On Neighbourhood Zagreb index of product graphs

Sourav Mondal\textsuperscript{a}, Nilanjan De\textsuperscript{b}, Anita Pal\textsuperscript{c}

\textsuperscript{a}Department of mathematics, NIT Durgapur, India.
\textsuperscript{b}Department of Basic Sciences and Humanities (Mathematics), Calcutta Institute of Engineering and Management, Kolkata, India.
\textsuperscript{c}Department of mathematics, NIT Durgapur, India.

Abstract

There is powerful relation between the chemical behaviour of chemical compounds and their molecular structures. Topological indices defined on these chemical molecular structures are capable to predict physical properties, chemical reactivity and biological activity. In this article, a new topological index named as Neighbourhood Zagreb index ($M_N$) is presented. Here the chemical importance of this newly introduced index is studied and some explicit results for this index of different product graphs such as Cartesian, Tensor and Wreath product is derived. Some of these results are applied to obtain the Neighbourhood Zagreb index of several chemically important graphs and nano-structures.

MSC (2010): Primary: 05C35; Secondary: 05C07, 05C40

Keywords: Topological index, Zagreb index, Neighbourhood Zagreb index, Cartesian product, Tensor product, Wreath product.

1. Introduction

A chemical graph [1, 2] is a connected graph where loops and parallel edges are not allowed and in which nodes and edges are supposed to be atoms and chemical bonds of compound respectively. Through this work we use only chemical graphs. Consider a graph $G$ having $V(G)$ and $E(G)$ as node set and edge set respectively. The degree(valency) of a node $v \in V(G)$, written as $deg_G(v)$, is the total number of edges associated with $v$. The set of neighbours of a node $v$ is written as $N_G(v)$. For molecular graph, $|N_G(v)| = deg_G(v)$.

Email addresses: souravmath94@gmail.com (Sourav Mondal), de.nilanjan@radifmail.com (Nilanjan De), anitabuei@gmail.com (Anita Pal)
In mathematical chemistry, molecular descriptors play a leading role specifically in the field of QSPR/QSAR modelling. Amongst them, an outstanding area is preserved for the well-known topological indices or graph invariant. A real valued mapping considering graph as argument is called a graph invariant if it gives same value to graphs which are isomorphic. The order (total count of nodes) and size (total count of edges) of a graph are examples of two graph invariants. In mathematical chemistry, the graph invariants are named as topological indices. Some familiar topological indices are Wiener index, Randić index, connectivity indices, Schultz index, Zagreb indices etc.. The idea of topological indices was initiated when the eminent chemist Harold Wiener found the first topological index, known as Wiener index [3], in 1947 for searching boiling points of alkanes. Amidst the topological indices invented on initial stage, the Zagreb indices belong to the well known and well researched molecular descriptors. It was firstly presented by Gutman and Trinajstić [4], where they investigated how the total energy of π-electron depends on the structure of molecules and it was recognized on [6]. The first ($M_1$) and second ($M_2$) Zagreb indices are as follows:

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

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

$M_1(G)$ can also be expressed as

$$M_1(G) = \sum_{uv \in E(G)} \left[\text{deg}_G(u) + \text{deg}_G(v)\right].$$

For more discussion on these indices, we encourage the readers to consult the articles [7, 8, 9, 3, 10, 11, 12].

Let the sum of the degrees of all neighbours of $v$ in $G$ be denoted by $\delta_G(v)$, i.e.,

$$\delta_G(v) = \sum_{u \in N_G(v)} \text{deg}_G(u).$$

Following the construction of first Zagreb index, we present here a new degree based topological index named as the Neighbourhood Zagreb index ($M_N$) which is defined as follows:

$$M_N(G) = \sum_{v \in V(G)} \delta_G(v)^2.$$
In mathematical chemistry, graph operations are very significant since certain graphs of chemical interest can be evaluated by various graph operations of different simple graphs. H. Yousefi Azari and co-authors [13] derived some exact formulae of PI index for Cartesian product of bipartite graphs. P. Paulraja and V.S. Agnes [14] evaluated some explicit expressions of the degree distance for the cartesian and wreath products. De et al. [17] found explicit expressions of the $F$-index under several graph operations. For further illustration on this area, interested readers are suggested some articles [5, 15, 16, 18, 21]. We continue this progress for $M_N$ index. The objective of this work is to shed some attention on establishing some exact results for the Neighbourhood Zagreb index $M_N$ under different product graphs and applying these results for some significant family of chemical graphs and nano-materials.

2. Chemical significance of the Neighbourhood Zagreb index ($M_N$)

According to the instruction of the International Academy of Mathematical Chemistry (IAMC), in order to determine the effectiveness of a topological index to predict physiochemical behaviour, we use regression analysis. Usually octane isomers are helpful for such investigation, since they represent a sufficiently large and structurally diverse group of alkanes for the preliminary testing of indices [19]. Furtula et al. [20] derived that the correlation coefficient of both $M_1$ and $F$ for octane isomers is greater than 0.95 with acentric factor and entropy. They also enhanced the skill of prediction of these indices by devising a linear model ($M_1 + \lambda F$), where $\lambda$ was varied from -20 to 20. De et al. found that the correlation coefficient of $F$-coindex for octanes in case of the n-octanes/water partition coefficient (LogP) is 0.966.

In this article, we find the correlation of entropy ($S$) and acentric factor (Acent Fac.) with the corresponding Neighbourhood Zagreb index of octanes. The datas of octanes (table:1) are collected from www.moleculardescriptors.eu/dataset/dataset.htm. Here we computed that the correlation coefficient ($r$) between acentric factor (Acent Fac.) and $M_N$ is -0.99456 (figure.1) and between entropy ($S$) and $M_N$ is -0.95261 (figure.2). Thus $M_N$ can help to predict the Entropy ($r^2 = 0.98915$) and acentric factor ($r^2 = 0.90746$) with powerful accuracy. These results confirm the suitability of the indices in QSPR analysis.

A major drawback of most topological indices is their degeneracy, i.e., two or more isomers possess the same topological index. But this novel index is exceptional for octane isomers. Bonchev et al. [22] defined the mean isomer degeneracy as
Follows:

\[ d = \frac{n}{t} \]

where \( n \) and \( t \) are the number of isomers considered and the number of distinct values that the index assumes for these isomers respectively. Clearly the minimum value of \( d \) is 1. As much as \( d \)' increases the isomer-discrimination power of topological indices decreases. Thus \( d \) has a significant role for the discriminating power of an index. For octane isomers \( M_N \) index (table:2) exhibits good response \((d = 1)\).

Table 1: Experimental values of the acentric Factor, entropy(S) and the corresponding values of \( M_N \).

| Octanes                     | Acent Fac. | S  | \( M_N(G) \) |
|-----------------------------|------------|----|--------------|
| 2,2,3,3-tetramethyl butane  | 0.255294   | 93.06 | 194         |
| 2,3,4-trimethyl pentane     | 0.317422   | 102.39 | 144         |
| 2,3,3-trimethyl pentane     | 0.293177   | 102.06 | 164         |
| 2,2,3-trimethyl pentane     | 0.300816   | 101.31 | 162         |
| 3-methyl-3-ethyl pentane    | 0.306899   | 101.48 | 152         |
| 2-methyl-3-ethyl pentane    | 0.332433   | 106.06 | 132         |
| 3,4-dimethyl hexane         | 0.340345   | 106.59 | 130         |
| 3,3-dimethyl hexane         | 0.322596   | 104.74 | 146         |
| 2,5-dimethyl hexane         | 0.35683    | 105.72 | 118         |
| 2,4-dimethyl hexane         | 0.344223   | 106.98 | 124         |
| 2,3-dimethyl hexane         | 0.348247   | 108.02 | 126         |
| 2,2-dimethyl hexane         | 0.339426   | 103.42 | 138         |
| 3-ethyl hexane              | 0.362472   | 109.43 | 114         |
| 4-methyl heptane            | 0.371504   | 109.32 | 110         |
| 3-methyl heptane            | 0.371002   | 111.26 | 108         |
| 2-methyl heptane            | 0.377916   | 109.84 | 104         |
| n-octane                   | 0.397898   | 111.67 | 90          |

3. Main Result

In this section, we evaluate the newly introduced index of different product graphs such as Cartesian, Wreath and Tensor product of graphs. Here \( V_i \) and
Figure 1: Experimental values of Acent Fac. vs. calculated values of $M_N$.

Figure 2: Experimental values of entropy(S) vs. calculated values of $M_N$. 
Table 2: Mean isomer degeneracy \((d)\) of different indices for octane isomers.

| Indices                              | Mean isomer degeneracy \((d)\) |
|--------------------------------------|---------------------------------|
| First Zagreb index \((M_1)\)         | 3.000                           |
| Second Zagreb index \((M_2)\)        | 1.286                           |
| Forgotten topological index \((F)\)  | 2.571                           |
| Hosoya index \((Z)\)                 | 1.286                           |
| Merrifield-Simmons index \((\sigma)\)| 1.200                           |
| Connectivity index \((\chi)\)        | 1.125                           |
| Harary index \((\eta)\)              | 1.059                           |
| Neighbourhood Zagreb index \((M_N)\) | **1.000**                       |

\(E_i\) denote vertex set and edge set of \(G_i\) respectively. Also for path, cycle and complete graphs with \(n\) nodes, we use \(P_n\), \(C_n\) and \(K_n\) respectively. We proceed with the following lemma directly followed from definitions.

**Lemma 1.** For graph \(G\), we have

\[
\begin{align*}
(i) \quad & \sum_{v \in V(G)} \delta_G(v) = M_1(G), \\
(ii) \quad & \sum_{v \in V(G)} \deg_G(v) \delta_G(v) = 2M_2(G).
\end{align*}
\]

### 3.1. Cartesian product

**Definition 1.** The Cartesian product of \(G_1, G_2\), written as \(G_1 \times G_2\), containing node set \(V_1 \times V_2\) and \((u_1, v_1)\) is adjacent with \((u_2, v_2)\) iff \([u_1 = u_2\) and \(v_1 v_2 \in E_2]\) or \([v_1 = v_2\) and \(u_1 u_2 \in E_1]\).

Clearly the above definition yield the lemma stated below.

**Lemma 2.** For graphs \(G_1\) and \(G_2\), we have

\[
\begin{align*}
(i) \quad & \delta_{G_1 \times G_2}(u, v) = \delta_{G_1}(u) + \delta_{G_2}(v) + 2\deg_{G_1}(u)\deg_{G_2}(v), \\
(ii) \quad & |E(G_1 \times G_2)| = |V_2||E_1| + |V_1||E_2|.
\end{align*}
\]

In [23, 24] different topological indices for Cartesian product of graphs were studied. Here we move to calculate the Neighbourhood Zagreb index of Cartesian product graphs.
**Proposition 1.** The Neighbourhood Zagreb index of $G_1 \times G_2$ is given by

$$M_N(G_1 \times G_2) = 6M_1(G_1)M_1(G_2) + |V_2|M_N(G_1) + |V_1|M_N(G_2) + 16|E_2|M_2(G_1) + |E_1|M_2(G_2).$$

*Proof.* From definition of Neighbourhood Zagreb index and applying lemma 2 and lemma 1, we get

$$M_N(G_1 \times G_2) = \sum_{(u,v) \in V_1 \times V_2} \delta_{G_1 \times G_2}^2(u,v)$$

$$= \sum_{u \in V_1} \sum_{v \in V_2} \left(\delta_{G_1}(u) + \delta_{G_2}(v) + 2deg_{G_1}(u)deg_{G_2}(v)\right)^2$$

$$= 6M_1(G_1)M_1(G_2) + |V_2|M_N(G_1) + |V_1|M_N(G_2) + 16|E_2|M_2(G_1) + |E_1|M_2(G_2).$$

Hence the result. Using the proposition 1, we have the following results.

**Example 1.** The Cartesian product of $P_2$ and $P_{n+1}$ produces the ladder graph $L_n$ (figure 3). By the above proposition, we derive the following result.

$$M_N(L_n) = 162n - 132.$$

![Figure 3: The ladder graph $L_n$.](image)

**Example 2.** For a $C_4$-nanotorus $TC_4(m, n) = C_m \times C_n$, the Neighbourhood Zagreb index is given by

$$M_N(TC_4(m, n)) = 256mn.$$

**Example 3.** The Cartesian product of $P_n$ and $C_4$ yields a $C_4$-nanotube $TUC_4(m, n) = P_n \times C_m$. Its $M_N$ index is as follows:

$$M_N(TUC_4(m, n)) = 256mn - 374m, n \geq 4.$$
Example 4. The Neighbourhood Zagreb index of the grids \((P_n \times P_m)\) is given by

\[ M_N(P_n \times P_m) = 256mn - 310m - 310n + 216, m, n \geq 4. \]

Example 5. For a n-prism\((K_2 \times C_n)\) (figure 4), the Neighbourhood Zagreb index is given below.

\[ M_N(K_2 \times C_n) = 162n. \]

Example 6. The Cartesian product of \(K_n\) and \(K_m\) yields the Rook’s graph (figure 4). Applying the above proposition we have the following.

\[ M_N(K_m \times K_n) = mn[6(m-1)^2(n-1)^2 + (n-1)^4 + (m-1)^4 + 4(m-1)(n-1)((m-1)^2 + (n-1)^2)]. \]

Now we generalize the Proposition 1. We begin with the following lemma.

Lemma 3. If \(G_1, G_2, \ldots, G_n\) be \(n\) graphs and \(V = V(\bigotimes_{i=1}^{n} G_i), E = E(\bigotimes_{i=1}^{n} G_i)\), then we have

(i) \(|E(\bigotimes_{i=1}^{n} G_i)| = |V| \sum_{i=1}^{n} |E_i| / |V_i|,\)

(ii) \(M_1(\bigotimes_{i=1}^{n} G_i) = |V| \sum_{i=1}^{n} M_1(G_i) / |V_i| + 4|V| \sum_{i \neq j, j=1}^{n-1} |E_i| / |V_i|^2,\)

(iii) \(M_2(\bigotimes_{i=1}^{n} G_i) = |V| \sum_{i=1}^{n} M_2(G_i) / |V_i| + 3 \sum_{i=1}^{n} M_1(G_i) (|E_i| / |V_i|) - |V| |E_i| / |V_i|^2 + 4|V| \sum_{i \neq j, k, i, j, k=1}^{n} |E_i| / |V_i|^2 / |V_k|^2.\)
Proof. Applying lemma 2(ii) and an inductive argument, (i) is clear. In order to proof (ii) and (iii), we refer to [15].

Proposition 2. If $G_1, G_2, \ldots, G_n$ be $n$ graphs, then we have

$$M_N(\bigotimes_{i=1}^n G_i) = |V| \sum_{i=1}^n \frac{M_N(G_i)}{|V_i|} + 3|V| \sum_{i \neq j, j=1}^n \frac{M_1(G_i)M_1(G_j)}{|V_i||V_j|}$$

$$+ 24|V| \sum_{i \neq j, i, j, k=1}^n \frac{M_1(G_i)E_jE_k}{|V_i||V_j||V_k|} + 16|V| \sum_{i \neq j, i, j=1}^n \frac{M_2(G_i)E_j}{|V_i||V_j|}$$

$$+ 16|V| \sum_{i \neq j, i, j, k, l=1}^n \frac{|E_i||E_j||E_k||E_l|}{|V_i||V_j||V_k||V_l|}.$$

Proof. We derive the formula by mathematical induction. Evidently the result holds for $n = 2$. Let us take the proposition to be true for $(n - 1)$ graphs. Then we obtain

$$M_N(\bigotimes_{i=1}^n G_i) = M_N(\bigotimes_{i=1}^{n-1} G_i \times G_n)$$

$$= 6M_1(\bigotimes_{i=1}^{n-1} G_i)M_1(G_n) + |V_n|M_N(\bigotimes_{i=1}^{n-1} G_i) + |V(\bigotimes_{i=1}^{n-1} G_i)|M_N(G_n)$$

$$+ 16[M_2(\bigotimes_{i=1}^{n-1} G_i)E_n + M_2(G_n)E(\bigotimes_{i=1}^{n-1} G_i)].$$

Now applying lemma 3, we get

$$M_N(\bigotimes_{i=1}^n G_i) = 6|V| \sum_{i=1}^{n-1} \frac{M_1(G_i)}{|V_i|} \sum_{i=1}^{n-1} M_1(G_i) + 4 \sum_{i \neq j, j=1}^{n-1} \frac{|E_i||E_j|}{|V_i||V_j|}$$

$$+ |V| \sum_{i=1}^{n-1} \frac{M_N(G_i)}{|V_i|} + 3 \sum_{i \neq j, j=1}^{n-1} \frac{M_1(G_i)M_1(G_j)}{|V_i||V_j|}$$

$$+ 24 \sum_{i \neq j, i, j, k=1}^{n-1} \frac{M_1(G_i)E_jE_k}{|V_i||V_j||V_k|} + 16 \sum_{i \neq j, i, j=1}^{n-1} \frac{M_2(G_i)E_j}{|V_i||V_j|}$$

$$+ 16 \sum_{i \neq j, i, j, k, l=1}^{n} \frac{|E_i||E_j||E_k||E_l|}{|V_i||V_j||V_k||V_l|} + |V| \frac{M_N(G_n)}{|V_n|}.$$
Hence the derived result follows.

After simplification, we have

\[
M_N \left( \bigotimes_{i=1}^n G_i \right) = |V| \sum_{i=1}^n \frac{M_N(G_i)}{|V_i|} + 3 |V| \sum_{i \neq j, j=1}^{n-1} \frac{M_1(G_i)M_1(G_j)}{|V_i||V_j|} + 24 |V| \sum_{i \neq j, j=1}^{n-1} \frac{M_1(G_i)|E_j||E_k|}{|V_i||V_j||V_k|} + 2 \sum_{i \neq j, j=1}^{n-1} \frac{M_1(G_i)|E_j||E_n|}{|V_i||V_j||V_n|} + 16 |V| \sum_{i \neq j, j=1}^{n-1} \frac{M_2(G_i)|E_j|}{|V_i||V_j|} + \sum_{i=1}^{n-1} \frac{M_2(G_n)|E_i|}{|V_n||V_i|} + \sum_{i=1}^{n-1} \frac{M_2(G_j)|E_n|}{|V_i||V_n|} + 16 |V| \sum_{i \neq j, j=1}^{n-1} \frac{|E_i||E_j||E_k||E_n|}{|V_i||V_j||V_k||V_n|} + 4 \sum_{i \neq j, j=1}^{n-1} \frac{|E_i||E_j||E_k||E_n|}{|V_i||V_j||V_k||V_n|} + 16 |V| \sum_{i \neq j, j=1}^{n-1} \frac{|E_i||E_j||E_k||E_n|}{|V_i||V_j||V_k||V_n|}.
\]

Hence the derived result follows.
Definition 2. Consider the graph $G$ containing $m$-tuples $b_1, b_2, ..., b_m$ with $b_i \in \{0, 1, ..., n_i - 1\}, n_i \geq 2$, as vertices and let whenever the difference of two tuples is exactly one place, the corresponding two vertices are adjacent. Such a graph is known as Hamming graph. The necessary and sufficient criteria for a graph $G$ to be a Hamming graph is that $G = \bigotimes_{i=1}^{m} K_{n_i}$ and that is why such a graph $G$ is naturally written as $H_{n_1, n_2, ..., n_m}$.

Hamming graph is very useful in coding theory specially in error correcting codes. Also such type of graph is effective in association schemes. Applying proposition 2, we have the corollary stated below.

Corollary 1. The Neighbourhood Zagreb index of Hamming graph is given by

$$M_N(G) = \prod_{i=1}^{m} n_i \left[ \sum_{i=1}^{m} (n_i - 1)^4 + 3 \sum_{i \neq j, j=1}^{m} (n_i - 1)^2(n_j - 1)^2 ight]
+ 6 \sum_{i \neq j, k, l=1}^{m} (n_i - 1)^2(n_j - 1)(n_k - 1) + 4 \sum_{i \neq j, l=1}^{m} (n_i - 1)^3(n_j - 1)$$

+ \sum_{i \neq j, k, l=1}^{m} (n_i - 1)(n_j - 1)(n_k - 1)(n_l - 1)].$$

Example 7. When $n_1, n_2, ..., n_m$ are all equal to 2, the hamming graph $G$ is known as a hypercube (figure.5) with dimension $m$ and written as $Q_m$. We compute the following.

$$M_N(Q_m) = 2^m m^4.$$

3.2. Tensor product

Definition 3. The tensor product of $G_1$, $G_2$, written as $G_1 \otimes G_2$, is a graph containing node set $V_1 \times V_2$ and $(u_1, v_1)$ is adjacent with $(u_2, v_2)$ iff $u_1 u_2 \in E_1$ and $v_1 v_2 \in E_2$.

Clearly the definition gives the lemma as follows:

Lemma 4. For graphs $G_1$ and $G_2$, we have

$$\delta_{G_1 \otimes G_2}(u, v) = \delta_{G_1}(u) \delta_{G_2}(v).$$
Proposition 3. The Neighbourhood Zagreb index of tensor product for two graphs is given by

\[ M_N(G_1 \otimes G_2) = M_N(G_1)M_N(G_2). \]

Proof. By the definition of the \( M_N \) index and applying lemma 4, we get

\[
M_N(G_1 \otimes G_2) = \sum_{(v_1,v_2) \in V_1 \times V_2} \delta_{G_1 \times G_2}^2(v_1,v_2)
= \sum_{v_1 \in V_1} \sum_{v_2 \in V_2} [\delta_{G_1}(v_1)\delta_{G_2}(v_2)]^2
= M_N(G_1)M_N(G_2).
\]

Which is the required result.

Example 8. Using the proposition 3, we have the following computations.

(i) \( M_N(P_n \otimes P_m) = (16n - 38)(16m - 38), m, n \geq 4. \)
(ii) \( M_N(C_n \otimes C_m) = 256mn. \)
(iii) \( M_N(K_n \otimes K_m) = mn(m - 1)^4(n - 1)^4. \)
(iv) \( M_N(P_n \otimes C_m) = 16m(16n - 38), n \geq 4. \)
(v) \( M_N(P_n \otimes K_m) = m(m - 1)^4(16n - 38), n \geq 4. \)
(vi) \( M_N(C_n \otimes K_m) = 16mn(m - 1)^4. \)
3.3. Wreath Product

**Definition 4.** The Wreath product (also known as composition) of $G_1$ and $G_2$ having $V_1$ and $V_2$ as vertex sets with no common vertex and edge sets $E_1$ and $E_2$ is the graph $G_1[G_2]$ containing node set $V_1 \times V_2$ and $(u_1, v_1)$ is adjacent to $(u_2, v_2)$ iff $(u_1u_2 \in E_1)$ or $(u_1 = u_2$ and $v_1v_2 \in E_2)$.

The following lemma is obvious from the definition.

**Lemma 5.** For graphs $G_1$ and $G_2$, we have

$$\delta_{G_1[G_2]}(u, v) = |V_2|^2 \delta_{G_1}(u) + \delta_{G_2}(v) + 2|E_2| \deg_{G_1}(u) + |V_2| \deg_{G_1}(u) \deg_{G_2}(v).$$

In [17, 21, 28] different topological indices for Wreath product of graphs are derived. Here we preserve this movement to find the $M_N$ index of Wreath product of two graphs.

**Proposition 4.** The Neighbourhood Zagreb index of Wreath product for two graphs is given by

$$M_N(G_1[G_2]) = |V_2|^4 M_N(G_1) + M_N(G_2) + 12|V_2|^2 |E_2|^2 M_1(G_1) + 8|E_1||E_2|M_1(G_2) + 8|V_2|^2 |E_2|(|V_2| - 1)M_2(G_1) + 8|V_2||E_1|M_2(G_2) + 3|V_2|^2 M_1(G_1) M_1(G_2).$$

**Proof.** From definition of Neighbourhood Zagreb index and using lemma 5, we have

$$M_N(G_1[G_2]) = \sum_{(u, v) \in V_1 \times V_2} \delta_{G_1[G_2]}^2(u, v)$$

$$= \sum_{u \in V_1} \sum_{v \in V_2} [|V_2|^2 \delta_{G_1}(u) + \delta_{G_2}(v) + 2|E_2| \deg_{G_1}(u) + |V_2| \deg_{G_1}(u) \deg_{G_2}(v)]^2$$

$$= \sum_{u \in V_1} \sum_{v \in V_2} [|V_2|^4 \delta_{G_1}(u)^2 + |V_2|^2 \deg_{G_1}(u)^2 \deg_{G_2}(v)^2 + 4|E_2|^2 \deg_{G_1}(u)^2$$

$$+ \delta_{G_1}(v)^2 + 2|V_2|^3 \delta_{G_1}(u) \deg_{G_1}(u) \deg_{G_2}(v)$$

$$+ 4|V_2|^2 |E_2| \delta_{G_1}(u) \deg_{G_1}(u) + 2|V_2|^2 \delta_{G_1}(u) \delta_{G_2}(v)$$

$$+ 4|V_2||E_2| \deg_{G_1}(u)^2 \deg_{G_2}(v) + 2|V_2| \delta_{G_2}(v) \deg_{G_1}(u) \deg_{G_2}(v)$$

$$+ 4 \deg_{G_1}(u) |E_2| \delta_{G_2}(v)].$$
Applying lemma 1, we have

\[
M_N(G_1[G_2]) = |V_2|^dM_N(G_1) + M_N(G_2) + 12|V_2||E_2|^2M_1(G_1) + 8|E_1||E_2|M_1(G_2)
+ 8|V_2|^2|E_2|(|V_2| + 1)M_2(G_1) + 8|V_2||E_1|M_2(G_2)
+ 3|V_2|^2M_1(G_1)M_1(G_2).
\]

Which is the desired result.

**Example 9.** The Wreath product of the path graphs \(P_n\) and \(P_2\) yield the Fence graph (figure 6), whereas the Wreath product of the cycle \(C_n\) and the path \(P_2\) gives the closed Fence graph (figure 6). Thus from the proposition 4, we compute the following results.

(i) \(M_N(P_n[P_2]) = 864n - 1694, n \geq 4.\)
(ii) \(M_N(C_n[P_2]) = 816n + 2, n \geq 3.\)

![Figure 6: Fence graph (\(P_4[P_2]\)) and closed Fence graph (\(C_n[P_2]\)).](image-url)
4. Conclusion

In this article, we introduce the Neighbourhood Zagreb index ($M_N$), investigate chemical applicability, compute some exact formulae for $M_N$ of some product graphs and apply the results on some chemical graphs. As a future work, we derive the results for some other graph operations, compute some bounds of this index and create some linear models with another indices having good correlation with different physiochemical properties of molecules. As the pharmacological activity of a compound depends on its physiochemical properties and the correlations of $M_N$ index with some of these properties are good, there is nothing to be surprised that $M_N$ index can be used in designing new drugs.

5. Acknowledgements

The first author is very obliged to the Department of Science and Technology (DST), Government of India for the Inspire Fellowship [IF170148].

References

[1] N. Trinajstić, Chemical Graph Theory, *CRC Press, Boca Raton*, (1983).

[2] I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry *Springer, Berlin*, (1986).

[3] K. C. Das, K. Xu and I. Gutman, On Zagreb and Harary Indices, *MATCH Commun. Math. Comput. Chem.*, 70,(2013), 301-314.

[4] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total $\pi$-electron energy of alternate hydrocarbons, *Chem. Phys. Lett.*, 17,(1972), 535-538.

[5] M. Ghorbani, M. A. Hossainzadeh, The Third Version Of Zagreb Index, *Discrete Math. Algorithm. Appl.*, 5, (2013), doi:10.1142/S1793830913500390.

[6] I. Gutman, B. Ručić, N.Trinajstić and C. F. Wilcox, Graph theory and molecular orbitals.XII.Acyclic Polyenes, *J. Chem. Phys.* 62,(1975), 3399-3405.

[7] M. Azari, A. Iranmanesh, Chemical graphs constructed from rooted product and their Zagreb indices, *MATCH Commun. Math. Comput. Chem.*, 70,(2013), 901-919.
[8] M. Azari, A. Iranmanesh and I. Gutman, Zagreb indices of bridge and chain graphs, *MATCH Commun. Math. Comput. Chem.*, 70,(2013), 921-938.

[9] C. M. D. Fonseca, D. Stevanovic, Further Properties of the Second Zagreb Index, *MATCH Commun. Math. Comput. Chem.*, 72,(2014), 655-668.

[10] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.*, 50,(2004), 83-92.

[11] A. Hamzeh, T. Reti, An analogue of Zagreb Index Inequality Obtained from Graph Ir-regularity measures, *MATCH Commun. Math. Comput. Chem.*, 72,(2014), 669-683.

[12] S. Li, M. J. Zhang, Sharp bounds for the Zagreb indices of bipartite graphs with a given diameter, *Appl. Math. Lett.*, 24,(2011), 131-137.

[13] H. Yousefi-Azari, B. Manoochehrian and A. R. Ashrafi, The PI index of product graphs, *Appl. Math. Lett.*, 21,(2008), 624-627.

[14] P. Paulraja, V. S. Agnes, Degree distance of product graphs, *Discrete Math. Algorithm. Appl.*, 6,(2014), DOI: 10.1142/S1793830914500037.

[15] M. H. Khalifeh, H. Yousefi-Azari and A. R. Ashrafi, The first and second Zagreb indices of some graph operations, *Discret. Appl. Math.*, 157,(2009), 804-811.

[16] N. De, A. Pal and S. M. A. Nayeem, On some bounds and exact formulae for connective eccentric indices of graphs under some graph operations, *Int. J. Comb.*, (2014), DOI:10.1155/2014/579257.

[17] N. De, S. M. A. Nayeem and A. Pal, F-index of some graph operations, *Discrete Math. Algorithm. Appl.*, 8,(2016), doi:10.1142/S1793830916500257.

[18] S. Akhtera, M. Imran, Computing the forgotten topological index of four operations on graphs, *AKCE Int. J. Graphs Comb.*, 14,(2017), 70-79.

[19] M. Randić, N. Trinajstič, In search for graph invariants of chemical interest, *J. Mol. Struct.* 300, (1993), 551-571.

[20] B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.*, 53(4), (2015), 11841190, doi:10.1007/s10910-015-0480-z.
[21] N. De, S. M. A. Nayeem and A. Pal, The F-coindex of some graph operations, Springer Plus, (2016 Feb 29), doi: 10.1186/s40064-016-1864-7.

[22] D. Bonchev, O. Mekenyan and N. Trinajstić, Isomer discrimination by topological information approach, J. Comput. Chem., 2, (1981), 127-148.

[23] S. Klavzar, A. Rajapakse and I. Gutman, The Szeged and the Wiener Index of Graphs, Appl. Math. Lett., 9, (1996), 45-49.

[24] M. H. Khalifeh, H. Yousefi-Azari and A. R. Ashrafi, Vertex and edge PI indices of Cartesian product graphs, Discret. Appl. Math., 156, (2008), 1780-1789.

[25] Z. Yarahmadi, Computing Some topological Indices of Tensor product of graphs, Iranian J. Math. Chem., 2, (2011), 109-118.

[26] K. Pattabiraman, P. Paulraja, On some topological indices of the tensor products of graphs, Discret. Appl. Math., 160, (2012), 267-279.

[27] M. J. Nadjafi-Arani, H. Khodashenas, Distance-based topological indices of tensor product of graphs, Iranian J. Math. Chem., 3, (2012), 45-53.

[28] A. Donno, Spectrum, distance spectrum, and Wiener index of wreath products of complete graphs, Ars Math. Contemp., 13, (2017), 207-225.