International Journal of Applied Mathematics

Volume 32 No. 6 2019, 1037-1049

ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

doi: http://dx.doi.org/10.12732/ijam.v32i6.10

ON SOME GENERAL NEIGHBORHOOD DEGREE BASED TOPOLOGICAL INDICES

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Abstract: Newly developing territories of mathematical chemistry is computational technique to get accurate analytical expressions for various topological indices of different networks. Among different topological indices, neighborhood degree based indices have significant predictive ability of physico-chemical properties. In this work, we generalize the neighborhood degree based topological indices and obtain their exact expressions for the benzene ring embedded in P-type-surface in 2D network.

AMS Subject Classification: 05C35, 05C07, 05C40

Key Words: topological index, degree, benzene ring embedded in P-type-surface in 2D network

1. Introduction

Graph theory provides an important tool called topological index [1] to correlate the physico-chemical properties of chemical compounds with their molecular structure. Topological index is a mapping from the collection of all molecular graphs (simple connected graphs) to the set of real numbers that characterizes

Received: June 17, 2019

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the topology of the molecular graph and remains unchanged for isomorphic graphs. It is widely used in various field of chemistry and nanotechnology in isomer discrimination, QSPR/QSAR analysis and pharmaceutical drug design etc. Utilization of such indices in chemistry and biology started in 1947 when chemist Harold Wiener [2] introduced 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 [3], where they investigated the dependence of total π-electron energy on molecular structure. Throughout this article, we consider simple connected graph. Let $V(G)$ and $E(G)$ denote the vertex set and edge set of a graph G respectively. By $deg_G(u)$, we mean degree of vertex $u \in V(G)$.

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

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

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

For detail discussion see [4, 5]. Recently some researchers put their attention on the degree of neighborhood vertices. Two nodes $u, v \in V(G)$ are neighbors if $uv \in E(G)$. Here $\delta_G(v)$ represents the sum of degrees of all neighborhood nodes of v in G. Based on the neighborhood degree, many topological descriptors have been developed which are discussed below.

The neighborhood Zagreb index [6] of a graph G is defined as

$$M_N(G) = \sum_{u \in V(G)} [\delta_G(u)]^2.$$

In [7], some novel topological indices have been introduced. They are named as neighborhood version of forgotten topological index (F_N), modified neighborhood version of Forgotten topological index (F_N^*), and neighborhood version of second Zagreb index (M_2^*), which are defined as follows:

$$F_N(G) = \sum_{u \in V(G)} [\delta_G(u)]^3, \qquad F_N^*(G) = \sum_{uv \in E(G)} [\delta_G(u)^2 + \delta_G(v)^2],$$

$$M_2^*(G) = \sum_{uv \in E(G)} [\delta_G(u)\delta_G(v)].$$

In [8] some new indices have been presented, named as first NDe index (ND_1), second NDe index (ND_2), third NDe index (ND_3), fourth NDe index (ND_4), and fifth NDe index (ND_5) and defined as:

$$ND_1(G) = \sum_{uv\in E(G)} \sqrt{\delta_G(u)\delta_G(v)},$$

$$ND_2(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{\delta_G(u)+\delta_G(v)}},$$

$$ND_3(G) = \sum_{uv\in E(G)} \delta_G(u)\delta_G(v)[\delta_G(u)+\delta_G(v)],$$

$$ND_4(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{\delta_G(u)\delta_G(v)}},$$

$$ND_5(G) = \sum_{uv\in E(G)} [\frac{\delta_G(u)}{\delta_G(v)} + \frac{\delta_G(v)}{\delta_G(u)}].$$

Kulli [9] introduced some new indices, known as modified first neighborhood index (${}^mNM_1$), neighborhood inverse degree index (NID), neighborhood zeroth order index (NZ), and defined as

$${}^mNM_1(G) = \sum_{u\in V(G)} \frac{1}{\delta_G(u)^2}, \qquad NID(G) = \sum_{u\in V(G)} \frac{1}{\delta_G(u)},$$

$$NZ(G) = \sum_{u\in V(G)} \frac{1}{\sqrt{\delta_G(u)}}.$$

In addition, Kulli [10] presented some novel multiplicative neighborhood degree based topological indices which are described below.
The fifth multiplicative M_1 and M_2 Zagreb indices are defined as

$$M_1G_5\Pi(G) = \prod_{uv\in E(G)} [\delta_G(u)+\delta_G(v)],$$

$$M_2G_5\Pi(G) = \prod_{uv\in E(G)} [\delta_G(u)\delta_G(v)].$$

The multiplicative total neighborhood index ($T_n\Pi$), the multiplicative first neighborhood index ($NM_1\Pi$), and the multiplicative F_1-neighborhood index ($F_1N\Pi$) are defined as

$$T_n\Pi(G) = \prod_{u\in V(G)} \delta_G(u), \qquad NM_1\Pi(G) = \prod_{u\in V(G)} \delta_G(u)^2,$$

$$F_1N\Pi(G) = \prod_{u\in V(G)} \delta_G(u)^3.$$

In this work, we put some effort to generalize the neighborhood degree based topological indices described below. We consider here three parameters α, β, and γ, which are all belong to the set of real numbers. The neighborhood general Zagreb index of a graph G is given by

$$NM_\alpha(G) = \sum_{u\in V(G)} [\delta_G(u)]^\alpha.$$

The neighborhood general Randić index of a graph G is given by

$$NR_\alpha(G) = \sum_{uv\in E(G)} [\delta_G(u)\delta_G(v)]^\alpha.$$

The neighborhood general sum connectivity index of a graph G is given by

$$N\chi_\alpha(G) = \sum_{uv\in E(G)} [\delta_G(u) + \delta_G(v)]^\alpha.$$

The (β, γ)-Zagreb index of a graph G is given by

$$Z_{(\beta,\gamma)}(G) = \sum_{uv\in E(G)} [\delta_G(u)^\beta\delta_G(v)^\gamma + \delta_G(u)^\gamma\delta_G(v)^\beta].$$

The multiplicative neighborhood general Zagreb index of a graph G is given by

$$PNM_\alpha(G) = \prod_{u\in V(G)} [\delta_G(u)]^\alpha.$$

The multiplicative neighborhood general Randić index of a graph G is given by

$$PNR_\alpha(G) = \prod_{uv\in E(G)} [\delta_G(u)\delta_G(v)]^\alpha.$$

The multiplicative neighborhood general sum connectivity index of a graph G is given by

$$PN\chi_\alpha(G) = \prod_{uv\in E(G)} [\delta_G(u) + \delta_G(v)]^\alpha.$$

The multiplicative (β, γ)-Zagreb index of a graph G is given by

$$PZ_{(\beta,\gamma)}(G) = \prod_{uv\in E(G)} [\delta_G(u)^\beta \delta_G(v)^\gamma + \delta_G(u)^\gamma \delta_G(v)^\beta].$$

Different neighborhood degree based indices can be obtained (Table 1) from the novel general indices by assigning particular values to α, β, and γ.

TI	**CGTI**	**TI**	**CGTI**	**TI**	**CGTI**
$M_1(G)$	$NM_1(G)$	$NID(G)$	$NM_{-1}(G)$	$ND_5(G)$	$Z_{(1,-1)}(G)$
$M_N(G)$	$NM_2(G)$	$NZ(G)$	$NM_{-\frac{1}{2}}(G)$	$T_n\Pi(G)$	$PNM_1(G)$
$M_2^*(G)$	$NR_1(G)$	$ND_1(G)$	$NR_{\frac{1}{2}}(G)$	$NM_1\Pi(G)$	$PNM_2(G)$
$F_N(G)$	$NM_3(G)$	$ND_2(G)$	$N\chi_{-\frac{1}{2}}(G)$	$F_1N\Pi(G)$	$PNM_3(G)$
$F_N^*(G)$	$Z_{(2,0)}(G)$	$ND_3(G)$	$Z_{(2,1)}(G)$	$M_1G_5\Pi(G)$	$PN\chi_1(G)$
${}^mNM_1(G)$	$NM_{-2}(G)$	$ND_4(G)$	$NR_{-\frac{1}{2}}(G)$	$M_2G_5\Pi(G)$	$PNR_1(G)$

Table 1: The relation between the neighborhood degree based indices and the newly introduced general indices. Here TI and CGTI represent topological index and corresponding general topological index, respectively.

Ahmed [11] obtained the degree based topological indices of benzene ring embedded in P-type-surface network. Liu et al. [12] studied the topological properties of Boron nanotubes. For more discussions related to such work, readers are referred to [13, 14]. Inspired by these works, we study here the topological properties of the benzene ring embedded in P-type-surface network in terms of the neighborhood degree based indices.

2. Main result

About a quarter of a century ÓKeeffe et al. [15] distributed a letter managing two 3D systems of benzene one of the structure (figure 1) called 6.82P (additionally polybenzene) and has a space gathering place Im3m, compared to the

P-type surface. This actually inserts the hexagon-fix into the negative ebb and flow P surface. The P-type surface in the Euclidean space is coordinated with the Cartesian arrangements. The peruser can find out more about this intermittent surface in [16, 17]. This structure had to be combined as 3D carbon solids. This goal was to awaken researchers' enthusiasm for the atomic recognition in carbon nanoscience of such pleasant thoughts. The graph of the benzene ring embedded in P-type-surface in 2D network, shown in Figure 1, contains $24mn$ nodes and $32mn-2m-2n$ edges. The vertex and edge partitions of this graph are shown in Table 2 and Table 3, respectively.

For vertex and edge partitions, we consider $V_i = \{u \in V(G) : \delta_G(u) = i\}$, $E_{(i,j)} = \{uv \in E(G) : \delta_G(u) = i, \delta_G(v) = j\}$, n_i = the number of nodes in V_i, and $m_{(i,j)}$ = the number of edges in $E_{(i,j)}$.

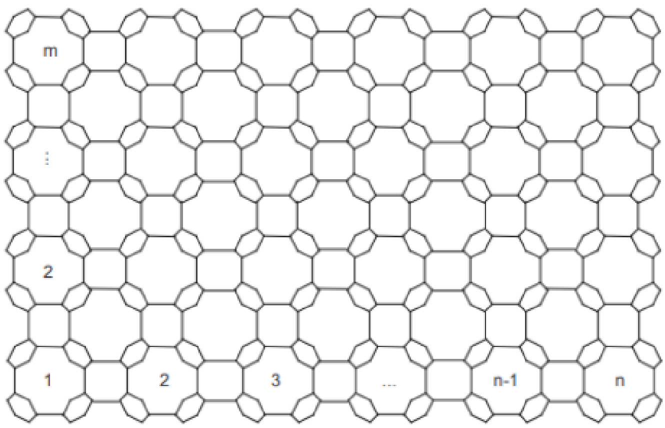

Figure 1: Benzene ring embedded in the P-type-surface network.

Theorem 1. *Let G be the benzene ring embedded in the P-type-surface network. Then we have*

(i) $NM_\alpha(G) = 4^{\alpha+1} + 8(m+n-1)5^\alpha + 4(2mn-m-n+1)6^\alpha + 4(m+n)7^\alpha + (2mn-m-n)8^{\alpha+1}$,

(ii) $NR_\alpha(G) = 8(20^\alpha) + 4(m+n-2)25^\alpha + 4(m+n)35^\alpha + 4(m+n-2)40^\alpha + 4(m+n)42^\alpha + 4(4mn-3m-3n+2)48^\alpha + 2(m+n)49^\alpha + 8(2mn-m-n)64^\alpha$,

V_i	n_i
V_4	4
V_5	8(m+n-1)
V_6	8mn-4m-4n+4
V_7	4m+4n
V_8	16mn-8m-8n

Table 2: The vertex partition of the benzene ring embedded in P-type-surface network based on degree sum of neighborhood nodes.

$E_{(i,j)}$	$m_{(i,j)}$
$E_{(4,5)}$	8
$E_{(5,5)}$	4m+4n-8
$E_{(5,7)}$	4m+4n
$E_{(5,8)}$	4m+4n-8
$E_{(6,7)}$	4m+4n
$E_{(6,8)}$	16mn-12m-12n+8
$E_{(7,7)}$	2m+2n
$E_{(8,8)}$	16mn-8m-8n

Table 3: The edge partition of the benzene ring embedded in P-type-surface network based on degree sum of neighborhood nodes.

(iii) $N\chi_\alpha(G) = 8(9^\alpha) + 4(m+n-2)10^\alpha + 4(m+n)12^\alpha + 8(m+n-1)13^\alpha + 2(8mn-5m-5n+4)14^\alpha + 8(2mn-m-n)16^\alpha$,

(iv) $Z_{(\beta,\gamma)}(G) = 8(4^\beta 5^\gamma + 4^\gamma 5^\beta) + 8(m+n-2)5^{\beta+\gamma} + 4(m+n)(5^\beta 7^\gamma + 5^\gamma 7^\beta) + 4(m+n-2)(5^\beta 8^\gamma + 5^\gamma 8^\beta) + 4(m+n)(6^\beta 7^\gamma + 6^\gamma 7^\beta) + 4(4mn-3m-3n+2)(6^\beta 8^\gamma + 6^\gamma 8^\beta) + 4(m+n)7^{\beta+\gamma} + 16(2mn-m-n)8^{\beta+\gamma}$,

where α, β, γ are real numbers.

Proof. The formula of neighborhood general Zagreb index is given by

$$NM_\alpha(G) = \sum_{u\in V(G)} [\delta_G(u)]^\alpha.$$

Now using the vertex partition, we obtain

$$NM_\alpha(G) = \sum_{u\in V_4} [\delta_G(u)]^\alpha + \sum_{u\in V_5} [\delta_G(u)]^\alpha + \sum_{u\in V_6} [\delta_G(u)]^\alpha$$

$$+\sum_{u\in V_7}[\delta_G(u)]^\alpha+\sum_{u\in V_8}[\delta_G(u)]^\alpha$$
$$=n_4(4)^\alpha+n_5(5)^\alpha+n_6(6)^\alpha+n_7(7)^\alpha+n_8(8)^\alpha$$
$$=4^{\alpha+1}+8(m+n-1)5^\alpha+4(2mn-m-n$$
$$+1)6^\alpha+4(m+n)7^\alpha+(2mn-m-n)8^{\alpha+1}.$$

The neighborhood general Randić index is defined as

$$NR_\alpha(G)=\sum_{uv\in E(G)}[\delta_G(u)\delta_G(v)]^\alpha.$$

Using the edge partition, we get

$$\begin{aligned}NR_\alpha(G) &= \sum_{uv\in E_{(4,5)}}[\delta_G(u)\delta_G(v)]^\alpha+\sum_{uv\in E_{(5,5)}}[\delta_G(u)\delta_G(v)]^\alpha\\ &\quad+\sum_{uv\in E_{(5,7)}}[\delta_G(u)\delta_G(v)]^\alpha+\sum_{uv\in E_{(5,8)}}[\delta_G(u)\delta_G(v)]^\alpha\\ &\quad+\sum_{uv\in E_{(6,7)}}[\delta_G(u)\delta_G(v)]^\alpha+\sum_{uv\in E_{(6,8)}}[\delta_G(u)\delta_G(v)]^\alpha\\ &\quad+\sum_{uv\in E_{(7,7)}}[\delta_G(u)\delta_G(v)]^\alpha+\sum_{uv\in E_{88}}[\delta_G(u)\delta_G(v)]^\alpha\end{aligned}$$

$$\begin{aligned}&= m_{(4,5)}(20)^\alpha+m_{(5,5)}(25)^\alpha+m_{(5,7)}(35)^\alpha+m_{(5,8)}\\ &\quad(40)^\alpha+m_{(6,7)}(42)^\alpha+m_{6,8)}(48)^\alpha+m_{(7,7)}(49)^\alpha\\ &\quad+m_{(8,8)}(64)^\alpha\\ &= 8(20^\alpha)+4(m+n-2)25^\alpha+4(m+n)35^\alpha+4(m\\ &\quad+n-2)40^\alpha+4(m+n)42^\alpha+4(4mn-3m-3n+\\ &\quad 2)48^\alpha+2(m+n)49^\alpha+8(2mn-m-n)64^\alpha.\end{aligned}$$

The neighborhood general sum connectivity index is formulated as

$$N\chi_\alpha(G)=\sum_{uv\in E(G)}[\delta_G(u)+\delta_G(v)]^\alpha.$$

Now applying the edge partition, we obtain

$$\begin{aligned}N\chi_\alpha(G) &= m_{(4,5)}(9)^\alpha+m_{(5,5)}(10)^\alpha+m_{(5,7)}(12)^\alpha+m_{(5,8)}(13)^\alpha+\\ &\quad m_{(6,7)}(13)^\alpha+m_{(6,8)}(14)^\alpha+m_{(7,7)}(14)^\alpha+m_{(8,8)}(16)^\alpha.\end{aligned}$$

Now putting the values of m_{ij}'s, we can easily obtain the required result after some simple calculation.
Similarly, applying the edge partition on the definition of (β,γ)-Zagreb index, the required result can be obtained easily. □

Now using Table 1, we obtain the following corollary.

Corollary 1. *Different neighborhood degree based topological indices for the benzene ring embedded in the P-type-surface network are given by*

(i) $M_1(G) = 176mn - 20m - 20n,$

(ii) $M_N(G) = 1312mn - 260m - 260n + 8,$

(iii) $M_2^*(G) = 1792mn - 422m - 422n + 24,$

(iv) $F_N(G) = 9920mn - 2588m - 2588m + 120,$

(v) $F_N^*(G) = 3648mn - 836m - 836n + 16,$

(vi) ${}^{m}NM_1(G) = 0.472mn + 0.166m + 0.166n + 0.041,$

(vii) $NID(G) = 3.333mn + 0.505m + 0.505n + 0.067,$

(viii) $NZ(G) = 8.923mn + 0.628m + 0.628n + 0.055,$

(ix) $ND_1(G) = 155.713mn - 38.253m - 38.253n + 0.076,$

(x) $ND_2(G) = 8.276mn - 0.034m - 0.034n + 0.056,$

(xi) $ND_3(G) = 27136mn + 252m + 252n - 784,$

(xii) $ND_4(G) = 8.928mn - 3.185m - 3.185n + 2.388,$

(xiii) $ND_5(G) = 65.333mn - 3.548m - 3.548n - 0.733.$

Theorem 2. *Let G be the benzene ring embedded in the P-type-surface network. Then we have*

(i) $PNM_\alpha(G) = 2^{4(14mn-7m-7n+3)\alpha}3^{4(2mn-m-n+1)\alpha}5^{8(m+n-1)\alpha}$
$7^{4(m+n)\alpha},$

(ii) $PNR_\alpha(G) = 2^{8(20mn-10m-10n+3)\alpha}3^{8(2mn-m-n+1)\alpha}5^{16(m+n-1)\alpha}$
$7^{12(m+n)\alpha},$

(iii) $PN\chi_\alpha(G) = 2^{10(8mn-3m-3n)\alpha}3^{4(m+n+4)\alpha}5^{4(m+n-2)\alpha}$
$7^{2(8mn-5m-5n+4)\alpha}13^{8(m+n-1)\alpha}$,

(iv) $PZ_{(\beta,\gamma)}(G) = 2^{[\{48(\beta+\gamma)+16\}mn-\{24(\beta+\gamma)+2\}m-\{24(\beta+\gamma)+2\}n]}$
$5^{4(\beta+\gamma)(m+n-2)}7^{2(\beta+\gamma)(m+n)}(4^\beta 5^\gamma + 4^\gamma 5^\beta)^8(5^\beta 7^\gamma +$
$5^\gamma 7^\beta)^{4(m+n)}(5^\beta 8^\gamma + 5^\gamma 8^\beta)^{4(m+n-2)}(6^\beta 7^\gamma + 6^\gamma 7^\beta)^{4(m+n)}$
$(6^\beta 8^\gamma + 6^\gamma 8^\beta)^{4(4mn-3m-3n+2)}$,

where α, β, γ are real numbers.

Proof. Applying vertex partition on the definition of multiplicative neighborhood general Zagreb index, we obtain

$$\begin{aligned}
PNM_\alpha(G) &= \prod_{u\in V_4}[\delta_G(u)]^\alpha \times \prod_{u\in V_5}[\delta_G(u)]^\alpha \times \prod_{u\in V_6}[\delta_G(u)]^\alpha \\
&\quad \times \prod_{u\in V_7}[\delta_G(u)]^\alpha \times \prod_{u\in V_8}[\delta_G(u)]^\alpha \\
&= (4)^{n_4\alpha} \times (5)^{n_5\alpha} \times (6)^{n_6\alpha} \times (7)^{n_7\alpha} \times (8)^{n_8\alpha} \\
&= (4)^{4\alpha} \times (5)^{8(m+n-1)\alpha} \times (6)^{4(2mn-m-n+1)\alpha} \\
&\quad \times (7)^{4(m+n)\alpha} \times (8)^{8(2mn-m-n)\alpha}.
\end{aligned}$$

After simplification, we can obtain the required result.
Using the edge partition on the formula of multiplicative neighborhood general Randić index, we get

$$\begin{aligned}
PNR_\alpha(G) &= \prod_{uv\in E_{(4,5)}}[\delta_G(u)\delta_G(v)]^\alpha \times \prod_{uv\in E_{(5,5)}}[\delta_G(u)\delta_G(v)]^\alpha \\
&\quad \times \prod_{uv\in E_{(5,7)}}[\delta_G(u)\delta_G(v)]^\alpha \times \prod_{uv\in E_{(5,8)}}[\delta_G(u)\delta_G(v)]^\alpha \\
&\quad \times \prod_{uv\in E_{(6,7)}}[\delta_G(u)\delta_G(v)]^\alpha \times \prod_{uv\in E_{(6,8)}}[\delta_G(u)\delta_G(v)]^\alpha \\
&\quad \times \prod_{uv\in E_{(7,7)}}[\delta_G(u)\delta_G(v)]^\alpha \times \prod_{uv\in E_{(8,8)}}[\delta_G(u)\delta_G(v)]^\alpha \\
&= (20)^{m_{(4,5)}\alpha} \times (25)^{m_{(5,5)}\alpha} \times (35)^{m_{(5,7)}\alpha} \times (40)^{m_{(5,8)}\alpha} \\
&\quad \times (42)^{m_{6,7)}\alpha} \times (48)^{m_{(6,8)}\alpha} \times (49)^{m_{(7,7)}\alpha} \times (64)^{m_{(8,8)}\alpha}.
\end{aligned}$$

Putting the values of m_{ij}'s, we can easily obtain the required result after simplification.

Applying the edge partition on the formulation of multiplicative neighborhood general sum connectivity index, we obtain

$$\begin{aligned} PN\chi_\alpha(G) &= (9)^{m_{(4,5)}\alpha} \times (10)^{m_{(5,5)}\alpha} \times (12)^{m_{(5,7)}\alpha} \times (13)^{m_{(5,8)}\alpha} \\ &\quad \times (13)^{m_{(6,7)}\alpha} \times (14)^{m_{(6,8)}\alpha} \times (14)^{m_{(7,7)}\alpha} (16)^{m_{(8,8)}\alpha}. \end{aligned}$$

Now putting the values of m_{ij}'s, we can easily obtain the required result after some simple calculation.

Similarly, applying the edge partition on the definition of (β, γ)-Zagreb index, the required result can be obtained easily. □

Now using Table 1, we obtain the following corollary.

Corollary 2. *Different neighborhood degree based topological indices for the benzene ring embedded in the P-type-surface network are given by*

(i) $T_n\Pi(G) = 2^{4(14mn-7m-7n+3)} 3^{4(2mn-m-n+1)} 5^{8(m+n-1)} 7^{4(m+n)}$,

(ii) $NM_1\Pi(G) = 2^{8(14mn-7m-7n+3)} 3^{8(2mn-m-n+1)} 5^{16(m+n-1)} 7^{8(m+n)}$,

(iii) $F_1N\Pi(G) = 2^{12(14mn-7m-7n+3)} 3^{12(2mn-m-n+1)} 5^{24(m+n-1)} 7^{12(m+n)}$,

(iv) $M_1G_5\Pi(G) = 2^{10(8mn-3m-3n)} 3^{4(m+n+4)} 5^{4(m+n-2)} 7^{2(8mn-5m-5n+4)} 13^{8(m+n-1)}$,

(v) $M_2G_5\Pi(G) = 2^{8(20mn-10m-10n+3)} 3^{8(2mn-m-n+1)} 5^{16(m+n-1)} 7^{12(m+n)}$.

3. Conclusion

In this work, we have introduced some general neighborhood degree based topological indices. We have found those indices for the benzene ring embedded in P-type-surface in 2D network. Also we have obtained different neighborhood degree based topological indices by considering some values of the parameters on the general formula. This work will help researchers working on network science to understand the topology of the aforesaid network. In future, we would like to compute these indices for some other networks, trees, dendrimers etc.

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