On Topological Indices of Dual Graph of Benzene Ring Embedded in P-Type Surface in 2D Network

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ABSTRACT

The structure of any finite molecular graph which represent numerical quantities are known as topological indices. The importance of topological indices is generally linked with QSAR/QSPR. In this paper, we compute general Zagreb $(M_{\alpha-})$ index, general Randic connectivity $(R_{\alpha-})$ index, general sum-connectivity (χ_{α}) index, atom-bond connectivity (ABC) index, and geometric-arithmetic (GA) index, ABC_4, GA_5, multiple Zagreb indices and Zagreb polynomial indices of the of dual graph of benzene ring embedded in P-type-surface in 2D network.

Key words: Topological Indices, Multiple Zagreb Indices, Zagreb Polynomials, Benzene Ring.

1 INTRODUCTION AND DEFINITIONS

In this paper all graphs are finite, simple and undirected. Let V(G) and E(G) be the vertex set and edge set of a graph. We follow the basic notation and terminologies of graph theory as in [1]. The vertices u, v ϵ V (G) are adjacent (or neighbors) if u and v are end points of e ϵ E(G) and is incident with the vertices of u and v and e is said to be connect u and v. The set of all neighbors of a vertex u of G denoted by N (u), is called the neighborhood of v. The degree of a vertex is an undirected simple graph is the number of edges incident with it. The degree of the vertex u is denoted by d_u and S_u is the sum of degrees of all vertices adjacent to the vertex u. In other words

$$S_u = \sum_{v \epsilon N(u)} d_v,$$

Where $N(u) = \{v \epsilon V(G) : uv \, \epsilon E(G)\}$

The application of molecular structure descriptors in nowadays a standard procedure in the study of structure-property relations, especially in QSPR/QSAR study. In the latest couple of years, the amount of proposed nuclear descriptors is rapidly getting to be a result of the creation significance of these descriptors. They interface the particular physico-substance properties of mixture blends. A most seasoned, most considered and most prominent topological record among all degree based topological lists is Randic index, which was presented by Randic in 1975 [2]). This record was discovered reasonable with the end goal of medication plan [2], [3]. The numerical elements of Randic index incorporates its association with the standardized Laplacian framework [4], [5],[6],[9]. The formal definition of Randic index of a graph G is given as follows:

$$R(G) = \sum_{uv \epsilon E(G)} \frac{1}{\sqrt{d_u d_v}}$$

Soon after the discovery of Randic index was introduced a general Randic index. It is denoted by R_(G) and its formula is given as

$$R_\alpha(G) = \sum_{uv \epsilon E(G)} (d_u d_v)^\alpha$$

where α is a non zero real number. Zhou et al. [7] introduced the general sum connectivity index χ_α(G) and defined as

$$\chi_\alpha(G) = \sum_{uv \epsilon E(G)} (d_u + d_v)^\alpha$$

where α is a real number. Shirdel et al. introduced a new degree based Zegreb index named as " hyper-Zegreb index " which is defined in [8], which is also known as general sum-connectivity index χ_2(G). The first general Zagreb index studies in [9].

$$M_\alpha(G) = \sum_{uv \epsilon E(G)} (d_u)^\alpha$$

Estrada et al. invented atom-bond connectivity index which is abbreviated as ABC index [10]. ABC index is much importance due to its correlation with the thermodynamic properties of alkanes, see [11], [12]. The definition for ABC index is as follows

$$ABC(G) = \sum_{uv \epsilon E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

The fourth version of ABC index was introduced by Ghorbani and Hosseinzadeh [13] and defined as

$$ABC_4(G) = \sum_{uv \epsilon E(G)} \sqrt{\frac{S + S_v - 2}{S_u S_v}}$$

Recently the fifth version of GA is introduced by Graovac et al. [15] and defined as:

$$GA_5(G) = \sum_{uv \epsilon E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}$$

In [16], Ghorbani and Azimi defined first multiple Zagreb index P $M_1(G)$ and second multiple Zagreb index PM_2 defined as:

$$PM_1(G) = \prod_{uv \epsilon E(G)} (d_u + d_v),$$

$$PM_2(G) = \prod_{uv \epsilon E(G)} (d_u d_v)$$

These multiple Zagreb indices are studied for some chemical structures in [17], [18],[19],[20],[21] first Zagreb polynomial $M_1(G; x)$ and second Zagreb polynomial $M_2(G; x)$ are defined as:

$$M_1(G, x) = \prod_{uv \epsilon E(G)} x(d_u + d_v),$$

$$M_2(G, x) = \prod_{uv \epsilon E(G)} x(d_u d_v)$$

The interested readers to be focused on the recent collection of topological indices [21], [22], [23],[24],[25],[26], [27].

2 RESULTS AND DISCUSSION

Keeffe et al. [28] have distributed around a quarter century a letter managing two 3D systemsof benzene one of the structure (Figure 1) was called 6.82P (additionally polybenzene) and has a place with the space gather Im3m, comparing to the P-type surface. Actually this is inserting of the hexagon fix in the surface of negative ebb and flow P. The P-type surface is coordinated to the Cartesian arranges in the Euclidean space. More about this intermittent surface the peruser can discover in [29],[30]. This structure was required to be combined as 3D carbon solids: be that as it may, in our best learning, no such a combination was accounted for as such. This goal was to awaken the enthusiasm of researchers to the atomic acknowledgment of such pleasant thoughts in carbon nanoscience, as much as the graphenes were picked up a moment Nobel prize after C60, also the immediate union of fullerenes is currently a reality see detail in [31].

The graph G of benzene ring embedded in the P-type-surface network is shown in Figure 1
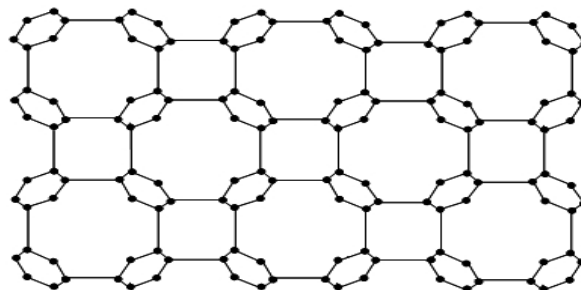
Figure 1: Benzene ring embedded in P-type surface in 2D-network

A graph G' is called dual of a plane graph G if the set of all faces of the graph G forms the vertex set of G'. It is represented by $D_u(G)$. If an edge e is shared by faces f and g in planar graph G then e' joined respective vertices f' and g' in $D_u(G)$. Bounded dual is constructed if we delete the vertex which represents the unbounded face. It is not necessary that bounded dual of a simple plane graph is simple. If the bounded of simple plane graph is not simple then we remove the multiple edges in $Bd_u(G)$ to make it simple graph. We will denote the simple bounded dual of plane graph G by $Sbd_u(G)$. The simple bounded dual of benzene ring embedded in P-type surface is shown in figure 2 and in more discrete form shown in figure 3
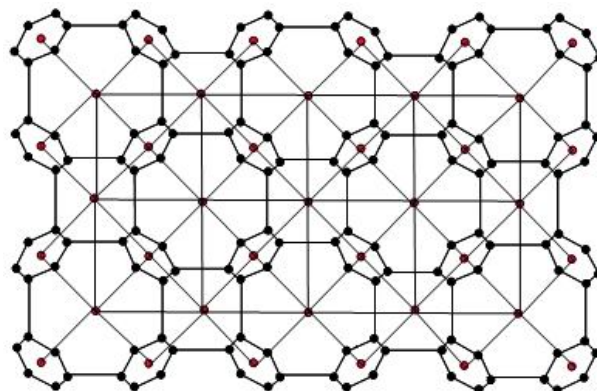
Figure 2: Construction of simple bounded dual of benzene ring embedded in P-type surface in 2D-network The number of total vertices in simple bounded dual of benzene ring embedded in P-type
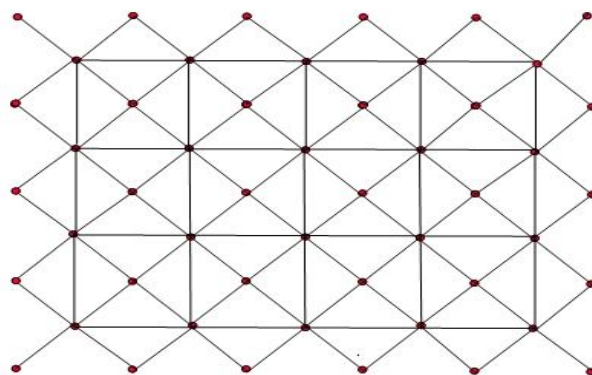
Figure 3: Simple bounded dual of benzene ring embedded in P-type surface in 2D-network

surface in 2D are $8mn - 2m - 2n + 1$, where m is number of columns and n number of rows of benzene ring embedded in P-type surface in 2D. Vertices of different degrees are presented in Table 1.

Let $\delta(G)$ and $\Delta(G)$ be the minimum and maximum degree of G, respectively. The edge set E(G) can be divided into several partitions: for any i and j , $\delta(G) \leq i, j \leq \Delta(G)$, let $E_{i,j} = \{e = uv \epsilon\ E(G): d_v = i, d_u = j\}$, $e_{i,j} = |E_{i,j}|$ and $V_i = \{v \epsilon\ V(G): d_v = i\}$

Table 1: The vertex partition of graph $\mathrm{Sb}d_u$(G) based on degree of vertices, where m, n $\geq$ 2.

Degree of vertex	Number of vertices
1	4
2	4m+4n-8
4	4mn-4m-4n+4
6	4
7	4m+4n-12
8	4mn-6m-6n+9
Total	8mn-2n-2n+1

Table 2: The edge partition of graph Sbdu(G) based on degree of end vertices of each edge, where m, n $\geq$ 2

(d_u, d_v),where uv ϵ $E(Bd_u(G))$	Number of edges
(1,6)	4
(2,6)	8
(2,7)	8m+8n-24
(4,6)	4
(4,7)	8m+8n-24
(4,8)	16mn-24m-24n+36
(6,7)	8
(7,7)	4m+4n-16
(7,8)	4m+4n-12
(8,8)	8mn-14m-14n+24
Total	24mn-14m-14n+8

3 MAIN RESULTS

Theorem 1. Let $\mathrm{Sb}d_u$(G) be a simple bounded dual of G, G be a benzene ring embedded in P-type-surface on 2D-network, then

$M_\alpha(Sbd_u\ (G))$ $= (4m + 4n\text{-}8)2^\alpha + (4mn\text{-}4m\text{-}4n + 4)4^\alpha + (4)6^\alpha + (4m + 4n\text{-}12)7^\alpha + (4mn\text{-}6m\text{-}6n + 9)8^\alpha + 4,$

$R_\alpha(Sbd_u\ (G))$ $= (4)6^\alpha + (8)12^\alpha + (8m + 8n\text{-}24)14^\alpha + (4)24^\alpha + (8m + 8n\text{-}24)28^\alpha$
$+ (16mn\text{-}24m\text{-}24n + 36)2^{5\alpha} + (8)42^\alpha$
$+ (4m + 4n\text{-}16)7^{2\alpha}$
$+ (4m + 4n\text{-}12)56^\alpha + (8mn\text{-}14m\text{-}14n + 24)2^{6\alpha},$

$\chi_\alpha(Sbd_u\ (G))$ $= (4)7^\alpha + (8)2^{3\alpha} + (8m + 8n\text{-}24)3^{2\alpha} + (4)10^\alpha + (8m + 8n\text{-}24)11^\alpha$
$+ (16mn\text{-}24m\text{-}24n + 36)12^\alpha + (8)13^\alpha$
$+ (4m + 4n\text{-}16)14^\alpha$
$+ (4m + 4n\text{-}12)15^\alpha + (8mn\text{-}14m\text{-}14n +$

24)$2^{4\alpha}$,

where α is a real number.

Proof. The number of vertices in $\mathrm{Sb}d_u$(G) are given in Table 1. Since the formula for M_(G) is given

$$.M_\alpha(G) = \sum_{u \epsilon V(G)} (d_u)^\alpha$$
$.M_\alpha(G) = V_1(1)^\alpha + V_2(2)^\alpha + V_4(4)^\alpha + V_6(6)^\alpha + V_7(7)^\alpha + V_8(8)^\alpha,$

where V_i represents the cardinality of vertex of degree i.

$M_\alpha(Sbd_u(G))= 4 + (4m + 4n\text{-}8)2^\alpha + (4mn\text{-}4m\text{-}4n + 4)4^\alpha + (4)6^- + (4m + 4n\text{-}12)7^\alpha + (4mn\text{-}6m\text{-}6n + 9)8^\alpha:$

The number of edges in Sbdu(G) are 24mn-14m-14n + 8. The edge partition based on the degree of the end vertices of each edge are shown in Table 2. Since, the formula of general Randic index is this implies that and the formula of general sum-connectivity is

$$R_\alpha(G) = \sum_{uv \epsilon E(G)} (d_u d_v)^\alpha$$

$R_\alpha(\mathrm{Sbdu}(G))$ $= e_{1,6}(1 * 6)^\alpha + e_{2,6}(2 * 6)^\alpha + e_{2,7}(2 * 7)^\alpha + e_{4,6}(4 * 6)^\alpha + e_{4,7}(4 * 7)^\alpha + e_{4,8}(4 * 8)^\alpha + e_{6,7}(6 * 7)^\alpha + e_{7,7}(7 * 7)^\alpha + e_{7,8}(7 * 8)^\alpha + e_{8,8}(8 * 8)^\alpha, = (4)6^\alpha + (8)12^\alpha + (8m + 8n\text{-}24)14^\alpha + (4)24^\alpha + (8m + 8n\text{-}24)28^\alpha + (16mn\text{-}24n\text{-}24n + 36)2^{5\alpha} + (8)42^\alpha + (4m + 4n\text{-}16)7^{2\alpha} + (4m + 4n\text{-}12)56^\alpha + (8mn\text{-}14m\text{-}14n + 24)2^{6\alpha},$

$$\chi_\alpha(G) = \sum_{uv \epsilon E(G)} (d_u + d_v)^\alpha$$

$\chi_\alpha(\mathrm{Sbdu}(G))$ $= e_{1,6}(1 + 6)^\alpha + e_{2,6}(2 + 6)^\alpha + e_{2,7}(2 + 7)^\alpha + e_{4,6}(4 + 6)^\alpha + e_{4,7}(4 + 7)^\alpha + e_{4,8}(4 + 8)^\alpha + e_{6,7}(6 + 7)^\alpha + e_{7,7}(7 + 7)^\alpha + e_{7,8}(7 + 8)^\alpha + e_{8,8}(8 + 8)^\alpha, = (4)7^\alpha + (8)2^{3\alpha} + (8m + 8n\text{-}24)3^{2\alpha} + (4)10^\alpha + (8m + 8n\text{-}24)11^\alpha + (16mn\text{-}24n\text{-}24n + 36) 12^\alpha + (8)13^\alpha + (4m + 4n\text{-}16)14^\alpha + (4m + 4n\text{-}12)15^\alpha + (8mn\text{-}14m\text{-}14n)2^{4\alpha}$

This completes the proof.

Theorem 2. The atom-bond connectivity index ABC of simple bounded dual of the benzene ring embedded in the P-type-surface network is given by

$\mathrm{ABC}\ (Sbd_u(G))= (4\sqrt{5} + \sqrt{14})mn + (4\sqrt{2} - 6\sqrt{5} + (12\sqrt{7} + \sqrt{182} + 8\sqrt{3})/7)(m + n) + (-8\sqrt{2} + 9\sqrt{5} + 3\sqrt{14} + (2\sqrt{30} + 4\sqrt{3})/3 - (36\sqrt{7} - 32\sqrt{3} + 3\sqrt{182})/7 + 4\sqrt{462}/21$

Proof. The number of edges are mentioned in Table. 2.,

By using Table. 2., after simplification we get

ABC $(Sbd_u(G))= (4\sqrt{5}+\sqrt{14})mn + (4\sqrt{2}-6\sqrt{5}+ (12\sqrt{7}+\sqrt{182}+8\sqrt{3})/7(m+n) + (-8\sqrt{2}+9\sqrt{5}+ 3\sqrt{14}+(2\sqrt{30}+4\sqrt{3})/3 - (36\sqrt{7}-32\sqrt{3}+ 3\sqrt{182})/7 + 4\sqrt{462}/21$

This completes the proof.

Theorem 3. The geometric-arithmetic index GA of simple bounded dual of benzene ring embedded in the P-type-surface network is given by

$$GA(Sbdu\,(G) = ((32\sqrt{3}+8)/3)mn + \left(\frac{128\sqrt{14}}{45}- \frac{32\sqrt{7}}{11}-16\sqrt{2}-10\right)(m+n) + (4\sqrt{13}+24\sqrt{2}+8- \frac{96\sqrt{7}}{11}+\frac{16\sqrt{42}}{13}+96\frac{\sqrt{6}}{35}-128\frac{\sqrt{14}}{15}$$

Proof. The number of edges are mentioned in Table 2. Since, the geometric-arithmetic index is defined as after simplifications we get

$$GA(G) = \sum_{uv\in E(G)}\frac{2\sqrt{d_u d_v}}{d_u+d_v}$$

By using Table. 2, after simplification we get

$$GA(Sbdu\,(G) = (\frac{32\sqrt{3}+8}{3})mn + \left(\frac{128\sqrt{14}}{45}-\frac{32\sqrt{7}}{11}- 16\sqrt{2}-10\right)(m+n) + (4\sqrt{13}+24\sqrt{2}+8-\frac{96\sqrt{7}}{11}+ \frac{16\sqrt{42}}{13}+96\frac{\sqrt{6}}{35}-128\frac{\sqrt{14}}{15}$$

In the next two theorems we calculated the fourth atom-bond connectivity index ABC_4 and the fifth geometric-arithmetic index GA_5. There are twenty four types of edges on degree based sum of neighbors vertices of each edge in the simple bounded dual of benzene ring embedded in the P-type-surface network.

Table 3: The edge partition of graph Sbdu(G) based on degree sum of neighbor vertices of end vertices of each edge. where m; n ≥3.

(S_u,S_v); where uv ≥2E (Sbdu (G))	Number of edges
(6,23)	4
(13,23)	8
(13,33)	8
(14,33)	8
(14,34)	8m+8n-40
(23,28)	4
(23,33)	8
(28,33)	8
(28,46)	4
(30,33)	8
(30,34)	8m+8n-40
(30,46)	8
(30,47)	8m+8n-40
(32,46)	4
(32,47)	8m+8n-40

(32,48)	16mn-40m-40n+100
(33,34)	8
(33,46)	8
(34,34)	4m+4n-24
(34,47)	4m+4n-20
(46,47)	8
(47,47)	4m+4n-24
(47,48)	4m+4n-20
(48,48)	8mn-22m-22n+60
Total	24mn-14m-14n+8

Theorem 4. Let G be a benzene ring embedded in the P-type-surface network, then

1. HM (Sbdu(G)) = 4352mn-3740(m + n) + 3104,

2. PM_1(Sbdu(G))= $2^{(64mn-100m-100n+180)}* 3^{(16mn-4m-4n-24)} * 5^{(4m+4n-8)} *7^{(4m+4n\,-12)} * 11^{(8m+8n\,-24)} * 13^{(8)}$,

PM_2(Sbdu(G)) = $2^{(128mn-168m-168n+256)} * 3^{(24)} * 7^{(28m+28n\,-84)}$,

M1(Sbdu(G), x) = $(4)x^7 + (8)x^8 + (8m + 8n-24)x^9 + (4)x^{10} + (8m + 8n-24)x^{11}+ (16mn-24m-24n + 36)x^{12} + (8)x^{13} + (4m + 4n-16)x^{14}+ (4m + 4n-12)x^{15} + (8mn-14m-14n + 24)x^{16}$;

M2(Sbdu(G), x) = $(4)x^6 + (8)x^{12} + (8m + 8n-24)x^{14} + (4)x^{24} + (8m + 8n-24)x^{28}+ (16mn-24n-24n + 36)x^{32} + (8)x^{42} + (4m + 4n-16)x^{49}+ (4m + 4n-12)x^{56} + (8mn-14m-14n + 24)x^{64}$

Proof. Let G be a benzene ring embedded in the P-type-surface network. The edge set E(Sbdu(G)) divided into ten edge partitions based on degree of end vertices. The number of edges of edges partitions are given in Table 1 . By using Table 1 and Table 3, after simplification we get,

HM (Sbdu(G)) = 4352mn-3740(m + n) + 3104, Since,

$$PM_1(G) = \prod_{uv\in E(G)}(d_u+d_v)$$

After simplification we get

PM_1(Sbdu(G)) = $2^{(64mn-100m\quad-100n+180)}3^{(16mn-4m-4n-24)}5^{(4m+4n-\,8)} 7^{(4m+4n\,-12)} 11^{(8m+8n\,-24)} 13^{(8)}$,

We know that

$$PM_2(G) = \prod_{uv\in E(G)}(d_u d_v),$$

so using this and simplification we get
$PM_2(Sbdu(G)) = 2^{(128mn-168m-168n+256)} * 3^{(24)} * 7^{(28m+28n\ -84)}$.

Similarly

$M1(Sbdu(G),x)$ $= (4)x^7 + (8)x^8 + (8m + 8n-24)x^9 + (4)x^{10} + (8m + 8n-24)x^{11} + (16mn-24m-24n + 36)x^{12} + (8)x^{13} + (4m + 4n-16)x^{14} + (4m + 4n-12)x^{15} + (8mn-14m-14n + 24)x^{16}$,

and

$M2(Sbdu(G), x)$ $= (4)x^6 + (8)x^{12} + (8m + 8n-24)x^{14} + (4)x^{24} + (8m + 8n-24)x^{28} + (16mn-24n-24n + 36)x^{32} + (8)x^{42} + (4m + 4n-16)x^{49} + (4m + 4n-12)x^{56} + (8mn-14m-14n + 24)x^{64}$

Hence proved.

4 CLOSING REMARKS

In this paper, we deal with simple bounded dual of benzene ring embedded in the P- type-surface network and studies their topological indices. We determined first general Zagreb index M, general Randic connectivity index R_-, general sum-connectivity index χ_α, atom-bond connectivity index ABC, geometric-arithmetic index GA, fourth atom bound connectivity index ABC_4, fifth geometric-arithmetic index GA_5, hyper-Zagreb index HM (Sbdu(G)); first multiple Zagreb index $PM_1(Sbdu(G))$, second multiple Zagreb index $PM_2(Sbdu(G))$ and Zagreb polynomials $M_1(Sbdu(G); x)$, $M_2(Sbdu(G); x)$.

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