# Topological Indices And Topological Polynomials of Triangular Benzenoid System

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Abstract - Degree-based topological indices of benzenoid system are widely studied due to its use as an intermediate to make various synthetic compounds. Topological polynomials give topological indices which are used in QSPR/QSAR study. In this paper ABC<sub>4</sub>(G), GA<sub>5</sub>(G), fourth, fifth Zagreb indices, first and second forgotten polynomials and topological indices of triangular benzenoid system are studied.

**Keywords** -  $ABC_4(G)$ ,  $GA_5(G)$ , F-polynomial, F-index, Zagreb index.

#### I. INTRODUCTION

The application of molecular structure descriptors is nowadays a standard procedure in the study of structure-property relations, especially in the QSPR/QSAR study. Molecules and molecular compounds often model by molecular graph. A molecular graph is a representation of the structure of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms and edges correspond to chemical bonds [1].A topological index is a numerical parameter mathematically derived from the graph structure. All graphs considered in this paper are finite, connected, loop less, and without multiple edges. The topological indices has huge appilcaions in pharmacy, theoretical chemistry and especially in QSPR/QSAR [2]. Let G(V, E) be a graph with vertex set V and edge set E. The degree of a vertex u belong to E(G) is denoted by d<sub>u</sub> and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [3]. There are five different types of topological indices: degree, distance, Eigen value, matching and mixed [4,5]. In the field of mathematical chemistry, topological index is a number associated with molecular graph of a compound that depends on topology of that compound [6].

New Arithmetic-geometric indices of some chemical graphs are studied by V.R.Kulli [7]. Sanskriti index of nanostructures is studied by S.Prabhu [8], GA index for TUC<sub>4</sub>C<sub>8</sub>(S) nanotube are studied by M.Ghorbani et al. [9]. ABC<sub>4</sub>(G) and GA<sub>5</sub>(G) of some special graph are studied by M.S.Abdelgader et al. [10]. ABC<sub>4</sub>(G) and GA<sub>5</sub>(G) indices of paraline graph of some convex polytropes are studied by Z.Foruzanfar et al. [11]. ABC<sub>4</sub>(G) and GA<sub>5</sub>(G) of certain nanotubes are studied by S.Hayat et al. [12].F-indices and F-polynomials of the carbon nanocones are studied by N.K.Raut et al.[13].Sum of degrees of all edge incident to a vertex v based first and second and modified Kulli-Basava indices are stidied by V.R.Kulli [14].Sanskruti and harmonic indices of graph structure are studied by Z.S.Mufti et al. [15]. The sum of degrees of all the edges incident on a vertex Kulli-Basava indices of wheel graph  $(W_n)$  and gear graph  $(G_n)$  are studied by V.R.Kulli [16].  $ABC_4(G)$  and  $GA_5(G)$  topological indices of Nicotine are studied by H.L.Parashivmurthy et al. [17]. Harmonic index and harmonic polynomials of caterpillar with diameter four are studied by Iranmanesh M.A.[18]. Gaurava indices of line graph of subdivision of triangular benzenoid are studied by G.Keerthi et al. [19].

In a wheel graph, the hub has degree n-1 and other nodes have degree 3. Consider graph G depicted in figure 1. This triangular benzenoid graph has 13 vertices and 15 edges [20]. The notations used in this paper are mainly taken from books [21-23]. We consider triangular benzenoid which is a family of benzenoid molecular graphs, and is generalization of benzene molecule

 $C_6H_6$  in which, benzene rings form a triangular shape. These graphs consist of a hexagonal cycles arranged in rows and in each row one hexagon increases. We denote the triangular benzenoid molecular graph by  $T_p$  in which p is the number of hexagons in the base of a graph. A benzenoid system is to be a connected planar graph obtained by regular hexagons, with two such hexagons sharing a common edge or disjoint. Benzenoid systems are actually hydrogen depleted benzenoid hydrocarbons. Let  $T_p$  be a triangular benzenoid system where p shows the number of hexagons in the base graph and has total number of hexagons  $T_p = \frac{1}{2}p(p+1)$  and  $p^2+4p+1$  vertices and  $\frac{3}{2}p(p+3)$  edges. Different authors describe edge distribution and computation of topological indices for triangular benzenoid systems by various methods but by algebraic method the edge distribution and thereby computation of topological indices gives different results. Here we carry out actual counting of edges between different degrees of vertices.

The edge partition based on the degree of end vertices are given in table 1 and based on degree sum of neighbors of end vertices of each edge is represented in table 2.

ABC<sub>4</sub>(G) and GA<sub>5</sub>(G) are defined by W.Gao et al.[24] as,

ABC<sub>4</sub>(G) = 
$$\sum_{uv \in E(G)} \frac{\sqrt{S_u + S_v - 2}}{S_u S_v}$$
 and the fifth version of GA index is defined as

$$\mathrm{GA}_5(\mathrm{G}) = \sum_{uv \in E(G)} \ \frac{2\sqrt{S_u S_v}}{S_u + S_v} \quad \text{.} \quad \text{Where } \mathrm{S}_\mathrm{u} = \sum_{uv \in E(G)} \ S_v \quad \text{and} \quad \mathrm{S}_\mathrm{v} = \sum_{uv \in E(G)} \ S_u.$$

Bindusree A.R.et al. [25] defined the fourth and fifth Zagreb polynomials as,

$$M_4(G,x) = \sum_{uv \in E(G)} x^{d_u(d_u + d_v)} \text{ and } M_5(G,x) = \sum_{uv \in E(G)} x^{d_v(d_u + d_v)}$$

The first forgotten polynomial is defined as,  $F_1(G,x) = \sum_{uv \in E(G)} x^{(d_u^2 + d_v^2)}$ 

and the second forgotten polynomial is, $F_2(, \boldsymbol{G}, \boldsymbol{x}) = \sum_{uv \in E(\boldsymbol{G})} x^{(d_u^2 d_v^2)}$ 

Using the edge dividing technology the distribution of edges given by W.Wao et al. is  $n_{22} = 6$ ,  $n_{23} = 3n(n-1)/2$  and  $n_{33} = 6(n-1)$  [26]. But by algebraic method, we obtain the edge set E(G) which is divided into three particulars cases as,

$$E_{\{2,2\}} = \{uv \in E_G(T_p) | d_u = 2, d_v = 2\}, |E_{\{2,2\}}| = 6$$

$$E_{\{2,3\}} = \{uv \in E_G(T_p) | d_u=2, d_v=3\}, |E_{\{2,3\}}| = 6p-6$$

$$E_{\{3,3\}} = \{uv \in E_G(T_p) | d_u=3, d_v=3\}, |E_{\{3,3\}}| = \frac{3}{2}p(p-1)$$

This difference of observation gives motivation for the present investigation of triangular benzenoid system for some topological indices.

## II. Materials and Methods

A molecular graph is constructed by representing nodes and edges. A topological index Top(G) of a graph G is a number with the property that for every graph H isomorphic to G, Top(H) = Top(G).



Figure 1.Graph of triangular benzenoid G(2).

Degree of a vertex is the number of vertices adjacent to a vertex v.A vertex can form an edge with all the vertices except by itself. So the degree of a vertex will be up to the number of vertices in the graph minus 1. This 1 is for the self vertex as it cannot form a loop at any of the vertices, then it is not a simple graph. Graph of triangular benzenoid G(2) is shown in figure 1. It has 13 vertices and 15 edges. This is the simplest case for triangular benzenoid system studied by M. Ghorbani. The graph of triangular benzenoid is shown in figure 2.

It is observed from figure 2, there are  $|E_{\{2,2\}}|=6$ ,  $|E_{\{2,3\}}|=36$  and  $|E_{\{3,3\}}|=63$  edges, with the partition as,

 $E_{\{2,2\}} = \{uv \in E(T_p) | d_u = 2, d_v = 2\},$ 

 $E_{\{2,3\}} = \{uv \in E(T_p) | d_u = 2, d_v = 3\},\$ 

 $E_{3,3} = \{uv \in E(T_p) | d_u = 3, d_v = 3\}.$ 

The first, second forgotten indices and fourth, fifth Zagreb indices are studied by knowing degree of each vertex and for  $GA_5(G)$ ,  $ABC_4(G)$  the sum of degrees of neighbors is required.

### III. Results and discussion

**Theorem 3.1.** Let  $T_p$  be the graph of triangular benzenoid system then its fifth version of the geometric-arithmetic index is equal to  $GA_5(T_p) = 104.6$ .

**Proof.** The graph of the triangular benzenoid contains  $p^2+4p+1$  vertices and  $\frac{3}{2}p(p+3)$  edges. From figure 2 we notice that there five separate cases and where the number of edges are different: namely  $E_{\{4,5\}}$ ,  $E_{\{5,7\}}$ ,  $E_{\{6,7\}}$ ,  $E_{\{7,9\}}$ , and  $E_{\{9,9\}}$ . Using degree sum of neighbors of end vertices of each edge. We have the partition as,

 $E_{\{4,5\}} = \{uv \in E(T_p) | d_u = 4, d_v = 5\}.$ 

 $E_{(5,7)} = \{uv \in E(T_p) | d_u = 5, d_v = 7\}.$ 

 $E_{\{6,7\}} = \{uv \in E(T_p) | d_u = 6, d_v = 7\}.$ 

 $E_{(7,9)} = \{uv \in E(T_p) | d_u = 7, d_v = 9\}.$ 

 $E_{9,9} = \{uv \in E(T_p) | d_u = 9, d_v = 9\}.$ 

The number of edges  $E_{(4,5)}$ ,  $E_{(5,7)}$ ,  $E_{(6,7)}$ ,  $E_{(7,9)}$  and  $E_{(9,9)}$  are 6,8,28,18 and 45 respectively.

The GA<sub>5</sub>(T<sub>p</sub>) = 
$$\sum_{uv \in E(Tp)} \frac{2\sqrt{S_uS_v}}{S_u + S_v}$$

$$==\sum_{(4,5)\in E(Tp)}\frac{2\sqrt{S_uS_v}}{S_u+S_v}+\sum_{(5,7)\in E(Tp)}\frac{2\sqrt{S_uS_v}}{S_u+S_v}+\sum_{(6,7)\in E(Tp)}\frac{2\sqrt{S_uS_v}}{S_u+S_v}+\sum_{(7,9)\in E(Tp)}\frac{2\sqrt{S_uS_v}}{S_u+S_v}+\sum_{(9,9,)\in E(Tp)}\frac{2\sqrt{S_uS_v}}{S_u+S_v}$$

$$\begin{split} &= \sum_{(4,5) \in E} \frac{2\sqrt{4.5}}{4+5} + \sum_{(5,7) \in E(Tp)} \frac{2\sqrt{5.7}}{5+7} + \sum_{(6,7) \in E(Tp)} \frac{2\sqrt{6.7}}{6+7} + \sum_{(7,9) \in E(Tp)} \frac{2\sqrt{7.9}}{7+9} + \sum_{(9,9) \in E(Tp)} \frac{2\sqrt{9.9}}{9+9} \\ &= |E_{\{4,5\}}(T_p)|0.9938 + |E_{\{5,7\}}(T_p)|0.9861 + |E_{\{6,7\}}(T_p)|0.9971 + |E_{(7,9)}(T_p)|0.9922 + |E_{\{9,9\}}(T_p)|.1 \\ &= 104.6. \end{split}$$

**Theorem 3.**2. Let  $T_p$  be the graph of triangular benzenoid system then its fourth version of the ABC index is equal to  $ABC_4(T_p) = 50.65$ .

**Proof.** The graph of the triangular benzenoid contains  $p^2+4p+1$  vertices and  $\frac{3}{2}p(p+3)$  edges. From figure 2 we notice that there five separate cases and where the number of edges are different: namely  $E_{\{4,5\}}$ ,  $E_{\{5,7\}}$ ,  $E_{\{6,7\}}$ ,  $E_{\{7,9\}}$ , and  $E_{\{9,9\}}$ . Using degree sum of neighbors of end vertices of each edge we have,

$$E_{\{4,5\}} = \{uv \in E(T_p) | d_u = 4, d_v = 5\}.$$

$$E_{(5,7)}\!=\{uv\!\!\in\!\!E(T_p)|d_u\!\!=\!\!5,\!d_v\!\!=\!\!7\}.$$

$$E_{\{6,7\}} = \{uv \in E(T_p) | d_u = 6, d_v = 7\}.$$

$$E_{(7,9)} = \{uv \in E(T_p) | d_u = 7, d_v = 9\}.$$

$$E_{9,9} = \{uv \in E(T_p) | d_u = 9, d_v = 9\}.$$

= 50.65.

The number of edges  $E_{(4,5)}$ ,  $E_{(5,7)}$ ,  $E_{(6,7)}$ ,  $E_{(7,9)}$  and  $E_{(9,9)}$  are 6,8,28,18 and 45 respectively.

The ABC<sub>4</sub>(T<sub>p</sub>) = 
$$\sum_{uv \in E(Tp)} \frac{\sqrt{S_u + S_v - 2}}{S_u S_v}$$
  
== $\sum_{45 \in E(Tp)} \frac{\sqrt{S_u + S_v - 2}}{S_u S_v} + \sum_{57 \in E(Tp)} \frac{\sqrt{S_u + S_v - 2}}{S_u S_v} + \sum_{67 \in E(Tp)} \frac{\sqrt{S_u + S_v - 2}}{S_u S_v} + \sum_{79 \in E(Tp)} \frac{\sqrt{S_u + S_v - 2}}{S_u S_v} + \sum_{99 \in E(Tp)} \frac{\sqrt{S_u + S_v - 2}}{S_u S_v}$   
== $\sum_{45 \in E(Tp)} \frac{\sqrt{4 + 5 - 2}}{4 \cdot 5} + \sum_{57 \in E(Tp)} \frac{\sqrt{5 + 7 - 2}}{5 \cdot 7} + \sum_{67 \in E(Tp)} \frac{\sqrt{6 + 7 - 2}}{6 \cdot 7} + \sum_{79 \in E(Tp)} \frac{\sqrt{7 + 9 - 2}}{7 \cdot 9} + \sum_{99 \in E(Tp)} \frac{\sqrt{9 + 9 - 2}}{9 \cdot 9}$   
=  $|E_{\{4,5\}}(T_p)| \cdot 0.3945 + |E_{\{5,7\}}(T_p)| \cdot 0.5345 + |E_{\{6,7\}}(T_p)| \cdot 0.5117 + |E_{\{7,9\}}(T_p)| \cdot 0.4715 + |E_{\{9,9\}}(T_p)| \cdot 0.4445$ 

**Theorem 3.3.** Let  $T_p$  be the graph of triangular benzenoid system then its fourth Zagreb index is equal to  $M_4(T_p) = 1542$ .

**Proof.** The graph of the triangular benzenoid contains  $p^2+4p+1$  vertices and  $\frac{3}{2}p(p+3)$  edges. From figure 2 we notice that there three separate cases and where the number of edges are different: namely  $E_{\{2,2\}}$ ,  $E_{\{2,3\}}$  and  $E_{\{3,3\}}$ .

The number of edges are  $E_{\{2,2\}} = 6$ ,  $E_{\{2,3\}} = 36$  and  $E_{\{3,3\}} = 63$ .

The fourth Zagreb polynomial is,

$$\begin{split} & M_4(T_p, x) = \sum_{uv \in E(Tp)} x^{d_u(d_u + d_v)} \\ & = \sum_{22 \in E(Tp)} x^{2(2+2)} + \sum_{23 \in E(Tp)} x^{2(2+3)} + \sum_{33 \in E(Tp)} x^{3(3+3)} \\ & = |E_{(2,2)}(T_p)| x^8 + |E_{(2,3)}(T_p)| x^{10} + |E_{(3,3)}(T_p)| x^{18} \end{split}$$

$$=6x^8+36x^{10}+63x^{18}$$

$$M_5(T_p,x) = 6x^8 + 36x^{10} + 63x^{18}$$

The fourth Zagreb index

$$= \frac{\delta M_4(Tp)}{\delta x}|_{x=1} = 6.8 + 36.10 + 63.18 = 1542.$$

**Theorem 3.4.** Let  $T_p$  be the graph of triangular benzenoid system then its fifth Zagreb index is equal to  $M_5(T_p) = 1722$ .

**Proof.** The graph of the triangular benzenoid contains  $p^2+4p+1$  vertices and  $\frac{3}{2}p(p+3)$  edges. From figure 2 we notice that there three separate cases and where the number of edges is different:namely  $E_{\{2,2\}}, E_{\{2,3\}}$  and  $E_{\{3,3\}}$ .

The number of edges are  $E_{\{2,2\}} = 6$ ,  $E_{\{2,3\}} = 36$  and  $E_{\{3,3\}} = 63$ .

The fifth Zagreb polynomial is,

$$\begin{split} &M_5(T_p,x) = \sum_{uv \in E(Tp)} x^{d_v(d_u + d_v)} \\ &= \sum_{22 \in E(Tp)} x^{2(2+2)} + \sum_{23 \in E(Tp)} x^{3(2+3)} + \sum_{33 \in E(Tp)} x^{3(3+3)} \\ &= |E_{\{2,2\}}(T_p)| x^8 + |E_{\{2,3\}}(T_p)| x^{15} + |E_{\{3,3\}}(T_p)| x^{18} \\ &= 6x^8 + 36 x^{15} + 63x^{18}. \end{split}$$

$$M_5(T_p,x) = 6x^8 + 36x^{15} + 63x^{18}$$

The fifth Zagreb index

$$= \frac{\delta M_5(Tp)}{\delta x}|_{x=1} = 6.8 + 36.15 + 63.18 = 1722.$$

**Theorem 3.5.** Let  $T_p$  be the graph of triangular benzenoid system then its first forgotten index is equal to  $F_1(T_p) = 1650$ .

**Proof.** The graph of the triangular benzenoid contains  $p^2+4p+1$  vertices and  $\frac{3}{2}p(p+3)$  edges. From figure 2 we notice that there three separate cases and where the number of edges are different:namely  $E_{\{2,2\}}$ ,  $E_{\{2,3\}}$  and  $E_{\{3,3\}}$ .

The number of edges are  $E_{\{2,2\}} = 6$ ,  $E_{\{2,3\}} = 36$  and  $E_{\{3,3\}} = 63$ .

The first forgotten polynomial is,

$$\begin{split} &F_{1}(T_{p},x) = \sum_{uv \in E(Tp)} x^{(d_{u}^{2} + d_{v}^{2})} \\ &= \sum_{22 \in E(Tp)} x^{(d_{u}^{2} + d_{v}^{2})} + \sum_{23 \in E(Tp)} x^{(d_{u}^{2} + d_{v}^{2})} + \sum_{33 \in E(Tp)} x^{(d_{u}^{2} + d_{v}^{2})} \\ &= \sum_{22 \in E(Tp)} x^{(2^{2} + 2^{2})} \sum_{23 \in E(Tp)} x^{(2^{2} + 3^{2})} \sum_{33 \in E(Tp)} x^{(3^{2} + 3^{2})} \\ &= |E_{\{2,2\}}(T_{p})|x^{8} + |E_{\{2,3\}}(T_{p})|x^{13} + |E_{\{3,3\}}(T_{p})|x^{18} \\ &= 6x^{8} + 36 x^{13} + 63x^{18} \\ &F_{1}(T_{p},x) = 6x^{8} + 36 x^{13} + 63x^{18} \end{split}$$

The first forgotten index

$$= \frac{\delta F_1(Tp)}{\delta x}|_{x=1} = 6.8 + 36.13 + 63.18 = 1650.$$

**Theorem 3.6.** Let T<sub>p</sub> be the graph of, triangular benzenoid system then its second forgotten index is equal to

$$F_2(T_p) = 6495.$$

**Proof.** The graph of the triangular benzenoid contains  $p^2+4p+1$  vertices and  $\frac{3}{2}p(p+3)$  edges. From figure 2 we notice that there three separate cases and where the number of edges are different:namely  $E_{\{2,2\}}$ ,  $E_{\{2,3\}}$  and  $E_{\{3,3\}}$ .

The number of edges are  $|E_{\{2,2\}}|=6$ ,  $|E_{\{2,3\}}|=36$  and  $|E_{\{3,3\}}|=63$ .

The second forgotten polynomial is,  $F_2(T_p, x) = \sum_{uv \in E(T_p)} \chi^{(d_u^2 d_v^2)}$ 

$$= \sum_{22 \in E(\text{Tp})} x^{(d_u^2 d_v^2)} + \sum_{23 \in E(\text{Tp})} x^{(d_u^2 d_v^2)} + \sum_{33 \in E(\text{Tp})} x^{(d_u^2 d_v^2)}$$

$$= \sum_{22 \in E(\text{Tp})} x^{(2^2 \, 2^2)} + \sum_{23 \in E(\text{Tp})} x^{(2^2 \, 3^2)} + \sum_{33 \in E(\text{Tp})} x^{(3^2 \, 3^2)}$$

$$= |E_{\{2,2\}}(T_p)| x^{16} + |E_{\{2,3\}}(T_p)| |x^{36} + |E_{\{3,3\}}(T_p)| x^{81}$$

$$=6x^{16}+36x^{36}+63x^{81}$$

$$F_2(T_p,x) = 6x^{16} + 36x^{36} + 63x^{81}$$

The second forgotten index

$$=\frac{\delta F_2(Tp)}{\delta r}|_{x=1} = 6.16 + 36.36 + 63.81 = 6495.$$

Table 1.Edge partition of triangular benzenoid system.

$(d_u,d_v),uv \in E(Tp)$	(2,2)	(2,3)	(3,3)
No. of edges	6	6(p-1)	$\frac{3}{2}$ p(p-1)

Table 2.Edge partition of triangular benzenoid system based on degree sum of neighbors of end vertices of each edge.

$(S_u, S_v), uv \in E(Tp)$	(4,5)	(5,7)	(6,7)	(7,9)	(9,9)
No. of edges	6	8	28	18	45

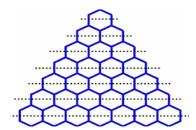


Figure 2.Graph of triangular benzenoid (Tp).

# IV. CONCLUSIONS

The fourth and fifth Zagreb polynomials and indices, first and second Forgotten polynomials and indices and fifth version of GA(G) index and fourth version of ABC(G) are studied for triangular benzenoid system

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