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NEW RESULTS ON LEAP ZAGREB INDICES

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Abstract. In this paper, we investigate the chemical importance of the leap Zagreb indices, and it is shown that the third leap Zagreb index is useful in predicting the boiling point of benzenoid hydrocarbons with high accuracy (with the co-efficient of correlation R=0.9788). We express the leap Zagreb indices in terms of first-degree based indices, instead of second-degree. We also obtain explicit formulae for the third leap Zagreb index of some derived graphs.

1. Introduction

Throughout this article, we consider graphs that are simple, finite, connected and undirected. Let G be a graph with the vertex set $V(G)$ and the edge set $E(G)$. For a vertex u in G, $d_G(u)$ denotes the degree of vertex u in G and $d_2(u/G)$ denotes the number of vertices at distance 2 from u in G. The neighbours degree sum of a vertex u in G, denoted by $\delta_G(u)$, is defined as $\delta_G(u) = \sum_{v\in N_G(u)} d_G(v)$, where $N_G(u) = \{v : uv \in E(G)\}$.

A molecular graph is a graph-theoretic representation of a chemical compound's structural formula. In mathematical chemistry, molecular descriptors (numerical functions related with molecule structure) play an important role. To share chemical features, they are used in QSAR and QSPR investigations. Graph invariants are significant types of molecular descriptors because they are numerical functions from the underlying molecular graph to positive real numbers $\mathbb{R}^+$.

The first and second Zagreb indices are graph invariants based on vertex-degree that were first presented in the 1970s [7, 8]:

$$M_1(G) = \sum_{u\in V(G)} d_G(u)^2 \text{ and } M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v).$$

The first Zagreb index has been discovered to be expressed, alternatively, as [4]

$$M_1(G) = \sum_{uv\in E(G)} \Big(d_G(u) + d_G(v)\Big).$$

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Many degree based indices were introduced after then: the forgotten index $F(G)$ [5], the re-defined third Zagreb index $ReZ(G)$ [16], the neighbourhood first Zagreb index $NM_1(G)$ [10] and the neighbourhood second Zagreb index [10] $NM_2(G)$, etc.

$$\begin{aligned} F(G) &= \sum_{u\in V(G)} d_G(u)^3 = \sum_{uv\in E(G)} \left[d_G(u)^2 + d_G(v)^2\right] \\ ReZ(G) &= \sum_{uv\in E(G)} \Big(d_G(u) + d_G(v)\Big)\, d_G(u)\, d_G(v) \\ NM_1(G) &= \sum_{u\in V(G)} \delta_G(u)^2 \\ NM_2(G) &= \sum_{uv\in E(G)} \delta_G(u)\delta_G(v). \end{aligned}$$

In 2017, Naji et al. [11] introduced the leap Zagreb indices based on second-degree, which are analogous to the Zagreb indices, and studied their basic properties.

Definition 1.1. [11] For a graph G, the first, second, and third leap Zagreb indices are:

$$LM_1(G) = \sum_{u\in V(G)} d_2(u/G)^2 \tag{1.1}$$

$$LM_2(G) = \sum_{uv\in E(G)} d_2(u/G)\, d_2(v/G) \tag{1.2}$$

$$LM_3(G) = \sum_{u\in V(G)} d_G(u) d_2(u/G). \tag{1.3}$$

In 2019, Maji et al. [9] correlated the third leap Zagreb index with the physico-chemical properties of octane isomers, and studied the same under different graph products. See [12, 17] for more works on the leap Zagreb indices.

In this paper, we investigate the chemical importance of the leap Zagreb indices, and it is shown that the third leap Zagreb index is useful in predicting the boiling point of benzenoid hydrocarbons with high accuracy. We express the leap Zagreb indices in terms of first-degree based indices, instead of second-degree. And we find explicit formulae for the third leap Zagreb index of some derived graphs.

2. Regression model for boiling point

Here, we look into the relationship between the leap Zagreb indices of the relevant molecular graphs and the boiling points (BP) of benzenoid hydrocarbons.

Experimental values for the boiling points of the benzenoid hydrocarbons shown in Table 1 are acquired from [13].

Molecular graphs of benzenoid hydrocarbons taken under consideration are shown in Figure 1. The scatter plot between BP and indices LM_1, LM_2 and LM_3 are shown in Figures 2, 3 and 4.

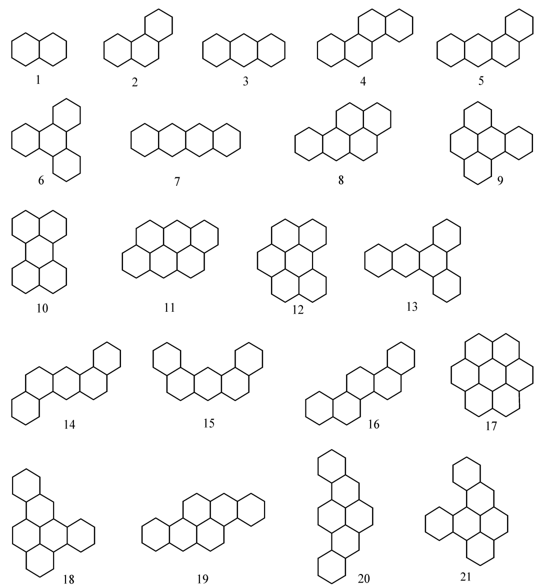

FIGURE 1. Molecular graphs of benzenoid hydrocarbons under consideration.

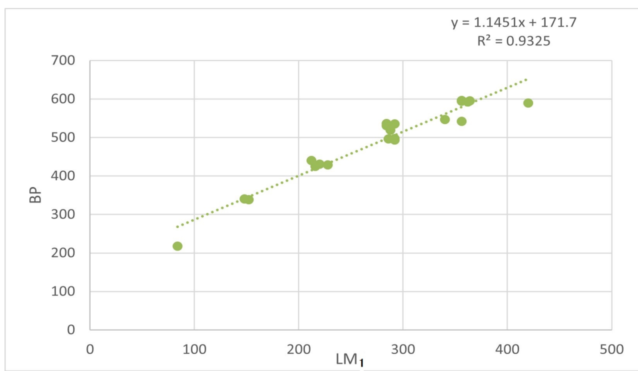

FIGURE 2. Scatter plot between the boiling point (BP) and the first leap Zagreb index (LM_1).

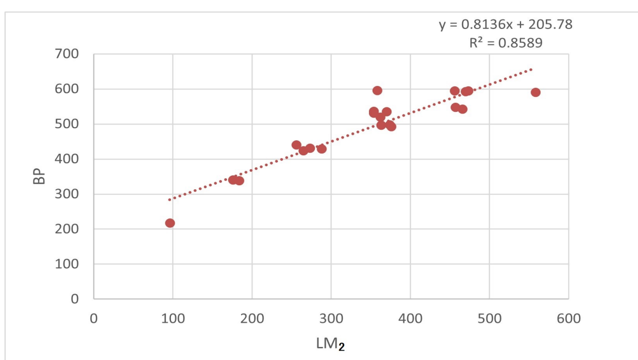

FIGURE 3. Scatter plot between the boiling point (BP) and the second leap Zagreb index (LM_2).

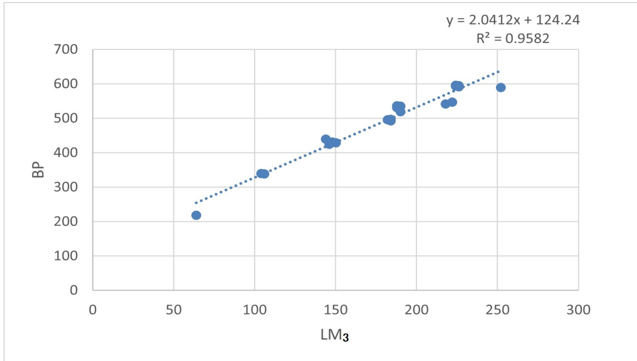

FIGURE 4. Scatter plot between the boiling point (BP) and the third leap Zagreb index (LM_3).

TABLE 1. The values of experimental boiling points and the leap Zagreb indices of 21 benzenoid hydrocarbons.

Benzenoid hydrocarbon	$BP(°C)$	LM_1	LM_2	LM_3
1	218	84	96	64
2	338	152	184	106
3	340	148	176	104
4	431	220	273	148
5	425	216	265	146
6	429	228	288	150
7	440	212	256	144
8	496	286	363	182
9	493	292	376	184
10	497	292	374	184
11	547	340	457	222
12	542	356	466	218
13	535	292	370	190
14	536	284	354	188
15	531	284	354	188
16	519	288	362	190
17	590	420	558	252
18	592	362	470	226
19	596	356	358	224
20	594	356	456	224
21	595	364	473	226

Using the data in Table 1 as input, the following linear regression models for the boiling point (BP) were created using the least squares fitting method in the SPSS Statistics programme.

Table 2. Correlation coefficient and standard error of the estimation.

Index	Correlation coefficient (R) with boiling point	Standard error of the estimate
LM_1	0.9656	26.64330
LM_2	0.9267	38.50440
LM_3	0.9788	20.97238

$$BP = 171.6991(\pm 20.4775) + 1.1451(\pm 0.0707)LM_1 \tag{2.1}$$
$$BP = 205.7777(\pm 27.7020) + 0.8136(\pm 0.0756)LM_2 \tag{2.2}$$
$$BP = 124.2412(\pm 18.1101) + 2.0412(\pm 0.0979)LM_3 \tag{2.3}$$

The model (2.3) demonstrates that the experimentally determined boiling point of benzenoid hydrocarbons has a stronger association with the third leap Zagreb index (R=0.9788) than it does with the other leap Zagreb indices.

Hence, the leap Zagreb indices have a strong chemical application. Therefore, in the following sections, we will discuss some new theoretical studies on them.

3. Leap Zagreb indices in terms of first-degree based indices

Lemma 3.1. [11] *Let G be a connected graph with n vertices and m edges. Then*

$$d_2(u/G) \leq \left(\sum_{v \in N_G(u)} d_G(v) \right) - d_G(u).$$

Equality holds if and only if G is a $\{C_3, C_4\}$-free graph.

Theorem 3.2. *For a $\{C_3, C_4\}$-free graph G,*

$$d_2(u/G) = \delta_G(u) - d_G(u). \tag{3.1}$$

Proof. Result follows immediately from Lemma 3.1 and definition of $\delta_G(u)$. □

Lemma 3.3. [10] *For a graph G,*

$$\sum_{u \in V(G)} \delta_G(u) = M_1(G).$$

Lemma 3.4. [14] *For a graph G,*

$$M_2(G) = \frac{1}{2} \sum_{u \in V(G)} d_G(u)\delta_G(u).$$

Lemma 3.5. [14] *For a graph G,*

$$NM_1(G) = \sum_{uv \in E(G)} \left(\delta_G(u)\, d_G(v) + \delta_G(v)\, d_G(u) \right).$$

Now, we express the leap Zagreb indices in terms of the first-degree based indices, instead of second-degree, in the form of following theorems.

Theorem 3.6. *For a $\{C_3, C_4\}$-free graph G,*

$$LM_1(G) = M_1(G) - 4M_2(G) + NM_1(G). \tag{3.2}$$

Proof. Let G be a $\{C_3, C_4\}$-free graph. Then, by definition

$$\begin{aligned}
LM_1(G) &= \sum_{u\in V(G)} d_2(u/G)^2 \\
&= \sum_{u\in V(G)} (\delta_G(u) - d_G(u))^2 \\
&= \sum_{u\in V(G)} \big(\delta_G(u)^2 + d_G(u)^2 - 2\delta_G(u)d_G(u)\big) \\
&= \sum_{u\in V(G)} \delta_G(u)^2 + \sum_{u\in V(G)} d_G(u)^2 - 2\sum_{u\in V(G)} \delta_G(u)d_G(u) \\
&= NM_1(G) + M_1(G) - 2(2M_2(G)) \\
&= M_1(G) - 4M_2(G) + NM_1(G).
\end{aligned}$$

□

Theorem 3.7. *For a $\{C_3, C_4\}$-free graph G,*

$$LM_2(G) = M_2(G) - NM_1(G) + NM_2(G). \tag{3.3}$$

Proof. Let G be a $\{C_3, C_4\}$-free graph. Then, by definition

$$\begin{aligned}
LM_2(G) &= \sum_{uv\in E(G)} d_2(u/G)\, d_2(v/G) \\
&= \sum_{uv\in E(G)} \Big(\delta_G(u) - d_G(u)\Big)\Big(\delta_G(v) - d_G(v)\Big) \\
&= \sum_{uv\in E(G)} \begin{pmatrix}\delta_G(u)\delta_G(v) - (\delta_G(u)d_G(v) + \delta_G(v)d_G(u)) \\ +d_G(u)d_G(v)\end{pmatrix} \\
&= \sum_{uv\in E(G)} \delta_G(u)\delta_G(v) - \sum_{uv\in E(G)} (\delta_G(u)d_G(v) + \delta_G(v)d_G(u)) \\
&\quad + \sum_{uv\in E(G)} d_G(u)d_G(v) \\
&= NM_2(G) - NM_1(G) + M_2(G).
\end{aligned}$$

□

Theorem 3.8. *For a $\{C_3, C_4\}$-free graph G,*

$$LM_3(G) = 2M_2(G) - M_1(G). \tag{3.4}$$

Proof. Let G be a $\{C_3, C_4\}$-free graph. Then, by definition

$$\begin{aligned}
LM_3(G) &= \sum_{u\in V(G)} d_G(u) d_2(u/G) \\
&= \sum_{u\in V(G)} d_G(u)\left(\delta_G(u) - d_G(u)\right) \\
&= \sum_{u\in V(G)} \left(d_G(u)\delta_G(u) - d_G(u)^2\right) \\
&= \sum_{u\in V(G)} d_G(u)\delta_G(u) - \sum_{u\in V(G)} d_G(u)^2 \\
&= 2M_2(G) - M_1(G).
\end{aligned}$$

□

4. Third leap Zagreb index of some derived graphs

The following graphs, which are derived from G, are considered here:

- The *line graph*, denoted by $L = L(G)$, is a graph with $V(L(G)) = E(G)$ and two vertices in $L(G)$ are adjacent if and only if their corresponding edges are adjacent in G.
- The *subdivision graph*, denoted by $S = S(G)$, is obtained by introducing a vertex of degree 2 on every edge of G.
- The *paraline*, denoted by $PL = PL(G)$, is defined as $PL(G) = L(S(G))$.

We need the second degree of an edge in a graph G, as a vertex in $L(G)$ is in association with its corresponding edge in G.

Proposition 4.1. *For any edge $e = uv$ of a $\{C_3, C_4\}$-free graph G,*

$$d_2(e/G) = \delta_G(u) + \delta_G(v) - 2\left(d_G(u) + d_2(v/G)\right) + 2.$$

Proof. Let $e = uv$ be an any edge of $\{C_3, C_4\}$-free graph G. Then,

$$\begin{aligned}
d_2(e/G) &= d_2(uv/G) \\
&= \begin{pmatrix}\text{Number of vertices at distance 2} \\ \text{from } u \text{ not through } v\end{pmatrix} + \begin{pmatrix}\text{Number of vertices at distance 2} \\ \text{from } v \text{ not through } u\end{pmatrix} \\
&= \left(d_2(u/G) - (d_G(v) - 1)\right) + \left(d_2(v/G) - (d_G(u) - 1)\right) \\
&= d_2(u/G) + d_2(v/G) - d_G(u) - d_G(v) + 2.
\end{aligned}$$

From Eqn. (3.1), the above equation becomes

$$\begin{aligned}
d_2(e/G) &= \left(\delta_G(u) - d_G(u)\right) + \left(\delta_G(v) - d_G(v)\right) - d_G(u) - d_G(v) + 2 \\
&= \delta_G(u) + \delta_G(v) - 2\left(d_G(u) + d_2(v/G)\right) + 2.
\end{aligned}$$

□

Theorem 4.2. *For a $\{C_3, C_4\}$-free graph G with n vertices and m edges,*

$$LM_3(L) = 6M_1(G) - 8M_2(G) - 2F(G) + ReZ(G) + NM_1(G) - 4m.$$

Proof. Let G be a $\{C_3, C_4\}$-free graph and $e = uv$ be any edge of G. Then

$$\begin{aligned}
LM_3(L) &= \sum_{e\in V(L)} d_L(e)\, d_2(e/L) \\
&= \sum_{uv\in E(G)} d_G(uv)\, d_2(uv/G) \\
&= \sum_{uv\in E(G)} \begin{array}{c}(d_G(u)+d_G(v)-2) \\ (\delta_G(u)+\delta_G(v)-2\,(d_G(u)+d_2(v/G))+2)\end{array} \\
&= \sum_{uv\in E(G)} \Big((d_G(u)\delta_G(u)+d_G(v)\delta_G(v)) \\
&\qquad +(d_G(u)\delta_G(v)+d_G(v)\delta_G(u)) \\
&\qquad -2(d_G(u)^2+d_G(v)^2)-2(\delta_G(u)+\delta_G(v)) \\
&\qquad -4d_G(u)d_G(v)+6(d_G(u)+d_G(v))-4\Big) \\
&= \sum_{uv\in E(G)} (d_G(u)\delta_G(u)+d_G(v)\delta_G(v)) \\
&\quad + \sum_{uv\in E(G)} (d_G(u)\delta_G(v)+d_G(v)\delta_G(u)) \\
&\quad -2\sum_{uv\in E(G)} (d_G(u)^2+d_G(v)^2) - 2\sum_{uv\in E(G)} (\delta_G(u)+\delta_G(v)) \\
&\quad -4\sum_{uv\in E(G)} d_G(u)d_G(v) \\
&\quad +6\sum_{uv\in E(G)} (d_G(u)+d_G(v)) - \sum_{uv\in E(G)} 4 \\
&= ReZ(G)+NM_1(G)-2F(G)-2(M_2(G))-4M_2(G)+6M_1(G)-4m \\
&= 6M_1(G)-8M_2(G)-2F(G)+ReZ(G)+NM_1(G)-4m.
\end{aligned}$$

□

Theorem 4.3. *For any graph G with n vertices and m edges,*

$$LM_3(S) = 3M_1(G) - 4m.$$

Proof. Let G be any graph. Then the subdivision graph $S = S(G)$ of G is always free from $\{C_3, C_4\}$. For $u \in V(G)$, $d_S(u) = d_G(u)$ and $d_2(u/S) = d_G(u)$. For $e = uv \in E(G)$, $d_S(uv) = 2$ and $d_2(uv/S) = (d_G(u) + d_G(v) - 2)$.

$$\begin{aligned}
LM_3(S) &= \sum_{x\in V(S)} d_S(x)\, d_2(x/S) \\
&= \sum_{x\in V(G)\cup E(G)} d_S(x)\, d_2(x/S) \\
&= \sum_{u\in V(G)} d_S(u)\, d_2(u/S) + \sum_{e\in E(G)} d_S(e)\, d_2(e/S)
\end{aligned}$$

$$
\begin{aligned}
LM_3(S) &= \sum_{u\in V(G)} d_G(u)d_G(u) + \sum_{uv\in E(G)} 2\left(d_G(u)+d_G(v)-2\right)\\
&= \sum_{u\in V(G)} d_G(u)^2 + 2\left(\sum_{uv\in E(G)} \left(d_G(u)+d_G(v)\right) - \sum_{uv\in E(G)} 2\right)\\
&= M_1(G) + 2\left(M_1(G)-2m\right)\\
&= 3M_1(G) - 4m.
\end{aligned}
$$

□

Lemma 4.4. [6] *Let S be the subdivision graph of the graph G. Then*

$$M_1(S) = M_1(G) + 4m.$$

Lemma 4.5. [2] *Let S be the subdivision graph of the graph G. Then*

$$M_2(S) = 2M_1(G).$$

Lemma 4.6. [3] *Let S be the subdivision graph of the graph G. Then*

$$F(S) = F(G) + 8m.$$

Lemma 4.7. [1] *Let S be the subdivision graph of the graph G. Then*

$$NM_1(S) = 4M_1(G) + 2M_2(G) + F(G).$$

Proposition 4.8. *Let S be the subdivision graph of the graph G. Then*

$$ReZ(S) = 2F(G) + 4M_1(G).$$

Proof.

$$
\begin{aligned}
ReZ(S) &= \sum_{xy\in E(S)} \big(d_S(x)+d_S(y)\big) d_S(x)\, d_S(y)\\
&= \sum_{uv\in E(G)} \big(\left(d_G(u)+2\right) d_G(u)2 + \left(2+d_G(v)\right) 2d_G(v)\big)\\
&= \sum_{uv\in E(G)} \left(2\left(d_G(u)^2+d_G(v)^2\right) + 4\left(d_G(u)+d_G(v)\right)\right)\\
&= 2\sum_{uv\in E(G)} \left(d_G(u)^2+d_G(v)^2\right) + 4\sum_{uv\in E(G)} \left(d_G(u)+d_G(v)\right)\\
&= 2F(G) + 4M_1(G).
\end{aligned}
$$

□

Theorem 4.9. *For any graph G with n vertices and m edges,*

$$LM_3(PL) = 2M_2(G) - 2M_1(G) + F(G).$$

Proof. Clearly, $PL(G) = L(S(G))$. Also, for any graph G, the subdivision graph $S = S(G)$ of G is always free from $\{C_3, C_4\}$. Therfore, applying Theorem 4.2 on

$S(G)$, we have

$$\begin{aligned} LM_3(PL) &= LM_3(L(S)) \\ &= 6M_1(S) - 8M_2(S) - 2F(S) + ReZ(S) + NM_1(S) - 4m_s \\ &= 6(M_1(G) + 4m) - 8(2M_1(G)) - 2(F(G) + 8m) + (2F(G) + 4M_1(G)) \\ &\quad + (4M_1(G) + F(G) + 2M_2(G)) - 4(2m) \\ &= 2M_2(G) - 2M_1(G) + F(G). \end{aligned}$$

□

5. Conclusions

In this paper, the chemical importance of the leap Zagreb indices is investigated, and it is shown that the third leap Zagreb index is useful in predicting the boiling point of benzenoid hydrocarbons with high accuracy (with the coefficient of correlation R=0.9788). We expressed the leap Zagreb indices in terms of first-degree based indices, instead of second-degree. Using all these, we obtained explicit formulae for the third leap Zagreb index of some derived graphs.

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References

1. B. Basavanagoud and A. P. Barangi, First neighbourhood Zagreb index of derived graphs and F-sums of graphs, *Bull. Int. Math. Virtual Inst.* **10** (2020), 325–337.
2. B. Basavanagoud, I. Gutman, and C. S. Gali, On second Zagreb index and coindex of some derived graphs, *Kragujevac J. Sci.* **37** (2015), 113–121.
3. N. De, F-index and coindex of some derived graphs, *Bull. Int. Math. Virtual Inst.* **8** (2018), 81–88.
4. T. Došlić, Vertex–weighted Wiener polynomials for composite graphs, *Ars Math. Contemp.* **1** (2008), 66–80.
5. B. Furtula and I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015), 1184–1190.
6. I. Gutman, B. Furtula, Z. K. Vukićević, and G. Popivoda, On Zagreb indices and coindices, *MATCH Commun. Math. Comput. Chem.* **74** (2015), 5–16.
7. I. Gutman, B. Ruščič, N. Trinajstić, and C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62**(9) (1975), 3399–3405.
8. I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17**(4) (1972), 535–538.
9. D. Maji and G. Ghorai, A novel graph invariant: The third leap Zagreb index under several graph operations, *Discrete Math. Algorithms Appl.* **11** (2019), #1950054.
10. S. Mondal, N. De, and A. Pal, On neighbourhood Zagreb index of product graphs, *J. Mol. Struct.* **1223** (2021), #129210.
11. A. M. Naji, N. D. Soner, and I. Gutman, On leap Zagreb indices of graphs, *Commun. Comb. Optim.* **2**(2) (2017), 99–117.
12. A. M. Naji and N. D. Soner, The first leap Zagreb index of some graph operations, *Int. J. Appl. Graph Theory* **2** (2018), 07–18.

13. S. Nikolić, A. Miličević, N. Trinajstić, and A. Jurić, On use of the variable Zagreb ${}^{v}M_2$ index in QSPR: boiling points of benzenoid hydrocarbons, *Molecules* **9** (2004), 1208–1221.
14. H. S. Ramane, K. S. Pise, R. B. Jummannaver, and D. D. Patil, On neighbourhood Zagreb indices and coindices of graphs, (pre-print).
15. H. S. Ramane, K. S. Pise, R. B. Jummannaver, and D. D. Patil, Application of neighbor degree sum of a vertex on Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **85** (2021), 329–348.
16. P. S. Ranjini, V. Lokesha, and A. Usha, Relation between phenylene and hexagonal squeeze using harmonic index, *Int. J. Graph Theory* **1** (2013), 116–121.
17. J. Zhu, N. Dehgardi, and X. Li, The third leap Zagreb index for trees, *J. Chem.* **2019** (2019), #9296401.

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