|\,(2^{(n+1)} - 3) &= (2^{(n+1)} - 2)(2^{(n+1)} - 3) \\
PI(G_n) &= |E|\,(2^{(n+1)} - 3) = (2^{(n+1)} - 2)(2^{(n+1)} - 3)
\end{aligned}$$

Proposition 2.6. The hyper–Wiener index of G_n in Figure 1 is:

$$WW(G_n) = 4^{n}\,(4n^2 - 14n + 24) + 2^{n}\,(n^2 - 3n - 31) - 1.$$

Proof. By definition we have:

$$WW(G) = \frac{1}{2}\Big(W(G) + \sum_{\{u,v\}\subseteq V} d^2(u,v)\Big). \qquad (5)$$

Because of the symmetric structure of the graph G_n in Figure l, d(u) for every vertex u in the n'–th branch is constant and doesn't depend on u, so we choose u_i as representative of the i'–th branch ($0 \le i \le 1$).

$$d^2(u_n) = \sum_{v\in V} d^2(u_n, v) = \sum_{v\in\bigcup_{i=0}^{n-1}V_i} d^2(u_n, v) + \sum_{v\in Vn} d^2(u_n, v). \qquad (6)$$

The graph G_n is a tree, so, for every vertex, $v \in \bigcup\limits_{i=0}^{n-1} V_i$:

$$d(u_n, v) = 1 + d(u_{n-1}, v) .$$

Now by (6) we have:

$$\begin{aligned} d^2(u_n) &= \sum_{v\in\bigcup_{i=0}^{n-1}V_i} (d\ (u_{n-1}, v) + 1)^2 + \sum_{v\in Vn} d^2(u_n, v) \\ &= \sum_{v\in\bigcup_{i=0}^{n-1}V_i} d^2(u_{n-1}, v) + 2\sum_{v\in\bigcup_{i=0}^{n-1}V_i} d\ (u_{n-1}, v) + \sum_{v\in V_n} d^2(u_n, v) + 2^n - 1 \qquad (7) \\ &= d^2(u_{n-1}) + 2d(u_{n-1}) + \sum_{v\in Vn} d^2(u_n, v) + 2^n - 1. \end{aligned}$$

2^n vertices are in the n'–th branch and by symmetric structure of the graph G_n we have :

$$\begin{aligned} \sum_{v\in V_n} d^2(u_n, v) &= 2^{n-1}(2n)^2 + 2^{n-2}(2n-2)^2 + \ldots + 2^0(2)^2 \\ &= \sum_{i=1}^{n} 2^{i+1} i^2 = 2^{n+2}(n^2 - 2n + 3) - 12. \end{aligned} \qquad (8)$$

By (4) in the proof of the proposition 2.1, and considering (7), (8):

$$\begin{aligned} d^2(u_n) &= \sum_{i=1}^{n} d^2(u_i) - d^2(u_{i-1}) \\ &= \sum_{i=1}^{n} (4i^2 - 4i + 3)2^i + 2i - 3 = 2^{n+1}(4n^2 - 12n + 19) + n^2 - 2n - 38 \end{aligned}$$

Therefore:

$$\begin{aligned} \Sigma_{\{u,v\}\subseteq V} d^2(u,v) - \Sigma_{\{u,v\}\subseteq\bigcup_{i=0}^{n-1}V_i} d^2(u,v) &= 2^n\ \ d^2(u_n) - \Sigma_{\{u,v\}\subseteq V_n} d^2(u,v) \\ &= 2^n\ \ d^2(u_n) - 2^{n-1}\Sigma_{v\in V_n} d^2(u_n, v) \\ &= 2^{2n+1}(3n^2 - 10n + 16) + 2n(n^2 - 2n - 32). \end{aligned}$$

Now let,

$$F(i) = \sum_{\{u,v\}\subseteq\bigcup_{i=0}^{i}V_j} d^2(u,v).$$

So,

$$\sum_{\{u,v\}\subseteq V} d^2(u,v) = \sum_{i=1}^{n} (F(i) - F(i-1)) = \sum_{i=1}^{n} 2^{2i+1}(3i^2 - 10i + 16) + 2^i(i^2 - 2i - 32)$$

$$= 4^{n+1}.2(n^2 - 4n + 7) + 2^{n+1}(n^2 - 4n - 27) - 2. \qquad (9)$$

Now considering (9) and the formula of $W(G_n)$ which was computed in proposition 2.1, and replacing those in (5), the proof is done. ■

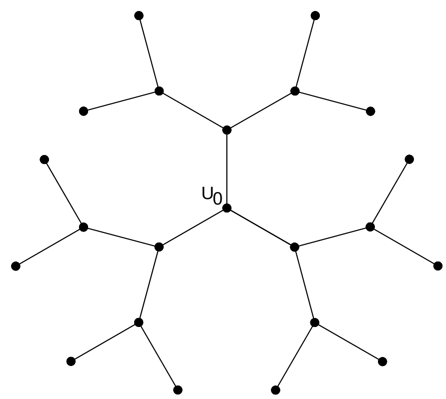

Figure 2. The second dendrimer graph H_n.

3. CALCULATING THE WIENER, HYPER–WIENER AND PI INDICES OF THE SECOND DENDRIMER GRAPH H_n

Let $G = (V,E)$ be the graph with vertex set V and edge set E, that begins with one vertex u_0 in Figure 2 that connects to three vertices which form the first branch and each one of these three vertices connects to two other vertices in second branch and so on. It means that any vertex but u_0 in the i'–th branch joins to the two vertices in the (i+1)'–th branch, so the vertices which have the same distance from u_0 are located on one branch. Let G have $n+1$ branches therefore, there are $3\times 2^{i-1}$vertices in the i'–th branch ($0 < \mathrm{i} \le n$). The graph G is another kind of dendrimer graph which have $n+1$ branches, which is denoted by H_n.

Proposition 3.1. Let $H_n = (V, E)$ be the dendrimer graph in Figure 2, then:

$$W(H_n) = 3(3\mathrm{n}-5)4^{\mathrm{n}} + 18\times 2^{\mathrm{n}} - 3.$$

Proof. The graph H_n consists of a starting vertex u_0 and n+1 branches such that the vertex set of the i'–th branch ($i > 0$), has $3\times 2^{i-1}$ vertices and is denoted by V_i and $|V_0|=1$. So we have:

$$|V| = 1 + |\bigcup_{i=0}^{n} V_i| = 1 + 3\sum_{i=0}^{n-1} 2^i = 3\times 2^n - 2.$$

Because of the symmetric structure of the graph G in Figure 2, $d(u)$ for every vertex u in the n'–th branch is constant and doesn't depend on u, so we choose u_i as representative of the i'–th branch ($0 \leq \mathrm{i} \leq n$).

$$d(u_n) = \sum_{v \in V_n} d(u_n, v) + \sum_{v \in V - V_n} d(u_n, v). \tag{10}$$

2/3 vertices in n'–th branch have the same distance from u_i which is:

$$2d(u_n, u_0) = 2n .$$

And the distance of 1/2 of the rest vertices in this branch from u_n is:

$$2d(u_n, u_1) = 2(n-1) .$$

By continuing in this way we have:

$$\begin{aligned}
\sum_{v \in V_n} d(u_n, v) &= \frac{2}{3}(3 \times 2^{n-1}) \times 2d(u_n, u_0) + \frac{1}{2} \times \frac{1}{3}(3 \times 2^{n-1}) \times 2d(u_n, u_1) \\
&+ \frac{1}{4} \times \frac{1}{3}(3 \times 2^{n-1}) \times 2d(u_n, u_2) + \ldots + \frac{1}{2^{n-1}} \times \frac{1}{3}(3 \times 2^{n-1}) 2d(u_n, u_{n-1}) \\
&2n \times 2^n + 2(n-1) \times 2^{n-2} + 2(n-2) \times 2^{n-3} + \ldots + 2 \times 2^0 \\
&n \times 2^n + \sum_{i=1}^{n} i 2^i = 2 + (3n-2) \times 2^n.
\end{aligned} \tag{11}$$

Now because H_n is a tree, the path between any two vertices is unique and for every vertex $v \in \bigcup_{i=0}^{n} V_i$ we have:

$$d(u_n, v) = 1 + d(u_{n-1}, v) .$$

So:

$$\sum_{v \in \bigcup_{i=0}^{n-1} V_i} d(u_n, v) - \sum_{v \in \bigcup_{i=0}^{n-1} V_i} d(u_{(n-1)}, v) = \left| \bigcup_{i=0}^{n-1} V_i \right| = 3 \times 2^{n-1} - 2. \tag{12}$$

By (10), (11) and (12) we have:

$$\begin{aligned}
d(u_n) - d(u_{n-1}) &= \sum_{v \in V_n} d(u_n, v) - \sum_{v \in V - V_n} d(u_{(n-1)}, v) \\
2 + (3n-2)2^n + (3 \times 2^{(n-1)}) - 2 &= (6n-1)2^{n-1} - 2^n + 1 \\
d(u_n) &= \sum_{i=1}^{n} d(u_i) - d(u_{i-1}) = 7 + (6n-7)2^n
\end{aligned}$$

If the Wiener index of H_n with $n+1$ branches is denoted by $W(n)$, we have:

$$\begin{aligned}
W(n) - W(n-1) &= 3 \times 2^{(n-1)} \left(7 + (6n-7)2^n\right) - \frac{1}{2}(3 \times 2^{n-1})(2 + (3n-2)2^n) \\
&18 \times 2^{n-1}((3n-4).2^{n-2} + 1)
\end{aligned}$$

Therefore,

$$W(n) = \sum_{i=0}^{n} 18 \times 2^{i-1}((3i-4).2^{i-2} + 1) = 3(3n-5)4^n + 18 \times 2^n - 3 .$$

And the proof is completed. ■

Corollary 3.2. $Sz(H_n) = 3(3\mathrm{n} - 5)4^{\mathrm{n}} + 18\times 2^{\mathrm{n}} - 3$.

Proof. The graph H_n is a tree so, by [11] the result is obtained. ■

Corollary 3.3. $S(H_n) = 4^{\mathrm{n}}(36\mathrm{n} - 69) + 87(2^{\mathrm{n}}) - 18$.

Proof. Because H_n is a tree by [11] we have, $S(G_n) = 4W(G_n) - \mathrm{n}(\mathrm{n}-1)$, where *n* is the number of vertices of H_n. Now by replacing the closed form of $W(H_n)$ which was obtained from proposition 3.1, the proof is completed. ■

Corollary 3.4. $Gut(G_n) = 4^{\mathrm{n}}(36\mathrm{n} - 78) + 105(2^{\mathrm{n}}) - 97$.

Proof. Because H_n is a tree by [11] we have, $Gut(G_n) = 4W(G_n) - (2\mathrm{n}-1)(\mathrm{n}-1)$ which *n* is the number of vertices of H_n and by proposition 3.1 it is done. ■

Corollary 3.5. $PI(H_n) = (3\times 2^{\mathrm{n}} - 3)\,(3\times 2^{\mathrm{n}} - 4)$.

Proof. Because H_n is a tree so for every edge $e = uv$ of H_n we have:

$$n_u(e\,|\,\mathrm{H_n}) + n_v(e\,|\,\mathrm{H_n}) = |V| = 3\times 2^{\mathrm{n}} - 2.$$

Subgraphs of H_n with vertex sets $N_u(e\,|\,\mathrm{H_n})$ and $N_v(e\,|\,H_n)$ both are trees, so the number of edges of them are $n_u(e\,|\,\mathrm{H_n}) - 1$ and $n_v(e\,|\,\mathrm{H_n}) - 1$ respectively. Then we have*:*

$$\begin{aligned} n_{eu}(e\,|\,\mathrm{H_n}) + n_{ev}(e\,|\,\mathrm{H_n}) &= n_u(e\,|\,\mathrm{H_n}) + n_v(e\,|\,\mathrm{H_n}) - 2 = 3\times 2^{\mathrm{n}} - 2 \\ PI(H_n) = |E|\,(3\times 2^{\mathrm{n}} - 4) &= (3\times 2^{\mathrm{n}} - 3)(3\times 2^{\mathrm{n+1}} - 4) \end{aligned}$$

Proposition 3.6. The hyper–Wiener index of H_n is:

$$WW(H_n) = \frac{1}{2}\left((18\mathrm{n}^2 - 51\mathrm{n} + 81)4^{\mathrm{n}} - 87(2^{\mathrm{n}}) + 6\right).$$

Proof. By the definition we have:

$$WW(H_n) = \frac{1}{2}\big(W(H_n) + \sum\nolimits_{\{u,v\}\subseteq V} d^2(u,v)\big). \tag{14}$$

Because of the symmetric structure of the graph H_n Figure 2, *d(u)* for every vertex *u* in the *n*'–th branch is constant and doesn't depend on *u*, so we choose u_i as representative of the *i*'–th branch ($0 \le \mathrm{i} \le 1$).

$$d^2(u_n) = \sum\nolimits_{v\in V} d^2(u_n, v) = \sum\nolimits_{v\in\bigcup_{i=0}^{n-1} V_i} d^2(u_n, v) + \sum\nolimits_{v\in Vn} d^2(u_n, v). \tag{15}$$

The graph H_n is a tree so, for any vertex $v \in \bigcup_{i=0}^{n-1} V_i$:

$$d(u_n, v) = 1 + d(u_{n-1}, v)$$

Now by (15) we have:

$$\begin{aligned} d^2(u_n) &= \sum_{v\in\bigcup_{i=0}^{n-1}V_i} (d\ (u_{n-1}, v)+1)^2 + \sum_{v\in Vn} d^2(u_n, v) \\ &= \sum_{v\in\bigcup_{i=0}^{n-1}V_i} d^2(u_{n-1}, v) + 2\sum_{v\in\bigcup_{i=0}^{n-1}V_i} d\ (u_{n-1}, v) + \sum_{v\in V_n} d^2(u_n, v) + 3\times 2^{n-1} - 2 \\ &= d^2(u_{n-1}) + 2d(u_{n-1}) + \sum_{v\in Vn} d^2(u_n, v) + 3\times 2^{n-1} - 2. \end{aligned} \tag{16}$$

2/3 vertices of the n'–th branch have the same distance from u_n which is:

$$2d(u_n, u_0) = 2n,$$

and the distance of 1/2 of the rest vertices in this branch from u_n is:

$$\begin{aligned} \sum_{v\in V_n} d^2(u_n, v) &= \frac{2}{3}(3\times 2^{n-1})(2n)^2 + \frac{1}{2}.\frac{1}{3}(3\times 2^{n-1})(2n-2)^2 \\ &+ \frac{1}{4}.\frac{1}{3}(3\times 2^{n-1})(2n-4)^2 + \ldots + 2^0(2)^2 \\ &2^{n+2}n^2 + 2^n(n-1)^2 + 2^{(n-1)}(n-2)^2 + \ldots + 2^0(2)^2 \\ &= 2^{n+1}n^2 + \sum_{i=1}^{n} 2^{i+1}i^2 = 2^{n+1}(3n^2 - 4n + 6) - 12. \end{aligned} \tag{17}$$

By (13) in the proof of the proposition 3.1, and considering (16), (17):

$$\begin{aligned} d^2(u_n) &= \sum_{i=1}^{n} d^2(u_i) - d^2(u_{i-1}) \\ &= \sum_{i=1}^{n} 2^{i-1}(12i^2 - 4i + 1) = (12n^2 - 28n + 41)2^n - 41 \end{aligned}$$

Therefore:

$$\begin{aligned} \sum_{\{u,v\}\subseteq V} d^2(u, v) - \sum_{\{u,v\}\subseteq\bigcup_{i=0}^{n-1}V_i} d^2(u, v) &= (3\times 2^n\ - 2)d^2(u_n) - \sum_{\{u,v\}\subseteq V_n} d^2(u, v) \\ &= (3\times 2^n\ - 2)d^2(u_n) - (3\times 2^{n-2})\sum_{v\in V_n} d^2(u_n, v). \end{aligned}$$

Now let,

$$F(i) = \sum_{\{u,v\}\subseteq\bigcup_{j=0}^{i}V_j} d^2(u, v).$$

So, we have:

$$\sum_{\{u,v\}\subseteq V} d^2(u, v) = \sum_{i=1}^{n} F(i) - F(i-1) = 6(3n^2 - 10n + 16)4^n - 105(2^n) + 9. \tag{18}$$

Now considering (18) and the formula of $W(H_n)$ which was computed in Proposition 3.1, and replacing those in (14), the proof is done. ■

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On the Multiplicative Zagreb Indices of Bucket Recursive Trees

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ABSTRACT

Bucket recursive trees are an interesting and natural generalization of ordinary recursive trees and have a connection to mathematical chemistry. In this paper, we give the lower and upper bounds for the moment generating function and moments of the multiplicative Zagreb indices in a randomly chosen bucket recursive tree of size n with maximal bucket size $b \geq 1$. Also, we consider the ratio of the multiplicative Zagreb indices for different values of n and b. All our results reduce to the ordinary recursive trees for $b = 1$.

1. INTRODUCTION

Trees are defined as connected graphs without cycles. Recursive trees are rooted labelled trees, where the root is labelled by 1 and the labels of all successors of any node v are larger than the label of v [8]. It is of particular interest in applications to assume the random recursive tree model and to speak about a random recursive tree with n nodes, which means that one of the $(n-1)!$ possible recursive trees with n nodes is chosen with equal probability, i.e., the probability that a particular tree with n nodes is chosen is always $1/(n-1)!$. An interesting and natural generalization of random recursive trees has been introduced in [7], and these are called bucket recursive trees. In this model the nodes of a bucket recursive tree are buckets, which can contain up to a fixed integer amount of $b \geq 1$ labels. A probabilistic description of random bucket recursive trees is given by a generalization of the stochastic growth rule for ordinary random recursive trees (which is the special instance $b = 1$). In fact, a tree grows by progressive attraction of increasing integer labels: when inserting label $n+1$ into an existing bucket recursive tree containing n

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labels (i.e., containing the labels $\{1,2,\ldots,n\}$) all n existing labels in the tree compete to attract the label $n+1$, where all existing labels have equal chance to recruit the new label. If the label winning this competition is contained in a node with less than b labels (an unsaturated bucket), label $n+1$ is added to this node, otherwise if the winning label is contained in a node with b labels already (a saturated bucket), label $n+1$ is attached to this node as a new bucket containing only the label $n+1$. Starting with a single bucket as the root node containing only the label 1, after $n-1$ insertion steps, where the labels $2,3,\ldots,n$ are successively inserted according to this growth rule, results in a so called random bucket recursive tree with n labels and maximal bucket size b. For an existing bucket recursive tree T with n labels, the probability that a certain node $v \in T$ with capacity $1 \le c(v) \le b$ attracts the new label $n+1$ is equal to the number of labels contained in v, i.e., $c(v)/n$ (see [7]). Figure 1 illustrates a bucket recursive tree of size $n = 11$ with maximal bucket size $b = 2$. For a connection to chemistry, suppose n atoms in a dendrimer (a repetitively branched molecule) are stochastically labelled with integers $1,2,\ldots,n$, then labelled atoms in a functional group can be considered as the labels of a bucket in a bucket recursive tree. It is obvious that the number of nodes (here buckets) in a bucket recursive tree T is less than n for $b > 1$. Thus we can show the size of the tree as a function of n and b. Let $h(b)$ be a real valued function of b, where $h(1) = 0$ and $h(b) \ge 1$ for all $b \ge 2$. Now, we can write the size of the tree as $n - h(b)$, i.e., $|V(T)| = n - h(b)$. We choose the function $h(b)$ in this form for relation between the bucket recursive trees and ordinary recursive trees.

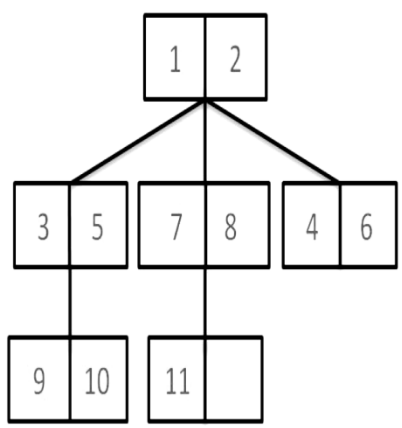

Figure 1: A bucket recursive tree of size 11 with maximal bucket size 2 [6].

Two vertices of graph G, connected by an edge, are said to be adjacent. The number of vertices of G, adjacent to a given vertex v, is the degree of this vertex, and will be denoted by $d(v)$. Todeschini *et al.* [9, 10] have suggested to consider multiplicative variants of additive graph invariants, which applied to the Zagreb indices would lead to the multiplicative Zagreb indices of a graph G, denoted by $\Pi_1(G)$ and $\Pi_2(G)$, under the name first and second multiplicative Zagreb index, respectively. These are defined as

$$\Pi_1(G) = \prod_{v \in V(G)} (d(v))^2 \tag{1}$$

and

$$\Pi_2(G) = \prod_{uv \in E(G)} d(u)d(v), \tag{2}$$

where $V(G)$ and $E(G)$ are the vertex set and edge set of G, respectively [3].

In probability theory and statistics, the moment generating function of a random variable is an alternative specification of its probability distribution. Thus, it provides the basis of an alternative route to analytical results compared with working directly with probability density functions or cumulative distribution functions. There are particularly simple results for the moment generating functions of distributions defined by the weighted sums of random variables. Note, however, that not all random variables have moment generating functions.

Definition 1.1 The moment generating function of a random variable X is defined as

$$M_X(t) = \mathbf{E}(\exp(tX)), \quad t \in \mathrm{R},$$

wherever this expectation exists.

The reason for defining this function is that it can be used to find all the moments of the distribution. In fact,

$$M_X(t) = \sum_{k=0}^{\infty} \frac{\mu_k}{k!} t^k,$$

where μ_k $(k \geq 1)$ is the kth moment of X, i.e., $\mu_k = \mathbf{E}(X^k)$ [1].

2. RESULTS

Let $d_n(v)$ denote the degree of bucket v in our model of size n with maximal bucket size *b*, and $Z_{1,n,b}$ be the first multiplicative Zagreb index. We also define M_n to be the sigma–field generated by the first n stages [1]. If label n is attached to an unsaturated bucket, then $Z_{1,n,b} = Z_{1,n-1,b}$. But if label n is attached to a saturated bucket, then by the stochastic growth rule of the tree and by definition of the first multiplicative Zagreb index,

$$\frac{Z_{1,n,b}}{Z_{1,n-1,b}} = \left(\frac{d_{n-1}(U)+1}{d_{n-1}(U)}\right)^2, \tag{3}$$

where U is uniformly distributed on buckets set.

Theorem 2.1 Let $M(t) = \mathbf{E}(\exp(tZ_{1,n,b}))$ be the moment generating function of $Z_{1,n,b}$ of a bucket recursive tree of size n with maximal bucket size b. Then

$$M(t) \le \exp\left(\left(4b^{\frac{1}{k}}\right)^{n-b-1}\left(\prod_{j=b+1}^{n-1}\frac{j-h(b)}{j}\right)^{\frac{1}{k}} t\right).$$

Proof. We have

$$M(t) = \sum_{k=0}^{\infty}\frac{\mu_{k,n,b}}{k!}t^k,$$

where $\mu_{k,n,b}\ (k \ge 1)$ is the kth moment of $Z_{1,n,b}$. For $k \ge 1$,

$$\begin{aligned}\mathbf{E}(Z_{1,n,b}^k \mid \mathsf{M}_{n-1}) &= \mathbf{E}(Z_{1,n,b}^k \mid d_{n-1}(v_j),\ j \le n-1-h(b)) \\ &= \frac{Z_{1,n-1,b}^k}{n-1}\sum_{j=1}^{|V(T_{n-1})|}\left(\frac{d_{n-1}(v_j)+1}{d_{n-1}(v_j)}\right)^{2k} c(v_j),\end{aligned}$$

since $Z_{1,n-1,b}^k$ is M_{n-1}-measurable and the label n is attached to any saturated bucket v of the already grown tree T_{n-1} with probability $\frac{c(v)}{n-1}$. Thus

$$\mathbf{E}(Z_{1,n,b}^k \mid \mathsf{M}_{n-1}) \le \frac{n-1-h(b)}{n-1}4^k b Z_{1,n-1,b}^k. \tag{4}$$

Taking expectation of the inequality (4):

$$\mu_{k,n,b} \le 4^k b\frac{n-1-h(b)}{n-1}\mu_{k,n-1,b}, \quad k \ge 1. \tag{5}$$

Also $Z_{1,b+1,b} = 1$. Thus (5) leads to

$$\mu_{k,n,b} \le (4^k b)^{n-b-1}\prod_{j=b+1}^{n-1}\frac{j-h(b)}{j} \tag{6}$$

and proof is completed.

If we replace t by $\ln t$, then we obtain the upper bound for the probability generating function [1].

Let $Z_{2,n,b}$ be the second multiplicative Zagreb index of a bucket recursive tree of size n with maximal bucket size b. Then by definition of the second multiplicative Zagreb index,

$$\frac{Z_{2,n,b}}{Z_{2,n-1,b}} = \left(\frac{d_{n-1}(U)+1}{d_{n-1}(U)}\right)^{d_{n-1}(U)} \times (d_{n-1}(U)+1). \tag{7}$$

Theorem 2.2 Let $N(t) = \mathbf{E}(\exp(tZ_{2,n,b}))$ be the moment generating function of $Z_{2,n,b}$ of a bucket recursive tree of size n with maximal bucket size b. Then

$$N(t) \geq \exp\left(\left(4b^{\frac{1}{k}}\right)^{n-b-1}\left(\prod_{j=b+1}^{n-1}\frac{j-h(b)}{j}\right)^{\frac{1}{k}} t\right).$$

Proof. Let $\gamma_{k,n,b}$ $(k \geq 1)$ be the kth moment of $Z_{2,n,b}$ of a bucket recursive tree of size n with maximal bucket size b. For $k \geq 1$, similar to the first multiplicative Zagreb index,

$$\begin{aligned}
\mathbf{E}(Z_{2,n,b}^{k} \mid \mathsf{M}_{n-1}) &= \mathbf{E}(Z_{2,n,b}^{k} \mid d_{n-1}(v_j),\ j \leq n-1-h(b)) \\
&= \frac{Z_{2,n,b}^{k}}{n-1}\sum_{j=1}^{n-1-h(b)}\left(\frac{d_{n-1}(v_j)+1}{d_{n-1}(v_j)}\right)^{d_{n-1}(v_j)} \\
&\quad \times (d_{n-1}(v_j)+1)c(v_j).
\end{aligned}$$

Thus

$$\mathbf{E}(Z_{2,n,b}^{k} \mid \mathsf{M}_{n-1}) \geq \frac{n-1-h(b)}{n-1}4^{k} bZ_{2,n-1,b}^{k}. \tag{8}$$

Taking expectation of the inequality (8):

$$\gamma_{k,n,b} \geq 4^{k} b\frac{n-1-h(b)}{n-1}\gamma_{k,n-1,b}, \quad k \geq 1.$$

Now, proof is completed just similar to the proof of Theorem 2.1.

In passing, we consider the ratio of the multiplicative Zagreb indices for different values of n and b.

Theorem 2.3 Suppose

$$Z^{*}_{t_1,t_2,n,b;k} = \frac{Z^{k}_{t_1,n,b}}{Z^{k}_{t_2,n,b}}, \quad t_i \in \{1,2\}, t_1 \neq t_2$$

and

$$\mathsf{P}_{t_1,t_2,n,b;k} = \mathbf{E}(Z^{*}_{t_1,t_2,n,b;k}).$$

Then

$$\mathsf{P}_{2,1,n,b;k} \geq \frac{4^k}{b^{n-b-1}} \prod_{j=b+1}^{n-1} \frac{j}{j-h(b)}$$

and

$$\mathsf{P}_{1,2,n,b;k} \leq \frac{b^{n-b-1}}{4^k} \prod_{j=b+1}^{n-1} \frac{j-h(b)}{j}.$$

Proof. We have $Z^{k}_{2,n,b} \geq Z^{k}_{2,n-1,b}$. Let $g(x) = x^{-1}$ for $x > 0$. Then g is convex because $g''(x) = 2x^{-3} \geq 0$ and by Jensen's inequality $\mathbf{E}(\frac{1}{X}) \geq \frac{1}{\mathbf{E}(X)}$. Thus

$$\begin{aligned}
\mathsf{P}_{2,1,n,b;k} &= \mathbf{E}\left(\mathbf{E}\left(\frac{Z^{k}_{2,n,b}}{Z^{k}_{1,n,b}} \,|\, \mathsf{M}_{n-1}\right)\right) \\
&\geq \mathbf{E}\left(\mathbf{E}\left(\frac{Z^{k}_{2,n-1,b}}{Z^{k}_{1,n,b}} \,|\, \mathsf{M}_{n-1}\right)\right) \\
&\geq \mathbf{E}\left(Z^{k}_{2,n-1,b}\mathbf{E}\left(\frac{1}{Z^{k}_{1,n,b}} \,|\, \mathsf{M}_{n-1}\right)\right) \\
&\geq \mathbf{E}\left(4^k Z^{k}_{2,n-2,b}\mathbf{E}\left(\frac{1}{Z^{k}_{1,n,b}} \,|\, \mathsf{M}_{n-1}\right)\right) \\
&\geq \cdots \geq 4^{k(n-b)}\mathbf{E}\left(\frac{1}{Z^{k}_{1,n,b}}\right) \\
&\geq 4^{k(n-b)} \frac{1}{\mu_{n,b,k}} \\
&\geq \frac{4^k}{b^{n-b-1}} \prod_{j=b+1}^{n-1} \frac{j}{j-h(b)}.
\end{aligned}$$

With the same manner, we can obtain the upper bound for $\mathsf{P}_{1,2,n,b;k}$.

Theorem 2.4 Suppose

$$Z^{*}_{1,2,n,b_1,b_2;k} = \frac{Z^{k}_{1,n,b_1}}{Z^{k}_{2,n,b_2}}, \quad Z^{*}_{2,1,n,b_1,b_2;k} = \frac{Z^{k}_{2,n,b_1}}{Z^{k}_{1,n,b_2}}, \; b_1 \neq b_2,$$

and

$$\mathsf{K}_{1,2,n,b_1,b_2;k} = \mathbf{E}(Z^*_{1,2,n,b_1,b_2;k}), \qquad \mathsf{S}_{2,1,n,b_1,b_2;k} = \mathbf{E}(Z^*_{2,1,n,b_1,b_2;k}).$$

Then

$$\mathsf{K}_{1,2,n,b_1,b_2;k} \le 4^{k(b_2-b_1-1)} b_1^{n-b_1-1} \prod_{j=b_1+1}^{n-1} \frac{j-h(b_1)}{j},$$

and

$$\mathsf{S}_{2,1,n,b_1,b_2;k} \ge \frac{4^{k(b_2-b_1+1)}}{b_2^{n-b_2-1}} \prod_{j=b_2+1}^{n-1} \frac{j}{j-h(b_2)}.$$

Proof. By definition of the conditional expectation,

$$\begin{aligned}
\mathsf{K}_{1,2,n,b_1,b_2;k} &= \mathbf{E}\left(\mathbf{E}\left(\frac{Z^k_{1,n,b_1}}{Z^k_{2,n,b_2}} \mid \mathsf{M}_{n-1}\right)\right) \\
&\le \mathbf{E}\left(\mathbf{E}\left(\frac{Z^k_{1,n,b_1}}{Z^k_{2,n-1,b_2}} \mid \mathsf{M}_{n-1}\right)\right) \\
&\le \cdots \le \frac{1}{4^{k(n-b_2)}} \mu_{n,b_1,k} \\
&\le 4^{k(b_2-b_1-1)} b_1^{n-b_1-1} \prod_{j=b_1+1}^{n-1} \frac{j-h(b_1)}{j}.
\end{aligned}$$

With the same manner, we can obtain the lower bound for $\mathsf{S}_{2,1,n,b_1,b_2;k}$.

Corollary 2.5 The presented results in Theorem 4 reduce to the previous results in Theorem 2 for $b_1 = b_2 = b$.

Theorem 2.6 Suppose

$$Z^*_{t,i,b} = \frac{Z^k_{t,i,b}}{Z^k_{t,i-1,b}}, \quad t = 1,2,\ Z_{t,i,b} \ne Z_{t,i-1,b}$$

and

$$\mathsf{E}_{t,i,j,b} = \mathsf{E}(Z^*_{t,i,b} Z^*_{t,j,b}), \quad i < j.$$

Then

$$\mathsf{E}_{1,i,j,b,k} \le \frac{(i-1-h(b))(j-1-h(b))}{(i-1)(j-1)} (4^k b)^2$$

and

$$\mathsf{E}_{2,i,j,b,k} \ge \frac{(i-1-h(b))(j-1-h(b))}{(i-1)(j-1)} (4^k b)^2.$$

Proof. From (4),

$$
\begin{aligned}
\mathsf{E}_{1,i,j,b,k} &= \mathbf{E}(\mathbf{E}(Z^*_{1,i,b} Z^*_{1,j,b} \mid \mathsf{M}_{j-1})) \\
&= \mathbf{E}(Z^*_{1,i,b} \mathbf{E}(Z^*_{1,j,b} \mid \mathsf{M}_{j-1})) \\
&\le 4^k b \frac{j-1-h(b)}{j-1} \mathbf{E}(Z^*_{1,i,b}) \\
&= 4^k b \frac{j-1-h(b)}{j-1} \mathbf{E}(\mathbf{E}(Z^*_{1,i,b} \mid \mathsf{M}_{i-1})) \\
&\le \frac{(i-1-h(b))(j-1-h(b))}{(i-1)(j-1)} (4^k b)^2.
\end{aligned}
$$

With the same manner, we can obtain the lower bound of $\mathsf{E}_{2,i,j,b,k}$.

We can study the ratio of the multiplicative Zagreb indices for different values of k as n and d are different with the above presented approach.

Corollary 2.7 For ordinary recursive trees,

$$
\begin{aligned}
\mu_{k,n,1} &\le 4^{k(n-2)}, \quad M(t) \le \exp(4^{n-2} t), \\
\gamma_{k,n,1} &\ge 4^{k(n-2)}, \quad N(t) \ge \exp(4^{n-2} t)
\end{aligned}
$$

.

Also, let $r, k \in [1, \infty]$ with $1/r + 1/k = 1$. By Holder's inequality,

$$
\begin{aligned}
\mathbf{E}(Z_{1,n,b} Z_{1,m,b}) &\le (\mu_{k,n,1})^{\frac{1}{k}} (\mu_{r,n,1})^{\frac{1}{r}} \\
&\le 4^{m+n-4}.
\end{aligned}
$$

Also

$$
\mathsf{P}_{1,2,n,1;k} \le 4^{-k}, \quad \mathsf{P}_{2,1,n,1;k} \ge 4^{k}
$$

and

$$
\mathsf{E}_{1,i,j,1,k} \le 16^k, \quad \mathsf{E}_{2,i,j,1,k} \ge 16^k.
$$

Then the bounds does not depend on i and j in ordinary recursive trees.

3. DISCUSSION AND CONCLUSION

So far, the multiplicative Zagreb indices have been studied vastly in literature from mathematical point of view. In this paper, we introduced the first probabilistic analysis of the multiplicative Zagreb indices in the random bucket recursive trees. Through the recurrence equations, an upper bound related to the first multiplicative Zagreb index and a lower bound related to the second multiplicative Zagreb index are obtained. As an interesting result it is shown that these bounds are the same in this model. It is difficult to find a lower bound in Theorem 2.1 and an upper bound in Theorem 2.2, since the maximum degree of buckets of our model might not change for different values of n. However, we can study some probabilistic characteristics of these indices such as martingales, asymptotic normality and so on (see [4, 5, 6] for details). The lower and upper bounds for the moment generating function and moments are very important. For example, by Markov's inequality,

$$P(Z_{1,10,1} \geq 4^9) \leq \frac{1}{4}.$$

Eliasi *et al.* [2] considered a multiplicative version of the first Zagreb index defined as

$$\Pi_1^*(G) = \prod_{uv \in E(G)} (d(u) + d(v)).$$

With the same approach, we can obtain the lower and upper bounds related to this index. Generally, one can extend this approach to another indices and tree structures.

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The Conditions of the Violations of Le Chatlier's Principle in Gas Reactions at Constant T and P

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ABSTRACT

Le Chatelier's principle is used as a very simple way to predict the effect of a change in conditions on a chemical equilibrium. However, several studies have been reported the violation of this principle, still there is no reported simple mathematical equation to express the exact condition of violation in the gas phase reactions. In this article, we derived a simple equation for the violation of Le Chatelier's principle for the ideal gas reactions at the constant temperature and pressure.

1. INTRODUCTION AND PRELIMINARIES

Le Chatelier principle (LCP) is a very simple way of predicting the direction of a disturbed chemical equilibrium [1]. LCP is often expressed as follows: In a system at equilibrium, a change in one of the variables that determines the equilibrium will shift the equilibrium in the direction counteracting the change of that variable. However, the LCP has led to some wrong predictions and thus caused to some controversial discussions among many students and teachers [2−7].

The industrial synthesis of ammonia is shown below:

$$N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g)$$

This is a traditional example used by teachers when the LCP is discussed. In this reaction, at constant pressure and temperature, when the mole fraction of nitrogen in the equilibrium mixture exceeds 0.5, the LCP predicts that this change should shift the equilibrium to the right in order to moderate the excess of nitrogen. However, in contrast to LCP prediction this disturbance shifts the reaction to the left, producing more N_2.

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Although many discussions and examples of the failure of LCP have been reported, a simple inquiry to predict the conditions of the failure of LCP in gas phase reaction (at constant T and P) is still missing. The inquiries discussed by Jeffrey E. Lacy [10] are not general and only limited to special cases, where $\Delta \upsilon < 0$.

In this work, we mathematically derive the criteria in which LCP fails to predict the correct direction of a reaction at equilibrium upon changing the mole number of a species at constant T and P.

2. THEOREM AND DERIVATION

Theorem 1. In the ideal gas reaction $\sum_i \nu_i A_i(g) = 0$ where $\frac{\Delta \mathrm{n}}{\mathrm{mol}} = \sum_{\mathrm{i}} \nu_{\mathrm{i}}$ and ν_i is the stoichiometric factor of species $A_i(g)$ in the reaction (where it is positive for products and negative for reactants). At constant temperature (T) and pressure (P), by changing n_j of the j-th species, the reaction proceeds towards the direction that offsets this perturbation unless: $x_j \geq \left|\frac{\nu_j}{\Delta n}\right| mol$ and $\Delta n \neq 0$, where, x_j is the mole fraction of j-th species at the reaction equilibrium before perturbation. In equal st ate, the reaction equilibrium does not change. However, in non-equal state, the perturbation factor is elevated.

Derivation 2. The expression for the chemical potential (μ_i) at equilibrium is given as $\sum \upsilon_i \mu_i = 0$. This term leads to $\Delta G^0 = RTlnK_p^0$, where $\Delta G^0 = \sum \upsilon_i \mu_i^0$ and the standard equilibrium constant $K_P^0 = \prod_i (P_i/P_0)^{\upsilon_i}$ is a function of T only.

For a closed system in equilibrium (at constant P and T), if we perturb the system by adding (or removing) n_i mole of A_j, the equilibrium will shift to the direction to counteract this perturbation. Because in this condition K_{eq} is constant, we use Q_p as a parameter to find the direction of shift. We know from thermodynamic if $Q_p<K_{eq}$, the reaction proceeds forward (producing more product) and if $Q_p > K_{eq}$, the reaction proceeds backward (producing more reactant). At constants T and P, Q depend only on $n_j Q_P = Q_P(n_1, n_2, \ldots, n_j \ldots)$. Let us add small mole of A_j (dn_j) to this system. The term $\frac{\partial Q_P}{\partial n_j}$ represents the change in Q_p upon addition of A_j. As dn_j is positive, the sign of dQ_P illustrates the direction of reaction. The term $dQ_P > 0$ denotes the elevation of Q_p upon addition of species. This is the case where reaction proceeds backward to reach the new equilibrium (because K_{eq} is constant). In the same way, the reaction proceeds forward if $dQ_P < 0$. However, there is no change in the reaction equilibrium upon addition of n_j if $dQ = 0$. Before going step forward to the final statement, let us discuss the following required expressions:

$$\frac{\Delta n}{mol} = \sum_i \nu_i \tag{1}$$

$$Q_P = \prod_i (P_i)^{\nu_i} \tag{2}$$

$$P_i = x_i P \tag{3}$$

$$x_i = \frac{n_i}{n_t} \tag{4}$$

$$n_t = \sum_i n_i \tag{5}$$

where in these equations, P_i , x_i, and n_i are partial pressure, mole faction, and mole numbers of A_i, respectively. The n_t is the total mole numbers of all gases in the reaction. By substituting the equations 1, 3, 4 into Eq. 2, we get:

$$\begin{aligned} Q_P &= \prod_i (P_i)^{\nu_i} = \prod_i (x_i P)^{\nu_i} \\ &= \left(\prod_i (x_i)^{\nu_i}\right)\left(\prod_i (P)^{\nu_i}\right) \\ &= \left(\prod_i \left(\frac{n_i}{n_t}\right)^{\nu_i}\right)\left((P)^{\sum_i \nu_i}\right) \\ &= \left(\frac{\prod_i (n_i)^{\nu_i}}{\prod_i (n_t)^{\nu_i}}\right)\left((P)^{\frac{\Delta n}{mol}}\right) \\ &= \left(\frac{\prod_i (n_i)^{\nu_i}}{(n_t)^{\sum_i \nu_i}}\right)(P)^{\frac{\Delta n}{mol}} \\ &= \left(\frac{\prod_i (n_i)^{\nu_i}}{(n_t)^{\frac{\Delta n}{mol}}}\right) P^{\frac{\Delta n}{mol}} \\ &= P^{\frac{\Delta n}{mol}} n_t^{-\frac{\Delta n}{mol}} \prod_i (n_i)^{\nu_i} \end{aligned} \tag{6}$$

The final statement is used to obtain $\left(\frac{\partial Q_P}{\partial n_j}\right)_{T,P,n_{i\neq j}}$

$$\begin{aligned} \left(\frac{\partial Q_P}{\partial n_j}\right)_{T,P,n_{i\neq j}} &= \left(\frac{\partial}{\partial n_j}\right)_{T,P,n_{i\neq j}} \left[P^{\frac{\Delta n}{mol}} n_t^{-\frac{\Delta n}{mol}} \left(\prod_i (n_i)^{\nu_i}\right)\right] = P^{\frac{\Delta n}{mol}} \left(\frac{\partial}{\partial n_j}\right)_{T,P,n_{i\neq j}} \left[n_t^{-\frac{\Delta n}{mol}} \left(\prod_i (n_i)^{\nu_i}\right)\right] \\ &= P^{\frac{\Delta n}{mol}} \left[\left(-\frac{\Delta n}{mol}\right)\left((n_t)^{-\frac{\Delta n}{mol}-1}\right)\left(\prod_i (n_i)^{\nu_i}\right) + \left((n_t)^{-\frac{\Delta n}{mol}}\right)(\nu_j)\left((n_j)^{\nu_j-1}\right)\left(\prod_{i\neq j} (n_i)^{\nu_i}\right)\right] \\ &= P^{\frac{\Delta n}{mol}} \left[\left(-\frac{\Delta n}{mol}\right)\left(\frac{(n_t)^{-\frac{\Delta n}{mol}}}{n_t}\right)\left(\prod_i (n_i)^{\nu_i}\right) + \left((n_t)^{-\frac{\Delta n}{mol}}\right)(\nu_j)\left(\frac{(n_j)^{\nu_j}}{n_j}\right)\left(\prod_{i\neq j} (n_i)^{\nu_i}\right)\right] \\ &\times \left(\frac{P}{n_t}\right)^{\frac{\Delta n}{mol}} \left[\left(-\frac{\Delta n}{mol}\right)\frac{1}{n_t}\prod_i (n_i)^{\nu_i} + (\nu_j)\frac{1}{n_j}\prod_i (n_i)^{\nu_i}\right] \\ &= \left(\frac{P}{n_t}\right)^{\frac{\Delta n}{mol}} \prod_i (n_i)^{\nu_i} \left[\left(-\frac{\Delta n}{mol}\right)\frac{1}{n_t} + (\nu_j)\frac{1}{n_j}\right] \end{aligned} \tag{7}$$

By Eq. 4 into the final term of Eq. 7, we have:

$$x_j = \frac{n_j}{n_t} \rightarrow n_t = \frac{n_j}{x_j}$$

$$\left(\frac{\partial Q_P}{\partial n_j}\right)_{T,P,n_{i\neq j}} = \left(\frac{P}{n_t}\right)^{\frac{\Delta n}{mol}} \prod_i (n_i)^{\nu_i} \left[-\frac{\Delta n}{mol}\frac{1}{n_j/_{x_j}} + \frac{\nu_j}{n_j}\right]$$
$$= \left(\frac{P}{n_t}\right)^{\frac{\Delta n}{mol}} \prod_i (n_i)^{\nu_i} \left[-\frac{\Delta n}{mol}\frac{x_j}{n_j} + \frac{\nu_j}{n_j}\right] = \left(\frac{P}{n_t}\right)^{\frac{\Delta n}{mol}} \left(\frac{\prod_i (n_i)^{\nu_i}}{n_j}\right)\left[\nu_j - x_j\frac{\Delta n}{mol}\right] \tag{8}$$

The statement before bracket is denoted as ω for simplicity. It is clear that this statement is positive.

$$\left(\frac{P}{n_t}\right)^{\frac{\Delta n}{mol}} \left(\frac{\prod_i (n_i)^{\nu_i}}{n_j}\right) \equiv \omega > 0$$

Now Eq. 8 will be written as:

$$\left(\frac{\partial Q_P}{\partial n_j}\right)_{T,P,n_{i\neq j}} = \omega\left[\nu_j - x_j\frac{\Delta n}{mol}\right] \tag{9}$$

$$(\partial Q_P)_{T,P,n_{i\neq j}} = \omega\left[\nu_j - x_j\frac{\Delta n}{mol}\right](\partial n_j)_{T,P,n_{i\neq j}} \tag{10}$$

We now assume $(\partial n_j)_{T,P,n_{i\neq j}}$ is positive, which means that n_j is added to the system. Therefore, the only parameter which effects the sign of $(\partial Q_P)_{T,P,n_{i\neq j}}$ is the statement inside the bracket,i.e. $\nu_j - x_j\frac{\Delta n}{mol}$. We now try to determine the sign of this statement. To do it, let us refer to the absolute property as follows:

$$|\theta| = \begin{cases} +\theta, & \theta > 0 \\ -\theta, & \theta < 0 \end{cases} \tag{11}$$

We now distribute Eq. 10 vs. sign of ν_j and Δn to find in which condition $(\partial Q_P)_{T,P,n_{i\neq j}}$ is positive, negative or zero. For simplicity, we omit subscript T, P and $n_{i\neq j}$.

$$\begin{cases}
\nu_j > 0 \to \partial Q_P = \omega\left[+|\nu_j| - x_j\frac{\Delta n}{mol}\right]\partial n_j \begin{cases}
\Delta n > 0 \to \partial Q_P = \omega\left[+|\nu_j| - x_j\left|\frac{\Delta n}{mol}\right|\right]\partial n_j \to \begin{cases} |\nu_j| > x_j\left|\frac{\Delta n}{mol}\right| \to \partial Q_P > 0 \\ |\nu_j| < x_j\left|\frac{\Delta n}{mol}\right| \to \partial Q_P < 0 \\ |\nu_j| = x_j\left|\frac{\Delta n}{mol}\right| \to \partial Q_P = 0 \end{cases} \\
\Delta n = 0 \to \partial Q_P = \omega[+|\nu_j|]\partial n_j > 0 \\
\Delta n < 0 \to \partial Q_P = \omega\left[+|\nu_j| + x_j\left|\frac{\Delta n}{mol}\right|\right]\partial n_j > 0
\end{cases} \\
\nu_j < 0 \to \partial Q_P = \omega\left[-|\nu_j| - x_j\frac{\Delta n}{mol}\right]\partial n_j \begin{cases}
\Delta n > 0 \to \partial Q_P = \omega\left[-|\nu_j| - x_j\left|\frac{\Delta n}{mol}\right|\right]\partial n_j < 0 \\
\Delta n = 0 \to \partial Q_P = \omega[-|\nu_j|]\partial n_j < 0 \\
\Delta n < 0 \to \partial Q_P = \omega\left[-|\nu_j| + x_j\left|\frac{\Delta n}{mol}\right|\right]\partial n_j \to \begin{cases} |\nu_j| > x_j\left|\frac{\Delta n}{mol}\right| \to \partial Q_P < 0 \\ |\nu_j| < x_j\left|\frac{\Delta n}{mol}\right| \to \partial Q_P > 0 \\ |\nu_j| = x_j\left|\frac{\Delta n}{mol}\right| \to \partial Q_P = 0 \end{cases}
\end{cases}
\end{cases} \tag{12}$$

For conditions 1, 4 and 5 of Eq. 12, where $\nu_j > 0$ and $Q_P > 0$, by adding more species from products ($\nu_j > 0$) Q_p increases. Therefore, the reaction shifts backward to reach the equilibrium, which is in agreement with the LCP. The conditions 6, 7 and 8 are also in agreement with LCP; where by adding more reactants reaction proceeds forward. For conditions 3 and 10, no effect will be appeared by adding n_j while $\partial Q_P = 0$. The condition 2 (where $\nu_j > 0$ and $\partial Q_P < 0$) reveals that by adding more product to the reaction at equilibrium, the reaction shifts to the right to produce more product, which is in contradiction to the LCP. The situation 9 is also contradictory to the LCP; where by adding more reactant, the reaction shifts to the left. For these conditions we can write:

$$|\nu_j| < x_j \left|\frac{\Delta n}{mol}\right| \Rightarrow x_j > \left|\frac{\nu_j}{\Delta n}\right| mol \tag{13}$$

By combining conditions 2, 3, 9 and 10, we obtain:

$$x_j \geq \left|\frac{\nu_j}{\Delta n}\right| mol \tag{14}$$

This is the equation we were searching for. From this equation we conclude that the term $x_j = \left|\frac{\nu_j}{\Delta n}\right| mol$ represents the critical mole fraction; where if x_j increases ($x_j > \left|\frac{\nu_j}{\Delta n}\right| mol$), LCP would be broken. For NH_3 production from N_2 and H_2, Posthumus [8] found that when the system is initially in chemical equilibrium and has more than 50% N_2, the addition of N_2 as reactant would result in an internal reaction forming more reactant at constant T and P. Using Eq. 14 we also found the critical mole fraction as:

$$x_j = \left|\frac{\nu_j}{\Delta n}\right| mol = \left|\frac{-1}{-2}\right| = \frac{1}{2}.$$

Now, let's obtain a general perquisite for reactions where the LCP is broken. To do so, we use the fundamental property of the mole fraction which cannot be exceeded unity. Hence the first perquisite is as follows:

$$\left|\frac{\nu_j}{\Delta n}\right| < 1 \tag{15}$$

Using this statement, we will find plenty of reactions where the LCP could be broken.

3. CONCLUSIONS

We achieved a simple term for the situations that LCP fails to predict the correct direction of the reaction change after suffering a perturbation caused by adding species in gas phase reactions at constant T and P. If the term of Eq. 15 is met, the reaction can go toward the direction of added substrate (reactant or product) only if the mole fraction is larger than the critical mole fraction of $\left|\frac{\nu_j}{\Delta n}\right| mol$ (Eq. 14). As an example in the following reaction:

$$CH_4(g) + 2H_2S(g) \rightleftharpoons CS_2(g) + 4H_2(g)$$

For both $CH_4(g)$ and $CS_2(g)$, *the term* $\left|\frac{\nu_j}{\Delta n}\right| = \frac{1}{2}$ represents that the first prerequisite is fulfilled, that is $\left|\frac{\nu_j}{\Delta n}\right| < 1$. In the reaction at equilibrium, if the mole fraction of $CH_4(g)$ or

$CS_2(g)$ is 0.5 or higher, then by adding one of these species to the reaction at constant T and P, the reaction shifts in the direction to produce more of that species, in contradictory to LCP.

Finally, from Eqs. 14 and 15, we also conclude that for the reactions in which Δn is 0 or 1, the LCP will never be broken while υ_j is an integer number.

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Neighbourly Irregular Derived Graphs

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ABSTRACT

A connected graph G is said to be neighbourly irregular graph if no two adjacent vertices of G have same degree. In this paper, we obtain neighbourly irregular derived graphs such as semitotal-point graph, *k-th* semitotal-point graph, semitotal-line graph, paraline graph, quasi-total graph and quasivertex-total graph and also neighbourly irregular of some graph products.

1. INTRODUCTION AND PRELIMINARIES

In this paper, we are concerned with finite, simple, connected graph G with vertex set $V(G)=\{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)=\{e_1, e_2, \ldots, e_m\}$. If v_i and v_j are vertices of G, then the edge connecting them will be denoted by v_iv_j. The *degree* of a vertex v in G is denoted by $d_G(v)$. The *complement* of G, denoted by $\overline{G}$, is a graph which has the same vertex set as G, in which two vertices are adjacent if and only if they are not adjacent in G and $d_{\overline{G}}(v) = n - 1 - d_G(v)$ holds for all $v \in V(G)$. Definitions not given here may be found in [4].

A graph G is said to be *regular* if all its vertices have the same degree. A connected graph G is said to be *highly irregular* if each neighbor of any vertex has different degree [1]. The graph G is said to be *neighbourly irregular graph*, abbreviated as *NI* graph, if no

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two adjacent vertices of G have the same degree. This concept was introduced by Bhragsam and Ayyaswamy [2]. In [2, 12], authors constructed *NI* graphs of order n for a given n and a partition of n with distinct parts and proved some properties of *NI* graphs related to graphoidal covering number, gracefulness, ply number, lace number, clique graph, minimal edge covering and studied the neighbourly irregularity of some graph products.

The *line graph* $L(G)$ of a graph G is the graph with vertex set as the edge set of G and two vertices of $L(G)$ are adjacent whenever the corresponding edges in G have a vertex in common. The *subdivision graph* $S(G)$ of a graph G whose vertex set is $V(G) \cup E(G)$ where two vertices are adjacent if and only if one is a vertex of G and other is an edge of G incident with it.

2. DERIVED GRAPHS

In this paper we considered the following graphs derived from the parent graph G:

1. The ***semitotal-point graph*** $T_2(G)$ as the graph [8] whose vertex set is $V(G) \cup E(G)$ where two vertices are adjacent if and only if (i) they are adjacent vertices of G or (ii) one is a vertex of G and other is an edge of G incident with it. If u is a vertex of G, then $d_{T_2(G)}(u) = 2d_G(u)$. If e is an edge of G, then $d_{T_2(G)}(e) = 2$.
2. The ***k-th semitotal-point graph*** $T_2^k(G)$ of G [6] is the graph obtained by adding k vertices to each edge of G and joining them to the endvertices of the respective edge. Obviously, this is equivalent to adding k triangles to each edge of G.
3. The ***semitotal-line graph*** $T_1(G)$ as the graph [8] whose vertex set is $V(G) \cup E(G)$ where two vertices are adjacent if and only if (i) they are adjacent edges of G or (ii) one is a vertex of G and other is an edge of G incident with it. If u is a vertex of G, then $d_{T_1(G)}(u) = d_G(u)$. If $e=uv$ is an edge of G, then $d_{T_1(G)}(e) = d_G(u) + d_G(v)$.
4. The ***paraline graph*** $PL(G)$ is a line graph of subdivision graph of G.
5. The ***quasi-total graph*** $P(G)$ as the graph [9] whose vertex set is $V(G) \cup E(G)$ where two vertices are adjacent if and only if (i) they are nonadjacent vertices of G or (ii) they are adjacent edges of G or (iii) one is a vertex of G and other is an edge of G incident with it. If u is a vertex of G, then $d_{P(G)}(u) = n - 1$. If $e = uv$ is an edge of G, then $d_{P(G)}(u) = d_G(u) + d_G(v)$.
6. The ***quasivertex-total graph*** $Q(G)$ as the graph [7] whose vertex set is $V(G) \cup E(G)$ where two vertices are adjacent if and only if (i) they are adjacent vertices of G or (ii) they are nonadjacent vertices of G (iii) they are adjacent edges of G or (iv) one is a vertex of G and other is an edge of G incident with it. If u is a vertex of G, then $d_{Q(G)}(u) = n - 1 + d_G(u)$. If $e = uv$ is an edge of G, then $d_{Q(G)}(e) = d_G(u) + d_G(v)$.

In Figure 1 self-explanatory examples of these derived graphs are depicted.

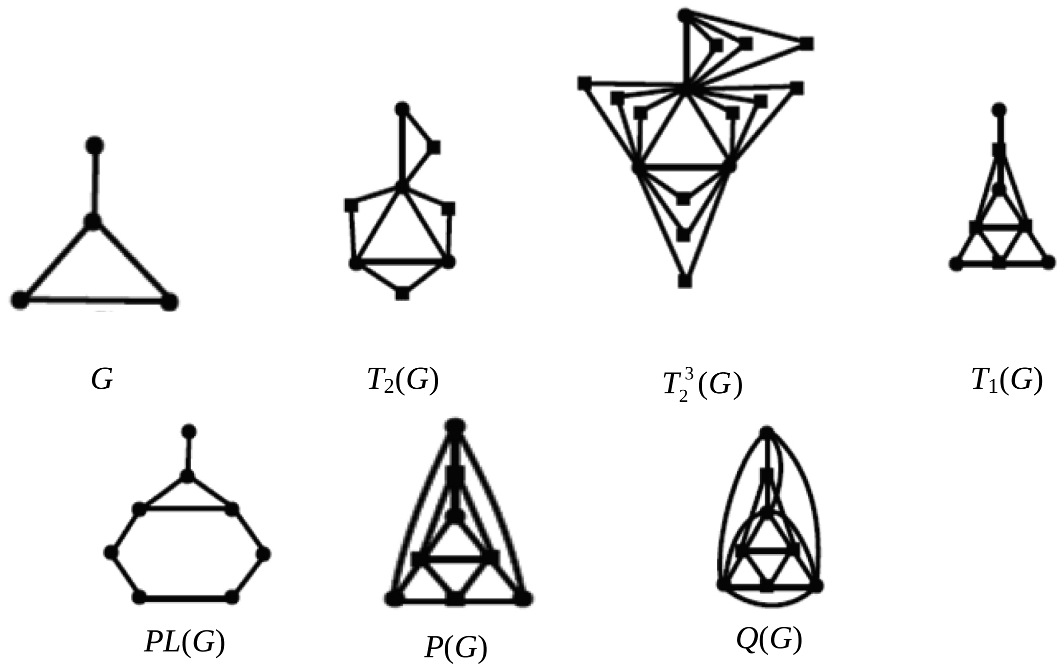

Figure 1. Various graphs derived from the graph G and $T_2^3(G)$ is *k-th* semitotal-point graph of G for k = 3.

The vertices of derived graphs depicted in Figure 1 except from the paraline graph *PL*, corresponding to the vertices of the parent graph *G*, are indicated by circles. The vertices of these graphs corresponding to the edges of the parent graph *G* are indicated by squares. In this paper we obtain neighbourly irregular derived graphs.

Theorem 2.1 [12] Let G be a graph. The subdivision graph S(G) is NI if and only if G does not have any vertex of degree two.

Theorem 2.2 [12] For any graph G, its line graph L(G) is NI graph if and only if N(u) contains all vertices of different degree for all u $\in$ V(G).

Theorem 2.3 [2] If G is NI graph, then $\overline{G}$ is not NI graph.

Theorem 2.4 [12] If G is NI graph, then L(G) is not NI graph.

Theorem 2.5 [12] For each integer k $\geq$ 1, there exist a graph G with maximum degree Δ(G) = k such that L(G) is NI graph.

3. RESULTS

Theorem 3.1 For any graph G, the semitotal-point graph $T_2(G)$ is NI if and only if G is NI graph and no vertex of degree one is in G.

Proof. Suppose G is NI graph and no vertex of degree one is in G. In $T_2(G)$, let e = xy be an edge. Then x, y ∈ V(G) or x ∈ V(G) and y ∈ E(G).

(a) x, y ∈ V(G). Since $d_G(x) \neq d_G(y)$, $d_{T_2(G)}(x) = 2d_G(x) \neq 2d_G(y) = d_{T_2(G)}(y)$.

(b) x ∈ V(G) and y ∈ E(G). Since no vertex of degree is one in G and $d_{T_2(G)}(y) = 2$, $d_{T_2(G)}(x) = 2d_G(x) \neq 2 = d_{T_2(G)}(y)$. Thus from all the cases $T_2(G)$ is NI graph.

Conversely, suppose G is not NI graph. Then $d_G(x) = d_G(y)$ for some vertices x and y are adjacent in G. So, $d_{T_2(G)}(x) = d_{T_2(G)}(y)$. A contradiction to $T_2(G)$ is NI graph. Suppose $d_G(v) = 1$ for some v ∈ V(G). Let e = vy be an edge in $T_2(G)$. Then $d_{T_2(G)}(v) = 2d_G(v) = 2 = d_{T_2(G)}(y)$. Again a contradiction to $T_2(G)$ is NI graph. □

Theorem 3.2 For any graph G, the k^{th} semitotal-point graph is NI if and only if G is NI graph and $k \geq 2$.

Proof. The proof of this theorem is similar to the proof of the Theorem 3.1, so is omitted. □

Theorem 3.3 For any graph G, its $T_1(G)$ is NI if and only if L(G) is NI graph.

Proof. Suppose L(G) is NI graph. In $T_1(G)$, let e = xy be an edge. Then x, y ∈ E(G) or x ∈ V(G) and y ∈ E(G).

(a) x, y ∈ E(G). Let $x = v_iv_j$ and $y = v_iv_k$, so that x and y are adjacent in $T_1(G)$. Since L(G) is NI graph, we have $d_{L(G)}(x) \neq d_{L(G)}(y)$, $d_G(v_i) + d_G(v_j) - 2 \neq d_G(v_i) + d_G(v_k) - 2$ or $d_G(v_i) + d_G(v_j) \neq d_G(v_i) + d_G(v_k)$. Therefore $d_{T_1(G)}(x) \neq 2d_{T_1(G)}(y)$.

(b) x ∈ V(G) and y ∈ E(G). Let $e = xy = v_ie_j$ for some $v_i \in V(G)$ and $e_j \in E(G)$. Therefore $d_{T_1(G)}(x) = d_{T_1(G)}(v_i) = d_G(v_i)$ and $d_{T_1(G)}(y) = d_{T_1(G)}(e_j) = d_G(v_i) + d_G(v_k)$ where $e_j = v_iv_k \neq d_G(v_i)$ as $d_G(v_k) \neq 0 = d_G(x) = d_{T_1(G)}(x)$. Therefore for every pair of adjacent vertices in $T_1(G)$ have different degree. Thus $T_1(G)$ is NI graph.

Conversely, suppose L(G) is not NI graph. Then $d_{L(G)}(e_i) = d_{L(G)}(e_j)$ for some $e_i = v_rv_s$ and $e_j = v_rv_k$ are adjacent vertices in L(G). Hence, $d_G(v_r) + d_G(v_s) - 2 = d_G(v_r) + d_G(v_k) - 2$, $d_G(v_r) + d_G(v_s) = d_G(v_r) + d_G(v_k)$. Therefore $d_{T_1(G)}(e_i) = d_{T_1(G)}(e_j)$. A contradiction to $T_1(G)$ is NI graph. □

From Theorems 2.4, 2.5 and 3.3, we have the following corollaries.

Corollary 3.4 If G is NI graph, then $T_1(G)$ is not NI graph.

Corollary 3.5 For each integer $k \geq 1$, there exists a graph G with maximum degree $\Delta(G) = k$ such that $T_1(G)$ is NI graph.

Theorem 3.6 For any graph $G \neq K_2$, the paraline graph PL(G) is not NI graph.

Proof. Let v be a vertex of degree at least two in G. Then neighbourhood of v in S(G) has at least two vertices of degree two. By Theorem 2.2, L(S(G))=PL(G) is not NI graph. □

Theorem 3.7. For any graph $G \neq K_2$, the quasi-total graph P(G) is not NI graph.

Proof. Let $G \neq K_2$ be a graph. We have the following cases:

Case 1. If G is not a complete graph, then there exist at least two vertices $u, v \in V(G)$ such that $d_{P(G)}(u) = d_{P(G)}(v) = n - 1$. Therefore P(G) is not NI graph.

Case 2. If G is a complete graph, then there exist at least two edges $e_i, e_j \in E(G)$ such that $d_{P(G)}(e_i) = d_{P(G)}(e_j)$. Therefore P(G) is not NI graph. □

Theorem 3.8 For any graph G with n vertices, the quasivertex-total graph Q(G) is NI if and only if G, $\overline{G}$ and L(G) all are NI graphs and $\Delta(G) \neq n - 1$.

Proof. Suppose G, $\overline{G}$ and L(G) all are NI graphs. In Q(G), let e = xy be an edge, then $x, y \in V(G)$ or $x, y \in V(\overline{G})$ or $x, y \in E(G)$ or $x \in V(G)$ and $y \in E(G)$.

(a) $x, y \in V(G)$. Since $d_G(x) \neq d_G(y)$, $d_{Q(G)}(x) = n - 1 + d_G(x) \neq n - 1 + d_G(y) = d_{Q(G)}(y)$.

(b) $x, y \in V(\overline{G})$. Since $d_{\overline{G}}(x) \neq d_{\overline{G}}(y)$, $d_{Q(G)}(x) = n - 1 + d_G(x) \neq n - 1 + d_G(y) = d_{Q(G)}(y)$.

(c) $x, y \in E(G)$. Let $x = v_iv_j$ and $y = v_iv_k$. So that x and y are adjacent in Q(G). Therefore $d_{Q(G)}(x) = d_G(v_i) + d_G(v_j)$ and $d_{Q(G)}(x) = d_G(v_i) + d_G(v_k)$. But $d_{L(G)}(x) \neq d_{L(G)}(y)$ as L(G) is NI graph, $d_{L(G)}(x) = d_G(v_i) + d_G(v_j) - 2$ and $d_{L(G)}(y) = d_G(v_i) + d_G(v_k) - 2$. Therefore $d_{Q(G)}(x) \neq d_{Q(G)}(y)$.

(d) $x \in V(G)$ and $y \in E(G)$. Let $e = xy = v_ie_j$ for some $v_i \in V(G)$ and $e_j \in E(G)$. Then $d_{Q(G)}(y) = d_{Q(G)}(e_j) = d_{L(G)}(e_j) + 2$ where $e_j = v_iv_j = d_G(v_i) + d_G(v_j) \neq n - 1 + d_G(v_i)$ as $\Delta(G) \neq n - 1 \neq d_{Q(G)}(x)$. Thus in all the cases Q(G) is NI graph.

Conversely, suppose Q(G) is NI graph. We have to prove that G, $\overline{G}$ and L(G) are all NI graphs. If G is not NI graph, then there exists an edge $e_k = v_iv_j$ in G such that $d_G(v_i) = d_G(v_j)$. Therefore $n - 1 + d_G(v_i) = n - 1 + d_G(v_j)$. So, $d_{Q(G)}(v_i) = d_{Q(G)}(v_j)$. A contradiction to Q(G) is NI graph. Suppose $\overline{G}$ is not NI graph, then there exists an edge $e_k = v_iv_j$ in $\overline{G}$ such that $d_{\overline{G}}(v_i) = d_{\overline{G}}(v_j)$. Therefore $n - 1 + d_G(v_i) = n - 1 + d_G(v_j)$ and so $d_{Q(G)}(v_i) = d_{Q(G)}(v_j)$. A contradiction to Q(G) is NI graph.

Suppose L(G) is not NI graph, then there exists two adjacent vertices $e_i = v_rv_s$ and $e_j = v_rv_k$ in L(G) with $d_{L(G)}(e_i) = d_{L(G)}(e_j)$. Thus $d_G(v_r) + d_G(v_s) - 2 = d_G(v_r) + d_G(v_k) - 2$. Hence $d_G(v_r) + d_G(v_s) = d_G(v_r) + d_G(v_k)$ and so $d_{Q(G)}(e_i) = d_{Q(G)}(e_j)$. Again a contradiction to Q(G) is NI graph. Suppose $\Delta(G) = n - 1 = d_G(v)$ and let $e = uv$ be an edge. Then $d_{Q(G)}(e) = d_{Q(G)}(u)$. Again a contradiction to Q(G) is NI graph. □

From Theorems 2.3, 2.4 and 3.8 we have following result.

Theorem 3.9 There is no nontrivial graph G whose quasivertex-total graph Q(G) is NI graph.

4. NEIGHBOURLY IRREGULAR GRAPH PRODUCTS

The corona [10] of two graphs G and H is the graph obtained by taking one copy of G, |V(G)| copies of H and joining each i-th vertex of G to every vertex in the i-th copy of H. The edge corona [5] of two graphs G and H denoted by $G \Diamond H$ is obtained by taking one copy of G and |E(G)| copies of H and joining each end vertices of i-th edge of G to every vertex in the i-th copy of H.

Theorem 4.1 Let G and H be nontrivial graphs. Then $G \Diamond H$ is NI graph if and only if both G and H are NI graphs and, G does not have pendent vertex or $\Delta(H) < |V(H)| - 1$, where $\Delta(H)$ is the maximum degree of the vertices of H.

Proof. To prove the result, we have to present some notations. Let G′ be the copy of G and H_i be the i-th copy of H in $G \Diamond H$, $1 \le i \le |E(G)|$. A vertex of $G \Diamond H$ corresponding to the vertex u in H is denoted by u′. Also, we denote a vertex of $G \Diamond H$ corresponding to the vertex v in G by v′.

Let G and H be NI graphs and, G does not have pendent vertex or $\Delta(H) < |V(H)| - 1$. Then it is clear that $G \Diamond H$ is NI graph.

Conversely, let G and H be two nontrivial graphs and $G \Diamond H$ is NI graph. Suppose $u'v' \in E(G \Diamond H)$ such that $u', v' \in V(H_i)$, then $d_{G\Diamond H}(u') - d_{G\Diamond H}(v') = d_H(u) - d_H(v) \neq 0$ and so H is NI graph. Also, if $u'v' \in E(G \Diamond H)$ such that $u', v' \in V(G')$, then $d_{G\Diamond H}(u') - d_{G\Diamond H}(v') = (|V(H)| + 1)(d_G(u) - d_G(v)) \neq 0$. Thus, G is NI graph. On the other hand, if $u'v' \in E(G \Diamond H)$ such that $u' \in V(G')$, and $v' \in V(H_i)$, then $d_{G\Diamond H}(u') - d_{G\Diamond H}(v') = (|V(H)| + 1)$

$d_G(u) - (d_H(v) + 2) \neq 0$ and it shows that, G does not have pendent vertex or $\Delta(H) < |V(H)| - 1$. □

To present the next results, we need two definitions as follows: The cluster G{H} is obtained by taking one copy of G and |V(G)| copies of a rooted graph H, and by identifying the root of the i-th copy of H with the i-th vertex of G, i = 1, 2, …, |V(G)| [11].

Suppose G and H are graphs with disjoint vertex sets. Following Došlić [3], for given vertices $y \in V(G)$ and $z \in V(H)$ a splice of G and H by vertices y and z, $(G \cdot H)(y, z)$, is defined by identifying the vertices y and z in the union of G and H.

Theorem 4.2 Let G and H be graphs. Then G{H} is NI graph if and only if both G and $(H \cdot S_{d_G(u_i)})(r, x)$ are NI graphs, for each i = 1, 2, …, |V(G)|, where x is the vertex with maximum degree of the star $S_{d_G(u_i)}$ and r the root vertex of H.

Proof. Let G and $(H \cdot S_{d_G(u_i)})(r, x)$ be NI graphs, for each i = 1, 2, …, |V(G)|, where x is the vertex with maximum degree of the star $S_{d_G(u_i)}$ and r the root vertex of H. Then, it is clear that G{H} is NI graph.

Conversely, let G{H} be NI graph. Also, suppose $u'v' \in E(G\{H\})$ and u′, v′ are the vertices of G{H} corresponding to the vertices u, v in G, respectively. If u′ and v′ are vertices of a copy of G, then $d_{G\{H\}}(u') - d_{G\{H\}}(v') = d_G(u) - d_G(v) \neq 0$. So G is NI graph. On the other hand, suppose $u'v' \in E(G\{H\})$ and u′, v′ are the vertices of $G\{H\} \cap H_i$ corresponding to the vertices u, v in H, respectively. Then, it is not difficult to see that $dG\{H\}(u') - dG\{H\}(v') \neq 0$ if and only if

$$d_{(H \cdot S_{d_G(u_i)})(r,x)}(u) - d_{(H \cdot S_{d_G(u_i)})(r,x)}(v) \neq 0 .$$

So, $(H \cdot S_{d_G(u_i)})(r, x)$ is NI graph. □

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Splice Graphs and Their Vertex−Degree−Based Invariants

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ABSTRACT

Let G_1 and G_2 be simple connected graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$, respectively. For given vertices $a_1 \in V(G_1)$ and $a_2 \in V(G_2)$, a splice of G_1 and G_2 by vertices a_1 and a_2 is defined by identifying the vertices a_1 and a_2 in the union of G_1 and G_2. In this paper, we present exact formulas for computing some vertex-degree-based graph invariants of splice of graphs.

1. INTRODUCTION

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $u \in V(G)$, we denote by $N_G(u)$ the set of all first neighbors of u in G. The cardinality of $N_G(u)$ is called the *degree* of u in G and denoted by $d_G(u)$. A *graph invariant* (also known as *topological index* or *structural descriptor*) is any function on a graph that does not depend on a labeling of its vertices. Several hundreds of different invariants have been employed to date with various degrees of success in QSAR/QSPR studies. We refer the reader to [1−3] for review.

In 1975, Milan Randić [4] proposed a structural descriptor, based on the end-vertex degrees of edges in a graph, called the *branching index* that later became the well-known *Randić connectivity index*. The Randić index of a graph G is denoted by $R(G)$ and defined as

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$$R(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)d_G(v)}}.$$

The Randić index is one of the most successful molecular descriptors in QSPR and QSAR studies, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons.

A closely related variant of the Randić connectivity index called the *sum-connectivity index* was proposed by Zhou and Trinajstić [5] in 2009. The sum-connectivity index $\chi(G)$ of a graph G is defined as

$$\chi(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)+d_G(v)}}.$$

The sum-connectivity index has been found to correlate well with π-electronic energy of benzenoid hydrocarbons.

Another variant of the Randić connectivity index named the *harmonic index* was introduced by Fajtlowicz [6] in 1987. The harmonic index of a graph G is denoted by $H(G)$ and defined as

$$H(G)=\sum_{uv\in E(G)}\frac{2}{d_G(u)+d_G(v)}.$$

In 1998, Estrada et al. [7] introduced another vertex-degree-based descriptor called the *atom-bond connectivity index*. The atom-bond connectivity index of a graph G is denoted by $ABC(G)$ and defined as

$$ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}.$$

This index has been proved to be a valuable predictive index in the study of the formation heat in alkanes and it provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [7, 8].

Motivated by the success of the atom-bond connectivity index, Furtula et al. [9] put forward its modified version, that they somewhat inadequately named it *augmented Zagreb index*. The augmented Zagreb index of a graph G is denoted by $AZI(G)$ and defined as

$$AZI(G)=\sum_{uv\in E(G)}\left(\frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)-2}\right)^3.$$

Preliminary studies [9] indicate that *AZI* index has an even better correlation potential than *ABC* index.

Motivated by definition of the Randić connectivity index, Vukičević and Furtula [10] proposed another vertex-degree-based topological index, named the *geometric-arithmetic index*. The geometric-arithmetic index of a graph G is denoted by $GA(G)$ and defined as

$$GA(G) = \Sigma_{uv \in E(G)} \frac{\sqrt{d_G(u) d_G(v)}}{(d_G(u) + d_G(v))/2} = \Sigma_{uv \in E(G)} \frac{2\sqrt{d_G(u) d_G(v)}}{d_G(u) + d_G(v)}.$$

It has been proved that [10], for physico-chemical properties such as boiling point, entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation and acentric factor, the predictive power of *GA* index is somewhat better than the predictive power of the Randić connectivity index.

Recently, Deng et al. [11] proposed a general mathematical formulation for vertex-degree-based invariants which is defined for a graph G as

$$TI(G) = \Sigma_{uv \in E(G)} F(d_G(u), d_G(v)),$$

where $F(x, y)$ is an appropriately chosen function.

For an arbitrary vertex u of G, we define

$$TI_G(u) = \Sigma_{v \in N_G(u)} F(d_G(u), d_G(v)).$$

In particular,

$F(x, y) = \dfrac{1}{\sqrt{xy}}$ for the Randić index,

$F(x, y) = \dfrac{1}{\sqrt{x + y}}$ for the sum-connectivity index,

$F(x, y) = \dfrac{2}{x + y}$ for the harmonic index,

$F(x, y) = \sqrt{\dfrac{x + y - 2}{xy}}$ for the atom-bond connectivity index,

$F(x, y) = \left(\dfrac{xy}{x + y - 2} \right)^3$ for the augmented Zagreb index, and

$F(x,y)=\frac{2\sqrt{xy}}{x+y}$ for the geometric-arithmetic index.

In this paper, we present an exact formula for computing the general vertex-degree-based invariant of splice of graphs. Using this result, the Randić connectivity index, sum–connectivity index, harmonic index, atom-bond connectivity index, augmented Zagreb index, and geometric–arithmetic index of splice of graphs are computed. Readers interested in more information on computing topological indices of splice of graphs can be referred to [12−22].

2. RESULTS AND DISCUSSION

Let G_1 and G_2 be simple connected graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$, and edge sets $E(G_1)$ and $E(G_2)$, respectively, and let $a_1 \in V(G_1)$ and $a_2 \in V(G_2)$. Following Došlić [21], a *splice* or *coalescence* of G_1 and G_2 by vertices a_1 and a_2 is denoted by $(G_1 \bullet G_2)(a_1,a_2)$ and defined by identifying the vertices a_1 and a_2 in the union of G_1 and G_2 as shown in Fig. 1. For notational convenience, we denote by n_i, e_i, and δ_i the order of G_i, the size of G_i, and the degree of the vertex a_i in G_i, respectively, where $i \in \{1,2\}$. It is easy to see that, $|V((G_1 \bullet G_2)(a_1,a_2))| = n_1+n_2-1$ and $|E((G_1 \bullet G_2)(a_1,a_2))| = e_1+e_2$.

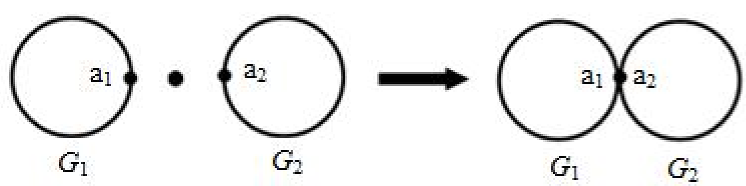

Figure 1. *A splice of* G_1 *and* G_2 *by vertices* a_1 *and* a_2.

In the following lemma, the degree of an arbitrary vertex of the splice of two graphs is computed. The result follows easily from the definition of the splice of graphs, so the proof is omitted.

Lemma 2.1 Let $G=(G_1 \bullet G_2)(a_1,a_2)$. For every vertex $u \in V(G)$,

$$d_G(u)=\begin{cases} d_{G_1}(u) & u\in V(G_1)-\{a_1\},\\ d_{G_2}(u) & u\in V(G_2)-\{a_2\},\\ \delta_1+\delta_2 & u=a_1 \text{ or } u=a_2.\end{cases}$$

In the following theorem, the general vertex-degree-based invariant of the splice of two graphs is computed.

Theorem 2.2 The general vertex-degree-based invariant of $G=(G_1\bullet G_2)(a_1,a_2)$ is given by

$$\begin{aligned} TI(G) &= TI(G_1)+TI(G_2)-TI_{G_1}(a_1)-TI_{G_2}(a_2)\\ &+\textstyle\sum_{v\in N_{G_1}(a_1)}F(\delta_1+\delta_2,d_{G_1}(v))\\ &+\textstyle\sum_{v\in N_{G_2}(a_2)}F(\delta_1+\delta_2,d_{G_2}(v)).\end{aligned} \tag{1}$$

Proof. By definition of the general vertex-degree-based invariant and Lemma 2.1,

$$\begin{aligned} TI(G) &= \textstyle\sum_{uv\in E(G)}F(d_G(u),d_G(v))\\ &= \textstyle\sum_{uv\in E(G_1);u,v\neq a_1}F(d_{G_1}(u),d_{G_1}(v))\\ &+\textstyle\sum_{uv\in E(G_2);u,v\neq a_2}F(d_{G_2}(u),d_{G_2}(v))\\ &+\textstyle\sum_{v\in N_{G_1}(a_1)}F(\delta_1+\delta_2,d_{G_1}(v))\\ &+\textstyle\sum_{v\in N_{G_2}(a_2)}F(\delta_1+\delta_2,d_{G_2}(v)).\end{aligned}$$

Now, using the fact that

$$\sum_{uv\in E(G_i);u,v\neq a_i}F(d_{G_i}(u),d_{G_i}(v))=TI(G_i)-TI_{G_i}(a_i),\qquad i\in\{1,2\},$$

we can get Eq. (1). ■

Using Eq. (1), one can easily compute the Randić connectivity index, sum–connectivity index, harmonic index, atom–bond connectivity index, augmented Zagreb index, geometric–arithmetic index, and some other vertex-degree-based invariants of splice of two graphs.

By setting $F(x,y)=\frac{1}{\sqrt{xy}}$ in Eq. (1), we easily arrive at:

Corollary 2.3 The Randić connectivity index of $G=(G_1\bullet G_2)(a_1,a_2)$ is given by

$$\begin{aligned} R(G) &= R(G_1) + R(G_2) - R_{G_1}(a_1) - R_{G_2}(a_2) \\ &\quad + \frac{1}{\sqrt{\delta_1 + \delta_2}} \left(\sum_{v \in N_{G_1}(a_1)} \frac{1}{\sqrt{d_{G_1}(v)}} + \sum_{v \in N_{G_2}(a_2)} \frac{1}{\sqrt{d_{G_2}(v)}} \right). \end{aligned}$$

As a direct consequence of Corollary 2.3, we obtain the following Corollary.

Corollary 2.4 Let G_1 be r_1–regular and G_2 be r_2–regular. The Randić connectivity index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$R(G) = \frac{e_1}{r_1} + \frac{e_2}{r_2} + \frac{\sqrt{r_1} + \sqrt{r_2}}{\sqrt{r_1 + r_2}} - 2.$$

By setting $F(x, y) = \frac{1}{\sqrt{x+y}}$ in Eq. (1), we easily arrive at:

Corollary 2.5 The sum–connectivity index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$\begin{aligned} \chi(G) &= \chi(G_1) + \chi(G_2) - \chi_{G_1}(a_1) - \chi_{G_2}(a_2) \\ &\quad + \sum\nolimits_{v \in N_{G_1}(a_1)} \frac{1}{\sqrt{\delta_1 + \delta_2 + d_{G_1}(v)}} \\ &\quad + \sum\nolimits_{v \in N_{G_2}(a_2)} \frac{1}{\sqrt{\delta_1 + \delta_2 + d_{G_2}(v)}}. \end{aligned}$$

As a direct consequence of Corollary 2.5, we obtain the following Corollary.

Corollary 2.6 Let G_1 be r_1–regular and G_2 be r_2–regular. The sum–connectivity index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$\chi(G) = \frac{e_1 - r_1}{\sqrt{2r_1}} + \frac{e_2 - r_2}{\sqrt{2r_2}} + \frac{r_1}{\sqrt{2r_1 + r_2}} + \frac{r_2}{\sqrt{2r_2 + r_1}}.$$

By setting $F(x, y) = \frac{2}{x+y}$ in Eq. (1), we easily arrive at:

Corollary 2.7 The harmonic index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$\begin{aligned} H(G) &= H(G_1)+H(G_2)-H_{G_1}(a_1)-H_{G_2}(a_2) \\ &+\Sigma_{v\in N_{G_1}(a_1)}\frac{2}{\delta_1+\delta_2+d_{G_1}(v)} \\ &+\Sigma_{v\in N_{G_2}(a_2)}\frac{2}{\delta_1+\delta_2+d_{G_2}(v)}. \end{aligned}$$

As a direct consequence of Corollary 2.7, we obtain the following Corollary.

Corollary 2.8 Let G_1 be r_1–regular and G_2 be r_2–regular. The harmonic index of $G=(G_1 \bullet G_2)(a_1,a_2)$ is given by

$$H(G)=\frac{e_1}{r_1}+\frac{e_2}{r_2}-\frac{r_1}{2r_2+r_1}-\frac{r_2}{2r_1+r_2}.$$

By setting $F(x,y)=\sqrt{\frac{x+y-2}{xy}}$ in Eq. (1), we easily arrive at:

Corollary 2.9 The atom bond connectivity index of $G=(G_1 \bullet G_2)(a_1,a_2)$ is given by

$$\begin{aligned} ABC(G) &= ABC(G_1)+ABC(G_2)-ABC_{G_1}(a_1)-ABC_{G_2}(a_2) \\ &+\frac{1}{\sqrt{\delta_1+\delta_2}}\left(\Sigma_{v\in N_{G_1}(a_1)}\sqrt{\frac{\delta_1+\delta_2+d_{G_1}(v)-2}{d_{G_1}(v)}}+\Sigma_{v\in N_{G_2}(a_2)}\sqrt{\frac{\delta_1+\delta_2+d_{G_2}(v)-2}{d_{G_2}(v)}}\right). \end{aligned}$$

As a direct consequence of Corollary 2.9, we obtain the following Corollary.

Corollary 2.10 Let G_1 be r_1–regular and G_2 be r_2–regular. The atom bond connectivity index of $G=(G_1 \bullet G_2)(a_1,a_2)$ is given by

$$ABC(G)=\sqrt{2(r_1-1)}\left(\frac{e_1}{r_1}-1\right)+\sqrt{2(r_2-1)}\left(\frac{e_2}{r_2}-1\right)+\frac{\sqrt{r_1(2r_1+r_2-2)}+\sqrt{r_2(2r_2+r_1-2)}}{\sqrt{r_1+r_2}}.$$

By setting $F(x,y)=\left(\frac{xy}{x+y-2}\right)^3$ in Eq. (1), we easily arrive at:

Corollary 2.11 The augmented Zagreb index of $G=(G_1 \bullet G_2)(a_1,a_2)$ is given by

$$\begin{aligned} AZI(G) &= AZI(G_1) + AZI(G_2) - AZI_{G_1}(a_1) - AZI_{G_2}(a_2) \\ &+ (\delta_1+\delta_2)^3 \left(\Sigma_{v\in N_{G_1}(a_1)} \left(\frac{d_{G_1}(v)}{\delta_1+\delta_2+d_{G_1}(v)-2} \right)^3 + \Sigma_{v\in N_{G_2}(a_2)} \left(\frac{d_{G_2}(v)}{\delta_1+\delta_2+d_{G_2}(v)-2} \right)^3 \right). \end{aligned}$$

As a direct consequence of Corollary 2.11, we obtain the following Corollary.

Corollary 2.12 Let G_1 be r_1–regular and G_2 be r_2–regular. The augmented Zagreb index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$AZI(G) = \frac{r_1^{\,6}(e_1 - r_1)}{8(r_1-1)^3} + \frac{r_2^{\,6}(e_2 - r_2)}{8(r_2-1)^3} + (r_1+r_2)^3 \left(\frac{r_1^{\,4}}{(2r_1+r_2-2)^3} + \frac{r_2^{\,4}}{(2r_2+r_1-2)^3} \right).$$

By setting $F(x,y) = \dfrac{2\sqrt{xy}}{x+y}$ in Eq. (1), we easily arrive at:

Corollary 2.13 The geometric–arithmetic index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$\begin{aligned} GA(G) &= GA(G_1) + GA(G_2) - GA_{G_1}(a_1) - GA_{G_2}(a_2) \\ &+ 2\sqrt{\delta_1+\delta_2} \left(\Sigma_{v\in N_{G_1}(a_1)} \frac{\sqrt{d_{G_1}(v)}}{\delta_1+\delta_2+d_{G_1}(v)} + \Sigma_{v\in N_{G_2}(a_2)} \frac{\sqrt{d_{G_2}(v)}}{\delta_1+\delta_2+d_{G_2}(v)} \right). \end{aligned}$$

As a direct consequence of Corollary 2.13, we obtain the following corollary.

Corollary 2.14 Let G_1 be r_1–regular and G_2 be r_2–regular. The geometric-arithmetic index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$GA(G) = e_1 + e_2 - r_1 - r_2 + 2\sqrt{r_1+r_2} \left(\frac{r_1\sqrt{r_1}}{2r_1+r_2} + \frac{r_2\sqrt{r_2}}{2r_2+r_1} \right).$$

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An Upper Bound on the First Zagreb Index in Trees

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ABSTRACT

The first Zagreb index $M_1(G)$ is equal to the sum of squares of the degrees of the vertices and the first Zagreb coindex $\overline{M_1}(G)$ is equal to the sum of sums of vertex degrees of the pairs of non-adjacent vertices. Kovijanić Vukićević and G. Popivoda (Iran. J. Math. Chem. **5** (2014) 19–29) proved that for any chemical tree of order n, $n \geq 5$,

$$M_1(T) \leq \begin{cases} 6n-12 & n \equiv 0,1 \pmod 3 \\ 6n-10 & \text{otherwise.} \end{cases}$$

In this paper, we generalize the aforementioned bound for all trees in terms of their order and maximum degree. Moreover, we give a lower bound on the first Zagreb coindex of trees.

1. INTRODUCTION

In this paper, G is a simple connected graph with vertex set $V = V(G)$ and edge set $E = E(G)$. The order $|V|$ of G is denoted by $n = n(G)$. For every vertex $v \in V$, the *open neighborhood* $N(v)$ is the set $\{u \in V(G) \mid uv \in E(G)\}$ and the *closed neighborhood* of v is the set $N[v] = N(v) \cup \{v\}$. The *degree* of a vertex $v \in V$ is $d_v = |N(v)|$. The *minimum* and *maximum degree* of a graph G are denoted by $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively. Trees with the property $\Delta \leq 4$ are called chemical trees.

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestić in [6]. They are important molecular descriptors and have been closely correlated with many chemical properties [6, 7]. Thus, it attracted more and more attention from chemists and mathematicians [2, 3, 4, 8, 10, 11].

The *first Zagreb index* $M_1(G)$ is defined as follows:

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$$M_1(G) = \sum_{v \in V} d_v^2.$$

The first Zagreb index can be also expressed as the sum of vertex degree over edges of G, that is, $M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$. Došlić in [5] introduced a new graph invariant called the *first Zagreb coindex*, as $\overline{M}_1(G) = \sum_{uv \notin E(G)} (d_u + d_v)$. Next we introduce a family of trees. For $n = (\Delta - 1)k + p$ $(k \geq 2)$, let T_n be the family of trees of order n with maximum degree Δ such that:

- If $p = 0$, $k-1$ vertices have degree Δ, 1 vertex has degree $\Delta - 2$ and remaining vertices are pendant.
- If $p = 1$, $k-1$ vertices have degree Δ, 1 vertex has degree $\Delta - 1$ and remaining vertices are pendant.
- If $p = 2$, k vertices have degree Δ and remaining vertices are pendant.
- If $p \geq 3$, k vertices have degree Δ, 1 vertex has degree $p-1$, and $n-k-1$ remaining vertices are pendant.

Kovijanić Vukićević and Popivoda [9] proved the following upper bound on the first Zagreb index of chemical trees and characterized all extreme chemical trees.

Theorem 1. Let T be a chemical tree with $n \geq 5$ vertices. Then

$$M_1(T) \leq \begin{cases} 6n - 12 & n \equiv 0,1 \,(\mathrm{mod}\ 3) \\ 6n - 10 & otherwise, \end{cases}$$

with equality if and only if $G \in \mathrm{T}_n$.

In this paper, we establish an upper bound on the first Zagreb index of trees in terms of the order and maximum degree, as a generalization of aforementioned bound. As a consequence, we obtain a lower bound on the first Zagreb coindex for trees.

2. MAIN RESULTS

In this section, we prove the following result:

Theorem 2. Let T be a tree of order n and maximum degree Δ. If $n \equiv p \pmod{\Delta - 1}$, then

$$M_1(T) \le \begin{cases} (\Delta+2)n-4\Delta+4 & p=0 \\ (\Delta+2)n-3\Delta & p=1 \\ (\Delta+2)n-2\Delta-2 & p=2 \\ (\Delta+2)n-2\Delta-3+p(p-2) & p\ge 3, \end{cases}$$

with equality if and only if $G \in \mathrm{T}_n$.

To prove Theorem 2, we proceed with some definitions and lemmas. If n is a positive integer, then an integer partition of n is a non-increasing sequence of positive integers $(a_1, a_2, \ldots, a_t)$ whose sum is n. If $1 \le a_1 \le a_2 \le \ldots \le a_t \le a$, then $(a_1, a_2, \ldots, a_t)$ is called an integer partition of n on $N_a = \{1,2,\ldots,a\}$. An integer partition $(a_1, a_2, \ldots, a_t)$ of n on N_a is called an integer a-partition if the number of a in this partition is as large as possible. In other words, if $n = ka$, then $(a, \ldots, a)$ is the integer a–partition and if $n = ka + b$ where $0 < b < a$ then $(b, a, \ldots, a)$ is the integer a–partition. The proof of the next result is straightforward and therefore omitted.

Lemma 3. *For positive integers n, t and a_i ($1 \le i \le t$), we have*

a) If $n = a_1 + a_2 + \ldots + a_t$ and $t > 1$, then $n^2 > a_1^2 + a_2^2 + \cdots + a_t^2$.

b) If $a_i \le a_j$, then $(a_i - 1)^2 + (a_j + 1)^2 \ge a_i^2 + a_j^2 + 2$.

Lemma 4. *If $(a_1, a_2, \ldots, a_t)$ is an integer partition of $n = ka + b$ $(0 \le b < a)$ on N_a, then*

$$\sum_{i=1}^{t} a_i^2 < ka^2 + b^2.$$

Proof. Let $(a_1, a_2, \ldots, a_t)$ be an partition of n on N_a. If $a_i \le a_j < a$ for some $1 \le i \ne j \le t$, then by switching (a_i, a_j) to $(a_i - 1, a_j + 1)$, we get a new integer partition of n on N_a. Note that if $a_i - 1 = 0$, then we will remove $a_i - 1$ from the new partition. Applying Lemma 3 (a), we obtain

$$\sum_{i=1}^{t} a_i^2 < a_1^2 + \cdots + (a_i - 1)^2 + \cdots + (a_j + 1)^2 + \cdots + a_t^2.$$

By repeating this process, we arrive at an integer a–partition of n on N_a. It follows from Lemma 2 that $\sum_{i=1}^{t} a_i^2 < ka^2 + b^2$ and the proof is complete.

Lemma 5. Let $n = ka + b$ where $0 \le b < a$ and let $(a_1, a_2, \ldots, a_t)$ be an integer partition of n on N_a which is not a–partition. Then the following statements holds:

a. If $b > 0$, then $\sum_{i=1}^{t}(a_i+1)^2 < k(a+1)^2 + (b+1)^2$.

b. If $b = 0$, then $\sum_{i=1}^{t}(a_i+1)^2 < k(a+1)^2$.

Proof. (a) Since $n = a_1 + \cdots + a_t = b + \underbrace{a + \cdots + a}_{\text{k}} = ka + b$, we have $t \ge k+1$. First let $t = k+1$. Then we have

$$\begin{aligned}(a_1+1)^2 + \cdots + (a_t+1)^2 &= (a_1^2 + \cdots + a_t^2) + t + 2(ka+b) \\ &< (ka^2 + b^2) + t + 2(ka+b) \qquad \text{(by Lemma3)} \\ &= k(a+1)^2 + (b+1)^2 + t - (k+1) \\ &= k(a+1)^2 + (b+1)^2,\end{aligned}$$

as desired. Now let $t > k+1$. Repeating the switching process described in the proof of Lemma 4, i.e. for any pair (a_i, a_j) where $1 \le a_i < a_j < a$ and using the fact that $a_i^2 + a_j^2 \le (a_i - 1)^2 + (a_j + 1)^2 - 2$, we get $a_i = 0$ or $a_j = a$. To achieving an integer a–partition, we need to apply the switching process at least $t-(k+1)$ times. This implies that

$$a_1^2 + \cdots + a_t^2 \le ka^2 + b^2 - 2(t-(k+1)). \tag{1}$$

Thus

$$\begin{aligned}(a_1+1)^2 + \ldots + (a_t+1)^2 &= (a_1^2 + \ldots + a_t^2) + t + 2(ka+b) \\ &\le ka^2 + b^2 - 2(t-(k+1)) + t + 2(ka+b) \quad \text{(by } \textit{inequality} \text{ (1))} \\ &= k(a+1)^2 + (b+1)^2 - (t-(k+1)) \\ &< k(a+1)^2 + (b+1)^2.\end{aligned}$$

(b) If $b = 0$,then $n = a_1 + \cdots + a_t = \underbrace{a + \cdots + a}_{\text{k}} = ka$. Since $(a_1, \ldots, a_t)$ is not a–partition, we have $t > k$. Applying (1), we obtain

$$\begin{aligned}(a_1+1)^2 + \cdots + (a_t+1)^2 &= (a_1^2 + \cdots + a_t^2) + t + 2ka \\ &\le ka^2 - 2(t-k) + t + 2ka \\ &= k(a+1)^2 + k - t \\ &< k(a+1)^2.\end{aligned}$$

This completes the proof.

Remark 6. Let T be a tree of order n and maximum degree Δ. For each $i \in \{1,2,\ldots,\Delta\}$, let n_i denote the number of vertices of degree i. Then

$$n_1 + n_2 + \ldots + n_\Delta = n \tag{2}$$

and

$$n_1 + 2n_2 + \ldots + \Delta n_\Delta = 2n-2. \tag{3}$$

Subtracting (2) from (3), yields

$$n_2 + 2n_3 + \ldots + (\Delta-1)n_\Delta = n-2. \tag{4}$$

By (4), we obtain the following integer partition

$$(\underbrace{1,\ldots,1}_{n_2}, \underbrace{2,\ldots,2}_{n_3}, \ldots, \underbrace{\Delta-1,\ldots,\Delta-1}_{n_\Delta}), \tag{5}$$

of $n-2$ on $N_{\Delta-1} = \{1,2,\ldots,\Delta-1\}$. It follows from Lemma 4 that $2^2 n_2 + 3^2 n_3 + \ldots + \Delta^2 n_\Delta$ is maximum if and only if the partition (5) obtained from (4), is an $(\Delta-1)-$partition of $n-2$ on $N_{\Delta-1}$. In that case, n_1 (the number of leaves) will be maximum.

Next result is an immediate consequence of above discussion.

Corollary 7. For any tree T of order n with maximum degree Δ, the first Zagreb index $M_1(T) = n_1 + 2^2 n_2 + \cdots + \Delta^2 n_\Delta$ is maximum if and only if the integer partition (5) is an $(\Delta-1)$–partition of $n-2$ on $N_{\Delta-1}$. In that case, the integer partition $(n_1, n_2, \ldots, n_\Delta)$ is called an optimal solution of (4).

Theorem 8. Let T be a tree of order n and maximum degree Δ with $n \equiv 0 \pmod{\Delta-1}$. Then $M_1(T) \le (\Delta+2)n - 4\Delta + 4$, with equality if and only if $T \in \mathsf{T}_n$.

Proof. Assume that $n = (\Delta-1)k$. By (4),

$$n_\Delta = k - \left(\frac{n_2 + 2n_3 + \cdots + (\Delta-2)n_{\Delta-1} + 2}{\Delta-1}\right) = k - r,$$

where $r = \dfrac{n_2 + 2n_3 + \cdots + (\Delta-2)n_{\Delta-1} + 2}{\Delta-1}$. Then $1 \le r \le k-1$ and $1 \le n_\Delta \le k-1$. We consider three cases as follows:

Case 1. $r = 1$. Then clearly $n_\Delta = k-1$. It follows that

$$n_2 + 2n_3 + \cdots + (\Delta-2)n_{\Delta-1} + (\Delta-1)(k-1) = (\Delta-1)k - 2$$

and so

$$n_2 + 2n_3 + \ldots + (\Delta - 2).n_{\Delta-1} = \Delta - 3.$$

Thus $n_{\Delta-1} = 0$ and so

$$n_2 + 2n_3 + \cdots + (\Delta - 3).n_{\Delta-2} = \Delta - 3. \tag{6}$$

According to Corollary 6, the optimal solution of (6) is $n_2 = n_3 = \cdots = n_{\Delta-3} = 0$ and $n_{\Delta-2} = 1$. Since $n_1 + n_2 + \cdots + n_\Delta = n$, we conclude that $n_1 = (\Delta - 2)k$. By Corollary 7,

$$(n_1, n_2, \ldots, n_{\Delta-3}, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k, 0, \ldots, 0, 1, 0, k - 1)$$

is the optimal solution and so $M_1(T)$ is maximum. Therefore,

$$\begin{aligned} M_1(T) &\le n_1 + 2^2 n_2 + \ldots + (\Delta - 2)^2 .n_{\Delta-2} + (\Delta - 1)^2 .n_{\Delta-1} + \Delta^2 .n_\Delta \\ &= (\Delta - 2)k + (\Delta - 2)^2 + \Delta^2 (k - 1) \\ &= (\Delta + 2)(\Delta - 1)k - 4\Delta + 4 \\ &= (\Delta + 2)n - 4\Delta + 4. \end{aligned}$$

Case 2. $2 \le r < \Delta$. Then $n_2 + 2n_3 + \ldots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)r + (r - 2)$. Since $r - 2 < \Delta - 2$, it follows from Corollary 7 that

$$(n_1, n_2, \ldots, n_{r-2}, n_{r-1}, n_r, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k - 1, 0, \ldots, 0, 1, 0, \ldots, 0, r, k - r)$$

is an optimal solution in this case. Since $2 \le r < \Delta$ and $4 \le \Delta$, we have $r(r - 2\Delta - 1) < -4\Delta + 4$ and so

$$\begin{aligned} M_1(T) &\le (\Delta - 2)k - 1 + (r - 1)^2 + (\Delta - 1)^2 r + \Delta^2 (k - r) \\ &= (\Delta + 2)(\Delta - 1)k + r(r - 2\Delta - 1) \\ &< (\Delta + 2)n - 4\Delta + 4. \end{aligned}$$

Case 3. $\Delta \le r \le k - 1$. Then $n_2 + 2n_3 + \ldots + (\Delta - 2).n_{\Delta-1} = (\Delta - 2)r + (r - 2)$. There are non-negative integers t, s such that $(r - 2) = t(\Delta - 2) + s$ and $0 \le s < \Delta - 2$. Hence $n_2 + 2n_3 + \ldots + (\Delta - 2).n_{\Delta-1} = (\Delta - 2)(r + t) + s.$ If $0 < s < \Delta - 2$, then

$$(n_1, n_2, \ldots, n_s, n_{s+1}, n_{s+2}, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k - (t + 1), 0, \ldots, 0, 1, 0, \ldots, 0, r + t, k - r)$$

is the optimal solution and since $(s - \Delta) < 0$ and $4 \le \Delta \le r$, we obtain

$$\begin{aligned} M_1(T) &\le (\Delta - 2)k - (t + 1) + (s + 1)^2 + (\Delta - 1)^2 (r + t) + \Delta^2 (k - r) \\ &= (\Delta + 2)(\Delta - 1)k + s(s + 2) + r(1 - 2\Delta) + t\Delta(\Delta - 2) \\ &= (\Delta + 2)n + (s - \Delta)(s + 2) - r\Delta + r \\ &< (\Delta + 2)n + (s - \Delta)(s + 2) - r\Delta + r \\ &< (\Delta + 2)n - 4\Delta + 4. \end{aligned}$$

If $s = 0$, then the optimal solution is

$$(n_1, n_2, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k - t, 0, \ldots, 0, r + t, k - r).$$

Since $t(\Delta-2)=r-2-s$, $(s+2)>0$ and $4\le\Delta\le r$, we conclude that

$$\begin{aligned} M_1(T) &\le n_1+4n_2+9n_3+\ldots+\Delta^2.n_\Delta \\ &=((\Delta-2)k-t)+(\Delta-1)^2(r+t)+\Delta^2(k-r) \\ &=\Delta k-2k-t+\Delta^2 r-2\Delta r+r+\Delta^2 t-2\Delta t+t+\Delta^2 k-\Delta^2 r \\ &=(\Delta+2)n-(s+2)-r\Delta+r \\ &<(\Delta+2)n-r\Delta+r \\ &<(\Delta+2)n-4\Delta+4. \end{aligned}$$

Therefore, in all cases $M_1(T)\le(\Delta+2)n-4\Delta+4$. If $T\in\mathsf{T}_n$, then clearly $M_1(T)=(\Delta+2)n-4\Delta+4$. Conversely, let T be a tree of order n with $n\equiv 0 \pmod{\Delta-1}$ and $M_1(T)=(\Delta+2)n-4\Delta+4$. This occurs only in Case 1, that is, T has $k-1=\dfrac{n-\Delta+1}{\Delta-1}$ vertices of degree Δ, one vertex of degree $\Delta-2$ and $(\Delta-2)k$ leaves. Hence $T\in\mathsf{T}_n$ and the proof is complete.

Theorem 9. Let T be a tree of order n with maximum degree Δ and $n\equiv 1\,(\mathrm{m}od\ \Delta-1)$. Then $M_1(T)\le(\Delta+2)n-3\Delta$, with equality if and only if $T\in\mathsf{T}_n$.

Proof. Let $n=(\Delta-1)k+1$. Set $r=\dfrac{n_2+2n_3+\ldots+(\Delta-2)n_{\Delta-1}+1}{\Delta-1}$. By (4),

$$n_\Delta=k-\Big(\frac{n_2+2n_3+\ldots+(\Delta-2)n_{\Delta-1}+1}{\Delta-1}\Big)=k-r.$$

Then clearly $1\le r\le k-1$ and $1\le n_\Delta\le k-1$. We consider three cases.

Case 1. $r=1$. Since $n_\Delta=k-1$, it follows from (4) that $n_2+\ldots+(\Delta-2).n_{\Delta-1}=(\Delta-2)$ and by Corollary 7

$$(n_1,n_2,\ldots,n_{\Delta-2},n_{\Delta-1},n_\Delta)=((\Delta-2)k+1,0,\ldots,0,1,k-1)$$

is the optimal solution. Thus

$$\begin{aligned} M_1(T) &\le n_1+2^2n_2+\ldots+(\Delta-2)^2.n_{\Delta-2}+(\Delta-1)^2.n_{\Delta-1}+\Delta^2.n_\Delta \\ &=((\Delta-2)k+1)+(\Delta-1)^2(1)+\Delta^2(k-1) \\ &=(\Delta+2)n-3\Delta. \end{aligned}$$

Case 2. $2\le r<\Delta-1$. As above, $n_2+\ldots+(\Delta-2).n_{\Delta-1}=(\Delta-2)r+(r-1)$. Since $r-1<\Delta-2$, it follows from Corollary 7 that

$$(n_1, n_2, \ldots, n_{r-1}, n_r, n_{r+1}, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k, 0, \ldots, 0, 1, 0, \ldots, 0, r, k-r)$$

is the optimal soloution. Since $2 \le r < \Delta - 1$, it is easy to see that $2\Delta(1-r) + (r^2 + r - 2) < 0$ and we have

$$\begin{aligned} M_1(T) &= n_1 + 4n_2 + \ldots + (\Delta-2)^2.n_{\Delta-2} + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\ &= (\Delta-2)k + r^2(1) + (\Delta-1)^2 r + \Delta^2(k-r) \\ &= (\Delta+2)(\Delta-1)k + r^2 + r - 2r\Delta \\ &= (\Delta+2)n - 3\Delta + 2\Delta(1-r) + (r^2 + r - 2) \\ &< (\Delta+2)n - 3\Delta. \end{aligned}$$

Case 3. $\Delta - 1 \le r \le k - 1$. There are non-negative integers t, s such that $r - 1 = t(\Delta-2) + s$, $t \ge 1$ and $s < \Delta - 1$. By substituting in (4), we have $n_2 + 2n_3 + \ldots + (\Delta-2)n_{\Delta-1} = (\Delta-2)(r+t) + s$. First let $0 < s$. Since $s \le \Delta - 2$, it follows from Corollary 7 that

$$(n_1, n_2, \ldots, n_s, n_{s+1}, n_{s+2}, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k - t, 0, \ldots, 0, 1, 0, \ldots, 0, 0, r+t, k-r)$$

is the optimal solution. Thus

$$\begin{aligned} M_1(T) &\le (\Delta-2)k - t + (s+1)^2 + (\Delta-1)^2(r+t) + \Delta^2(k-r) \\ &= (\Delta+2)(\Delta-1)k + (s+1)^2 + r(1-2\Delta) + t\Delta(\Delta-2) \\ &= (\Delta+2)n - 3\Delta - s(\Delta-s-2) - (r-1)(\Delta-1) \\ &< (\Delta+2)n - 3\Delta. \end{aligned}$$

Now let $s = 0$. Then the optimal solution is

$$(n_1, n_2, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k - t + 1, 0, \ldots, 0, r+t, k-r)$$

and we have

$$\begin{aligned} M_1(T) &\le (\Delta-2)k - t + 1 + (\Delta-1)^2(r+t) + \Delta^2(k-r) \\ &= (\Delta+2)(\Delta-1)k - r(2\Delta-1) + 1 + t\Delta(\Delta-2) \\ &= (\Delta+2)n - 3\Delta - (\Delta-1)(r-1) \\ &< (\Delta+2)n - 3\Delta. \end{aligned}$$

As in the proof of Theorem 8 we can see that $M_1(T) = (\Delta+2)n - 3\Delta$ if and only if $T \in \mathsf{T}_n$.

Theorem 10. Let T be a tree of order n with maximum degree Δ and $n \equiv p \pmod{\Delta-1}$ where $2 \le p \le \Delta - 2$. Then

$$M_1(T) \leq \begin{cases} (\Delta+2)n - 2\Delta - 2 & p = 2 \\ (\Delta+2)n - 2\Delta - 3 + p(p-2) & p \geq 3, \end{cases}$$

with equality if and only if $T \in \mathrm{T}_n$.

Proof. Let $n = (\Delta-1)k + p$. Suppose that $r = \dfrac{n_2 + 2n_3 + \ldots + (\Delta-2)n_{\Delta-1} + (2-p)}{\Delta-1}$. By (4), we have

$$n_\Delta = k - (\frac{n_2 + 2n_3 + \ldots + (\Delta-2)n_{\Delta-1} + (2-p)}{\Delta-1}) = k - r.$$

Then clearly $0 \leq r \leq k-1$ and $1 \leq n_\Delta \leq k$. We consider four cases.

Case 1. $r = 0$. Then $n_\Delta = k$ and by (4) we have

$$n_2 + 2n_3 + \cdots + (\Delta-2).n_{\Delta-1} = (n-2) - ((\Delta-1).n_\Delta) = ((\Delta-1)k + p - 2) - (\Delta-1)k = p - 2.$$

If $p = 2$, then $n_2 + 2n_3 + \ldots(\Delta-2).n_{\Delta-1} = 0$. This implies that $n_2 = n_3 = \ldots = n_{\Delta-1} = 0$ and $n_1 = n - k$ by (2). Thus

$$\begin{aligned} M_1(T) &\leq n_1 + 2^2 n_2 + \cdots + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\ &= (n-k) + \Delta^2 k \\ &= n + (\Delta+1)(\Delta-1)k \\ &= n + (\Delta+1)(n-2) \\ &= (\Delta+2)n - 2\Delta - 2. \end{aligned}$$

Now let $2 < p \leq \Delta - 2$. Since $1 \leq p - 2 \leq \Delta - 4$ and $n_2 + 2n_3 + \ldots(\Delta-2).n_{\Delta-1} = p - 2$, it follows from Corollary 7 that

$$(n_1, n_2, \ldots, n_{p-2}, n_{p-1} n_p, \ldots, n_{\Delta-1}, n_\Delta) = (n-k-1, 0, \ldots, 0, 1, 0, \ldots, 0, k)$$

is the optimal solution and so

$$\begin{aligned} M_{1_{max}}(T) &\leq n_1 + 4n_2 + \ldots + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\ &= (n-k-1) + (p-1)^2(1) + \Delta^2(k) \\ &= (\Delta+1)(\Delta-1)k + n + p^2 - 2p \\ &= (\Delta+1)(n-p) + n + p^2 - 2p \\ &= (\Delta+2)n - p\Delta + p^2 - 3p. \end{aligned}$$

Case 2. $r = 1$. Then $n_\Delta = k - 1$ and

$$(n_1, n_2, \ldots, n_{p-1}, n_p, n_{p+1}, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k + p - 1, 0, \ldots, 0, 1, 0, \ldots, 0, 1, k-1)$$

is the optimal solution and since $p \leq \Delta - 2$ we have

$$\begin{aligned} M_1(T) &= n_1 + 4n_2 + \ldots + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\ &= (\Delta-2)k + p - 1 + p^2 + (\Delta-1)^2 + \Delta^2(k-1) \\ &= \Delta k - 2k + p - 1 + p^2 + \Delta^2 - 2\Delta + 1 + \Delta^2 k - \Delta^2 \\ &= (\Delta+2)(\Delta-1)k + p + p^2 - 2\Delta \\ &= (\Delta+2)(n-p) + p + p^2 - 2\Delta \\ &< (\Delta+2)n - p\Delta + p^2 - 3p. \end{aligned}$$

Case 3. $2 \le r < \Delta - p$. By (4), we have $n_2 + 2n_3 + \ldots + (\Delta-2)n_{\Delta-1} = (\Delta-2)r + (p+r-2)$. Since $r-2 < \Delta-2$, it follows from Corollary 7 that

$(n_1, n_2, \ldots, n_{p+r-2}, n_{p+r-1}, n_{p+r}, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k + p - 1, 0, \ldots, 0, 1, 0, \ldots, 0, r, k-r)$

is the optimal solution. On the other hand, we deduce from $p \le \Delta - 2$ and $r < \Delta - p$ that $r - 1 + 2(p-\Delta) < \Delta - p - 1 + 2(p-\Delta) = p - \Delta - 1 < 0$ and so $r(r-1+2(p-\Delta)) < 0$. Thus

$$\begin{aligned} M_1(T) &\le n_1 + 4n_2 + \ldots + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\ &= ((\Delta-2)k + p - 1) + (p+r-1)^2(1) + (\Delta-1)^2(r) + \Delta^2(k-r) \\ &= \Delta k - 2k + p - 1 + p^2 + r^2 + 1 + 2rp - 2p - 2r + r\Delta^2 - 2\Delta r + r + \Delta^2 k - r\Delta^2 \\ &= (\Delta+2)(\Delta-1)k + p^2 - p - 2\Delta r + r(r + 2p - 1) \\ &= (\Delta+2)(n-p) + p^2 - p - 2\Delta r + r(r+2p-1) \\ &= (\Delta+2)n - p\Delta + p^2 - 3p + r(r - 1 + 2(p-\Delta)) \\ &< (\Delta+2)n - p\Delta + p^2 - 3p = M_{1_{max}}(T). \end{aligned}$$

Case 4. $\Delta - p \le r \le k-1$. Let $p + r - 2 = t(\Delta-2) + s$. By substituting in (4), we have $n_2 + 2n_3 + \ldots + (\Delta-2)n_{\Delta-1} = (\Delta-2)(r+t) + s$. If $s = 0$ then by Corollary 7,

$$(n_1, n_2, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k + p - t, 0, \ldots, 0, r+t, k-r)$$

is the optimal solution. Since $\Delta - p \le r$ and $p \le \Delta - 2$, we have

$$\begin{aligned} (2p - p^2 + p\Delta - \Delta r - 2\Delta + r) &= p(\Delta - p + 2) - \Delta r - 2\Delta + r \\ &\le p(r+2) - \Delta r - 2\Delta + r \\ &= (p-\Delta)(r+2) + r \\ &< (p-\Delta)(r+2) + (r+2) \\ &= (p - \Delta + 1)(r+2) < 0. \end{aligned}$$

Thus

$$\begin{aligned}
M_1(T) &= n_1 + 4n_2 + \ldots + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\
&= ((\Delta-2)k + p - t) + (\Delta-1)^2(r+t) + \Delta^2(k-r) \\
&= (\Delta^2 k + \Delta k - 2k) + \Delta t(\Delta-2) + p - 2\Delta r + r \\
&= (\Delta+2)(n-p) + \Delta t(\Delta-2) + p - 2\Delta r + r \\
&= (\Delta+2)n - p\Delta - 2p + p\Delta + \Delta r + p - 2\Delta - 2\Delta r + r \\
&= (\Delta+2)n - p\Delta + p^2 - 3p + (2p - p^2 + p\Delta - \Delta r - 2\Delta + r) \\
&< (\Delta+2)n - p\Delta + p^2 - 3p.
\end{aligned}$$

Now let $0 < s$. Since $s < \Delta - 2$, it follows from Corollary 7 that $(n_1, n_2, \ldots, n_s, n_{s+1}, n_{s+2}, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k + p - (t+1), 0, \ldots, 0, 1, 0, \ldots, 0, 0, r+t, k-r)$ is the optimal solution. Since $2 \le p \le \Delta - 2$ and $0 < s \le \Delta - 3$, it is straightforward to verify that $p\Delta - p^2 + 2p + s^2 + 2s - \Delta r + r - 2\Delta - \Delta s < 0$. Thus

$$\begin{aligned}
M_1(T) &= n_1 + 4n_2 + \cdots + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\
&= (\Delta-2)k + p - (t+1) + (s+1)^2 + (\Delta-1)^2(r+t) + \Delta^2(k-r) \\
&= (\Delta^2 k + \Delta k - 2k) + p + s^2 + 2s - 2\Delta r + r + \Delta^2 t - 2\Delta t \\
&= (\Delta+2)(\Delta-1)k + p + s^2 + 2s - 2\Delta r + r + \Delta t(\Delta-2) \\
&= (\Delta+2)(n-p) + p + s^2 + 2s - 2\Delta r + r + \Delta(p + r - 2 - s) \\
&= (\Delta+2)n - p + s^2 + 2s - \Delta r + r - 2\Delta - \Delta s \\
&= (\Delta+2)n - p\Delta + p^2 - 3p + (p\Delta - p^2 + 2p + s^2 + 2s - \Delta r + r - 2\Delta - \Delta s) \\
&< (\Delta+2)n - p\Delta + p^2 - 3p.
\end{aligned}$$

Therefore, in all cases $M_1(T) \le \Delta + 2)n - p\Delta + p^2 - 3p$. As in the proof of Theorem 8, we can see that

$$M_1(T) = \begin{cases} (\Delta+2)n - 2\Delta - 2 & p = 2 \\ (\Delta+2)n - 2\Delta - 3 + p(p-2) & p \ge 3, \end{cases}$$

if and only if $T \in \mathsf{T}_n$. This completes the proof.

We now present a lower bound on the first Zagreb coindex among all trees. Ashrafi et al. [1] proved that for any conneted graph G of order n and size m

$$\overline{M}_1(G) = 2m(n-1) - M_1(G).$$

Next result is an immediate consequence of this equality and Theorem 1.

Corollary 11. Let T be a tree of order n with maximum degree Δ. If $n \equiv p \pmod{\Delta - 1}$, then

$$\overline{M}_1(T) \leq \begin{cases} -(\Delta+6)n + 2n^2 + 4\Delta - 2 & p = 0 \\ -(\Delta+6)n + 2n^2 + 3\Delta + 2 & p = 1 \\ -(\Delta+6)n + 2n^2 + 2\Delta + 4 & p = 2. \\ -(\Delta+6)n + 2n^2 + p\Delta + 2 - p(p-3) & p \geq 3. \end{cases}$$

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Distance–Based Topological Indices and Double Graph

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ABSTRACT

Let G be a connected graph, and let $D[G]$ denote the double graph of G. In this paper, we first derive closed-form formulas for some distance based topological indices for $D[G]$ in terms of G. Finally, these formulas are applied for several special kinds of graphs, such as, the complete graph, the path and the cycle.

1. INTRODUCTION

Topological indices of molecules can be carried out through their molecular graphs. A molecular graph is a collection of points representing the atoms in the molecule and a set of lines representing the covalent bonds. In graph theory, these points and lines are called vertices and edges, respectively. The chemical graph theory is a branch of mathematical chemistry in which topological indices of chemical graphs relates the certain physical, biological or chemical properties of the corresponding molecules.

Many different topological indices have been investigated so far. Most of the useful topological indices are distance based or degree based. The Wiener index, the Harary index and the total eccentricity index are examples of distance based topological indices and the Zagreb indices and Randić [8] index are examples of degree based topological indices.

The Wiener index of a molecular graph is defined as the sum of all distances between different vertices. This topological index was introduced by Wiener [13]. It also

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gave rise to some modifications such as, the hyper-Wiener index and the Tratch-Stankevich-Zefirov index.

Plavšić [7] et. al. and Ivanciuc et. al. [4] independently introduced the Harary index in honor of Frank Harary. The Harary index is obtained from the reciprocal distance matrix and has a number of interesting physical and chemical properties. The Harary index and its related molecular descriptors have shown some success in structure-property correlations [2, 3]. Its modification has also been proposed and their use in combination with other molecular descriptors improves the correlations [10, 11].

In order to improve the interest of the Harary-type indices, many modification were proposed recently. In [1] authors introduced a correction that gives more weight to the contributions of pairs of vertices of high degrees, named as the additively weighted Harary index.

The eccentric connectivity index belongs to the family of distance based topological indices. This quantity has been recently used in several papers on structure-property and structure-activity relationship and its mathematical properties have been investigated [9]. Munarini et. al. [6] define the *double graph* of a simple graph denoted as $D[G]$. The double graph of a simple graph G can be build up taking two distinct copies of the graph G and joining every vertex v in one copy to every vertex w' in the other copy corresponding to a vertex w adjacent to v in the first copy. In this paper we study some distance based topological indices for general double graphs.

2. DEFINITIONS AND PRELIMINARY RESULTS

All the graphs G considered in this paper are finite and simple. For basic definitions and notation see [12]. Let $G(V,E)$ be a simple connected graph where $V(G)$ and $E(G)$ are the set of vertices and set of edges, respectively. By $d_G(v)$ we denote the degree of vertex v in G. The distance between two vertices u and v, in a graph G, is the length of any shortest path connecting u and v and denoted as $d_G(u,v)$. The eccentricity of a vertex v in G is the maximum distance between v and any other vertex in G, it is denoted $ecc_G(v)$. By P_n and S_n we denote the path with n vertices and the star graph $k_{1,n-1}$ respectively.

The Wiener index of a given graph G having $V(G)=\{v_1,\ldots,v_n\}$ is defined as the sum of distances between all unordered pairs of vertices of a graph G, i. e.,

$$W(G)=\sum\nolimits_{1\le i<j\le n} d_G(v_i,v_j).$$

The Harary index of G is defined as the sum of reciprocals of distances between all unordered pairs of vertices of a connected graph:

$$H(G)=\sum_{1\le i\le j\le n}\frac{1}{d_G(v_i,v_j)}.$$

The additively weighted Harary index for G is defined by

$$H_A(G) = \sum_{1\le i\le j\le n} \frac{d_G(v_i)+d_G(v_j)}{d_G(v_i,v_j)},$$

and multiplicative weighted Harary index for G is defined by

$$H_M(G) = \sum_{1\le i\le j\le n} \frac{d_G(v_i)\,d(v_j)}{d_G(v_i,v_j)}.$$

The eccentric connectivity index of G is

$$\zeta^c(G) = \sum_{v\in V(G)} d_G(v)\,ecc_G(v),$$

and the total eccentricity of G is defined by

$$\zeta(G) = \sum_{v\in V(G)} ecc_G(v).$$

The *direct product* of two graphs G and H is a graph $G\times H$ with $V(G\times H) = V(G) \times V(H)$ such that (u_1,v_1) is adjacent to (u_2,v_2) in $G\times H$ if and only if $u_1u_2\in E(G)$ and $v_1v_2\in E(H)$. By adding a loop to every vertex of K_2 we obtained the graph K_2^s. The double graph of a simple graph G can be expressed as $D[G] = G\times K_2^s$. Since the direct product of a simple graph with any graph is always a simple graph, it follows that the double of a simple graph is still a simple graph. Some of its elementary properties are discussed in [6]. If G has n vertices and m edges then $D[G]$ has $2n$ vertices and $4m$ edges. For illustration see figure1.

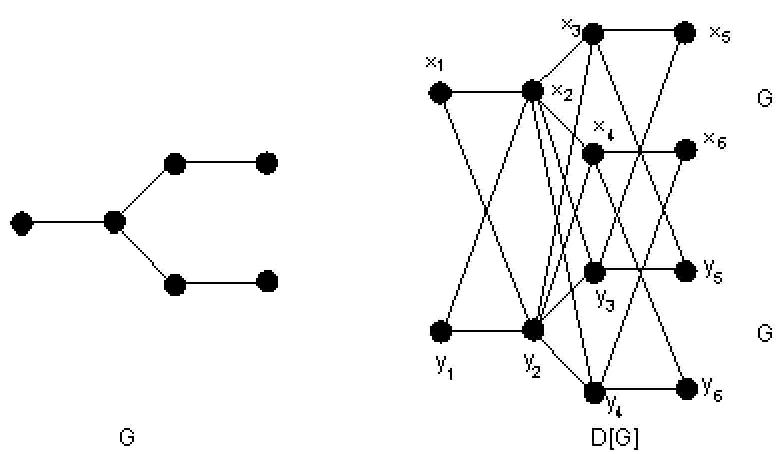

Figure 1 .A graph G and its double graph $D[G]$.

Let $G(V,E)$ be a simple graph and $G'(V', E')$ $'$ be its distinct copy. Let $D[G]$ be the double graph of G and $V(D[G]) = V(G) \cup V(G')$, where $V(G) = \{x_1, x_2, \ldots, x_n\}$ and $V(G') = \{y_1, y_2, \ldots, y_n\}$ and y_i is the corresponding vertex of x_i in $V(G')$.

Lemma 1. *For the above defined double graph $D[G]$*

$$d_{D[G]}(x_i, x_j) = d_G(x_i, x_j) \; ; i, j = 1, \ldots, n.$$

Proof. Clearly, $G \subset D[G]$. Let $\{x_i, \{x_i, x_j\} \subseteq V(G) \subset V(D[G])$ then $d_{D[G]}(x_i, x_j) \leq d_G(x_i, x_j)$. Suppose $l = d_{D[G]}(x_i, x_j) < d_G(x_i, x_j) = m$ and a shortest path in $D[G]$ from x_i to x_j is $x_i v_1 v_2 \ldots v_{l-1} x_j$. If $l = 1$ then the property is obvious. Suppose $1 \geq 2$. Since $l < m$, there exists some $v_k \in V(G')$. As v_{k-1} and v_{k+1} are adjacent to v_k, by definition of the double graph, v_{k-1} and v_{k+1} are adjacent to x_k (corresponding vertex of v_k in $V(G)$). Now we have obtained a path $x_i v_1 v_2 \ldots x_k \ldots v_{l-1} x_j$. In this way we can find a path in G of length l, which is a contradiction. It follows that $d_{D[G]}(x_i, x_j) = d_G(x_i, x_j)$. Similarly, $d_{D[G]}(y_i, y_j) = d_G(y_i, y_j)$.

Lemma 2. *For the double graph $D[G]$*

$$d_{D[G]}(x_i, x_j) = d_G(x_i, x_j) \; ; i, j = 1, \ldots, n.$$

Proof. Let $x_i \in V(G)$ and $y_j \in V(G')$. Suppose $l = d_{D[G]}(x_i, y_j) < d_G(x_i, x_j) = m$ and a shortest path in $D[G]$ is $x_i v_1 v_2 \ldots v_{l-1} y_j$. If $l=1$ the property is true. Let $l \geq 2$. It follows that there exists some $v_k \in V(G')$. Since v_{k-1} and v_{k+1} are adjacent to v_k, by construction v_{k-1} and v_{k+1} are adjacent to x_k (corresponding vertex of v_k in $V(G)$). We have obtained a path $x_i v_1 v_2 \ldots x_k \ldots v_{l-1} y_j$ in $D[G]$, which implies the existence of a path $x_i x_1 x_2 \ldots x_k \ldots x_{l-1} x_j$ in G of length l, a contradiction. If $l = d_{D[G]}(x_i, y_j) > d_G(x_i, x_j) = m$ we get a similar contradiction. Consequently, $d_{D[G]}(x_i, y_j) = d_G(x_i, x_j)$.

The following results are obvious from the construction of the double graph.

Lemma 3. *We have*

$$d_{D[G]}(x_i, y_i) = 2 \quad ; i = 1, \ldots, n.$$

Lemma 4 . *For the double graph $D[G]$*

$$d_{D[G]}(x_i) = d_{D[G]}(y_i) = 2 d_G(x_i) \qquad ; i = 1, \ldots, n.$$

Lemma 5 . *The eccentricities of the vertices of the double graph $D[G]$ are*

$$ecc_{D[G]}(x_i) = ecc_{D[G]}(y_i) = ecc_G(x_i) \;\; if \;\; ecc_G(x_i) \geq 2 \quad ; i = 1, \ldots, n$$

$$ecc_{D[G]}(x_i) = ecc_{D[G]}(y_i) = 2 \quad if \quad ecc_G(x_i) = 1 \quad ; i = 1, \ldots, n.$$

3. MAIN RESULTS

Theorem 1. *Let G be a simple graph with n vertices. Then the Wiener index of $D[G]$ is given by*

$$W(D[G]) = 4W(G) + 2n.$$

Proof. The Wiener index of $D[G]$ is

$$\begin{aligned} W(D[G]) &= \sum_{1 \leq i < j \leq n} d_{D[G]}(v_i, v_j) \\ &= \sum_{1 \leq i < j \leq n} d_{D[G]}(x_i, x_j) + \sum_{1 \leq i < j \leq n} d_{D[G]}(y_i, y_j) + \sum_{\substack{i, j = 1, \ldots, n \\ i = j}} d_{D[G]}(x_i, y_j) + \\ &+ \sum_{i = 1, \ldots, n} d_{D[G]}(x_i, y_i). \end{aligned}$$

By Lemmas 1 – 3 we deduce

$$\begin{aligned} W(D[G]) &= \sum_{1 \leq i < j \leq n} d_G(x_i, x_j) + \sum_{1 \leq i < j \leq n} d_G(x_i, x_j) + \sum_{\substack{i, j = 1, \ldots, n \\ i = j}} d_G(x_i, x_j) + 2n \\ &= W(G) + W(G) + 2W(G) + 2n \\ &= 4W(G) + 2n. \end{aligned}$$

A well known property of the Wiener index of trees implies the following corollary.

Corollary 1. *Suppose T_n is a tree with n vertices. Then*

$$W(D[S_n]) \leq W(D[T_n]) \leq W(D[P_n]).$$

Theorem 2. *Let G be a simple graph with n vertices. Then the Harary index of $D[G]$ is given by*

$$H(D[G]) = 4H(G) + \frac{n}{2}.$$

Proof. The Harary index of $D[G]$ is

$$\begin{aligned} H(D[G]) &= \sum_{1 \leq i < j \leq n} \frac{1}{d_{D[G]}(v_i, v_j)} \\ &= \sum_{1 \leq i < j \leq n} \frac{1}{d_{D[G]}(x_i, x_j)} + \sum_{1 \leq i < j \leq n} \frac{1}{d_{D[G]}(y_i, y_j)} \\ &+ \sum_{\substack{i, j = 1, \ldots, n \\ i = j}} \frac{1}{d_{D[G]}(x_i, y_j)} + \sum_{i = 1, \ldots, n} \frac{1}{d_{D[G]}(x_i, y_i)} \end{aligned}$$

By Lemmas 1 − 3 we have

$$H(D[G]) = \sum_{1\le i<j\le n} \frac{1}{d_G(x_i,x_j)} + \sum_{1\le i<j\le n} \frac{1}{d_G(x_i,x_j)} + \sum_{\substack{i,j=1,\ldots,n\\ i=j}} \frac{1}{d_G(x_i,x_j)} + \frac{n}{2}$$

$$= H(G) + H(G) + 2H(G) + \frac{n}{2}$$

$$= 4H(G) + \frac{n}{2}.$$

Corollary 2. *Let T_n be a tree with n vertices. Then*

$$H(D[P_n]) \le H(D[T_n]) \le H(D[S_n]).$$

Theorem 3. *Let G be a simple graph with m edges. Then the additively weighted Harary index of $D[G]$ is given by*

$$H_A(D[G]) = 8H_A(G) + 4m.$$

Proof. The additively Harary index of $D[G]$ is

$$H_A(D[G]) = \sum_{1\le i<j\le n} \frac{d_{D[G]}(v_i) + d_{D[G]}(v_j)}{d_{D[G]}(v_i,v_j)}$$

$$= \sum_{1\le i<j\le n} \frac{d_{D[G]}(x_i) + d_{D[G]}(x_j)}{d_{D[G]}(x_i,x_j)} + \sum_{1\le i<j\le n} \frac{d_{D[G]}(y_i) + d_{D[G]}(y_j)}{d_{D[G]}(y_i,y_j)}$$

$$+ \sum_{\substack{i,j=1,\ldots,n\\ i\ne j}} \frac{d_{D[G]}(x_i) + d_{D[G]}(y_j)}{d_{D[G]}(x_i,y_j)} + \sum_{i=1,\ldots,n} \frac{d_{D[G]}(x_i) + d_{D[G]}(y_i)}{d_{D[G]}(x_i,y_i)}.$$

by Lemmas 1 − 4 the last expression is equal to

$$\sum_{1\le i<j\le n} \frac{2d_G(x_i) + 2d_G(x_j)}{d_G(x_i,x_j)} + \sum_{1\le i<j\le n} \frac{2d_G(x_i) + 2d_G(x_j)}{d_G(x_i,x_j)}$$

$$+ \sum_{\substack{i,j=1,\ldots,n\\ i\ne j}} \frac{2d_G(x_i) + 2d_G(x_j)}{d_G(x_i,x_j)} + \sum_{x_i\in V(G)} \frac{2d_G(x_i) + 2d_G(x_i)}{2}$$

$$= 2H_A(G) + 2H_A(G) + 4H_A(G) + 2\sum_{x_{i\in V(G)}} d_G(x_i)$$

$$= 8H_A(G) + 4m.$$

Corollary 3. *Suppose T_n and U_n be tree and unicyclic graphs, respectively, with n vertices. Then*

$$H_A(D[T_n]) = 8H_A(T_n) + 4(n-1).$$
$$H_A(D[U_n]) = 8H_A(U_n) + 4n.$$

Corollary 4 . *Suppose T_n is a tree with n vertices. Then*

$$H_A(D[P_n]) \le H_A(D[T_n]) \le H_A(D[S_n]).$$

Theorem 4. *Let G be a simple graph. The multiplicative weighted Harary index of $D[G]$ is given by*

$$H_M(D[G]) = 16H_M(G) + 2\sum_{x_i \in V(G)} d_G(x_i)^2.$$

Proof. The multiplicative Harary index of $D[G]$ is

$$H_M(D[G]) = \sum_{1 \le i < j \le n} \frac{d_{D[G]}(v_i)\, d_{D[G]}(v_j)}{d_{D[G]}(v_i, v_j)}$$
$$= \sum_{1 \le i < j \le n} \frac{d_{D[G]}(x_i)\, d_{D[G]}(x_j)}{d_{D[G]}(x_i, x_j)} + \sum_{1 \le i < j \le n} \frac{d_{D[G]}(y_i)\, d_{D[G]}(y_j)}{d_{D[G]}(y_i, y_j)}$$
$$+ \sum_{\substack{i,j=1,\ldots,n \\ i \ne j}} \frac{d_{D[G]}(x_i)\, d_{D[G]}(y_j)}{d_{D[G]}(x_i, y_j)} + \sum_{i=1,\ldots,n} \frac{d_{D[G]}(x_i)\, d_{D[G]}(y_i)}{d_{D[G]}(x_i, y_i)}.$$

By Lemmas 1 − 4 this expression equals

$$\sum_{1 \le i < j \le n} \frac{2d_G(x_i)\, 2d_G(x_j)}{d_G(x_i, x_j)} + \sum_{1 \le i < j \le n} \frac{2d_G(x_i)\, 2d_G(x_j)}{d_G(x_i, x_j)}$$
$$+ \sum_{\substack{i,j=1,\ldots,n \\ i \ne j}} \frac{2d_G(x_i)\, 2d_G(x_j)}{d_G(x_i, x_j)} + \sum_{x_i \in V(G)} \frac{2d_G(x_i)\, 2d_G(x_i)}{2}$$
$$= 4H_M(G) + 4H_M(G) + 8H_M(G) + 2\sum_{x_i \in V(G)} d_G(x_i)^2$$
$$= 16H_M(G) + 2\sum_{x_i \in V(G)} d_G(x_i)^2.$$

Corollary 5 . *Suppose P_n , S_n ,C_n and K_n be the path, star cyclic and complete graphs with n vertices. Then*

$$H_M(D[P_n]) = 16H_M(P_n) + 8n - 12$$
$$H_M(D[S_n]) = 16H_M(S_n) + 2n(n-1)$$
$$H_M(D[C_n]) = 16H_M(C_n) + 8n$$
$$H_M(D[K_n]) = 16H_M(K_n) + 2n(n-1)^2.$$

Theorem 5. *Suppose G is a graph of order n, having k vertices v such that ecc*(*v*)=1 (*or equivalently, $d_G(v)=n$-1). The eccentric connectivity index of D*[*G*] *is given by*

$$\zeta^c(D[G]) = 4\zeta^c(G) + 4k(n-1).$$

Proof.

$$\zeta^c(D[G]) = \sum_{i=1}^{n} d_{D[G]}(x_i)\, ecc_{D[G]}(x_i) + \sum_{i=1}^{n} d_{D[G]}(y_i)\, ecc_{D[G]}(y_i).$$

By Lemmas 4 and 5 we have

Theorem 6. *Let G be a simple graph having k vertices with $ecc_G(v)$ = 1. The total eccentricity index of D*[*G*] *is given by*

$$\zeta(D[G]) = 2\zeta(G) + 2k.$$

Proof.

$$\zeta(D[G]) = \sum_{i=1}^{n} ecc_{D[G]}(x_i) \; + \sum_{i=1}^{n} ecc_{D[G]}(y_i).$$

By Lemma 5, we have

$$\zeta(D[G]) = 2\left(\sum_{i ecc_G(x_i)\geq 2} ecc_G(x_i) \; + \sum_{i ecc_G(x_i)=1} 2 \right) = 2\zeta(G) + 2k.$$

Corollary 6. *For the star and the complete graph we have:*

$$\zeta(D[S_n]) = 2\zeta(S_n) + 2;$$
$$\zeta(D[K_n]) = 2\zeta(K_n) + 2n.$$

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ABSTRACTS
IN
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Stirling Numbers and Generalized Zagreb Indices

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اعداد استرلینگ و شاخص‌های زاگرب تعمیم‌یافته

ادیتور رابط : سندی کلاوزار

چکیده

در این مقاله نشان می‌دهیم که چگونه می‌توان شاخص‌های زاگرب تعمیم‌یافته $M_1^k(G)$ را با استفاده از یک گراف چندجمله‌ای ساده و اعداد استرلینگ نوع دوم، محاسبه کرد. به این ترتیب، معنی یک مثلث از اعداد را که برای حصول نتیجه ای مشابه با یک مرجع قبلی، استفاده می‌شود را شرح می‌دهیم.

لغات کلیدی: گراف ساده، شاخص زاگرب، عدد استرلینگ

Relationship Between Coefficients of Characteristic Polynomial and Matching Polynomial of Regular Graphs and its Applications

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رابطه میان ضرایب چندجمله‌ای مشخصه و چندجمله‌ای جورسازی گراف‌های منظم و کاربردهای آن

ادیتور رابط : علیرضا اشرفی

چکیده

فرض کنید G یک گراف و A(G) ماتریس مجاورت آن است. فرض کنید چندجمله‌ای مشخصه گراف G به‌صورت $\chi(G,\lambda)=\lambda^n+\sum_{i=1}^{n}a_i\lambda^{n-i}$ است. چندجمله‌ای جورسازی گراف G به‌صورت زیر تعریف می‌شود:

$$M(G,x)=\sum_{k\geq 0}(-1)^k m(G,k)x^{n-2k}$$

که در آن $m(G,k)$ تعداد k-جورسازی‌های گراف G است. در این مقاله رابطه میان 2k-امین ضریب چندجمله‌ای مشخصه، a_{2k}، و k-امین ضریب چندجمله‌ای جورسازی، $(-1)^k m(G,k)$، در یک گراف منظم را مشخص می‌نماییم و سپس با استفاده از این روابط، تعداد 5 و 6-جورسازی‌ها را در گراف‌های فولرن به‌دست می‌آوریم.

لغات کلیدی: چندجمله‌ای مشخصه، چندجمله‌ای جورسازی، گراف فولرن.

The Topological Indices of some Dendrimer Graphs

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اندیس های توپولوژیکی برخی گراف‌های دندریمر

ادیتور رابط : حسن یوسفی آذری

چکیده

در این مقاله، اندیس‌های وینر و وینر بالایی دو نوع گراف دندریمر محاسبه شده است. با به‌کارگیری فرمول به دست آمده برای اندیس وینر، اندیس‌های سگد، شولز، پادماکار- ایوان و گوتمن نیز برای این گراف‌ها تعیین می‌شود.

لغات کلیدی: اندیس توپولوژیکی، دندریمر، اندیس وینر، اندیس وینر بالایی

On the Multiplicative Zagreb Indices of Bucket Recursive Trees

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شاخص‌های زاگرب ضربی درخت‌های بازگشتی سطلی

ادیتور رابط : علیرضا اشرفی

چکیده

درخت‌های بازگشتی سطلی یک تعمیم جالب و طبیعی از درخت‌های بازگشتی معمولی هستند و یک ارتباط با ریاضی-شیمی دارند. در این مقاله، کران‌های پایین و بالایی برای تابع مولد گشتاور و گشتاورهای شاخص‌های زاگرب ضربی در یک درخت بازگشتی سطلیِ به‌طور تصادفی انتخاب شده از اندازه‌ی n با اندازه‌ی سطل ماکسیمال $b \geq 1$ ارائه می‌شود. همچنین، به نسبت شاخص‌های زاگرب ضربی برای مقادیر مختلف n و b توجه می‌شود. همه‌ی نتایج ارائه شده برای $b = 1$ به درخت‌های بازگشتی معمولی تقلیل می‌یابد.

لغات کلیدی: درخت‌های بازگشتی سطلی، شاخص زاگرب ضربی، تابع مولد گشتاور، گشتاورها.

The Conditions of the Violations of Le Chatlier's Principle in Gas Reactions at Constant T and P

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شرایط نقض اصل لوشاتلیه در واکنش‌های گازی در دما و فشار ثابت

ادیتور رابط : ایوان گوتمن

چکیده

اصل لوشاتلیه به عنوان یک راه بسیار ساده برای پیش‌بینی اثر یک تغییر در شرایط تعادل شیمیایی استفاده می‌شود. به‌هرحال، چندین مطالعه، نقض‌شدن این اصل را گزارش کرده‌اند و هنوز هیچ معادله ریاضی‌ای برای بیان دقیق شرایط نقض در واکنش‌های فاز گازی گزارش نشده است. در این مقاله، ما یک معادله ساده را برای نقض اصل لوشاتلیه برای واکنش‌های گاز ایده‌آل در دما و فشار ثابت اثبات می‌کنیم.

لغات کلیدی: نقض اصل لوشاتلیه، واکنش گازی، مخلوط، تعادل شیمیایی، تعدیل پتانسیل شیمیایی

Neighbourly Irregular Derived Graphs

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گراف‌های مشتق‌شده همسایه‌وار نامنظم

ادیتور رابط : تومیسلاو داسلیک

چکیده

یک گراف همبند G، همسایه‌وار نامنظم نامیده می‌شود هرگاه هیچ دو رأس مجاور G، هم‌درجه نباشند. در این مقاله، گراف‌های مشتق‌شده همسایه وار نامنظم مانند گراف نیم‌کامل-نقطه، گراف نیم‌کامل-نقطه k-ام، گراف نیم‌کامل-خط، گراف خط‌خطی، گراف شبه‌کامل، گراف شبه‌رأس کامل و همچنین برخی گراف‌های حاصلضربی را به‌دست می‌آوریم.

لغات کلیدی: همسایه‌وار نامنظم، گراف‌های مشتق‌شده، گراف‌های حاصلضربی

Splice Graphs and Their Vertex-Degree-Based Invariants

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گراف های به‌هم پیوسته و پایاهای مبتنی بر درجه رأس آن‌ها

ادیتور رابط : تومیسلاو داسلیک

چکیده

فرض کنید G_1 و G_2 دو گراف همبند ساده به ترتیب با مجموعه رئوس مجزای $V(G_1)$ و $V(G_2)$ باشند. برای رأس‌های معین $a_1 \in V(G_1)$ و $a_2 \in V(G_2)$، به‌هم پیوستگی G_1 و G_2 توسط رأس‌های a_1 و a_2 با یکی‌کردن رأس‌های a_1 و a_2 در اجتماع G_1 و G_2 تعریف می‌شود. در این مقاله، فرمول‌های دقیقی برای محاسبه‌ی برخی پایاهای گرافی مبتنی بر درجه رأس به‌هم پیوستگی گراف‌ها ارائه می‌کنیم.

لغات کلیدی: درجه رأس، پایای گراف، به‌هم پیوستگی.

An upper bound on the first Zagreb index in trees

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کران بالای شاخص زاگرب اول در درخت‌ها

ادیتور رابط : علیرضا اشرفی

چکیده

شاخص زاگرب اول برابر مجموع مربعات درجات راس‌های گراف می‌باشد و با $M_1(G)$ نمایش داده می‌شود و هم‌اندیس اول گراف برابر مجموع درجات زوج راس‌های غیرمجاور است. ووکیسویچ و پاپیوودا در مرجع [Iran. J. Math. Chem. 5 (2014) 19-29] ثابت کردند که برای هر درخت شیمیایی از مرتبه n، $n \geq 5$،

$$M_1(T) \leq \begin{cases} 6n-12 & n \equiv 0,1 \pmod 3 \\ 6n-10 & otherwise. \end{cases}$$

در این مقاله کران بالای اندیس زاگرب اول در همه درخت‌ها بر حسب تعداد راس‌ها و ماکزیمم درجه، تعمیم یافته است. همچنین کران پایین برای هم‌اندیس زاگرب اول درخت‌ها محاسبه شده است.

لغات کلیدی: اندیس زاگرب اول، هم‌اندیس زاگرب اول، درخت، درخت شیمیایی

Distance-Based Topological Indices and Double Graph

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فاصله بر اساس شاخص‌های توپولوژیکی و گراف دوگانه

ادیتور رابط : علی رضا اشرفی

چکیده

فرض کنید G یک گراف همبند، و $D(G)$ بیانگر گراف دوگانه G باشد. دراین مقاله، ابتدا شکل بسته فرمول‌های برخی فواصل، برپایه‌ی شاخص‌های توپولوژیکی برای $D(G)$ برحسب G را نتیجه می‌گیریم. در پایان، این فرمول‌ها برای چند نوع خاص از گرافها مانند گراف کامل، مسیر و دور به‌کار گرفته می‌شوند.

لغات کلیدی: شاخص وینر، شاخص هراری، گراف دوگانه

این نشریه طبق مجوز شماره 89/3/11/104372 مورخه 89/11/27 دارای اعتبار **علمی -پژوهشی** از وزارت علوم ، تحقیقات و فناوری می باشد. همچنین این مجله در پایگاه اطلاعاتی ISC (Islamic World Science Citation Center) وابسته به وزارت علوم ، تحقیقات و فناوری نمایه می شود.

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