Iranian Journal of Mathematical Chemistry, Vol. 4,No.2, December 2013, pp. 221–230 **IJMC**

Applications of Some Graph Operations in Computing Some Invariants of Chemical Graphs

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(*Received October 20, 2013; Accepted October 29, 2013*)

ABSTRACT

In this paper, we first collect the earlier results about some graph operations and then we present applications of these results in working with chemical graphs.

Keywords: Topological index; graph operation; distance–balanced graph; chemical graph.

1. INTRODUCTION

Throughout this paper all graphs considered are finite, simple and connected. The distance $d_G(u,v)$ between the vertices u and v of a graph G is equal to the length of a shortest path that connects u and v. Suppose G is a graph with vertex and edge sets $V = V(G)$ and $E = E(G)$, respectively. For an edge $e = ab$ of G, let $n_a(e)$ be the number of vertices closer to a than to b. In other words, $n_a^G(e) = |\{u \in V(G) \mid d(u, a) < d(u, b)\}|$. In addition, let $n_0(e)$ be the number of vertices with equal distances to a and b, i.e., $n_0^G(e) = |\{u \in V(G) \mid d(u, a) = d(u, b)\}|$. We also denote the number of edges of G whose distance to the vertex a is smaller than the distance to the vertex b by $m_a(e)$. The Szeged, edge Szeged, revised Szeged, vertex–edge Szeged, vertex Padmakar–Ivan and edge Padmakar–Ivan indices of the graph G are defined as:

$Sz_v(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e)$ (see[1]),

$Sz_e(G) = \sum_{e=uv\in E(G)} m_u(e)m_v(e)$ (see[2]),

$Sz_v^*(G) = \sum_{e=uv\in E(G)} (n_u(e)+ \frac{n_0(e)}{2})(n_v(e)+ \frac{n_0(e)}{2})$ (see[3]),

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$Sz_{ev}(G) = \frac{1}{2}\sum_{e=uv\in E(G)}(m_u(e)n_v(e)+ m_v(e)n_u(e))$ (see[4]),
$PI_v(G) = \sum_{e=uv\in E(G)}(n_u(e)+n_v(e))$ (see[5]),
$PI_e(G) = \sum_{e=uv\in E(G)}(m_u(e)+m_v(e))$ (see[6]).

A graph G with a specified vertex subset $U\subseteq V(G)$ is denoted by $G(U)$. Suppose G and H are graphs and $U\subseteq V(G)$. The generalized hierarchical product, denoted by $G(U)\sqcap H$, is the graph with vertex set $V(G)\times V(H)$ and two vertices (g, h) and (g', h') are adjacent if and only if $g = g'\in U$ and $hh' \in E(H)$ or, $gg' \in E(G)$ and $h = h'$. This graph operation has been introduced by Barriére et al. [7,8] and it has some applications in computer science. To generalize this graph operation to n graphs, assume that $G_i = (V_i , E_i)$ is a graph with vertex set V_i , $1 \le i \le N$, having a distinguished or root vertex 0. The hierarchical product $H = G_N \sqcap\ldots\sqcap G_2\sqcap G_1$ is the graph with vertices the N–tuples $x_N \ldots x_3x_2x_1$, $x_i \in V_i$, and edges defined by the following adjacencies:

$$x_N\ldots x_3x_2x_1\sim\begin{cases} x_N\ldots x_3x_2y_1 & \text{if} \quad x_1y_1\in E(G_1),\\ x_N\ldots x_3y_2x_1 & \text{if} \quad x_2y_2\in E(G_2) \text{ and } x_1=0,\\ x_N\ldots y_3x_2x_1 & \text{if} \quad x_3y_3\in E(G_3) \text{ and } x_1=x_2=0,\\ \quad\vdots & \quad\vdots \qquad\qquad\qquad\qquad\qquad \vdots\\ y_N\ldots x_3x_2x_1 & \text{if} \quad x_Ny_N\in E(G_N) \text{ and } x_1=x_2=\ldots=x_{N-1}=0.\end{cases}$$

We encourage the reader to consult [9] for the mathematical properties of the hierarchical product of graphs.

The Cartesian product $G\times H$ of the graphs G and H has the vertex set $V(G\times H) = V(G)\times V(H)$ and $(a, x)(b, y)$ is an edge of $G\times H$ if $a = b$ and $xy \in E(H)$, or $ab \in E(G)$ and $x = y$, see[10].

The disjunction $G\vee H$ of graphs G and H is the graph with vertex set $V(G)\times V(H)$ such that (u_1, v_1) is adjacent to (u_2, v_2) whenever $u_1u_2\in E(G)$ or $v_1v_2\in E(H)$ [10].

Let $G=(V, E)$ be a simple graph of order $n=|V|$. Given $u, v \in V$, $u \sim v$ means that u and v are adjacent vertices. Given a set of vertices $S=\{v_1, v_2, \ldots, v_k\}$ of a connected graph G, the metric representation of a vertex $v \in V$ with respect to S is the vector $r(v|S)=(d_G(v, v_1), d_G(v, v_2), \ldots, d_G(v, v_k))$. We say that S is a resolving set for G if for every pair of distinct vertices $u, v \in V$, $r(u|S) \neq r(v|S)$. The metric dimension of G is the minimum cardinality of any resolving set for G, and it is denoted by $dim(G)$.

Now, we present some certain types of graphs that play prominent roles in this work. A graph G is called nontrivial if $|V(G)| > 1$. The n-cube Q_n $(n \geq 1)$ is the graph whose vertex set is the set of all n-tuples of 0s and 1s, where two n-tuples are adjacent if they differ in precisely one coordinate. A tree is an undirected graph in which any two vertices are connected by exactly one simple path. In other words, any connected graph without cycles is a tree. A regular graph is a graph where each vertex has the same number of neighbors. A regular graph with vertices of degree k is called a k–regular graph or regular graph of degree k. Note that the path graph, the complete and the cycle of order n are denoted by P_n, K_n and C_n, respectively.

2. MAIN RESULTS

In what follows, we assume that $\prod_i^j f_i = 1$ and $\sum_i^j f_i = 0$ for each $i, j \in \{0, 1, 2, \ldots\}$, that $i - j = 1$. Furthermore, let $\prod_i^j f_i = \sum_i^j f_i = 0$, for every $i, j \in \{0, 1, 2, \ldots\}$, such that $i - j > 1$. For a rooted graph G with root vertex r, we will use $\Gamma_v(G)$ to denote the sum of $n_v^G(e)$ over all edges $e = uv$ of G that $d_G(u, r) < d_G(v, r)$ and $\Gamma_v^c(G)$ to denote the sum of $n_u^G(e)$ over all edges $e = uv$ of G that $d_G(u, r) < d_G(v, r)$. Moreover, $\Gamma_e(G)$ denotes the sum of $m_v^G(e)$ over all edges $e = uv$ of G that $d_G(u, r) < d_G(v, r)$ and $\Gamma_e^c(G)$ denotes the sum of $m_u^G(e)$ over all edges $e = uv$ of G that $d_G(u, r) < d_G(v, r)$. In other words,

$$\Gamma_v(G) = \sum_{uv\in E(G), d_G(u,r)<d_G(v,r)} n_v^G(uv),$$

$$\Gamma_v^c(G) = \sum_{uv\in E(G), d_G(u,r)<d_G(v,r)} n_u^G(uv),$$

$$\Gamma_e(G) = \sum_{uv\in E(G), d_G(u,r)<d_G(v,r)} m_v^G(uv),$$

$$\Gamma_e^c(G) = \sum_{uv\in E(G), d_G(u,r)<d_G(v,r)} m_u^G(uv).$$

If the vertex r lies on no odd cycle of G, then one can easily seen that

$$PI_v(G) = \Gamma_v(G) + \Gamma_v^c(G) \quad \text{and} \quad PI_e(G) = \Gamma_e(G) + \Gamma_e^c(G).$$

Also, for a sequence of graphs, $G_1, G_2, \ldots, G_n$, we set $|V_{i,j}| = \prod_{k=i}^j |V(G_k)|$ and $|V_{i,j}^l| = \prod_{k=i,k\neq l}^j |V(G_k)|$. To say the next result, we have to present some notation. For a connected rooted graph G with root vertex r, let $N^G(r)$ be the set of vertices of G with the property that $u \in N^G(r)$ if there exists $v \neq u$ in $V(G)$ such that $d_G(u, r) = d_G(v, r)$. We say that

$S(N^G(r)) \subseteq V(G)$ is a resolving set for $N_G(r)$ if for each pair of distinct vertices $u, v \in N^G(r)$, $r(u|S(N^G(r))) \neq r(v|S(N^G(r)))$. Therefore, it is clear that $dim(N^G(r)) \leq dim(G)$. The metric dimension of $N^G(r)$ is the minimum cardinality of any resolving set for $N^G(r)$, and it is denoted by $dim(N^G(r))$.

Theorem 1. [9]. Suppose $G_1, G_2, \ldots, G_n$ are nontrivial connected rooted graphs with root vertices $r_1, \ldots, r_n$, respectively. Then

$$dim(G_n \sqcap \ldots \sqcap G_2 \sqcap G_1) = \begin{cases} \prod_{j=2}^{n} |V(G_j)| \, dim(N^{G_1}(r_1)) & \text{if } G_1 \ncong P_n \\ \prod_{j=3}^{n} |V(G_j)| \, dim(N^{G_2 \sqcap G_1}(r_2)) & \text{if } G_1 \cong P_n \end{cases}.$$

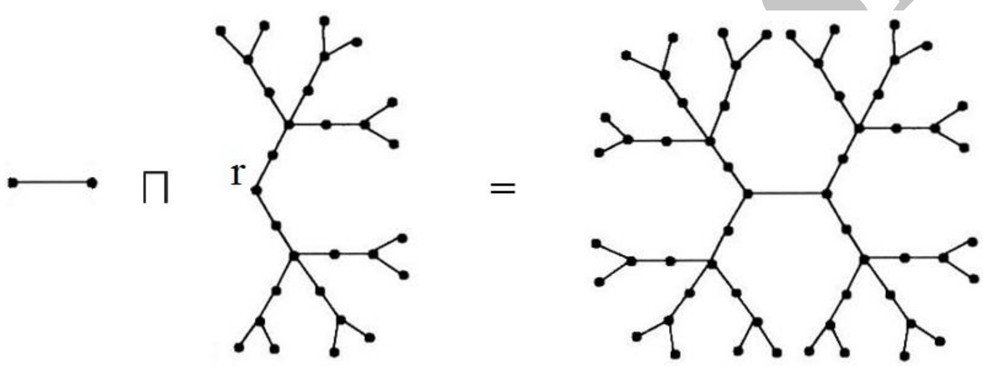

Figure 1: Irregular Dicentric $IDD_{5,(2,1,3,1,2)}$ Dendrimer.

Example 2. Let $IDD_{r,(p_1,\cdots,p_r)}$ be the graph of the irregular dicentric dendrimer that $p_i>1$, $i=1,.., r$, see [11] for more information. Then $IDD_{r,(p_1,\cdots,p_r)} = P_2 \sqcap H$, where H is a tree of progressive degrees p_i, $i=1,\ldots,r$, respectively, and generation r (see Figure 1). One can see that $dim(N^H(r)) = \prod_{i=1}^{r-1} p_i(p_r-1)$. Therefore, by Theorem 1, we have:

$$dim(IDD_{r,(p_1,\cdots,p_r)}) = |V(P_2)| \, dim(N^H(r)) = 2\prod_{i=1}^{r-1} p_i(p_r-1).$$

A graph G is said to be (vertex) distance-balanced, if $n_a^G(e) = n_b^G(e)$, for each edge $e = ab \in E(G)$, see [12, 13] for details. These graphs first studied by Handa [14] who considered distance-balanced partial cubes. In [15], Jerebic et al. studied distance-balanced graphs in the framework of various kinds of graph products. After that, in [16], the present authors introduced the concept of edge distance-balanced graphs. Such a graph G has this property that $m_a^G(e) = m_b^G(e)$ holds for each edge $e = ab \in E(G)$.

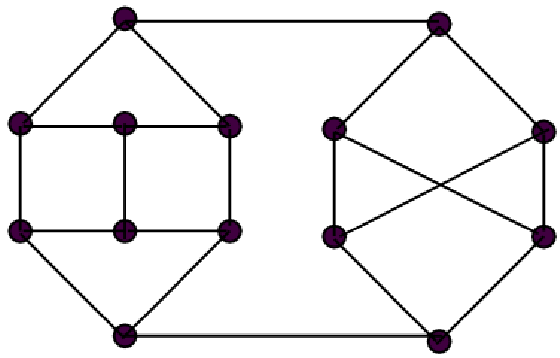

Figure 2: The Graph G'.

Proposition 3. [13]. Let G and H be arbitrary, nontrivial and connected graphs. Then $G \vee H$ is distance-balanced if and only if G and H are regular graphs.

Example 4. Consider G', see Figure 2, that was constructed in [17] as an example of a bipartite regular graph that is not distance-balanced. It would be interesting to know that we can produce a distance-balanced graph by two graphs which are not distance-balanced. Let G is arbitrary, nontrivial and connected regular graph then by the above proposition, $G' \vee G$ is distance-balanced (note that G can be not distance-balanced).

Theorem 5. [16]. Let G and H be edge and vertex distance–balanced graphs. Then $G \times H$ is edge distance-balanced graphs.

Example 6. Consider the N-cube Q_N. It is well-known fact that it can be written in the form $Q_N = \times_{i=1}^{N} K_2$. On the other hand, K_2 is edge and vertex distance-balanced graph. So, by the above theorem, Q_N is edge distance-balanced graph.

Theorem 7. [18]. Suppose $G_1, G_2, \ldots, G_n$ are connected rooted graphs with root vertices $r_1, \ldots, r_n$, respectively. Then

$$Sz_v(G_n \sqcap \ldots \sqcap G_2 \sqcap G_1) = \sum_{i=1}^{n} |V_{i+1,n}||V_{1,i-1}|^2 \, Sz_v(G_i)$$

$$+\sum_{i=1}^{n-1}\left(\sum_{j=i+1}^{n}(|V(G_j)|-1)|V_{1,j-1|}\right)|V_{1,n}^{i}|\,\Gamma_v(G_i).$$

Corollary 8. [18]. Suppose G_1, G_2, …, G_n are connected, rooted and distance-balanced graphs with root vertices r_1, …, r_n, respectively, such that r_i lies on no odd cycle of G_i, $i = 1, 2, \ldots, n$. Then

$$Sz_v(G_n\sqcap\ldots\sqcap G_2\sqcap G_1)=\sum_{i=1}^{n}|V_{i+1,n}||V_{1,i-1}|^2\,Sz_v(G_i)$$
$$+\frac{1}{2}\sum_{i=1}^{n-1}\left(\sum_{j=i+1}^{n}(|V(G_j)|-1)|V_{1,j-1|}\right)|V_{1,n}^{i}|\,PI_v(G_i).$$

Theorem 9. [18]. Suppose G_1, G_2, …, G_n are connected rooted graphs with root vertices r_1, …, r_n, respectively. Then

$$Sz_e(G_n\sqcap\ldots\sqcap G_2\sqcap G_1)=\sum_{i=1}^{n}|V_{i+1,n}|Sz_e(G_i)$$
$$+\sum_{i=1}^{n}|V_{i+1,n}|\left(\sum_{j=1}^{i-1}|E(G_j)||V_{j+1,i-1}|\right)^2 Sz_v(G_i)$$
$$+2\sum_{i=1}^{n}|V_{i+1,n}|\left(\sum_{j=1}^{i-1}|E(G_j)||V_{j+1,i-1}|\right)Sz_{ev}(G_i)$$
$$+\sum_{i=1}^{n}|V_{i+1,n}|\left(\Gamma_e(G_i)+\Gamma_v(G_i)\sum_{j=1}^{i-1}|E(G_j)||V_{j+1,i-1}|\right)$$
$$+\sum_{j=i+1}^{n}\left(\left(|V(G_j)|-1\right)\sum_{k=1}^{j-1}|E(G_k)||V_{k+1,j-1}|+|E(G_j)|\right).$$

Corollary 10. [18]. Suppose G_1, G_2, …, G_n are connected, rooted, distance-balanced and edge distance-balanced graphs with root vertices r_1, r_2, …, r_n, respectively, such that r_i lies on no odd cycle of G_i, $i = 1, 2, \ldots, n$. Then

$$Sz_e(G_n\sqcap\ldots\sqcap G_2\sqcap G_1)=\sum_{i=1}^{n}|V_{i+1,n}|Sz_e(G_i)$$

$$+\sum_{i=1}^{n}|V_{i+1,n}|\left(\sum_{j=1}^{i-1}|E(G_j)||V_{j+1,i-1}|\right)^2 Sz_v(G_i)$$

$$+2\sum_{i=1}^{n}|V_{i+1,n}|\left(\sum_{j=1}^{i-1}|E(G_j)||V_{j+1,i-1}|\right)Sz_{ev}(G_i)$$

$$+\frac{1}{2}\sum_{i=1}^{n}|V_{i+1,n}|\left(PI_e(G_i)+PI_v(G_i)\sum_{j=1}^{i-1}|E(G_j)||V_{j+1,i-1}|\right)$$

$$\times\sum_{j=i+1}^{n}\left(\left(|V(G_j)|-1\right)\sum_{k=1}^{j-1}|E(G_k)||V_{k+1,j-1}|+|E(G_j)|\right).$$

Theorem 11. [18]. Suppose $G_1, G_2, \ldots, G_n$ are connected rooted graphs with root vertices $r_1, r_2, \ldots, r_n$, respectively. Then

$$Sz_v^*(G_n \sqcap \ldots \sqcap G_2 \sqcap G_1) = \sum_{i=1}^{n}|V_{1,i-1}|^2|V_{i+1,n}|\ Sz_v^*(G_i)$$

$$+\sum_{i=1}^{n}\frac{|V_{1,n}^i|}{2}\left(\sum_{j=i+1}^{n}\left(|V(G_j)|-1\right)|V_{1,j-1}|\right)|V(G_i)||E(G_i)|$$

$$+\sum_{i=1}^{n}\frac{|V_{i+1,n}|}{4}\left(\sum_{j=i+1}^{n}\left(|V(G_j)|-1\right)|V_{1,j-1}|\right)^2 N_{r_i}$$

$$+\sum_{i=1}^{n}\frac{|V_{1,n}^i|}{2}\left(\sum_{j=i+1}^{n}\left(|V(G_j)|-1\right)|V_{1,j-1}|\right)\left(\Gamma_v(G_i)-\Gamma_v^c(G_i)\right)$$

where $N_{r_i} = |\{uv \in E(G_i) \mid d_{G_i}(u, r_i) = d_{G_i}(v, r_i)\}|$.

Corollary 12. [18]. Suppose $G_1, G_2, \ldots, G_n$ are connected, rooted, bipartite and distance-balanced graphs with root vertices $r_1, r_2, \ldots, r_n$, respectively. Then

$$Sz_v^*(G_n \sqcap \ldots \sqcap G_2 \sqcap G_1) = \sum_{i=1}^{n}|V_{1,i-1}|^2|V_{i+1,n}|\ Sz_v^*(G_i)$$

$$+\sum_{i=1}^{n}\frac{|V_{1,n}^i|}{2}\left(\sum_{j=i+1}^{n}\left(|V(G_j)|-1\right)|V_{1,j-1}|\right)PI_v(G_i).$$

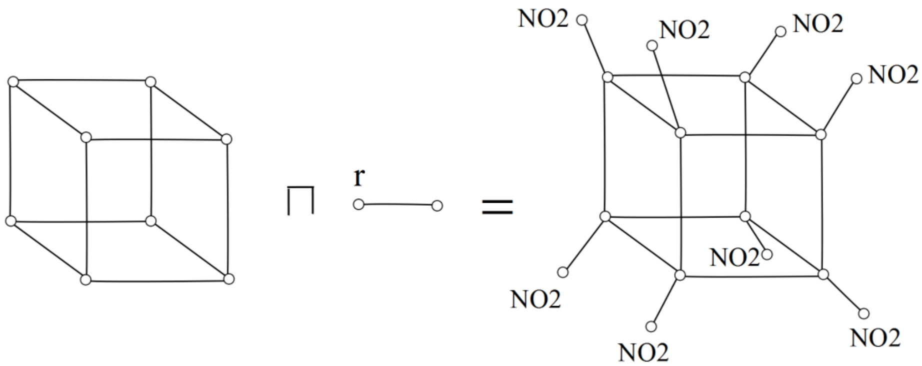

Figure 3: The Molecular Graph of Octanitrocubane.

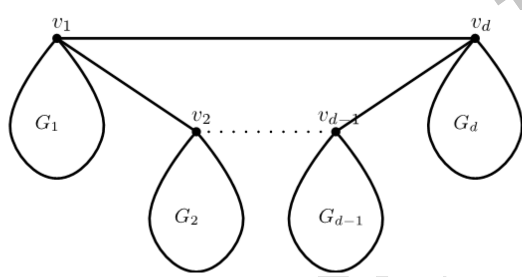

Figure 4: The Bridge–Cycle Graph.

Example 13. Octanitrocubane is the most powerful chemical explosive with formula $C_8(NO_2)_8$, Figure 3. Let H be the molecular graph of this molecule. Then obviously $H= Q_3 \sqcap P_2$. On the other hand, one can easily see that $Sz_v(Q_3)= Sz_e(Q_3)= Sz_{ev}(Q_3)=Sz^*(Q_3)=192$, $\Gamma_v(P_2) = 1$ and $\Gamma_e(P_2) = 0$ and so, by the above results, we have:

$$Sz_v(H) = Sz_v(Q_3 \sqcap P_2)=888,\ Sz_e(H) = Sz_e(Q_3 \sqcap P_2)=768,\ Sz_{ev}(H) = Sz_v(Q_3 \sqcap P_2)=888.$$

Example 14. Let $\{G_i\}_{i=1}^{d}$ be a set of finite pairwise disjoint graphs with $v_i \in V(G_i)$. The bridge–cycle graph $BC(G_1, G_2, \dots, G_d) = BC(G_1, G_2, \dots, G_d; v_1, v_2, \dots, v_d)$ of $\{G_i\}_{i=1}^{d}$ with respect to the vertices $\{v_i\}_{i=1}^{d}$ is the graph obtained from the graphs $G_1, \dots, G_d$ by connecting the vertices v_i and v_{i+1} by an edge for all $i = 1, 2, \dots, d-1$ and connecting the vertices v_1 and v_d by an edge, see Figure 4. Suppose that $G_1 = \dots = G_d = G$. Then we have $BC(G_1, G_2, \dots, G_d) \cong C_d \sqcap G$. On the other hand, It is not so difficult to check that $Sz_v(C_n)=\begin{cases} \frac{n^3}{4} & 2 \nmid n \\ \frac{n^2(n-1)}{4} & 2 \mid n \end{cases}$. Therefore, if $2 \mid n$, by Theorem 1, we have $Sz_v(C_n \sqcap G) = n$

$Sz_v(G) + \frac{n^3}{4}|V(G)|^2 + n(n-1)|V(G)|\Gamma_v(G)$ and if $2 \nmid n$, then $Sz_v(C_n \sqcap G) = n\, Sz_v(G) + \frac{n(n-1)^2}{4}|V(G)|^2 + n(n-1)|V(G)|\Gamma_v(G)$.

By replacing G with P_m (such that r is a pendant vertex of P_m) in the above relations, we obtain Sz_v of $Sun_{n,\,m-1}$, see [19], as follow:

$$Sz_v(Sun_{n\,,m-1}) = \begin{cases} \frac{1}{4}n^3m^2 + \frac{1}{2}n^2m^3 - \frac{1}{2}n^2m^2 - \frac{1}{3}nm^3 + \frac{1}{2}nm^2 - \frac{1}{6}nm & 2 \mid n \\ \frac{1}{4}n^3m^2 - n^2m^2 + \frac{3}{4}nm^2 + \frac{1}{2}n^2m^3 - \frac{1}{3}nm^3 - \frac{1}{6}nm & 2 \nmid n \end{cases}.$$

ACKNOWLEDGMENTS. This research was supported by a grant from Ferdowsi University of Mashhad; (No. MA91292RAH).

REFERENCES

1. I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes N. Y*. **27** (1994) 9–15.
2. I. Gutman, A. R. Ashrafi, The edge version of the Szeged index, *Croat. Chem. Acta* **81** (2008) 263–266.
3. T. Pisanski, M. Randić, Use of the Szeged index and the revised Szeged index for measuring network bipartivity, *Discrete Appl. Math.* **158** (2010) 1936–1944.
4. M. Randić, On generalization of Wiener index for cyclic structures, *Acta Chim. Slov*. **49** (2002) 483–496.
5. P. V. Khadikar, S. Karmarkar, V. K. Agrawal, A novel PI index and its applications to QSPR/QSAR studies, *J. Chem. Inf. Comput. Sci.* **41** (2001) 934–949.
6. M. H. Khalifeh, H. Yousefi−Azari, A. R. Ashrafi, Vertex and edge PI indices of Cartesian product graphs, *Discrete Appl. Math.* **156** (2008) 1780–1789.
7. L. Barriére, F. Comellas, C. Daflo and M. A. Fiol, The hierarchical product of graphs, *Discrete Appl. Math.* **157** (2009) 36–48.
8. L. Barriére, C. Daflo, M. A. Fiol and M. Mitjana, The generalized hierarchical product of *graphs*, *Discrete Math.* **309** (2009) 3871–3881.
9. M. Tavakoli, F. Rahbarnia and A. R. Ashrafi, Distribution of some graph invariants over hierarchical product of graphs, *Appl. Math. Comput*. **220** (2013) 405–413.

10. R. Hammack, W. Imrich and S. Klavžar, handbook of product graphs (Second edition), Taylor Francis Group, (2011).
11. M. V. Diudea, Molecular topology. 21. Hyper–Wiener index of dendrimers, *MATCH Commun. Math. Comput. Chem.* **32** (1995) 71–83.
12. M. Aouchiche, P. Hansen, on a conjecture about the Szeged index, *Eur. J. Combin.* **31** (2010) 1662–1666.
13. M. Tavakoli, F. Rahbarnia, A. R. Ashrafi, Further results on distance−balanced graphs, *U.P.B. Sci. Bull., Ser. A* **75** (2013) 77–84.
14. K. Handa, Bipartite graphs with balanced *(a,b)*–partitions, *Ars Combin.* **51** (1999) 113–119.
15. J. Jerebic, S. Klavžar, D.F. Rall, Distance−balanced graphs, *Ann. Combin.* **12** (2008) 71–79.
16. M. Tavakoli, H. Yousefi−Azari, A. R. Ashrafi, Note on edge distance-balanced graphs, *Trans. Comb.* **1** (2012) 1–6.
17. E. Chiniforooshan, B. Wu, Maximum values of Szeged index and edge−Szeged index of graphs, *Electron. Notes Discrete Math.* **34** (2009) 405–409.
18. M. Tavakoli, F. Rahbarnia and A. R. Ashrafi, Further results on hierarchical product of graphs, *Discrete Appl. Math*. **161** (2013) 1162–1167.
19. Y. N. Yeh and I. Gutman, On the sum of all distances in composite graphs, *Discrete Math*. **135** (1994) 359–365.