Computation of Zagreb and atom–bond connectivity indices of certain families of dendrimers by using automorphism group action

UZMA AHMAD[1]*, SARFRAZ AHMAD[2] and RABIA YOUSAF[1]

[1]*Department of Mathematics, University of the Punjab, New Campus, Lahore, Pakistan and* [2]*Department of Mathematics, COMSATS Institute of Information Technology, Lahore, Pakistan*

Abstract: In QSAR/QSPR studies, topological indices are utilized to predict the bioactivity of chemical compounds. In this paper, the closed forms of different Zagreb indices and atom–bond connectivity indices of regular dendrimers $G[n]$ and $H[n]$ in terms of a given parameter n are determined by using the automorphism group action. It was reported that these connectivity indices are correlated with some physicochemical properties and are used to measure the level of branching of the molecular carbon-atom skeleton.

Keywords: graph automorphism; orbits; dendrimer graphs; topological indices; QSAR/QSPR; wreath product.

INTRODUCTION

In the last few decades, computational methods have been used extensively in theoretical and physical chemistry for the prediction of molecular properties and the testing of theory. Recently, studies of quantitative structure–activity (QSAR) and structure–property (QSPR) relationships have been developing very rapidly by using many mathematical methods to predict the biological activities and properties of different chemical compounds with the help of topological indices.

The molecular graph theory is a significant area of mathematical chemistry with the help of which mathematical models of molecular structures can be developed. The graph theory converts chemical structures into mathematical invariants by associating mathematical object sets consisting of vertices that represents atoms and the edges that depicts covalent bonds between the atoms.

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The topological index of a molecular graph G is the real number denoted by *Top(G)* that describes the characteristics and the molecular topology of a chemical compound. Although by representing the molecular structures with topological indices (QSPR/QSAR study), there is substantial loss of information, but still these indices provide comprehensive knowledge in predicting many molecular properties and biological activities. Specifically, this study is helpful in predicting molecular properties that are either difficult to determine or may have health risk or in the case when the chemical substance is not available.

Some of the oldest and the most studied molecular descriptors are the Zagreb group indices. They found noteworthy applications in Chemistry. In 1972,[1] Gutman and Trinajstić introduced the Zagreb group indices, also known as the Zagreb group parameters. The level of branching of a molecular carbon-atom skeleton can be measured by these indices. Hence, they can be regarded as molecular structure-descriptors. The details and a historical overview of the Zagreb group indices are given in the Supplementary material to this paper.

Recently, Furtula *et al.*[2] introduced the atom–bond connectivity index (*ABC*), which has hitherto been applied to study the stability of alkanes and the strain energy of cycloalkanes.

The *ABC* index has a vast number of applications in chemical thermodynamics[2,3] and in chemistry[4–7]. This index is defined as follows:

$$ABC_1(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}} \tag{1}$$

where $E(G)$ is the number of edges of any graph G, and d_u and d_v denote the degree of vertex u and v, respectively.

$$ABC_2(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{m_u + m_v - 2}{m_u \times m_v}} \tag{2}$$

where m_u is the number of vertices whose distance from vertex u is smaller than to vertex v.

$$ABC_4(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u \times S_v}} \tag{3}$$

where $S_u = \sum_{v \in N_G(u)} d_v$ and $N_G(u) = \{v \in V(G) \,|uv \in E(G)\}$ and

$$ABC_5(G) = \sum_{e=uv \in E(G)} \sqrt{\frac{\epsilon_u + \epsilon_v - 2}{\epsilon_u \times \epsilon_v}} \tag{4}$$

here $\epsilon(u)$ is the eccentricity[8] of the vertex u, defined as:

$$\epsilon(u) = max_{v \in V(G)} d_G(u,v)$$

and $d_G(u,v)$ is the distance between u and v.

The connectivity index and its modifications, such as the group of Zagreb indices, ABC indices, *etc*., are used more often than any other topological indices in QSPR/QSAR. The mathematical properties of these topological indices can be found in some recent papers. The readers are encouraged to consult the literature[9–15] for the historical background, computational techniques and mathematical properties of the Zagreb and ABC indices. Since these indices represent mathematically attractive invariants, it is important to have some deeper studies on these indices for the advancement of this part of mathematical chemistry.

Dendrimers are star-shaped and pronged macromolecules with nanometer--scale measurements. Dendrimers were first investigated by Vogtle *et al*.[16] in 1978. They expand iteratively from a central core such that each succeeding phase depicts a new generation of the dendrimer that nearly doubles the molecular weight of the preceding generation. The heavily increasing growing structure of dendrimer leads to different shapes and sizes that protect the inner cores and hence are the best choice in biological and material sciences. Moreover, it is helpful in conjugating other chemical species to its surface, which acts like a detecting agent, targeting components, imaging agents, or pharmaceutically active compounds. The literature indicates that dendrimers have also been examined due to their vast applications in nanotechnology, drug delivery, gene transfection, catalysis, energy harvesting and other fields. The topological study of these macromolecules is the aim of this article.

In this article, the notations are standard for the hyper-Zagreb index, *HM*, and the augmented Zagreb index, *AZI*. In this paper, the closed form of first and second Zagreb indices, related Zagreb polynomials, augmented Zagreb, hyper--Zagreb and *ABC* indices of some dendrimers are studied and formulated by using group theoretical methods.[17,18]

RESULTS AND DISCUSSION

Zagreb indices of dendrimer G[n] *and* H[n]

In this section, the exact formulae for the first and second Zagreb indices, related Zagreb polynomials, augmented Zagreb index and hyper-Zagreb index of a family of regular dendrimers $G[n]$ and $H[n]$ are computed by using the action of an automorphism group of the graph on the vertices and edges of the dendrimer graphs.

Consider the molecular graphs of $G[n]$ and $H[n]$ of regular dendrimers with exactly n generations with the core isomorphic to the path graph on 6 and 4 vertices, respectively, as shown in Figs. 1 and 2.
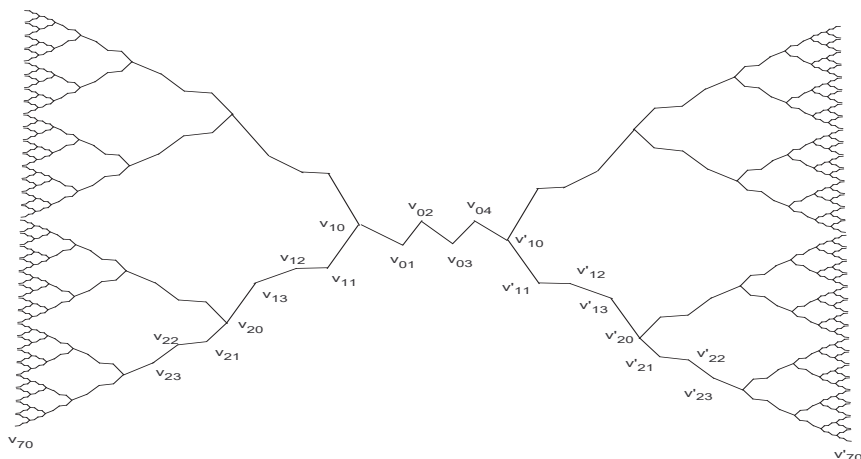
Fig. 1. 2-Dimensional representation of the Dendrimer graph $G[n]$ for n=6.
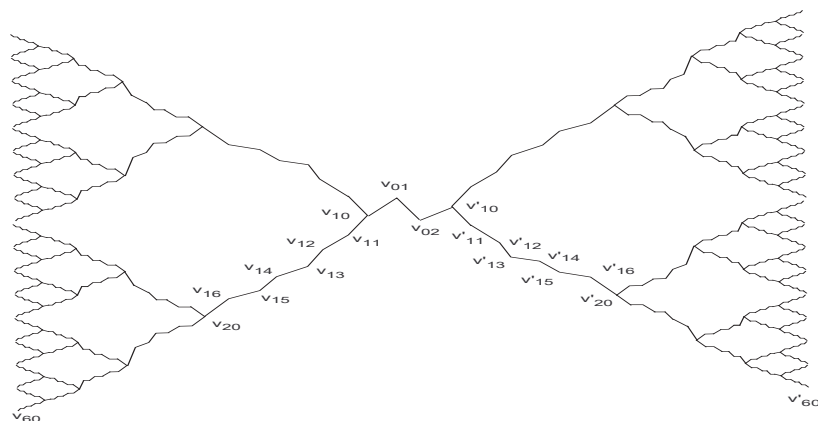

Fig.2. 2-Dimensional representation of the Dendrimer graph $H[n]$ for n=5.

Since the degree of any vertex is invariant under any automorphism of the graph, the first and second Zagreb indices, hyper-Zagreb and augmented Zagreb indices can be re-written using Lemma 1.

Lemma 1. Let Aut$(G) = \varphi_1$ act on the vertex set $V(G)$ and the edge set $E(G)$ of a molecular graph. Suppose further orbits of the vertices under this action are $U_1, U_2, \cdots, U_k$ and orbits of the edges under this action are $E_1, E_2, \cdots, E_s$. Then the first and second Zagreb indices, Zagreb variable indices, hyper-Zagreb, augmented Zagreb indices and ABC indices are given as follows:

$$M_1(G) = \sum_{i=1}^{k} |U_i| (d_{x_i})^2 \tag{5}$$

$$M_2(G) = \sum_{j=1}^{s} |E_j| (d_{x_{j-1}} d_{x_j}) \tag{6}$$

$$\bar{M}_1(G) = \sum_{u,v \in V(G)} (d_u + d_v) - \sum_{i=1}^{k} |E_i| (d_{x_{j-1}} + d_{x_j}) \tag{7}$$

$$\bar{M}_2(G) = \sum_{u,v \in V(G)} (d_u d_v) - \sum_{j=1}^{s} |E_j| (d_{x_{j-1}} d_{x_j}) \tag{8}$$

$$^{\upsilon}M_1(G) = \sum_{i=1}^{k} |U_i| (d_{x_i})^{2\upsilon} \tag{9}$$

$$^{\upsilon}M_2(G) = \sum_{j=1}^{s} |E_j| (d_{x_{j-1}} d_{x_j})^{\upsilon} \tag{10}$$

$$HM(G) = \sum_{j=1}^{k} |E_j| (d_{x_j} + d_{x_{j-1}})^2 \tag{11}$$

and

$$AZI(G) = \sum_{i=1}^{k} |E_j| \left(\frac{d_{x_{j-1}} d_{x_j}}{d_{x_j} + d_{x_{j-1}} - 2}\right)^3 \tag{12}$$

It is easy to see that $G[n]$ can be split into three parts, A, B and C, where C is the core as shown in the Fig. 3. It is noted that each of the sub-graphs A and B of $G[n]$ contains $n+1$ stages such that the first n stages consist of 4 levels and the last stage contains only one level. Thus, the number of levels of A and B are $4n+1$ each.

Let U_i and U_i' be the set of vertices of i-*th* stage of A and B, respectively and U_{it} and U_{it}' denote the t-th level of i-th stage in A and B, respectively. Then,

$$U_i = \bigcup_{t=0}^{3} U_{it} \text{ and } U_i' = \bigcup_{t=0}^{3} U_{it}'$$

The automorphism group of G[n] of vertices is isomorphic to $Z_2 \sim V_4$, where V_4 acts on the set $\cup_{i=1}^{n+1}(U_{i0} \cup U_{i0}')$, *i.e.*, on $2(2^{n+1} - 1)$ vertices and $\sim$ is the permutational wreath product. Label the vertices of the core as v_{01}, v_{02}, v_{03} and v_{04} and let v_{it} and v_{it}' be the first vertices of orbit U_{it} and U_{it}', as shown Fig. 1. Now it is easy to see that the orbits I_{it}, I_{01} and I_{02} under the action of automorphism group of G[n] on vertices can be written as:

$$I_{it} = \{U_{it} \cup U_{it}'\}$$

where $0 \leq t \leq 3$ for $1 \leq i \leq n$, and $t = 0$ for $i = n+1$ and $I_{01} = \{v_{01}, v_{03}\}$ and $I_{02} = \{v_{02}, v_{04}\}$. Thus $|I_{it}| = 2^{i+1-\delta_{0t}}$ and $|I_{01}| = |I_{02}| = 2$, where δ_{0s} is the Kronecker delta defined as:

$$\delta_{ij} = \begin{cases} 1, & i = j, \\ 0, & i \neq j, \end{cases}$$

Therefore:

$$V(G) = \bigcup_{i=1}^{n+1} \bigcup_{t=0}^{3} I_{it}(1 - \delta_{(n+1)i}(1 - \delta_{0t})) \bigcup I_{01} \bigcup I_{02}$$
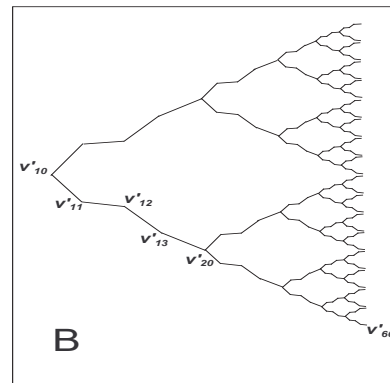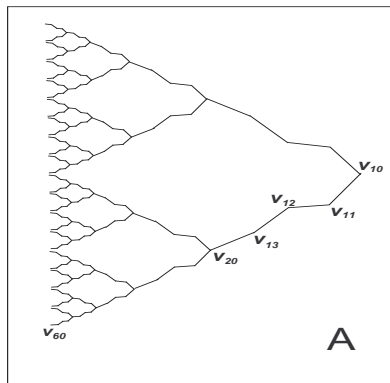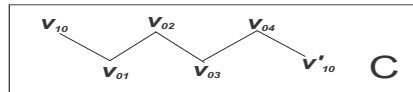

Fig.3. Three sub-graphs A, B and C of $G[n]$ for $n = 5$.

Now the action of Aut $(G[n])$ on $E(G)$ is considered. Let E_i and E_i' be the set of edges of i-th stages of A, B, respectively, and E_{it} and E_{it}' denote the set of edges joining the t and $t–1$ levels of i-th stage in A and B, respectively. Furthermore, F_i and F_i' are the set of edges joining the 3rd level of the i-th stage and 0-th level of $(i+1)$-th stage of A and B, respectively. Let:

$$E_i = \left\{ \bigcup_{t=1}^{3} E_{it}, F_i \right\} \quad \text{and} \quad E_i' = \left\{ \bigcup_{t=1}^{3} E_{it}', F_i' \right\}$$

Then, the orbits of the edges under this action are as follows:

$S_1 = \{v_{01}v_{10}, v_{10}'v_{04}\}, S_2 = \{v_{02}v_{01}, v_{04}v_{03}\}, S_3 = \{v_{02}v_{03}\}, M_{it} = \{E_{it} \cup E\}$

and

$$N_i = \{F_i \cup F_i^{'}\}$$

where $1 \leq t \leq 3$ and $1 \leq i \leq n$. Thus, $|M_{it}| = |N_i| = 2^{i+1}$, $|S_1| = 2 = |S_2|$ and $|S_3| = 1$.

Theorem 1: The first and the second Zagreb indices of $G[n]$ are:

$$M_1 G = 17 \times 2^{n+2} - 50 \tag{13}$$

$$M_2 G = 9 \times 2^{n+3} - 56 \tag{14}$$

The first and second Zagreb polynomials of $G[n]$ are:

$$Z_{g_1}(G, x) = (3 \times 2^{n+1} - 6)x^5 + (2^{n+3} - 5)x^4 + 2^{n+1}x^3 \tag{15}$$

$$Z_{g_2}(G, x) = (3 \times 2^{n+1} - 6)x^6 + (2^{n+3} - 5)x^4 + 2^{n+1}x^2 \tag{16}$$

The proof for Theorem 1 is given in the Supplementary material to this paper.

Theorem 2: The first and second Zagreb coincides of $G[n]$ are:

$$\bar{M}_1(G[n]) = 4096 \times 2^{3n} - 8192 \times 2^{2n} + 5388 \times 2^n - 1160 \tag{17}$$

$$\bar{M}_2(G[n]) = 4096 \times 2^{3n} - 8192 \times 2^{2n} + 5384 \times 2^n - 1154 \tag{18}$$

The proof for Theorem 2 is given in the Supplementary material.

Theorem 3: The first and second variable Zagreb indices of $G[n]$ are:

$$^{\upsilon}M_1(G[n]) = -2\{4 \times 2^{2\upsilon} + 3^{2\upsilon}\} + 2^{n+1}\{1 + 3^{2\upsilon} + 6 \times 2^{2\upsilon}\} \tag{19}$$

$$^{\upsilon}M_2(G[n]) = -6 \times 6^{\upsilon} - 5 \times 4^{\upsilon} + 2^{n+1}\{3 \times 6^{\upsilon} + 4 \times 4^{\upsilon} + 2^{\upsilon}\} \tag{20}$$

The proof for Theorem 3 is given in the Supplementary material.

Similarly, the hyper-Zagreb and augmented Zagreb indices of $G[n]$ can be calculated as in the following Theorem 4.

Theorem 4: The hyper-Zagreb and augmented Zagreb indices of $G[n]$ are:

$$HM(G[n]) = 37 \times 2^{n+3} - 230 \tag{21}$$

$$AZI(G[n]) = 2^{n+7} - 88 \tag{22}$$

The proof for Theorem 4 is given in the Supplementary material.

The automorphism group of $H[n]$ is isomorphic to $Z_2 \sim V_4$. $H[n]$ is shown in Fig. 2. Now the orbits I_{it} and I_{01} under the action of the automorphism group of $H[n]$ on vertices can be written as $I_{it} = \{U_{it} \cup U_{it}^{'}\}$, where for $0 \leq t \leq 6$ and $1 \leq i \leq n$ and $t = 0$ for $i = n+1$ and $I = \{v_{01}, v_{02}\}$. Thus $|I_{it}| = 2^{i+1-\delta_{0t}}$ and $|I| = 2$.

Similarly, the orbits of edges under this action are as follows:

$$S_1 = \{v_{01}v_{10}, v_{10}^{'}v_{02}\}, S_2 = \{v_{02}v_{01}\}, M_{it} = \{E_{it} \cup E_{it}^{'}\} \quad \text{and} \quad N_i = \{F_i \cup F_i^{'}\},$$

where $1 \leq t \leq 6$ and $1 \leq i \leq n$. Thus, $|M_{it}| = |N_i| = 2^{i+1}$, $|S_1| = 2$ and $|S_2| = 1$.

Theorem 5: The first and the second Zagreb indices of $H[n]$ are:

$$M_1\left(H[n]\right) = 29 \times 2^{n+2} - 106 \tag{23}$$

$$M_2\left(H[n]\right) = 15 \times 2^{n+3} - 112 \tag{24}$$

The first and second Zagreb polynomials of $H[n]$ are:

$$Z_{g_1}(H,x) = (3 \times 2^{n+1} - 6)x^5 + (5 \times 2^{n+2} - 19)x^4 + 2^{n+1}x^3 \tag{25}$$

$$Z_{g_2}(H,x) = (3 \times 2^{n+1} - 6)x^6 + (5 \times 2^{n+2} - 19)x^4 + 2^{n+1}x^2 \tag{26}$$

The proof for Theorem 5 is given in the Supplementary material.
Theorem 6: The first and second Zagreb co-indices of $H[n]$ are:

$$\bar{M}_1(H[n]) = 21952 \times 2^{3n} - 58016 \times 2^{2n} + 50984 \times 2^n - 14894 \tag{27}$$

$$\bar{M}_2(H[n]) = 21952 \times 2^{3n} - 58016 \times 2^{2n} + 50980 \times 2^n - 14888 \tag{28}$$

The proof for Theorem 6 is given in the Supplementary material.
Theorem 7: The first and second variable Zagreb indices of $H[n]$ are:

$$^vM_1(H[n]) = -2\{11 \times 2^{2v} + 3^{2v}\} + 2^{n+1}\{1 + 3^{2v} + 12 \times 2^{2v}\} \tag{29}$$

$$^vM_2(H[n]) = -6 \times 6^v - 19 \times 4^v + 2^{n+1}\{3 \times 6^v + 10 \times 4^v + 2^v\} \tag{30}$$

The Proof for Theorem 7 is given in the Supplementary material.
Similarly, the hyper-Zagreb and augmented Zagreb indices of H[n] can be calculated as in the following theorem:
Theorem 8: The hyper-Zagreb and augmented Zagreb indices of $H[n]$ are:

$$HM(H[n]) = 463 \times 2^n - 404 \tag{31}$$

$$AZI(H[n]) = 7 \times 2^{n+5} - 200 \tag{32}$$

The proof for Theorem 8 is given in the Supplementary material.

Atom–bond connectivity indices of G[n] *and* H[n]

Lemma 2. Let Aut(G) = φ_1 act on vertex set $V(G)$ and edge set $E(G)$ of a molecular graph and if the orbits of the vertices under this action are U_1, U_2,…, U_k and the orbits of the edges under this action are E_1, E_2, …, E_s, then the ABC indices are given as follows:

$$ABC_1 = \sum_{i=1}^{k} |E_j| \sqrt{\frac{d_{x_j} + d_{x_{j-1}} - 2}{d_{x_{j-1}} d_{x_j}}}, \tag{33}$$

$$ABC_2 = \sum_{i=1}^{k} |E_j| \sqrt{\frac{m_{x_j} + m_{x_{j-1}} - 2}{m_{x_{j-1}} m_{x_j}}}, \tag{34}$$

$$ABC_4 = \sum_{i=1}^{k} |E_j| \sqrt{\frac{S_{x_j} + S_{x_{j-1}} - 2}{S_{x_{j-1}} S_{x_j}}} \tag{35}$$

and

$$ABC_5 = \sum_{i=1}^{k} |E_j| \sqrt{\frac{\epsilon_{x_j} + \epsilon_{x_{j-1}} - 2}{\epsilon_{x_{j-1}} \epsilon_{x_j}}}, \tag{36}$$

where $x_i \in U_i$ and $x_{j-1}x_j \in E_j$.

Theorem 9: The first ABC index of $G[n]$ is:

$$ABC_1(G[n]) = \frac{-11}{\sqrt{2}} + 2^n \times \frac{16}{\sqrt{2}} \tag{37}$$

The proof for Theorem 9 is given in the Supplementary material.

Theorem 10: The second ABC index of $G[n]$ is:

$$ABC_2(G[n]) = \alpha_1 \left[\frac{2}{\sqrt{\beta_1}} + \frac{2}{\sqrt{\beta_1 + 3}} + \frac{1}{\sqrt{\beta_1 + 4}} + \right.$$

$$+ \sum_{i=1}^{n} \left\{ \frac{1}{\sqrt{\gamma_1 - 16(2^{n-i}) - 64(2^n) + 3}} + \frac{1}{\sqrt{\gamma_1 - 80(2^n) + 4}} + \right. \tag{38}$$

$$\left. + \frac{1}{\sqrt{\gamma_1 + 16(2^{n-i}) - 96(2^n) + 3}} + \frac{1}{\sqrt{\gamma_1 + 32(2^{n-i}) - 112(2^n)}} \right\} \right],$$

where $\alpha_1 = (16 \times 2^n - 12)^{0.5}$, $\beta_1 = 64(2^{2n}) - 80(2^n) + 21$ and $\gamma_1 = 128(2^{2n-i}) - 64(2^{2n-2i}) + 21$.

The proof for Theorem 10 is given in the Supplementary material.

Theorem 11: The fourth ABC index of $G[n]$ is:

$$ABC_4(G[n]) = \left\{ \sqrt{\frac{5}{18}} - 6\sqrt{\frac{11}{42}} - 6\sqrt{\frac{14}{63}} \right\} +$$

$$+ 2^n \left\{ 6\sqrt{\frac{14}{63}} + 6\sqrt{\frac{11}{42}} + 2\sqrt{\frac{9}{30}} + 2\sqrt{\frac{3}{4}} \right\} \tag{39}$$

The proof for Theorem 11 is given in the Supplementary material.

Theorem 12: The fifth ABC index of $G[n]$ is:

$$ABC_5(G[n]) = 2\sqrt{\frac{8n+7}{(4n+5)(4n+4)}} + 2\sqrt{\frac{8n+5}{(4n+3)(4n+4)}} + \frac{\sqrt{8n+4}}{4n+3}$$

$$+ \sum_{i=1}^{n} 2^{i+1} \left\{ \sqrt{\frac{8n+8i+7}{(4n+4i+4)(4n+4i+5)}} + \sum_{t=1}^{3} \sqrt{\frac{8n+8i+2t-2}{(4n+4i+t+1)(4n+4i+t)}} \right\} \tag{39}$$

The proof for Theorem 12 is given in the Supplementary material.

Similarly:

Theorem 13: The first ABC index of $H[n]$ is:

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$$ABC_1(H[n]) = \frac{-25}{\sqrt{2}} + 2^n \times \frac{28}{\sqrt{2}} \tag{40}$$

The proof for Theorem 13 is given in the Supplementary material.

Theorem 14: The second ABC index of $H[n]$ is:

$$ABC_2(H[n]) = \alpha_2 \left[\frac{2}{\sqrt{\beta_2}} + \frac{1}{\sqrt{\beta_2}+1} + \sum_{i=1}^{n} \left\{ \frac{1}{\sqrt{\gamma_2 - 140(2^{n-i}) - 196(2^n)}} \right. \right.$$

$$+ \frac{1}{\sqrt{\gamma_2 - 112(2^{n-i}) - 224(2^n) + 9}} + \frac{1}{\sqrt{\gamma_2 - 84(2^{n-i}) - 252(2^n) + 16}}$$

$$+ \frac{2}{\sqrt{\gamma_2 - 56(2^{n-i}) - 280(2^n) + 21}} + \frac{1}{\sqrt{\gamma_2 - 28(2^{n-i}) - 308(2^n) + 24}}$$

$$\left. \left. + \frac{1}{\sqrt{\gamma_2 - 336(2^n) + 25}} \right\} \right], \tag{41}$$

where $\alpha_2 = (28 \times 2^n - 26)^{0.5}$, $\beta_2 = 196(2^{2n}) - 336(2^n) + 143$ and $\gamma_2 = 392(2^{2n-i}) - 196(2^{2n-2i}) + 119$.

The proof for Theorem 14 is given in the Supplementary material.

Theorem 15: The fourth ABC index of $H[n]$ is:

$$ABC_4(H[n]) = \left\{ -2\sqrt{\frac{14}{63}} + 12\sqrt{\frac{12}{49}} - 8\sqrt{\frac{11}{42}} - 12\sqrt{\frac{5}{18}} \right\} +$$

$$+ 2^n \left\{ 8\sqrt{\frac{14}{63}} + 6\sqrt{\frac{11}{42}} + 12\sqrt{\frac{5}{18}} + 2\sqrt{\frac{2}{5}} \right\} \tag{42}$$

The proof for Theorem 15 is given in the Supplementary material.

Theorem 16: The fifth ABC index of $H[n]$ is

$$ABC_5(H[n]) = 2\sqrt{\frac{14n+3}{(7n+2)(7n+3)}} + \frac{\sqrt{14n+2}}{7n+2} +$$

$$+ \sum_{i=1}^{n} 2^{i+1} \left\{ \sqrt{\frac{14n+14i+3}{(7n+7i+2)(7n+7i+3)}} + \right.$$

$$\left. + \sum_{t=1}^{6} \sqrt{\frac{14n+14i+2t-11}{(7n+7i+t-5)(7n+7i+t-4)}} \right\} \tag{43}$$

The proof for Theorem 16 is given in the Supplementary material.

CONCLUSIONS

By using the definition of the Zagreb and atom–bond connectivity indices and the action of the automorphism group of graphs on the edges, this distance index was computed for regular dendrimer graphs $G[n]$ and $H[n]$. Even though the number of generations of such dendrimers was rather limited, the established formulae have a valuable diagnostic value, particularly in establishing composition rules of a global (topological) property by local contributions of the structural repeat units/monomers. In this respect, the Zagreb and atom–bond connectivity indices could be used both as a classifier of data downloaded from molecular structure databases and molecular descriptor in quantitative structure–property relationships.

SUPPLEMENTARY MATERIAL

Details about Zagreb group indices and proofs for theorems are available electronically at the pages of journal website: http://www.shd.org.rs/JSCS/, or from the corresponding author on request.

И З В О Д

ИЗРАЧУНАВАЊЕ ЗАГРЕБ ИНДЕКСА И ИНДЕКСА ПОВЕЗАНОСТИ АТОМ–ВЕЗА ОДРЕЂЕНИХ ПОРОДИЦА ДЕНДРИМЕРА КОРИСТЕЋИ ДЕЛОВАЊЕ ГРУПЕ АУТОМОРФИЗМА

UZMA AHMAD[1], SARFRAZ AHMAD[2] и RABIA YOUSAF[1]

[1]*Department of Mathematics, University of the Punjab, New Campus, Lahore, Pakistan u* [2]*Department of Mathematics, COMSATS Institute of Information Technology, Lahore, Pakistan*

У QSAR/QSPR студијама користе се тополошки индекси за предвиђање биоактивности хемијских једињења. У овом раду су одређене затворене форме различитих Загреб индекса и индекса повезаности атом–веза правилних дендримера $G[n]$ и $H[n]$ у зависности од датог параметра *n*, коришћењем дејства групе аутоморфизма. Нађено је да су ови индекси повезаности корелисани са неким физичко–хемијским својствима и коришћени су за мерење нивоа гранања молекулског скелета угљеникових атома.

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