Reduced second Zagreb index of product graphs

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The reduced second Zagreb index of a graph G is defined as $RM_2(G) = \sum\limits_{uv \in E(G)} (d_G(u) - 1)(d_G(v) - 1)$, where $d_G(v)$ denotes the degree of the vertex v of graph G. Recently Furtula et al. (Furtula B., Gutman I., Ediz S. *Discrete Appl. Math.*, 2014) characterized the maximum trees with respect to reduced second Zagreb index. The aim of this paper is to compute reduced second Zagreb index of the Cartesian product of k (≥ 2) number of graphs and hence as a consequence the reduced second Zagreb index of some special graphs applicable in various real world problems are computed. Topological properties of different nanomaterials like nanotube, nanotorus etc. are studied here graphically in terms of the aforesaid aforementioned index.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For a graph G, let $d_G(v)$ denote the degree of a vertex v in G, that is, the number of vertices adjacent with v. Throughout this article, we consider chemical graph [1,2]. By chemical graph we mean a simple connected graph where vertices and edges are supposed to be atoms and chemical bonds between them respectively.

Topological indices, also called molecular structure descriptors are used in theoretical chemistry for design of chemical compounds with given physico-chemical properties and also to model chemical biological and pharmacological properties of the molecules. A topological index is a real number and it does not depend on the labelling of a graph and must be a structural invariant. The first topological index, Wiener index, was published in 1947 [3]. Due to the importance of topological indices in chemical research, lots of topological indices are developed in the chemical graph theory. Degree based topological indices are one of them that is applicable in quantitative structure property relationship and quantitative structure activity relationship [4,5]. Among them Zagreb indices are most popular indices. First and second Zagreb indices are introduced by Gutman and Trinajestić [6], defined as follows:

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2,$$

$$M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v).$$

These graph invariants were proposed to measure the branching of carbon-atom skeleton [7]. For detail discussion on these indices, see [8–14]. Furtula et al. [15] proposed the reduced second Zagreb index of a graph G to study the difference between M_1 and M_2, which is defined as follows:

$$RM_2(G) = \sum_{uv \in E(G)} (d_G(u) - 1)(d_G(v) - 1).$$

The graphs having maximum and minimum reduced second Zagreb index in the class of cyclic graphs with cut edges are studied in [16]. Mahanta et al. [17] obtained Reduced the reduced second Zagreb index of four new graph operations based on tensor product. Several useful composite graphs can be obtained by operations of different graphs. The Cartesian product is one of that the operations and which is considered in the present work.

The Cartesian product $G_1 \otimes G_2$ of graphs G_1 and G_2 has the vertex set $V(G) \times V(G_2)$ and $(a, x)(b, y)$ is an edge of $G_1 \otimes G_2$ if $a = b$ and $xy \in E(H)$ or $ab \in E(G)$ and $x = y$. Using the Cartesian product of two graphs, the structure of several nanomaterials can be designed such as C_4-nanotube, C_4-nanotorus, multi-walled nanotorus etc. Carbon nanotube has diverse applications in cancer treatment, cardiac autonomic regulation, tissue regeneration etc. As topological index can predict different physico-chemical properties, it is worthy to compute that for different

structures of real world application. First and second Zagreb indices of the Cartesian product graph is presented in [18]. The PI index of the Cartesian product of bipartite graphs is computed in [19]. Klavzar et al. [20] computed the Szeged index of Cartesian product graph. In [21], the Wiener index of Cartesian product graphs are studied. The present author [22–24] studied F-index, F-coindex and reformulated first Zagreb index for Cartesian product graphs. The goal of this work is to obtain the reduced second Zagreb index of Cartesian product graphs. Using that results, RM_2 index of some chemical graphs is also derived.

2. Main results

Let G_i $(i = 1, 2, ..., k)$ be a connected graph with vertex set $V(G_i)$ and $E(G_i)$, so that, $|V(G_i)| = n_i$ and $|E(G_i)| = m_i$. In this section, we derive the reduced second Zagreb index of Cartesian product of k-number of connected graphs $G_1, G_2, ..., G_k$. To do this first we prove the result for two connected graphs G_1 and G_2.

Lemma 1. *[18] Let G_1 and G_2 be two connected graphs, then:*

$$
\begin{aligned}
(i)\ |V(G_1 \otimes G_2)| &= |V(G_1)| \times |V(G_2)|, \\
(ii)\ |E(G_1 \otimes G_2)| &= |E(G_1)||V(G_2)| + |E(G_2)||V(G_1)|, \\
(iii)\ d_{G_1 \otimes G_2}(a, b) &= d_{G_1}(a) + d_{G_2}(b).
\end{aligned}
$$

Lemma 2. *[18] Let $G_1, G_2, ..., G_k$ be k-number of graphs, then*

$$
M_1\left(\bigotimes_{i=1}^{k} G_i\right) = n \sum_{i=1}^{k} \frac{M_1(G_i)}{n_i} + 4n \sum_{i \neq j,\ i,j=1}^{k} \frac{m_i m_j}{n_i n_j}.
$$

Lemma 3. *[18] Let $G_1, G_2, ..., G_k$ be k-number of graphs, then*

$$
\begin{aligned}
(i)\ \left|V\left(\bigotimes_{i=1}^{k} G_i\right)\right| &= \prod_{i=1}^{k} n_i, \\
(ii)\ \left|E\left(\bigotimes_{i=1}^{k} G_i\right)\right| &= \prod_{i=1}^{k} n_i \sum_{i=1}^{k} \frac{m_i}{n_i}.
\end{aligned}
$$

Theorem 1. *Let G_1 and G_2 be two connected graphs with n_1 and n_2 number of vertices and, m_1 and m_2 number of edges respectively, then:*

$$
RM_2(G_1 \otimes G_2) = n_1 RM_2(G_2) + n_2 RM_2(G_1) + 3m_1 M_1(G_2) + 3m_2 M_1(G_1) - 8m_1 m_2.
$$

Proof. From definition of Cartesian product of two graphs, we have:

$$
\begin{aligned}
RM_2(G_1 \otimes G_2) &= \sum_{(a,b)(c,d) \in E(G_1 \otimes G_2)} (d_{G_1}(a,b) - 1)(d_{G_2}(c,d) - 1) \\
&= \sum_{u \in V(G_1)} \sum_{bd \in E(G_2)} (d_{G_1}(u) + d_{G_2}(b) - 1)(d_{G_1}(u) + d_{G_2}(d) - 1) \\
&\quad + \sum_{v \in V(G_2)} \sum_{ac \in E(G_1)} (d_{G_1}(a) + d_{G_2}(v) - 1)(d_{G_1}(c) + d_{G_2}(v) - 1) \\
&= C_1 + C_2,\ (Say).
\end{aligned}
$$

Where,

$$
\begin{aligned}
C_1 &= \sum_{u \in V(G_1)} \sum_{bd \in E(G_2)} (d_{G_1}(u) + d_{G_2}(b) - 1)(d_{G_1}(u) + d_{G_2}(d) - 1) \\
&= \sum_{u \in V(G_1)} \sum_{bd \in E(G_2)} (d_{G_2}(b) - 1)(d_{G_2}(d) - 1) + \sum_{bd \in E(G_2)} \sum_{u \in V(G_1)} d_{G_1}(u)^2 \\
&\quad + \sum_{bd \in E(G_2)} \sum_{u \in V(G_1)} d_{G_1}(u)(d_{G_2}(b) + d_{G_2}(d) - 2) \\
&= n_1 RM_2(G_2) + m_2 M_1(G_1) + 2m_1 M_1(G_2) - 4m_1 m_2.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
C_2 &= \sum_{v\in V(G_2)}\sum_{ac\in E(G_1)}(d_{G_1}(a)+d_{G_2}(v)-1)(d_{G_1}(c)+d_{G_2}(v)-1) \\
&= \sum_{v\in V(G_2)}\sum_{ac\in E(G_1)}(d_{G_1}(a)-1)(d_{G_1}(c)-1)+\sum_{ac\in E(G_1)}\sum_{v\in V(G_2)}d_{G_1}(v)^2 \\
&\quad+\sum_{ac\in E(G_1)}(d_{G_1}(a)+d_{G_1}(c)-2)\sum_{v\in V(G_2)}d_{G_1}(v) \\
&= n_2 RM_2(G_1)+m_1 M_1(G_2)+2m_2 M_1(G_1)-4m_1 m_2.
\end{aligned}
$$

Therefore, combining the contributions of C_1 and C_2 we get the desired results. $\qquad\square$

In the following, we calculate reduced second Zagreb index of the Cartesian product of k-number of graphs G_i for $i=1,2,....,k$.

Theorem 2. *Let G_1, G_2,.....,G_k be k-number of connected graphs, then*

$$
\begin{aligned}
RM_2(\bigotimes_{i=1}^{k}G_i) &= n\sum_{i=1}^{k}\frac{RM_2(G_i)}{n_i}+3\sum_{i=1}^{k}(\frac{m}{n_i}-\frac{nm_i}{n_i^2})M_1(G_i) \\
&\quad+4n\sum_{p,q,r=1,\,p\neq q\neq r}\frac{m_p m_q m_r}{n_p n_q n_r}-4n\sum_{i,j=1,\,i\neq j}\frac{m_i m_j}{n_i n_j}.
\end{aligned}
$$

Where, $n=|V(\bigotimes_{i=1}^{k}G_i)|$ and $m=|E(\bigotimes_{i=1}^{k}G_i)|$.

Proof. Let us assume that, $n'=|V(\bigotimes_{i=1}^{k-1}G_i)|$ and $m'=|E(\bigotimes_{i=1}^{k-1}G_i)|$ so that, $n'=\dfrac{n}{n_k}$ and $m'=\dfrac{mn_k-nm_k}{n_k^2}$. Now by Theorem 1 and an inductive argument, we can have

$$
\begin{aligned}
RM_2(\bigotimes_{i=1}^{k}G_i) &= RM_2(\bigotimes_{i=1}^{k-1}G_i\otimes G_k) \\
&= n_k RM_2(\bigotimes_{i=1}^{k-1}G_i)+|V(\bigotimes_{i=1}^{k-1}G_i)|RM_2(G_k)+3m_k M_1(\bigotimes_{i=1}^{k-1}G_i) \\
&\quad+3|E(\bigotimes_{i=1}^{k-1}G_i)|M_1(G_k)-8|E(\bigotimes_{i=1}^{k-1}G_i)||E(G_k)|
\end{aligned}
$$

Using Lemmas 1, 2, and 3 on the above result, we obtain:

$$
\begin{aligned}
RM_2(\bigotimes_{i=1}^{k}G_i) &= n_k[n'\sum_{i=1}^{k-1}\frac{RM_2(G_i)}{n_i}+3\sum_{i=1}^{k-1}(\frac{m'}{n_i}-\frac{n'm_i}{n_i^2})M_1(G_i) \\
&\quad+4n'\sum_{p,q,r=1,\,p\neq q\neq r}^{k-1}\frac{m_p m_q m_r}{n_p n_q n_r}-4n'\sum_{i,j=1}^{k-1}\frac{m_i m_j}{n_i n_j}]+n'RM_2(G_k) \\
&\quad+3m_k[n'\sum_{i=1}^{k-1}\frac{M_1(G_i)}{n_i}+4n'\sum_{i,j=1}^{k-1}\frac{m_i m_j}{n_i n_j}]+3n'\sum_{i=1}^{k-1}(\frac{m_i}{n_i}M_1(G_k) \\
&\quad-8m_k n'\sum_{i=1}^{k}\frac{m_i}{n_i}
\end{aligned}
$$

After arranging the terms, we have:

$$RM_2(\bigotimes_{i=1}^{k} G_i) = [n_k n' \sum_{i=1}^{k-1} \frac{RM_2(G_i)}{n_i} + n' RM_2(G_k)] + [3n_k \sum_{i=1}^{k-1} (\frac{m'}{n_i} - \frac{n' m_i}{n_i^2}) M_1(G_i)$$

$$+3m_k n' \sum_{i=1}^{k-1} \frac{M_1(G_i)}{n_i} + 3n' \sum_{i=1}^{k-1} (\frac{m_i}{n_i} M_1(G_k)]$$

$$+[4n_k n' \sum_{p,q,r=1,\ p\neq q\neq r}^{k-1} \frac{m_p m_q m_r}{n_p n_q n_r} + 12n' m_k \sum_{i,j=1}^{k-1} \frac{m_i m_j}{n_i n_j}]$$

$$-[4n \sum_{i,j=1}^{k-1} \frac{m_i m_j}{n_i n_j} + 8m_k n' \sum_{i=1}^{k} \frac{m_i}{n_i}]$$

After some calculations, we get:

$$RM_2(\bigotimes_{i=1}^{k} G_i) = [n \sum_{i=1}^{k-1} \frac{RM_2(G_i)}{n_i} + n \frac{RM_2(G_k)}{n_k}] + [3 \sum_{i=1}^{k-1} (\frac{m' n_k + m_k n'}{n_i}$$

$$- \frac{n' n_k m_i}{n_i^2}) M_1(G_i) + 3(\frac{mn_k - nm_k}{n_k^2}) M_1(G_k)]$$

$$+[4n \sum_{p,q,r=1,\ p\neq q\neq r}^{k-1} \frac{m_p m_q m_r}{n_p n_q n_r} + 12n \frac{m_k}{n_k} \sum_{i,j=1,i\neq j}^{k-1} \frac{m_i m_j}{n_i n_j}]$$

$$-[4n \sum_{i,j=1}^{k-1} \frac{m_i m_j}{n_i n_j} + 8n \frac{m_k}{n_k} \sum_{i=1}^{k} \frac{m_i}{n_i}]$$

$$= n \sum_{i=1}^{k} \frac{RM_2(G_i)}{n_i} + 3 \sum_{i=1}^{k} (\frac{m}{n_i} - \frac{nm_i}{n_i^2}) M_1(G_i)$$

$$+4n \sum_{p,q,r=1,p\neq q\neq r} \frac{m_p m_q m_r}{n_p n_q n_r} - 4n \sum_{i,j=1}^{k} \frac{m_i m_j}{n_i n_j}],$$

which is the desired result.   □

If $G_1 = G_2 = \dots = G_k = G$ then $\bigotimes_{i=1}^{k} G_i = G^k$. Hence from the above theorem, the following corollary follows:

Corollary 1. *If G be connected graph, then*

$$RM_2(G^k) = k|V(G)|^{k-3}[|V(G)|^2 RM_2(G) + 3(k-1)|V(G)||E(G)|M_1(G)$$
$$+4(k-1)(k-2)|E(G)|^3 - 4(k-1)|V(G)||E(G)|^2].$$

3. Applications

Using various unary and binary graph operations on different elementary graphs, such as the path graph, cycle graph, complete graph etc, we can obtain several significant composite graphs having excellent usage in modern science and technology. The Cartesian product is one of that binary operations capable to construct different special structure. Using Cartesian product of two graphs, one can get ladder graph, C_4-nanotube and nanotorus, rectangular grid, rook's graph, hamming graph etc. The Hamming graphs are interesting in connection with error-correcting codes and association schemes. The rook's graph represents all legal moves of rook on the chess board. So it is worth to investigate investigating topological indices for the above structures. In this section, the reduced second Zagreb index of aforesaid graphs is derived. For path, cycle, and complete graph of n vertices, the notations P_n, C_n, and K_n are used.

Example 1. *The Ladder graph L_n (Fig. 1) is the Cartesian product of P_2 and P_{n+1}, made by n sequences and $(2n + 2)$ vertices. So, using theorem 1, the reduced second Zagreb index of L_n is given by*
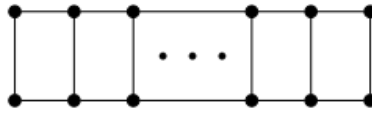
$$RM_2(L_n) = 12n - 10.$$

FIG. 1. The ladder graph L_n

Example 2. *The Cartesian product of P_n $(n \geq 2)$ and C_m $(m \geq 2)$ is a C_4-nanotube $TUC_4(m, n)$, whose reduced second Zagreb index can be calculated using theorem 1 as follows:*

$$RM_2(P_n \otimes C_m) = 18mn - 25m.$$

Example 3. *The Cartesian product of C_n $(n \geq 3)$ and C_m $(m \geq 3)$ is a C_4-nanotorus $TC_4(m, n)$, whose reduced second Zagreb index is calculated from Theorem 1 as follows:*

$$RM_2(C_n \otimes C_m) = 18mn.$$

Example 4. *The rectangular grid (Fig.2) is the Cartesian product of the P_n $(n \geq 2)$ and P_m $(m \geq 2)$. So, using Theorem 1, its reduced second Zagreb index is given by*
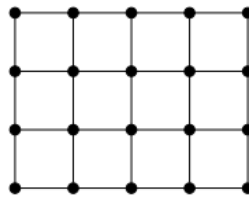
$$RM_2(P_n \otimes P_m) = 18mn - 25m - 25n + 28.$$

FIG. 2. The grid graph $P_5 \otimes P_4$

Example 5. *The Cartesian product of K_n and K_m yields the rook's graph (Fig. 3). So, using Theorem 1, its reduced second Zagreb index is given by*

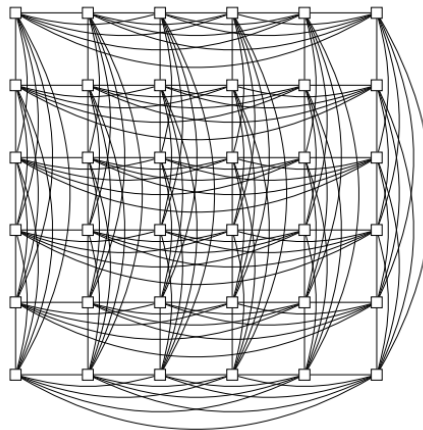$$RM_2(K_m \otimes K_n) = \frac{mn}{2}[(m + n)^3 - 8m^2 - 8n^2 - 16mn + 21m + 21n - 14].$$

FIG. 3. The rook's graph $K_6 \otimes K_6$

Example 6. *The graph* $G = \bigotimes_{i=1}^{N} K_{n_i}$ *is known as a Hamming graph and is denoted by* $H_{n_1,n_2,...,n_N}$*. so, applying previous theorem to compute reduced second Zagreb index of a Hamming graph as follows:*

$$
\begin{aligned}
RM_2(H_{n_1,n_2,...,n_N}) &= RM_2(\bigotimes_{i=1}^{N} K_{n_i}) \\
&= \frac{1}{2} \prod_{i=1}^{N} n_i \sum_{i=1}^{N} (n_i - 1)[\sum_{i=1}^{N}(n_i - 1) - 1]^2.
\end{aligned}
$$

If $n_1 = n_2 = ... = n_N = 2$*, then the graph* G *is known as a hypercube of dimension* N *and denoted by* Q_n *(Fig. 4). Thus from above, we directly get*
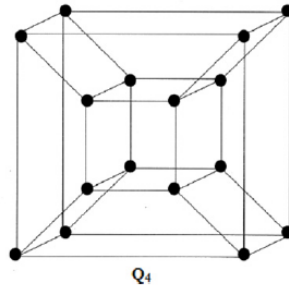
$$
RM_2(Q_n) = \frac{1}{2} N 2^N (N-1)^2.
$$

FIG. 4. Example of Hypercube

Example 7. *The reduced second Zagreb index of the torus* $C_{n_1} \otimes C_{n_2} \otimes .... \otimes C_{n_k}$ *is given by*

$$
RM_2(C_{n_1} \otimes C_{n_2} \otimes .... \otimes C_{n_k}) = k(2k-1)^2 \prod_{i=1}^{k} n_i.
$$

Example 8. *Let* $T = T[p,q]$ *be the molecular graph of a nanotorus (Fig. 5). Then* $|V(T)| = pq$*,* $|E(T)| = \dfrac{9pq}{2}$*,* $M_1(T) = 9pq$*. We consider a q-multi-walled nanotorus* $G_n = P_n \otimes T$*. It is easy to find that* $RM_2(P_n) = n - 3$*,* $RM_2(T) = 6pq$*, and* $M_1(P_n) = 4n - 6$*. Thus from theorem 1, we have the following result.*

$$
RM_2(G_n) = 5pq(8n - 9).
$$
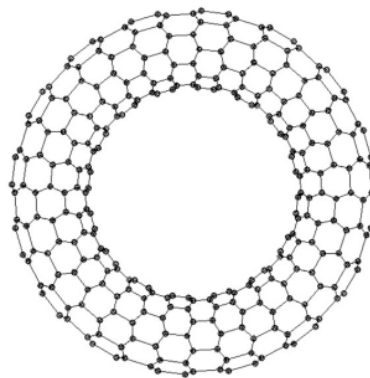
We have plotted the result in Fig. 6
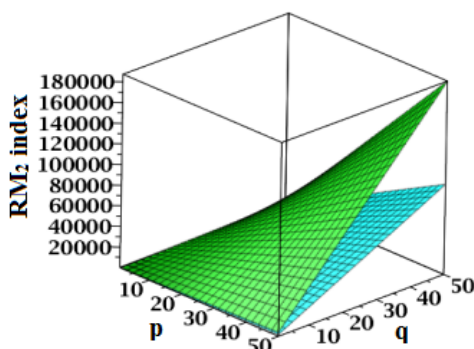

FIG. 5. The graph of a nanotorus

FIG. 6. Plotting of the RM_2 index for G_n, $n = 2, 3$. Cyan and green colors are used for $n = 2, 3$ respectively

4. Conclusion

In this article, reduced second Zagreb index of Cartesian product graph is studied. Firstly RM_2 index is obtained for the product of two graphs and then the general case is considered. Applying that results, RM_2 index is investigated for some special structures. As future work, some other graph operations like composition, tensor product, corona product, strong product, splice, link etc. can be discussed in terms of the reduced second Zagreb index.

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