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Bounds for neighborhood Zagreb index and its explicit expressions under some graph operations

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Abstract:

Topological indices are useful in QSAR/QSPR studies for modeling biological and physiochemical properties of molecules. The neighborhood Zagreb index (MN) is a novel topological index having good correlations with some physiochemical properties. For a simple connected graph G, the neighborhood Zagreb index is the totality of square of $\delta G(v)$ over the vertex set, where $\delta G(v)$ is the total count of degrees of all neighbors of v in G. In this report, some bounds are established for the neighborhood Zagreb index. Some explicit expressions of the index for some graph operations are also computed, which are used to obtain the index for some chemically significant molecular graphs.

Keywords: Topological index; First Zagreb index; Second Zagreb index; Neighbouhood Zagreb index; Graph operations.

MSC (2020): 05C35, 05C07, 05C40.

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1. Introduction

In theoretical chemistry molecular graphs [19,12] are often used to model different molecular structures. Molecular graphs are actually a graphical representation of molecular structure through vertices and edges so that each vertex corresponds to atoms and the edges represent the bonds between them. Throughout this article, we consider only the molecular graph. Let $V(G)$ and $E(G)$ be the vertex and edge sets of a graph G respectively. Here we use the notation $V(G_i)$, $E(G_i)$, n_i and m_i for vertex set, edge set, order and size of G_i respectively. Here $\delta_G(v)$ represents the totality of degrees of all neighbors of v in G. By neighbors of v, we mean the vertices that are connected to v. K_n and C_n represent complete and cycle graph with n vertices respectively. By $\bar{G}$, we mean the complement of any graph G.

Graph theory provides an important tool called topological index to correlate the physiochemical behavior of chemicals with their molecular structure. Topological index is nothing but a numeric amount gotten from molecular graphs that describes the topology of the molecular graph and is invariant for isomorphic graphs. It is widely used in various fields of chemistry, biochemistry and nanotechnology in isomer discrimination, QSAR, QSPR and pharmaceutical medication plan and so forth. Utilization of such indices in chemistry and biology started in 1947 when chemist Harold Wiener [20] presented the wiener index for searching boiling points of alkane. One of the most well used topological indices is the Zagreb index first introduced by Gutman and Trinajestić [13], where they investigated the total π-electron energy dependency on molecular structure.

The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ for a molecular graph (G) are as follows:

$$M_1(G) = \sum_{v\in V(G)} deg_G(v)^2 = \sum_{uv\in E(G)} [deg_G(u) + deg_G(v)],$$

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

Following first Zagreb index, we introduced a novel topological index named as neighborhood Zagreb index (M_N) [16]. To determine the usefulness of a topological index to predict physiochemical behavior of chemical compound, we compute correlation coefficient (r) between physiochemical properties and topological indices. Topological indices for which r^2 is greater than or equal to 0.8 is very useful in QSPR/QSAR analysis. In [16], it is shown that the correlations of neighborhood Zagreb index with Entropy ($r^2 = 0.98915$) and Acentric factor ($r^2 = 0.907460$) are excellent. Thus M_N can predict Entropy and Acentric factor with power full accuracy. The above correlations ensure the compatibility of the index in QSPR/QSAR analysis. A disadvantage of most topological indices is degeneracy, i.e. more than one isomer have same index. In case octane isomers, M_N index yields well response (mean isomer degeneracy = 1) [16]. It confirms the isomer-discrimination ability of this index with high accuracy. Consequently it is worth to discuss the mathematical properties of this chemically interesting index.

In [2,4,7], different bounds for topological descriptors are discussed. Analytical expressions of topological indices under some graph operations are derived in [1,6,8,15]. In this regard we obtain some bounds of the neighborhood Zagreb index and compute some exact expressions for the index under some graph operations. Also we apply them on some composite and chemically interesting graphs.

2. Some bounds of neighborhood Zagreb index

Throughout this section we obtain some upper and lower bounds of the neighborhood Zagreb index using some standard inequalities.

Lemma 1. *For a graph G, we have*

(i) $\sum_{i=1}^{n} \delta_G(v_i) = M_1(G)$,

(ii) $\sum_{i=1}^{n} \delta_G(v_i) deg_G(v_i) = 2M_2(G)$.

Lemma 2. *(Quadratic mean $\geq$ Arithmetic mean) For n positive numbers x_1, x_2,...,x_n, we have*

$$\sqrt{\frac{x_1^2 + x_2^2 + ... + x_n^2}{n}} \geq \frac{x_1 + x_2 + ... + x_n}{n}, \tag{2.1}$$

where equality holds iff $x_1 = x_2 = ... = x_n$.

Proposition 1. *For a graph G with n vertices, we have*

$$M_N(G) \geq \frac{M_1(G)^2}{n}, \tag{2.2}$$

where equality holds iff G is regular.

Proof 1. *Considering $x_i = \delta_G(v_i)$ for $i = 1, 2, ..., n$, inequality (2.1) becomes*

$$\sqrt{\frac{\delta_G(v_1)^2 + \delta_G(v_2)^2 + ... + \delta_G(v_n)^2}{n}} \geq \frac{\delta_G(v_1) + \delta_G(v_2) + ... + \delta_G(v_n)}{n} \tag{2.3}$$

Using lemma 1 and the definition of M_N index, we have from (2.2),

$$\sqrt{\frac{M_N(G)}{n}} \geq \frac{M_1(G)}{n}, \tag{2.4}$$

after squaring both sides of (2.4) we get the required result.
The equality in (2.2) holds iff $\delta_G(v_1) = \delta_G(v_2) = ... = \delta_G(v_n)$. Hence equality in (2.2) holds iff G is regular.

Lemma 3. *(Cauchy-Schwartz inequality) [14] Let x_i and y_i be real numbers for all $1 \leq i \leq n$. Then*

$$(\sum_{i=1}^{n} x_i y_i)^2 \leq (\sum_{i=1}^{n} x_i^2)(\sum_{i=1}^{n} y_i^2). \tag{2.5}$$

Equality holds iff $x_i = ky_i$ for some constant k and for each $1 \leq i \leq n$.

Proposition 2. *For a graph G, we have*

$$M_N(G) \geq \frac{4M_2(G)^2}{M_1(G)}, \tag{2.6}$$

where equality holds iff $\delta_G(v_i) = kdeg_G(v_i)$ for some constant k and for each $1 \leq i \leq n$.

Proof 2. *. For each $i = 1, 2, ..., n$, putting $x_i = \delta_G(v_i)$ and $y_i = deg_G(v_i)$ in (2.5), we have*

$$(\sum_{i=1}^{n} \delta_G(v_i) deg_G(v_i))^2 \leq \sum_{i=1}^{n} \delta_G(v_i)^2 \sum_{i=1}^{n} \mathrm{deg}_G(v_i)^2, \tag{2.7}$$

applying lemma 1 and the definition of M_N and M_1 index, we can rewrite the inequality (2.7) as

$$4M_2(G)^2 \leq M_N(G)M_1(G), \tag{2.8}$$

which gives the inequality (2.6).
Equality in (2.7) holds iff $\delta_G(v_i) = k deg_G(v_i)$ for some constant k and for each $1 \leq i \leq n$. Hence Equality in (2.6) holds iff $\delta_G(v_i) = k deg_G(v_i)$ for some constant k and for each $1 \leq i \leq n$.

Lemma 4. *(Bhatia and Davis's bound on variance)[3] Let x_1, x_2,...,x_n be real numbers such that $m \leq x_i \leq M$ for all $1 \leq i \leq n$ and $\mu = \frac{\sum_{i=1}^{n} x_i}{n}$. Then*

$$\frac{\sum_{i=1}^{n}(x_i - \mu)^2}{n} \leq (M - \mu)(\mu - m), \tag{2.9}$$

where equality holds iff each x_i is either M or m.

If we consider $x_i = \delta_G(v_i)$ for each $i(= 1, 2, ..., n)$, $m = \delta_N$ and $M = \Delta_N$, then $\mu = \frac{M_1(G)}{n}$ and inequality (2.9) gives the following bound.

Proposition 3. *Let G be a graph with n vertices. Also consider*

$$\Delta_N = max\{\delta_G(v) : v \in V(G)\},$$

$$\delta_N = min\{\delta_G(v) : v \in V(G)\}.$$

Then we have

$$M_N(G) \leq \frac{2}{n}M_1(G)^2 + (\delta_N + \Delta_N)M_1(G) - n\delta_N\Delta_N, \tag{2.10}$$

where equality holds iff each $\delta_G(v_i)$ $(1 \leq i \leq n)$ is either δ_N or Δ_N.

Lemma 5. *(Diaz-Metcalf inequality)[9] Let x_i and y_i be two sequence of real numbers with $x_i \neq 0 (i = 1, 2, ..., n)$ and such that $mx_i \leq y_i \leq My_i$, then we have*

$$\sum_{i=1}^{n} y_i^2 + mM\sum_{i=1}^{n} x_i^2 \leq (M + m)\sum_{i=1}^{n} x_i y_i, \tag{2.11}$$

where equality holds iff either $y_i = mx_i$ or $y_i = Mx_i$ $\forall i = 1, 2, ..., n$.

If we consider $x_i = deg_G(v_i)$, $y_i = \delta_G(v_i)$, $m = 1$, $M = \Delta_N$, inequality (2.11) yields the following bound.

Proposition 4. *Let G be a graph with $\Delta_N = max\{\delta_G(v) : v \in V(G)\}$, then we have*

$$M_N(G) \leq 2(\Delta_N + 1)M_2(G) - \Delta_N M_1(G), \tag{2.12}$$

where equality holds iff $\delta_G(v_i) = deg_G(v_i)$ or $\delta_G(v_i) = \Delta_N deg_G(v_i)$ $\forall i = 1, 2, ..., n$.

Lemma 6 (18). *Let $(x_1, x_2, ..., x_n)$ be positive n-tuple such that there exists positive numbers A, a satisfying $0 \leq a \leq x_i \leq A$, then we have*

$$\frac{n\sum\limits_{i=1}^{n} x_i^2}{(\sum\limits_{i=1}^{n} x_i)^2} \leq \frac{1}{4}(\frac{\sqrt{A}}{\sqrt{a}} + \frac{\sqrt{a}}{\sqrt{A}})^2, \tag{2.13}$$

where equality holds iff $a = A$ or $q = \frac{\frac{A}{a}}{\frac{A}{a}+1}n$ is an integer and q of the numbers x_i coincide with a and the remaining $(n-q)$ of the $x_i's$ coincide with $A(\neq a)$.

Considering $x_i = \delta_G(v_i)$, $a = \delta_N$ and $A = \Delta_N$ in lemma 6, we obtain the following upper bound of M_N.

Proposition 5. *Let G be a graph with n vertices. Also consider*

$$\Delta_N = max\{\delta_G(v) : v \in V(G)\},$$

$$\delta_N = min\{\delta_G(v) : v \in V(G)\}.$$

Then we have

$$M_N(G) \leq \frac{M_1^2(G)(\delta_N + \Delta_N)^2}{4n\delta_N\Delta_N}, \tag{2.14}$$

where equality holds iff $\delta_N = \Delta_N$ or $q = \frac{\frac{\Delta_N}{\delta_N}}{\frac{\Delta_N}{\delta_N}+1}n$ is an integer and q of the numbers x_i coincide with δ_N and the remaining $(n-q)$ of the $x_i's$ coincide with $\Delta_N(\neq \delta_N)$.

Lemma 7 (5). *Let $\vec{x} = (x_1, x_2, ..., x_n)$ and $\vec{y} = (y_1, y_2, ..., y_n)$ be sequences of real numbers. Also let $\vec{z} = (z_1, z_2, ..., z_n)$ and $\vec{w} = (w_1, w_2, ..., w_n)$ be non-negative sequences. Then*

$$\sum_{i=1}^{n} w_i \sum_{i=1}^{n} z_i x_i^2 + \sum_{i=1}^{n} z_i \sum_{i=1}^{n} w_i y_i^2 \geq 2 \sum_{i=1}^{n} z_i x_i \sum_{i=1}^{n} w_i y_i, \tag{2.15}$$

in particular, if z_i and w_i are positive, then the equality holds iff $\vec{x} = \vec{y} = \vec{k}$, where $\vec{k} = (k, k, ..., k)$, a constant sequence.

Proposition 6. *For a graph G with n vertices and m edges, we have*

$$M_N(G) > \frac{4m - n}{n} M_1(G). \tag{2.16}$$

Proof 3. *Considering $x_i = \delta_G(v_i)$, $y_i = \deg_G(v_i)$, $z_i = 1$, $w_i = 1$ in lemma 7, we have*

$$\sum_{i=1}^{n} 1 \sum_{i=1}^{n} \delta_G(v_i)^2 + \sum_{i=1}^{n} 1 \sum_{i=1}^{n} deg_G(v_i)^2 \geq 2 \sum_{i=1}^{n} deg_G(v_i) \sum_{i=1}^{n} \delta_G(v_i). \tag{2.17}$$

Now applying definition of M_N index, Handshaking lemma and inequality (2.17), we have the following result

$$M_N(G) \geq \frac{4m - n}{n} M_1(G). \tag{2.18}$$

From lemma 7, it is clear that equality in (2.18) is impossible. Hence the proof.

3. Neighborhood Zagreb index of graph operations

In this section, we discuss about different graph operations namely join, corona product, strong product, splice, link, disjunction and symmetric difference of graphs and explore the neighborhood Zagreb index for those operations. We start with the following obvious lemma.

Lemma 8. *For a graph G, we have*

(i) $\sum_{v \in V(G)} \delta_G(v) = M_1(G)$,

(ii) $\sum_{v \in V(G)} deg_G(v) \delta_G(v) = 2M_2(G)$.

3.1. Join

The join [15] of G_1 and G_2 having V_1 and V_2 as disjoint vertex sets, is the graph $G_1 + G_2$ which contains $V_1 \cup V_2$ as vertex set and $E_1 \cup E_2 \cup \{uv : u \in V_1, v \in V_2\}$ as edge set. Clearly we have the following lemma.

Lemma 9. *For join of two graphs G_1 and G_2, we have*

$$\delta_{G_1+G_2}(u) = \begin{cases} n_2 deg_{G_1}(u) + \delta_{G_1}(u) + n_1n_2 + 2m_2, \ if \ u \in V_1 \\ n_1 deg_{G_2}(u) + \delta_{G_2}(u) + n_1n_2 + 2m_1, \ if \ u \in V_2. \end{cases}$$

Now we obtain the neighborhood Zagreb index of join of two graphs.

Proposition 7. *The neighborhood Zagreb index of $G_1 + G_2$ is given by*

$$\begin{aligned} M_N(G_1+G_2) &= n_1^2n_2^2[n_1+n_2] + 8n_1n_2[n_1m_2+n_2m_1] + 8m_1m_2[n_1+n_2] + \\ &\quad 4[n_1m_2^2+n_2m_1^2] + M_N(G_1) + M_N(G_2) + [n_1^2M_1(G_2) + \\ &\quad n_2^2M_1(G_1)] + 2n_1n_2[M_1(G_1)+M_1(G_2)] + 4[n_1M_2(G_2) + \\ &\quad n_2M_2(G_1)] + 4[m_1M_1(G_2)+m_2M_1(G_1)]. \end{aligned}$$

Proof 4. *From the definition of neighborhood Zagreb index and using lemma 9, we have*

$$\begin{aligned} M_N(G_1+G_2) &= \sum_{u\in V_1\cup V_2} \delta^2_{G_1+G_2}(u) \\ &= \sum_{u\in V_1} \delta^2_{G_1+G_2}(u) + \sum_{u\in V_2} \delta^2_{G_1+G_2}(u) \\ &= \sum_{u\in V_1} [n_2deg_{G_1}(u) + \delta_{G_1}(u) + n_1n_2 + 2m_2]^2 \\ &\quad + \sum_{u\in V_2} [n_1deg_{G_2}(u) + \delta_{G_2}(u) + n_1n_2 + 2m_1]^2 \\ &= Z_1 + Z_2. \end{aligned}$$

Where Z_1 and Z_2 are the results of the terms above orderly. Then Z_1 and Z_2 will be computed individually. Now,

$$\begin{aligned} Z_1 &= \sum_{u\in V_1} [n_2deg_{G_1}(u) + \delta_{G_1}(u) + n_1n_2 + 2m_2]^2 \\ &= \sum_{u\in V_1} [n_1^2n_2^2 + 4m_2^2 + \delta_{G_1}(u)^2 + deg_{G_1}(u)^2n_2^2 + 4n_1n_2m_2 + 2n_1n_2\delta_{G_1}(u) + \\ &\quad 2n_1n_2^2deg_{G_1}(u) + 4\delta_{G_1}(u)m_2 + 4deg_{G_1}(u)n_2m_2 + 2deg_{G_1}(u)\delta_{G_1}(u)n_2]. \end{aligned}$$

Applying lemma 8, we get

$$\begin{aligned} Z_1 &= n_1^3n_2^2 + 4n_1m_2^2 + M_N(G_1) + n_2^2M_1(G_1) + 4n_1^2n_2m_2 + 2n_1n_2M_1(G_1) \\ &\quad +4n_1n_2^2m_1 + 4m_2M_1(G_1) + 8m_1n_2m_2 + 4n_2M_2(G_1). \end{aligned}$$

Similarly,

$$\begin{aligned} Z_2 &= \sum_{u\in V_2}[n_1deg_{G_2}(u) + \delta_{G_2}(u) + n_1n_2 + 2m_1]^2 \\ &= n_1^2n_2^3 + 4n_2m_1^2 + M_N(G_2) + n_1^2M_1(G_2) + 4n_1n_2^2m_1 + 2n_1n_2M_1(G_2) \\ &\quad +4n_1^2n_2m_2 + 4m_1M_1(G_2) + 8m_1n_1m_2 + 4n_1M_2(G_2). \end{aligned}$$

Addition of Z_1 and Z_2 yield the required result.

Example 1. *We can express the complete bipartite graph ($K_{n,t}$) as the join of $\bar{K_n}$ and $\bar{K_t}$. So the above proposition gives $M_n(K_{n,t}) = n^2t^2(n+t)$.*

By suspension of any graph G, we mean the join of G and a single vertex (K_1). So we have the corollary stated below followed directly from the above proposition.

Corollary 1. *The neighborhood Zagreb index for suspension of a graph G is given by*

$$\begin{aligned} M_N(G+K_1) &= |V(G)|^2(|V(G)|+1) + 8|V(G)||E(G)| + 4|E(G)|^2 + M_N(G) \\ &\quad +M_1(G)[1+2|V(G)|] + 4M_2(G). \end{aligned}$$

Example 2. *The suspension of $\bar{K_n}$ produces the star graph S_n having $(n+1)$ vertices (Figure 1). So its neighborhood Zagreb index can be computed using the above corollary as follows:*

$$M_N(S_n) = n^2(n+1).$$

Example 3. *The suspension of C_n yields the wheel graph W_n containing $n+1$ vertices (Figure 1). So by the above corollary the neighborhood Zagreb index of W_n is given by*

$$M_N(W_n) = n^3 + 21n^2 + 36n.$$

Example 4. *Considering the suspension of P_n, we get the Fan graph F_n having $(n+1)$ vertices (Figure 1). So using the corollary above, we can derive the following result.*

$$M_N(F_n) = n^3 + 21n^2 + 8n - 72, n \geq 4.$$

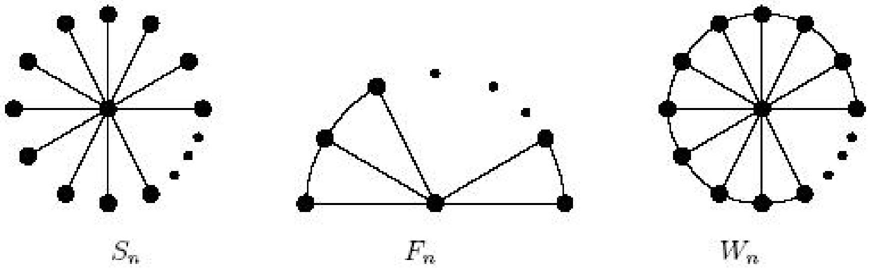

Figure 3.1: The example of star, fan and wheel graphs on $n+1$ vertices.

3.2. Corona product

For corona product [17] of G_1 and G_2, firstly one copy of G_1 and n_1 copies of G_2 are taken and then each node of ith copy of G_2 is joined to ith node of G_1, where $1 \leq i \leq n_1$. For such operation we denote ith copy of G_2 as $G_{2,i}$ and ith vertex of G_1 as u_i. We can state the following lemma.

Lemma 10. *For corona product of two graphs G_1, G_2, we have*

$$\delta_{G_1 \odot G_2}(u) = \begin{cases} \delta_{G_1}(u) + 3n_2 + 2m_2, \ if \ u \in V(G_1) \\ \delta_{G_{2,i}}(u) + \deg_{G_{2,i}}(u) + \deg_{G_1}(u_i) + n_2, \ if \ u \in V(G_{2,i}). \end{cases}$$

We obtain M_N index of corona product of two graphs in the following proposition.

Proposition 8. *The neighborhood Zagreb index for corona product is given by*

$$\begin{aligned} M_N(G_1 \odot G_2) &= M_N(G_1) + n_1 M_N(G_2) + (7n_2 + 4m_2)M_1(G_1) + (n_1 + 2n_1n_2 + \\ &\quad 4m_1)M_1(G_2) + 4n_1M_2(G_2) + n_1n_2^3 + 9n_1n_2^2 + 4n_1m_2^2 + 4n_2^2m_1 \\ &\quad +16n_1n_2m_2 + 8m_1m_2. \end{aligned}$$

Proof 5. *Applying the definition of neighborhood Zagreb index and using lemma 10, we have*

$$\begin{aligned}
M_N(G_1 \odot G_2) &= \sum_{v \in V(G_1 \odot G_2)} \delta_{G_1 \odot G_2}(v)^2 \\
&= \sum_{v \in V(G_1)} \delta_{G_1 \odot G_2}(v)^2 + \sum_{i=1}^{n_1} \sum_{v \in V(G_{2,i})} \delta_{G_1 \odot G_2}(v)^2 \\
&= \sum_{v \in V(G_1)} (\delta_{G_1}(v) + 2m_2 + 3n_2)^2 \\
&\quad + \sum_{i=1}^{n_1} \sum_{v \in V(G_{2,i})} (\delta_{G_{2,i}}(v) + deg_{G_{2,i}}(v)) + deg_{G_1}(v_i) + n_2)^2 \\
&= C_1 + C_2.
\end{aligned}$$

Where C_1 and C_2 are the above sums orderly. So applying lemma 8, we have

$$\begin{aligned}
C_1 &= \sum_{v \in V(G_1)} [\delta_{G_1}(v)^2 + 6n_2\delta_{G_1}(v) + 4m_2\delta_{G_1}(v) + 9n_2^2 + 12n_2m_2 + 4m_2^2] \\
&= M_N(G_1) + (6n_2 + 4m_2)M_1(G_1) + 9n_1n_2^2 + 4n_1m_2^2 + 12n_1n_2m_2.
\end{aligned}$$

$$\begin{aligned}
C_2 &= \sum_{i=1}^{n_1} \sum_{v \in V(G_{2,i})} [\delta_{G_{2,i}}(v)^2 + deg_{G_{2,i}}(v)^2 + deg_{G_1}(v_i)^2 + n_2^2 + 2\delta_{G_{2,i}}(v)deg_{G_{2,i}}(v) \\
&\quad 2\delta_{G_{2,i}}(v)deg_{G_1}(v_i) + 2n_2\delta_{G_{2,i}}(v) + 2deg_{G_{2,i}}(v)deg_{G_1}(v_i) + 2n_2deg_{G_{2,i}}(v) + \\
&\quad 2n_2deg_{G_1}(v_i)] \\
&= n_1M_1(G_2) + n_1M_N(G_2) + n_2M_1(G_1) + n_1n_2^3 + 4n_1M_2(G_2) + 8m_1m_2 + \\
&\quad 4n_1n_2m_2 + 4m_1M_1G_2 + 2n_1n_2M_1(G_2) + 4n_2^2m_1.
\end{aligned}$$

Adding C_1 and C_2, we obtain the required result.

Corollary 2. *The bottleneck graph of a graph G is nothing but the corona product of K_2 and G. By the proposition 8, M_N index of this graph is derived bellow.*

$$\begin{aligned}
M_N(K_2 \odot G) &= 2M_N(G) + (6 + 4|V(G)|)M_1(G) + 8M_2(G) + 2|V(G)|^3 + 22|V(G)|^2 \\
&\quad +8|E(G)|^2 + 32|V(G)||E(G)| + 14|V(G)| + 16|E(G)| + 2.
\end{aligned}$$

Corollary 3. *The t-fold bristled graph $Brs_t(G)$ of a graph G is obtained by the corona product of G and $\bar{K}_t$. Such type of graph is also called as t-throny graph. Using the proposition 8, the M_N index of t-throny graph is evaluated here.*

$$M_N(G \odot \bar{K}_t) \quad = \quad M_N(G) + 7tM_1(G) + t^3|V(G)| + 9t^2|V(G)| + 4t^2|E(G)|.$$

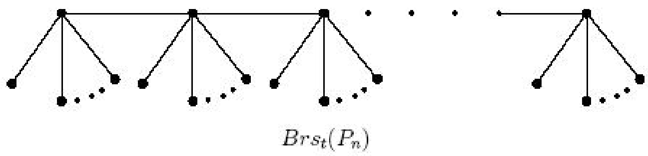

Figure 3.2: The t-throny graphs of P_n.

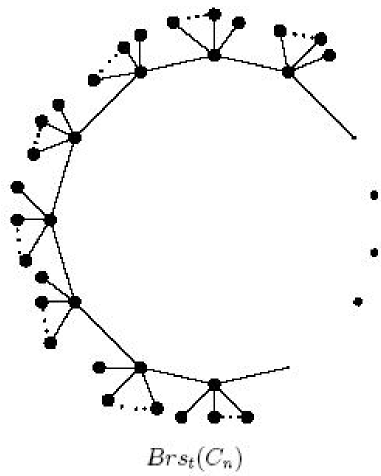

Figure 3.3: The t-throny graph of C_n.

Example 5. *The neighborhood Zagreb index of t-throny graph of path ($figure$ 2) and cycle ($figure$ 3) graphs on n vertices are computed bellow.*

(i) $M_N(P_n \odot \bar{K}_t) = nt^3 + 13nt^2 - 4t^2 + 28nt + 16n - 42t - 38, n \geq 4.$

(ii) $M_N(C_n \odot \bar{K}_t) = nt^3 + 13nt^2 + 28nt + 16n, n \geq 3.$

The M_N index of complete bipartite graph, t-throny graph of path and cycle graphs are depicted in Figure 3.4.

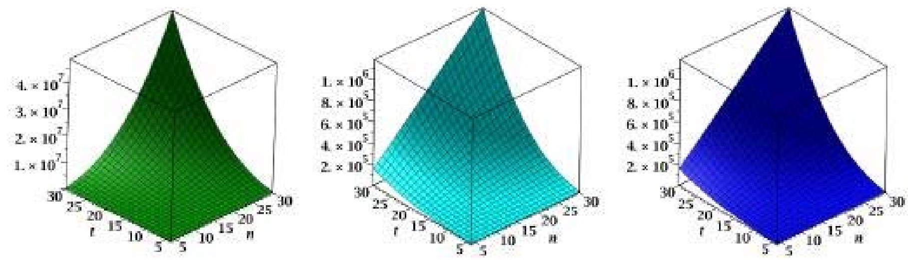

Figure 3.4: Plotting of M_N indices for $K_{n,t}$, $Brs_t(P_n)$ and $Brs_t(C_n)$ from left to right respectively.

3.3. Strong product

The strong product [8] G_1G_2 of G_1, G_2 is a graph with 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 $v_1v_2 \in E_2]$ or $[v_1 = v_2$ and $u_1u_2 \in E_1]$ or $[u_1u_2 \in E_1$ and $v_1v_2 \in E_2]$. Clearly we have the following lemma.

Lemma 11. *For strong product of G_1, G_1, we have*

$$\begin{aligned}\delta_{G_1G_2}(u,v) &= \delta_{G_1}(u)+\delta_{G_2}(v)+\delta_{G_1}(u)\delta_{G_2}(v)+2deg_{G_1}(u)\delta_{G_2}(v)\\ &\quad +2deg_{G_2}(v)\delta_{G_1}(u)+2deg_{G_1}(u)deg_{G_2}(v),\end{aligned}$$

where $u \in V(G_1), v \in V(G_2)$.

We obtain the neighborhood Zagreb index of strong product of two graphs in the following proposition.

Proposition 9. *The neighborhood Zagreb index of strong product of two graphs is given by*

$$\begin{aligned}M_N(G_1G_2) &= (n_2+8m_2)M_N(G_1)+(n_1+8m_1)M_N(G_2)+M_N(G_1)M_N(G_2)+\\ &\quad 6[M_1(G_1)M_N(G_2)+M_N(G_1)M_1(G_2)]+8[M_2(G_1)M_N(G_2)+\\ &\quad M_N(G_1)M_2(G_2)]+16[m_2M_2(G_1)+m_1M_2(G_2)]+6M_1(G_1)\\ &\quad M_1(G_2)+48M_2(G_1)M_2(G_2)+24M_1(G_1)M_2(G_2)+24M_2(G_1)M_1(G_2).\end{aligned}$$

Proof 6. *The proof is directly followed from the definition of neighborhood Zagreb index and lemma 8 and lemma 11.*

3.4. Splice

The splice [10] of G_1 and G_2 by nodes $v_1 \in V_1$ and $v_2 \in V_2$, denoted by $(G_1.G_2)(v_1,v_2)$, is constructed by identifying the vertices v_1 and v_2 in $G_1 \cup G_2$. Thus we have the following lemma.

Lemma 12. *For splice of two graphs, we have*

$$\delta_{(G_1.G_2)(v_1,v_2)}(u) = \begin{cases}\delta_{G_1}(v_1)+\delta_{G_2}(v_2),\ if\ u=v_i, v_i \in V(G_i), i=1,2\\ \delta_{G_i}(u)+deg_{G_j}(v_j),\ if\ u \in N_{G_i}(v_i), i\neq j, i,j=1,2\\ \delta_{G_i}(u),\ if\ u \in V(G_i), u \notin N_{G_i}(v_i), u \neq v_i, i=1,2.\end{cases}$$

We calculate the newly introduced index in the following proposition.

Proposition 10. *The neighborhood Zagreb index of splice of two graphs is given by*

$$\begin{aligned}M_N((G_1.G_2)(v_1,v_2)) &= M_N(G_1)+M_N(G_2)+|N_{G_1}(v_1)|deg_{G_2}(v_2)^2\\ &\quad +|N_{G_2}(v_2)|deg_{G_1}(v_1)^2+2[deg_{G_2}(v_2)\sum_{u\in N_{G_1}(v_1)}\delta_{G_1}(u)\\ &\quad +deg_{G_1}(v_1)\sum_{u\in N_{G_2}(v_2)}\delta_{G_2}(u)]+2\delta_{G_1}(v_1)\delta_{G_2}(v_2).\end{aligned}$$

Proof 7. *Applying the definition of neighborhood Zagreb index and using lemma 12, we have*

$$\begin{aligned} M_N((G_1.G_2)(v_1,v_2)) &= \sum_{u\in V((G_1.G_2)(v_1,v_2))} \delta_{(G_1.G_2)(v_1,v_2)}(u)^2 \\ &= (\delta_{G_1}(v_1)+\delta_{G_2}(v_2))^2 + \sum_{u\in N_{G_i}(v_i), i\neq j, i,j=1,2} [\delta_{G_i}(u)+deg_{G_j}(v_j)]^2 \\ &\quad + \sum_{u\in V(G_i), u\notin N_{G_i}(v_i), u\neq v_i, i=1,2} \delta_{G_i}(u)^2 \\ &= M_N(G_1)+M_N(G_2)+|N_{G_1}(v_1)|deg_{G_2}(v_2)^2+|N_{G_2}(v_2)|deg_{G_1}(v_1)^2 \\ &\quad +2[deg_{G_2}(v_2)\sum_{u\in N_{G_1}(v_1)}\delta_{G_1}(u)+deg_{G_1}(v_1)\sum_{u\in N_{G_2}(v_2)}\delta_{G_2}(u)]+ \\ &\quad 2\delta_{G_1}(v_1)\delta_{G_2}(v_2). \end{aligned}$$

Hence the proof.

3.5. Link

The link [10] of G_1, G_2 by nodes $v_1 \in V_1$ and $v_2 \in V_2$, written as $(G_1 \sim G_2)(v_1, v_2)$, is defined by joining the nodes v_1 and v_2 with an edge in $G_1 \cup G_2$. The following lemma is clear from above definition.

Lemma 13. *For link of two graphs G_1, G_2 by nodes $v_1 \in V_1$ and $v_2 \in V_2$, we have*

$$\delta_{(G_1\sim G_2)(v_1,v_2)}(u) = \begin{cases} \delta_{G_i}(v_i)+\deg_{G_j}(v_j)+1, \ if\ u=v_i, v_i\in V(G_i), i\neq j, i,j=1,2 \\ \delta_{G_i}(u)+1, \ if\ u\in N_{G_i}(v_i), i=1,2 \\ \delta_{G_i}(u), \ if\ u\in V(G_i), u\notin N_{G_i}(v_i), u\neq v_i, i=1,2. \end{cases}$$

The M_N index for link of graphs is obtained in the following proposition.

Proposition 11. *The neighborhood Zagreb index for link of two graphs is given by*

$$\begin{aligned} M_N((G_1\sim G_2)(v_1,v_2)) &= M_N(G_1)+M_N(G_2)+[deg_{G_1}(v_1)^2+deg_{G_2}(v_2)^2] \\ &\quad +3[deg_{G_1}(v_1)+deg_{G_2}(v_2)]+2[\delta_{G_1}(v_1)+\delta_{G_2}(v_2)] \\ &\quad +2[\delta_{G_1}(v_1)deg_{G_2}(v_2)+\delta_{G_2}(v_2)deg_{G_1}(v_1)] \\ &\quad +2[\sum_{u\in N_{G_1}(v_1)}\delta_{G_1}(u)+\sum_{u\in N_{G_2}(v_2)}\delta_{G_2}(u)]+2. \end{aligned}$$

Proof 8. *Applying the definition of neighborhood Zagreb index and using lemma 13, we have*

$$\begin{aligned} M_N((G_1 \sim G_2)(v_1, v_2)) &= \sum_{u \in V((G_1 \sim G_2)(v_1,v_2))} \delta_{(G_1 \sim G_2)(v_1,v_2)}(u)^2 \\ &= \sum_{i \neq j, i,j=1,2} [\delta_{G_i}(v_i) + \delta_{G_j}(v_j) + 1]^2 + \sum_{u \in N_{G_i}(v_i), i=1,2} [\delta_{G_i}(u) + 1]^2 \\ &\quad + \sum_{u \in V(G_i), u \notin N_{G_i}(v_i), u \neq v_i, i=1,2} \delta_{G_i}(u)^2 \\ &= M_N(G_1) + M_N(G_2) + [deg_{G_1}(v_1)^2 + deg_{G_2}(v_2)^2] \\ &\quad +3[deg_{G_1}(v_1) + deg_{G_2}(v_2)] + 2[\delta_{G_1}(v_1) + \delta_{G_2}(v_2)] \\ &\quad +2[\delta_{G_1}(v_1) deg_{G_2}(v_2) + \delta_{G_2}(v_2) deg_{G_1}(v_1)] \\ &\quad +2[\sum_{u \in N_{G_1}(v_1)} \delta_{G_1}(u) + \sum_{u \in N_{G_2}(v_2)} \delta_{G_2}(u)] + 2. \end{aligned}$$

Hence the proof.

Example 6. *Using link of graphs we can obtain the molecular graph of the nanostar dendrimers D_n as shown in Figure DC 5. Thus using above proposition we have the following result.*

$$M_N(D_n) = 624n - 102.$$

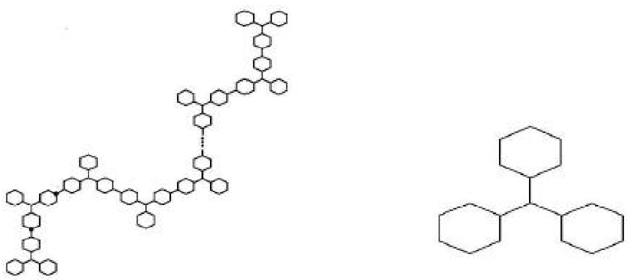

Figure 3.5: The molecular graph of the nanostar dendrimers D_n and D_1.

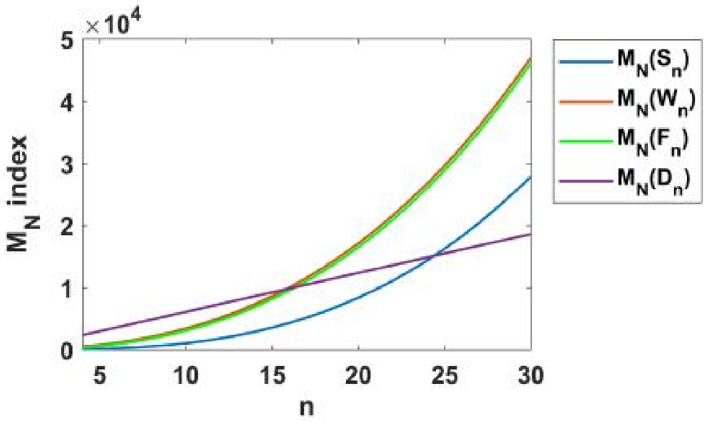

Figure 3.6: Plotting of M_N indices for S_n, W_n, F_n, and D_n.

The M_N indices of star graph, wheel graph, fan graph and nanostar dendrimer are depicted in Figure 3.6.

3.6. Disjunction

The disjunction [15] $G_1 \vee G_2$ of two graphs G_1, G_2 is the graph having node set $V_1 \times V_2$ and (u_1, v_1) is adjacent with (u_2, v_2) iff $u_1u_2 \in V_1$ or $v_1v_2 \in V_2$. Clearly we can state the following lemma.

Lemma 14. *For disjunction of two graphs*

$$\begin{aligned}\delta_{G_1 \vee G_2}(u,v) &= (n_2^2 - 2m_2)\delta_{G_1}(u) + (n_1^2 - 2m_1)\delta_{G_2}(v) + 2n_2m_1deg_{G_2}(v)\\ &\quad +2n_1m_2deg_{G_1}(u) - n_2\delta_{G_1}(u)deg_{G_2}(v) - n_1deg_{G_1}(u)\delta_{G_2}(v)\\ &\quad +\delta_{G_1}(u)\delta_{G_2}(v),\end{aligned}$$

where $u \in V(G_1), v \in V(G_2)$.

The M_N index for disjunction of two graphs can be computed like previous operations in the following proposition.

Proposition 12. *The neighborhood Zagreb index of disjunction of two graphs is given by*

$$\begin{aligned} M_N(G_1 \vee G_2) &= [(n_2^2-2m_2)(n_2^3-6n_2m_2)]M_N(G_1)+[(n_1^2-2m_1)(n_1^3-6n_1m_1)] \\ &\quad M_N(G_2)+[4n_1^2n_2m_2^2+8n_2m_1m_2(n_2^2-2m_2)]M_1(G_1)+[4n_1n_2^2m_1^2 \\ &\quad +8n_1m_1m_2(n_1^2-2m_1)]M_1(G_2)+[8n_1m_2(n_2^2-2m_2)-16n_1n_2m_2^2] \\ &\quad M_2(G_1)+[8n_2m_1(n_1^2-2m_1)-16n_1n_2m_1^2]M_2(G_2)+[3n_1^2-4m_1] \\ &\quad M_1(G_1)M_N(G_2)+[3n_2^2-4m_2]M_N(G_1)M_1(G_2)-4[n_1M_2(G_1) \\ &\quad M_N(G_2)+n_2M_N(G_1)M_2(G_2)]+[2(n_2^2-2m_2)(n_1^2-2m_1)-4n_2^2m_1 \\ &\quad -4n_1^2m_2]M_1(G_1)M_1(G_2)+[16n_2m_1-4n_1^2n_2]M_1(G_1)M_2(G_2)+ \\ &\quad [16n_1m_2-4n_1n_2^2]M_2(G_1)M_1(G_2)+8n_1n_2M_2(G_1)M_2(G_2)+ \\ &\quad M_N(G_1)M_N(G_2)+32n_1n_2m_1^2m_2^2. \end{aligned}$$

3.7. Symmetric difference

The symmetric difference [11] $G_1 \oplus G_2$ of two graphs G_1 and G_2 is the graph with node set $V_1 \times V_2$ and edge set $E(G_1 \oplus G_2) = \{\ (u_1,v_1)(u_2,v_2) : u_1u_2 \in E_1$ or $v_1v_2 \in E_2$ but not both $\}$. Clearly we have the following lemma.

Lemma 15. *For symmetric difference of two graphs*

$$\begin{aligned} \delta_{G_1 \oplus G_2}(u,v) &= (n_2^2-4m_2)\delta_{G_1}(u)+(n_1^2-4m_1)\delta_{G_2}(v)+2n_2m_1deg_{G_2}(v) \\ &\quad +2n_1m_2deg_{G_1}(u)-2n_2\delta_{G_1}(u)deg_{G_2}(v)-2n_1deg_{G_1}(u)\delta_{G_2}(v) \\ &\quad +4\delta_{G_1}(u)\delta_{G_2}(v), \end{aligned}$$

where $u \in V(G_1), v \in V(G_2)$.

In the following proposition, the Neighborhood Zagreb index of symmetric difference of two graphs can be achieved as before.

Proposition 13. *The neighborhood Zagreb index of symmetric difference of two graphs is given by*

$$\begin{aligned} M_N(G_1 \oplus G_2) &= [(n_2^2-4m_2)(n_2^3-12n_2m_2)]M_N(G_1)+[(n_1^2-4m_1)(n_1^3-12n_1m_1)] \\ &\quad M_N(G_2)+[4n_1^2n_2m_2^2+8n_2m_1m_2(n_2^2-4m_2)]M_1(G_1)+[4n_1n_2^2m_1^2 \\ &\quad +8n_1m_1m_2(n_1^2-4m_1)]M_1(G_2)+[8n_1m_2(n_2^2-4m_2)-32n_1n_2m_2^2] \\ &\quad M_2(G_1)+[8n_2m_1(n_1^2-4m_1)-32n_1n_2m_1^2]M_2(G_2)+[12n_1^2- \end{aligned}$$

$$32m_1]M_1(G_1)M_N(G_2) + [12n_2^2 - 32m_2]M_N(G_1)M_1(G_2) - 32[n_1M_2(G_1)M_N(G_2) + n_2M_N(G_1)M_2(G_2)] + [2(n_2^2 - 4m_2)(n_1^2 -4m_1) - 8n_2^2m_1 - 8n_1^2m_2]M_1(G_1)M_1(G_2) + [64n_2m_1 - 8n_1^2n_2] M_1(G_1)M_2(G_2) + [64n_1m_2 - 8n_1n_2^2]M_2(G_1)M_1(G_2) + 32n_1n_2 M_2(G_1)M_2(G_2) + 16M_N(G_1)M_N(G_2) + 32n_1n_2m_1^2m_2^2.$$

Conclusion

In this article, some bounds of the neighborhood Zagreb index are derived. Also some explicit expressions of the index for different graph operations are obtained and some results are applied to find the index of some composite and chemically interesting graphs. Still there are many other graph operations and special classes of graphs which are not studied here. For further work, the neighborhood Zagreb index of Mycielskis construction, generalized hierarchical product and different subdivision graphs can be obtained.

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References

[1] A. R. Ashrafi, T. Došlić, and A. Hamzeh, "The Zagreb coindices of graph operations", *Discrete applied mathematics,* vol. 158, no. 15, pp. 1571-1578, Aug. 2010, doi: 10.1016/j.dam.2010.05.017

[2] M. Azari, "Sharp lower bounds on the Narumi-Katayama index of graph operations", *Applied mathematics and computation*, vol. 239, pp. 409-421, Jul. 2014, doi: 10.1016/j.amc.2014.04.088

[3] R. Bhatia and C. Davis, "A Better Bound on the Variance", *The american mathematical monthly,* vol. 107, no. 4, pp. 353–357, Apr. 2000, doi: 10.2307/2589180

[4] Z. Che and Z. Chen, "Lower and upper bounds of the forgotten topological index", *MATCH communications in mathematical and in computer chemistry*, vol. 76, no. 3, pp. 635-648, 2016. [On line]. Available: https://bit.ly/3hvdXD4

[5] K. C. Das, "On geometrical-arithmetic index of graphs", *MATCH communications in mathematical and in computer chemistry*, vol. 64, no. 3, pp. 619-630, 2010. [On line]. Available: https://bit.ly/2N0M9sl

[6] K. C. Das, A. Yurttas, M. Togan, A. Cevik, and I. Cangul, "The multiplicative Zagreb indices of graph operations", *Journal of inequalities and applications,* vol. 2013, no. 1, Art ID. 90, Mar. 2013, doi: 10.1186/1029-242x-2013-90

[7] N. De, "Some bounds of reformulated Zagreb indices", *Applied mathematical sciences,* vol. 6, no. 101, pp. 5005-5012, 2012. [On line]. Available: https://bit.ly/3db09ds

[8] N. De, S. M. A. Nayeem, and A. Pal, "F-Index of some graph operations", Discrete mathematics, algorithms and applications, vol. 8, no. 2, Art ID. 1650025, 2006, doi: 10.1142/s1793830916500257

[9] J. B. Diaz and F. T. Metcalf, "Stronger forms of a class of inequalities of G. Pólya-G. Szegö, and L. V. Kantorovich", *Bulletin of the American Mathematical Society,* vol. 69, no. 3, pp. 415–419, May 1963, doi: 10.1090/s0002-9904-1963-10953-2

[10] T. Doslić, "Splices, links and their degree-weighted Wiener polynomials", *Graph theory notes New York,* vol. 48, pp. 47-55, 2005

[11] M. Ghorbani and M. A. Hosseinzadeh, "The third version Of Zagreb index", *Discrete mathematics, algorithms and applications,* vol. 05, no. 04, Art ID. 1350039, Dec. 2013, doi:10.1142/S1793830913500390

[12] I. Gutman and O. E. Polansky, Mathematical concepts in organic chemistry. Berlin: Springer, 1986, doi: 10.1007/978-3-642-70982-1

[13] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons", *Chemical physics letters,* vol. 17, no. 4, pp. 535-538, Dec. 1972, doi: 10.1016/0009-2614(72)85099-1

[14] G. H. Hardy, J. E. Littlewood, and P. George, *Inequalities*, 2nd ed. Cambridge: Cambridge University Press, 1988.

[15] M. H. Khalifeh, H. Yousefi-Azari, and A. R. Ashrafi, "The first and second Zagreb indices of some graph operations", *Discrete applied mathematics,* vol. 157, no. 4, pp. 804–811, Feb. 2009, doi:10.1016/j.dam.2008.06.015.

[16] S. Mondal, N. De, and A. Pal, "On neighborhood Zagreb index of product graphs", May 2018, arXiv:1805.05273

[17] K. Pattabiraman and P. Kandan, "Weighted PI index of corona product of graphs", *Discrete mathematics, algorithms and applications,* vol. 06, no. 04, Art ID.1450055, Oct. 2014, doi: 10.1142/S1793830914500554

[18] G. Pólya and G. Szegö, *Problems and theorems in analysis*. Berlin: Springer, 1972.

[19] N. Trinajstić, *Chemical graph theory*. Boca Raton, FL: CRC, 1983.

[20] H. Wiener, "Structural determination of the paraffin boiling points", *Journal of the American Chemical Society*, vol. 69, no. 1, pp. 17-20, Jan. 1947, doi: 10.1021/ja01193a005