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ON BOUNDS FOR CERTAIN CLOSED NEIGHBOURHOOD TOPOLOGICAL INDICES

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Abstract

Consider $G = (V, E)$ be a simple, finite, undirected and connected graph as having τ edges and η vertices. The vertices s and w are connected by the edge sw. The degree of a vertex $s \in V(G)$, denoted by $d_G(S)$ is the number of vertices that are adjacent to s and $N[w]$ is the closed neighbourhood set of a vertex w that includes w and its neighbours. Using this concept, we derived the lower and upper bounds for some closed neighbourhood topological indices in this paper.

1. Introduction

Topological indices are significant mathematical tools offered by graph theory to predict the physicochemical properties of molecular compounds [15, 16]. The degree-based index is the most studied topological index in structure-property relationships and bio-activity of chemical compounds [6].

In 1975, Milan Randić introduced the first degree-based index termed as Randić index $(R(G))$, which is applied in drug designing [11].

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$$R(G) = \sum_{sw \in E(G)} \frac{1}{\sqrt{d_G(s) \cdot d_G(w)}} \tag{1}$$

The first $(M_1(G))$ and second Zagreb $(M_2(G))$ indices were proposed by Gutman et al. [7] to predict the π electron energy of compounds.

$$M_1(G) = \sum_{s \in V(G)} d_G(s)^2 = \sum_{sw \in E(G)} (d_G(s) + d_G(w)) \tag{2}$$

$$M_2(G) = \sum_{sw \in E(G)} (d_G(s) d_G(w)) \tag{3}$$

Furtula et al. [5] proposed the Forgotten index $(F(G))$ for predicting the physicochemical properties of molecular compounds, which is another notable degree-based index.

$$F(G) = \sum_{s \in V(G)} d_G(s)^3 = \sum_{sw \in E(G)} (d_G(s)^2 + d_G(w)^2) \tag{4}$$

The first $(HM_1(G))$ and second hyper Zagreb $(HM_2(G))$ indices were established by Shirdel et al. [12].

$$HM_1(G) = \sum_{sw \in E(G)} (d_G(s) + d_G(w))^2 \tag{5}$$

$$HM_2(G) = \sum_{sw \in E(G)} (d_G(s) + d_G(w))^2 \tag{6}$$

For some latest reports on topological indices, we recommend the literatures [3, 4, 13, 14] to the enthusiastic readers.

2. Preliminaries

Below we enumerate the closed neighbourhood topological indices (neighbourhood Dakshayani indices [9]) that are needed to consider in the next section. Closed Neighbourhood degree-sum of a vertex $s \in V(G)$ is defined as

$$\Omega_G(s) = \sum_{w \in N[s]} d_G(w) \tag{7}$$

Closed neighbourhood first Zagreb index:

$$CM_1(G) = \sum_{sw \in E(G)} (\Omega_G(s) + \Omega_G(w)) \tag{8}$$

Modified closed neighbourhood first Zagreb index:

$$CM_1^*(G) = \sum_{s \in E(G)} \Omega_G(s)^2 \tag{9}$$

Closed neighbourhood second Zagreb index:

$$CM_2(G) = \sum_{sw \in E(G)} (\Omega_G(s)\Omega_G(w)) \tag{10}$$

Closed neighbourhood Forgotten index:

$$CF(G) = \sum_{sw \in E(G)} (\Omega_G(s)^2 + \Omega_G(w)^2) \tag{11}$$

Modified closed neighbourhood Forgotten index:

$$CF^*(G) = \sum_{s \in V(G)} \Omega_G(s)^3 \tag{12}$$

Closed neighbourhood first hyper Zagreb index:

$$CHM_1(G) = \sum_{sw \in E(G)} (\Omega_G(s) + \Omega_G(w))^2 \tag{13}$$

Closed neighbourhood second hyper Zagreb index:

$$CHM_2(G) = \sum_{sw \in E(G)} (\Omega_G(s)\Omega_G(w))^2 \tag{14}$$

The topological indices mentioned above are chemically beneficial as they have a significant correlation with the entropy, a centric factor, critical pressure, density, heats of vaporization, mean radius and standard enthalpy of vaporization of the octane isomers. Interestingly, these indices reveal exceptional degeneracy values (exactly 1) for various octane isomer structural formulae, demonstrating their superior discriminating behavior. At this juncture of the research, we primarily focus to reveal the mathematical behaviour of the closed neighbourhood indices reported in [9] by means of lower and upper bounds, which is exactly the contribution of this paper.

3. Main Results

In what follows, we obtain some lower and upper bounds of the closed neighbourhood topological indices using some well known inequalities.

Lemma 3.1. *For a graph G, we have,*

(i) $\sum_{i=1}^{\eta} \Omega_G(s_i) = M_1(G) + 2\tau.$

(ii) $\sum_{i=1}^{\eta} \Omega_G(s_i)\, d_G(s_i) = 2M_2(G) + M_1(G).$

(iii) $CM_1(G) = \sum_{sw \in E(G)} (\Omega_G(s) + \Omega_G(w)) = 2M_2(G) + M_1(G).$

Lemma 3.2 (Quadratic mean $\geq$ Arithmetic mean) [8]**.** *For n positive numbers* $z_1, z_2, \ldots, z_n$, *we have*

$$\sqrt{\frac{z_1^2 + z_2^2 + \ldots + z_n^2}{n}} \geq \frac{z_1 + z_2 + \ldots + z_n}{n}, \tag{15}$$

where equality holds iff $z_1 = z_2 = \ldots = z_n$.

Theorem 3.3. *For a graph G with* η *vertices, we obtain*

$$CM_1^*(G) \geq \frac{M_1(G)^2 + 4\tau M_1(G) + 4\tau^2}{\eta} \tag{16}$$

where equality holds iff G is regular.

Proof. Assuming $z_i = \Omega_G(s_i)$ for $i = 1, 2, \ldots, \eta$, from Equation (15), we have

$$\sqrt{\frac{\Omega_G(s_1)^2 + \Omega_G(s_2)^2 + \ldots + \Omega_G(s_\eta)^2}{\eta}} \geq \frac{\Omega_G(s_1) + \Omega_G(s_2) + \ldots + \Omega_G(s_\eta)}{\eta} \quad (17)$$

Using Lemma 3.1 and the definition of $CM_1^*(G)$ index, Equation (17) becomes

$$\sqrt{\frac{CM_1^*(G)}{\eta}} \geq \frac{(M_1(G) + 2\tau)}{\eta} \quad (18)$$

On squaring Equation (18) and simplifying, we get the desired result.

The equality holds iff $\Omega_G(s_1) = \Omega_G(s_2) = \ldots = \Omega_G(s_\eta)$. Therefore, equality in (16) holds iff G is regular.

Lemma 3.4 (Bhatia and Davis' bound on variance) [1]**.** *Let* $z_1, z_2, \ldots, z_n$ *be real numbers such that* $m \leq z_i \leq M$ *for all* $1 \leq i \leq n$ *and* $\theta = \frac{\sum_{i=1}^{n} z_i}{n}$. *Then*

$$\frac{\sum_{i=1}^{n}(z_i - \theta)^2}{n} \leq (M - \theta)(\theta - m), \quad (19)$$

where equality holds iff each z_i *is either* M *or* m.

Theorem 3.5. *For a graph G with* η *vertices, we have*

$$CM_1^*(G) \leq (\delta_{CN} + \Delta_{CN})(M_1(G) + 2\tau) - \eta\delta_{CN}\Delta_{CN} \quad (20)$$

and equality holds iff each $\Omega_G(s_i)(i = 1, 2, \ldots, \eta)$ *is either* δ_{CN} *or* Δ_{CN}, *where* $\delta_{CN} = \min\{\Omega_G(s) : s \in V(G)\}$ *and* $\Delta_{CN} = \max\{\Omega_G(s) : s \in V(G)\}$.

Proof. If we take $z_i = \Omega_G(s_i)$, for $1 \leq i \leq \eta$, $m = \delta_{CN}$ and $M = \Delta_{CN}$, then $\theta = \frac{M_1(G) + 2\tau}{\eta}$ and inequality Equation (19) yields

$$\frac{\sum_{i=1}^{\eta}\left(\Omega_G(s_i) - \left(\frac{M_1(G) + 2\tau}{\eta}\right)\right)}{\eta} \leq \left(\Delta_{CN} - \left(\frac{M_1(G) + 2\tau}{\eta}\right)\right)$$

$$\left(\left(\frac{M_1(G)+2\tau}{\eta}\right)-\delta_{CN}\right)$$

and then becomes $CM_1^*(G) \leq (\delta_{CN}+\Delta_{CN})(M_1(G)+2\tau)-\eta\delta_{CN}\Delta_{CN}$, where the equality in Equation (20) holds iff each $\Omega_G(s_i)(i = 1, 2, \ldots, \eta)$ is either δ_{CN} or Δ_{CN}.

Lemma 3.6 [8]. *Let* $(z_1, z_2, \ldots, z_n)$ *be positive n-tuple such that there exists positive numbers A, a satisfying* $0 \leq a \leq z_i \leq A$, *then we get*

$$\frac{n\sum_{i=1}^{n} z_i^2}{\left(\sum_{i=1}^{n} z_i\right)^2} \leq \frac{1}{4}\left(\frac{\sqrt{A}}{\sqrt{a}}+\frac{\sqrt{a}}{\sqrt{A}}\right)^2, \tag{21}$$

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* z_i, *coincide with a and remaining* $(n-q)$ *of the* z_i*'s coincide with* $A(\neq a)$.

Theorem 3.7. *Let G be a graph with* η *vertices. If* $\delta_{CN} = \min\{\Omega_G(s) : s \in V(G)\}$, *and* $\Delta_{CN} = \max\{\Omega_G(s) : s \in V(G)\}$, *then*

$$CM_1^*(G) \leq \frac{(M_1(G)+2\tau)^2(\Delta_{CN}+\delta_{CN})^2}{4\eta\Delta_{CN}\delta_{CN}}, \tag{22}$$

where equality holds iff $\delta_{CN} = \Delta_{CN}$ *or* $q = \frac{\frac{\Delta_{CN}}{\delta_{CN}}}{\frac{\Delta_{CN}}{\delta_{CN}}+1}\eta$ *is an integer and q of the numbers* $\Omega_G(s_i)$ *coincide with* δ_{CN} *and remaining* $(\eta-q)$ *of the* $\Omega_G(s_i)$*'s coincide with* $\Delta_{CN}(\neq \delta_{CN})$.

Proof. Applying $z_i = \Omega_G(s_i)(1 \leq i \leq \eta)$, $a = \delta_{CN}$ and $A = \Delta_{CN}$ in Equation (21), we attain

$$\frac{n\sum_{i=1}^{n}\Omega_G(s_i)^2}{\left(\sum_{i=1}^{n}\Omega_G(s_i)\right)^2} \leq \frac{1}{4}\left(\frac{\sqrt{\Delta_{CN}}}{\sqrt{\delta_{CN}}}+\frac{\sqrt{\delta_{CN}}}{\sqrt{\Delta_{CN}}}\right)^2$$

and simplifying, we have arrived the required result.

Also equality holds iff $\delta_{CN} = \Delta_{CN}$ or $q = \dfrac{\frac{\Delta_{CN}}{\delta_{CN}}}{\frac{\Delta_{CN}}{\delta_{CN}}+1}\eta$ is an integer and q of the numbers $\Omega_G(s_i)$ coincide with δ_{CN} and remaining $(\eta - q)$ of the $\Omega_G(s_i)$'s coincide with $\Delta_{CN}(\neq \delta_{CN})$.

Lemma 3.8 (Diaz-Metcalf inequality) [2]. *Let c_i and d_i be two sequences of real numbers with $c_i \neq 0 (1 \leq i \leq n)$ such that $mc_i \leq d_i \leq Md_i$, then*

$$\sum_{i=1}^{n} d_i^2 + mM\sum_{i=1}^{n} c_i^2 \leq (M+m)\sum_{i=1}^{n} c_i d_i, \tag{23}$$

where equality holds iff either $d_i = mc_i$ or $d_i = Mc_i$ $\forall i = 1, 2, \ldots, n$.

Theorem 3.9. *For a graph G of η vertices with $\Delta_{CN} = \max\{\Omega_G(s) : s \in V(G)\}$, we have*

$$CM_1^*(G) \leq M_1(G) + 2(\Delta_{CN}+1)M_2(G), \tag{24}$$

where equality holds iff either $\Omega_G(s_i) = d_G(s_i)$ or $\Omega_G(s_i) = \Delta_{CN} d_G(s_i)$ $\forall i = 1, 2, \ldots, \eta$.

Proof. Putting $c_i = d_G(s_i)$, $d_i = \Omega_G(s_i)$, $m = 1$, $M = \Delta_{CN}$ in inequality (23) of Lemma 3.8, we obtain

$$\sum_{i=1}^{\eta}\Omega_G(s_i)^2 + \Delta_{CN}\sum_{i=1}^{\eta} d_G(s_i)^2 \leq (\Delta_{CN}+1)\sum_{i=1}^{\eta}\Omega_G(s_i)\, d_G(s_i)$$

After simplifying, we attain the required proof.

Lemma 3.10 [10]. *Let* $\vec{a} = (a_1, a_2, \ldots, a_n)$ *and* $\vec{b} = (b_1, b_2, \ldots, b_n)$ *be* *sequences of real numbers. If* $\vec{c} = (c_1, c_2, \ldots, c_n)$ *and* $\vec{d} = (d_1, d_2, \ldots, d_n)$ *are non-negative sequences, then*

$$\sum_{i=1}^{n} d_i \sum_{i=1}^{n} c_i a_i^2 + \sum_{i=1}^{n} c_i \sum_{i=1}^{n} d_i b_i^2 \geq 2 \sum_{i=1}^{n} c_i a_i \sum_{i=1}^{n} d_i b_i, \tag{25}$$

In particular, if c_i *and* d_i *are positive, then equality holds iff* $\vec{a} = \vec{b} = \vec{k}$, *where* $\vec{k} = (k, k, \ldots, k)$, *a constant sequence.*

Theorem 3.11. *If G is a graph with* η *vertices and* τ *edges, then*

$$CM_1^*(G) > \frac{8\tau}{\eta} + \frac{4\tau - \eta}{\eta} M_1(G). \tag{26}$$

Proof. Assuming $a_i = \Omega_G(s_i)$, $b_i = d_G(s_i)$, $c_i = 1$ and $d_i = 1$ in inequality (25), we have

$$\sum_{i=1}^{\eta} 1 \sum_{i=1}^{\eta} \Omega_G(s_i)^2 + \sum_{i=1}^{\eta} 1 \sum_{i=1}^{\eta} d_G(s_i)^2 \geq 2 \sum_{i=1}^{\eta} \Omega_G(s_i) \sum_{i=1}^{\eta} d_G(s_i) \tag{27}$$

Using the result $\sum_{i=1}^{\eta} d_G(s_i) = 2\tau$ and Equation (27), we get

$$CM_1^*(G) \geq \frac{8\tau}{\eta} + \frac{4\tau - \eta}{\eta} M_1(G). \tag{28}$$

It is obvious from lemma 3.10 that equality in (28) is impossible.

Lemma 3.12 (Cauchy-Schwartz inequality) [1]. *If* c_i *and* d_i *are real numbers for* $i = 1, 2, \ldots, n$, *then*

$$\left(\sum_{i=1}^{n} c_i d_i\right)^2 \leq \left(\sum_{i=1}^{n} c_i^2\right)\left(\sum_{i=1}^{n} d_i^2\right). \tag{29}$$

Equality holds iff $c_i = kd_i$ *for some constant k and for* $i = 1, 2, \ldots, n$.

Theorem 3.13. *For a graph G*,

$$CM_1^*(G) \geq M_1(G) + 4M_2(G) + \frac{4M_2(G)^2}{M_1(G)}. \tag{30}$$

Equality holds iff $\Omega_G(s_i) = kd_G(s_i)$ *for some constant* k *and for* $i = 1, 2, \ldots, n$.

Proof. For $i = 1, 2, \ldots, \eta$, considering $c_i = \Omega_G(s_i), d_i = d_G(s_i)$ in Equation (29), we obtain

$$\left(\sum_{i=1}^{\eta} \Omega_G(s_i) d_G(s_i)\right)^2 \leq \left(\sum_{i=1}^{\eta} \Omega_G(s_i)^2\right)\left(\sum_{i=1}^{\eta} d_G(s_i)^2\right) \tag{31}$$

Applying lemma 3.1, we rewrite the Equation (31) as

$$(2M_2(G) + M_1(G))^2 \leq CM_1^*(G)M_1(G) \tag{32}$$

which yields the inequality given in Equation (30). Equality holds iff $\Omega_G(s_i) = kd_G(s_i)$ for some constant k and for $i = 1, 2, \ldots, \eta$.

Theorem 3.14. *Let G be a graph with* η *vertices and* τ *edges. Then*

$$CHM_1(G) \geq \frac{M_1(G)^2}{\tau} + \frac{4M_2(G)^2}{\tau} + \frac{4M_1(G)M_2(G)}{\tau}, \tag{33}$$

Equality holds iff $\Omega_G(s) + \Omega_G(w) = k$ *for some constant* $k, \forall sw \in E(G)$.

Proof. In Equation (29), putting $c_i = \Omega_G(s) + \Omega_G(w)$ and $d_i = 1$, we get

$$\left(\sum_{sw \in E(G)} [\Omega_G(s) + \Omega_G(w)]\right)^2 \leq \left(\sum_{sw \in E(G)} [\Omega_G(s) + \Omega_G(w)]^2\right)\left(\sum_{sw \in E(G)} 1^2\right)$$

Applying Lemma 3.1, we obtain

$$[2M_2(G) + M_1(G)]^2 \leq [CHM_1(s)][\tau]. \tag{34}$$

Hence the lower bound of $CHM_1(G)$ is

$$CHM_1(G) \geq \frac{M_1(G)^2}{\tau} + \frac{4M_2(G)^2}{\tau} + \frac{4M_1(G)M_2(G)}{\tau}.$$

It is elucidate that equality holds iff $\Omega_G(s) + \Omega_G(w) = k$ for some constant $k, \forall\ sw \in E(G)$.

Theorem 3.15. *Let the graph G have* η *vertices and* τ *edges. If* $\delta_{CN} = \min\{\Omega_G(s) : s \in V(G)\}$ *and* $\Delta_{CN} = \max\{\Omega_G(s) : s \in V(G)\}$, *then*

$$CHM_1(G) \leq \frac{[2M_2(G) + M_1(G)]^2[\delta_{CN} + \Delta_{CN}]}{4\tau\delta_{CN}\Delta_{CN}}. \tag{35}$$

Equality holds iff $\delta_{CN} = \Delta_{CN}$ *or* $q = \dfrac{\frac{\Delta_{CN}}{\delta_{CN}}}{\frac{\Delta_{CN}}{\delta_{CN}} + 1}\tau$ *is an integer and q of the numbers* $\Omega_G(s) + \Omega_G(w)$ *coincide with* $2\delta_{CN}$ *and remaining* $(\tau - q)$ *of the* $\Omega_G(s) + \Omega_G(w)$ *coincide with* $2\Delta_{CN}(\neq 2\delta_{CN})$.

Proof. Substituting $a = 2\delta_{CN}$, $A = 2\Delta_{CN}$ and $z_i = \Omega_G(s) + \Omega_G(w)$ in Equation (21), we attain

$$\frac{\tau\sum_{sw\in E(G)}[\Omega_G(s) + \Omega_G(w)]^2}{\left(\sum_{sw\in E(G)}[\Omega_G(s) + \Omega_G(w)]\right)^2} \leq \frac{1}{4}\left(\frac{\sqrt{2\Delta_{CN}}}{\sqrt{2\delta_{CN}}} + \frac{\sqrt{2\delta_{CN}}}{\sqrt{2\Delta_{CN}}}\right)^2 \tag{36}$$

Applying Lemma 3.1, we obtained the result.

$$CHM_1(G) \leq \frac{[2M_2(G) + M_1(G)]^2[\delta_{CN} + \Delta_{CN}]^2}{4\tau\delta_{CN}\Delta_{CN}}.$$

Also equality obtains iff $\delta_{CN} = \Delta_{CN}$ or $q = \dfrac{\frac{\Delta_{CN}}{\delta_{CN}}}{\frac{\Delta_{CN}}{\delta_{CN}} + 1}\tau$ is an integer and q of the numbers $\Omega_G(s) + \Omega_G(w)$ coincide with $2\delta_{CN}$ and remaining $(\tau - q)$ of the $\Omega_G(s) + \Omega_G(w)$ coincide with $2\Delta_{CN}(\neq 2\delta_{CN})$. Hence the proof.

Theorem 3.16. *For any graph G with* τ *edges*,

$$CF^*(G) > 2CM_1^*(G) - M_1(G) - 2\tau \tag{37}$$

Proof. Putting $a_i = \Omega_G(s)$, $b_i = 1$, $c_i = \Omega_G(s)$ and $d_i = 1$ in inequality (25), we obtain

$$\sum_{i=1}^{\eta} 1 \sum_{s \in V(G)} \Omega_G(s)^3 + \sum_{s \in V(G)} \Omega_G(s) \sum_{i=1}^{\eta} 1 \geq 2 \sum_{s \in V(G)} \Omega_G(s)^2 \sum_{i=1}^{\eta} 1 \tag{38}$$

Using Lemma 3.1, we get $CF^*(G) + M_1(G) + 2\tau \geq 2CM_1^*(G)$, and hence

$$CF^*(G) \geq 2CM_1^*(G) - M_1(G) - 2\tau. \tag{39}$$

Equality in Equation (39) is not possible. Hence the theorem is proved.

Lemma 3.17 (Radon's Inequality) [2, 10]**.** *If* $c_i, d_i > 0$, $i = 1, 2, \ldots, n$, $h > 0$, *then*

$$\sum_{i=1}^{n} \left(\frac{c_i^{h+1}}{d_i^h} \right) \geq \frac{\left(\sum_{i=1}^{n} c_i \right)^{h+1}}{\left(\sum_{i=1}^{n} d_i \right)^h}, \tag{40}$$

where equality holds iff $c_i = kd_i$ *for some constant* k, $\forall\ i = 1, 2, \ldots, n$.

Theorem 3.18. *Let the graph G have* η *vertices and* τ *edges. We attain*

$$CF^*(G) \geq \frac{(M_1(G) + 2\tau)^3}{\eta^2}, \tag{41}$$

Equality attains iff G is complete bipartite or regular graph.

Proof. Considering for $i = 1, 2, \ldots, \eta$, $c_i = \Omega_G(s_i)$, $d_i = 1$, and $h = 2$ in Equation (40) of Lemma 3.17, we attain $\sum_{i=1}^{n} \left(\frac{\Omega_G(s_i)^3}{1^2} \right) \geq \frac{\left(\sum_{i=1}^{n} \Omega_G(s_i) \right)^3}{\left(\sum_{i=1}^{n} 1 \right)^2}$.

Hence, $CF^*(G) \geq \frac{(M_1(G) + 2\tau)^3}{\eta^2}$. Equality attains iff $\Omega_G(s_i) = k$ for some constant k. i.e., equality attains iff G is complete bipartite or regular graph.

Theorem 3.19. *For graph G with τ edges,* $CF^*(G) \geq \frac{CM_1^*(G)^2}{M_1(G) + 2\tau}$. (42)

Proof. If G is a graph and $s \in V(G)$, then weighted arithmetic means of $\Omega_G(s)$ and that of $\Omega_G(s)^2$ are $\langle d \rangle_{WM} = \frac{\sum_{s \in V(G)} W_s \Omega_G(s)}{\sum_{s \in V(G)} W_s}$ and

$$\langle d^2 \rangle_{WM} = \frac{\sum_{s \in V(G)} W_s \Omega_G(s)^2}{\sum_{s \in V(G)} W_s},$$

where W_s is the weight of the vertex $s \in V(G)$.

For non-negative weight W_s,

$$\langle d^2 \rangle_{WM} \geq \langle d \rangle_{WM}^2 \tag{43}$$

Choosing $W_s = \Omega_G(s)$, inequality in Equation (43) has the form

$$\frac{\sum_{s \in V(G)} \Omega_G(s) \Omega_G(s)^2}{\sum_{s \in V(G)} \Omega_G(s)} \geq \left[\frac{\sum_{s \in V(G)} \Omega_G(s) \Omega_G(s)}{\sum_{s \in V(G)} \Omega_G(s)} \right]^2. \tag{44}$$

After making simplification, Equation (44) yields $CF^*(G) \geq \frac{CM_1^*(G)^2}{M_1(G) + 2\tau}$.

4. Conclusion

We successfully obtained the lower and upper bounds for some closed neighbourhood topological indices using certain standard inequalities.

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