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Benzenoid systems: a computational study of two topological indices

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Different versions of Geometric-arithmetic indices and Sum-connectivity index are the most important topological indices defined in *QSAR/QSPR*. In this paper, the first Geometric-arithmetic and Sum-connectivity indices of one important class of benzenoid systems are calculated.

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1. Introduction

Writing the mathematical model of a problem in various sciences is a helpful tool which helps a great deal to their progress. As an example, a graph can be drawn in chemistry based on atoms and the existing bonds between them for every molecule and the graph mathematical models can be defined in order to analyze the molecule. Topological indices are one of the mathematical models that can be defined by assigning a real number to the chemical molecule. The physical-chemical characteristics of the molecules can be analyzed by taking benefit from the topological indices and such properties as boiling point, entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, Acentric factor, etc can be predicted.

Consider the simple graph, G with the set of the following vertices $V = \{v_1, v_2, \ldots, v_n\}$. If $u \in V$, therefore the number of the edges ending in u is defined as the degree of vertex u and is denoted by $\deg(u)$ or simply by $d(u)$ or d_u. Various topological indices are being defined. From among the most important topological indices we can refer to the Sum-connectivity index and Geometric-arithmetic index. The Sum-connectivity index for graph G is shown by $\chi(G)$ and it is defined as follows:

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

In [1], the authors provided several basic properties for sum-connectivity index, especially lower and upper bounds in terms of sum-connectivity index, and they determined a unique tree with the given numbers of vertices and pendant vertices with the minimum value of the sum-connectivity index, and trees with the minimum, second minimum and third minimum, and with the maximum, second maximum and third maximum values of the sum-connectivity index. In [2], some properties of the sum-connectivity index were obtained for trees and unicycle graphs with given matching number. The most important works on Sum-connectivity index of molecular trees were done by Xing and his colleagues [3].

Vukicevic and Furtula [4] defined a topological index and named it first geometric–arithmetic index. They abbreviated this topological index as GA_1. The first geometric–arithmetic index of a graph G was defined as:

$$GA_1(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}.$$

The chemical applicability of the GA_1 index was examined and documented in detail in the paper [4] and the reviews [5, 6]. Some basic mathematical properties of the first geometric–arithmetic index have been established in [4, 7, 8].

Benzenoid systems form one of the most important classes of chemical graphs [9]. The benzenoid system is composed of a hexagonal mesh. Many studies have been conducted on benzenoid systems. Several topological indices are calculated for the family of benzenoid systems [10, 11, 12, 13]. Bagheri and his colleagues have calculated the Edge-Szeged and vertex-PI indices of some benzenoid systems in [14]. For further studies on benzenoid systems the readers are referred to [15, 16, 17, 18]. Yarahmadi deals with the first geometric-arithmetic for Hexagonal Systems and Phenylenes in [19].

In this article, a special kind of benzenoid systems is studied and the sum-connectivity and geometric-arithmetic indices are calculated for them. In section 2, we handle some of the fundamental subjects in mathematics and these will be taken advantage of in the next sections.

2. Preliminaries

Some basic concepts are necessary. Let G be a simple graph with n vertices, then the maximum possible vertex degree in such a graph is $n-1$. The number of vertices of degree i in G, for $i=1,2,\ldots,n-1$ is denoted by n_i and the number of edges joining the vertices of degrees i and j in graph G for $2\le i\le j\le n-1$ is denoted by $x_{i,j}\left(x_{i,j}\ge 0\right)$.Clearly, for every arbitrary graph G, we have $x_{i,j}=x_{j,i}$ and $n_0=0$. Then the sum-connectivity and the first geometric-arithmetic indices can be written as,

$$\chi(G)=\sum_{1\le i\le j\le n-1}\frac{1}{\sqrt{i+j}}x_{i,j}.$$

And,

$$GA_1(G)=\sum_{1\le i\le j\le n-1}\frac{2\sqrt{i\,j}}{i+j}x_{i,j}.$$

For any graph G there are,

$$n_1+n_2+\cdots+n_{n-1}=n.$$

And,

$$\begin{aligned}
2x_{1,1}+x_{1,2}+\cdots+x_{1,n-1}&=n_1\\
x_{1,2}+2x_{2,2}+\cdots+x_{2,n-1}&=2n_2\\
\vdots\qquad\qquad&\quad\vdots\\
x_{1,n-1}+x_{2,n-1}+\cdots+2x_{n-1,n-1}&=(n-1)x_{n-1}.
\end{aligned}$$

2. Main results

In this section, we investigate the sum-connectivity and first geometric-arithmetic indices for special types of benzenoid systems.

Example 1. Let $k\in N$ and let $L(k)$ be a benzenoid system which is depicted below. We calculated the sum-connectivity (χ) and first geometric-arithmetic indices (GA_1) for $L(k)$.

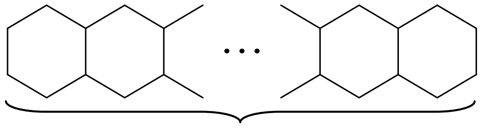


Fig. 1. benzenoid systems of $L(k)$.

In the benzenoid system $L(k)$, we have only vertices of degree 2 and 3. Therefore, by simple calculations we obtain,

$$n=\left|V(L(k))\right|=4k+2.$$
$$m=\left|E(L(k))\right|=5k+1.$$
$$n_2=2k+4.$$
$$n_3=2k-2.$$

And,

$$\begin{cases}x_{2,2}=6,\\ x_{2,3}=4k-4,\\ x_{3,3}=k-1.\end{cases}$$

The sum-connectivity and first geometric-arithmetic indices are calculated as follows,

$$\chi(L(k))=\frac{1}{\sqrt4}x_{2,2}+\frac{1}{\sqrt5}x_{2,3}+\frac{1}{\sqrt6}x_{3,3},$$
$$GA_1(L(k))=x_{2,2}+\frac{2\sqrt6}{5}x_{2,3}+x_{3,3}.$$

Therefore,

$$\chi(L(k))=3+\frac{4k-4}{\sqrt5}+\frac{k-1}{\sqrt6}=\left(\frac{\sqrt6}{6}+\frac{4\sqrt5}{5}\right)k$$
$$+3-\frac{\sqrt6}{6}-\frac{4\sqrt5}{5}.$$
$$GA_1(L(k))=6+\frac{2\sqrt6}{5}(4k-4)+k-1$$
$$=\left(\frac{8\sqrt6}{5}+1\right)k+5-\frac{8\sqrt6}{5}.$$

3.1. Hexagonal system $T(n,m)$

A hexagonal trapezoid $T(n,m),(m\ge n)$ is a hexagonal system consisting of rows $m-n+1$ of benzenoid chain in which every row has exactly one hexagon less than the its immediate lower row. For $m=4$ and $n=1,2,3,4$, the hexagonal systems $T(n,m)$ are shown in Fig. 2. It is clear that the hexagonal system $T(k,k)$ is the same as benzenoid system $L(k)$.

The number of vertices of $T(n,m)$ is equal to $\left|V(T(n,m))\right|=m^2-n^2+4m+2$ and the number of edges of $T(n,m)$ is equal to $\left|E(T(n,m))\right|=\frac{3}{2}\left(m^2-n^2\right)+\frac{9}{2}m+\frac{1}{2}n+1$. In the benzenoid system $T(n,m)$, we have only vertices of degree 2 and 3. Therefore by simple calculations we obtain,

$$\begin{cases} n_2 = 3m - n + 4, \\ n_3 = m^2 - n^2 + m + n - 2. \end{cases}$$

And,

$$\begin{cases} x_{2,2} = 6, \\ x_{2,3} = 6m - 2n - 4, \\ x_{3,3} = \frac{3}{2}\left(m^2 - n^2\right) - \frac{3}{2}m + \frac{5}{2}n - 1. \end{cases}$$

The sum-connectivity and first geometric-arithmetic indices are calculated as follows,

$$\chi(T(n,m)) = \frac{1}{\sqrt{4}} x_{2,2} + \frac{1}{\sqrt{5}} x_{2,3} + \frac{1}{\sqrt{6}} x_{3,3},$$

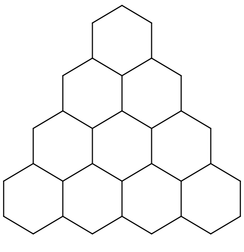
$$GA_1(T(n,m)) = x_{2,2} + \frac{2\sqrt{6}}{5} x_{2,3} + x_{3,3}.$$

Therefore,

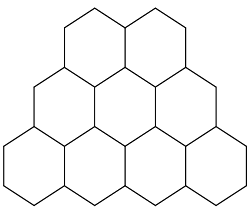
$$\chi(T(n,m)) = 3 + \frac{1}{\sqrt{5}}(6m - 2n - 4) + \frac{1}{\sqrt{6}}\left(\frac{3}{2}\left(m^2 - n^2\right) - \frac{3}{2}m + \frac{5}{2}n - 1\right).$$

$$GA_1(T(n,m)) = \frac{3}{2}\left(m^2 - n^2\right) - \frac{3}{2}m + \frac{5}{2}n + 5 + \frac{12\sqrt{6}}{5}m - \frac{4\sqrt{6}}{5}n - \frac{8\sqrt{6}}{5}.$$

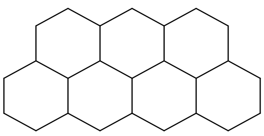
Table 1 exhibits the amount of sum-connectivity (χ) and the first geometric-arithmetic (GA_1) indices of the benzenoid system $T(n,m)$, for $m = 1,2,3,4$ and $n = 1,\ldots,m$.



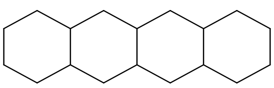
a) The graph $T(1,4)$



b) The graph $T(2,4)$



c) The graph $T(3,4)$



d) The graph $T(4,4)$

Fig. 2. The graph $T(n,4)$.

Table 1. The χ *and* GA_1 *indices of* $T(n,m)$.

m	n	$\chi(T(n,m))$	$GA_1(T(n,m))$
1	1	3.0000	6.0000
2	1	6.9080	14.8788
	2	5.1971	10.9192
3	1	12.0408	26.7576
	2	10.3299	22.7980
	3	7.3942	15.8384
4	1	18.3983	41.6363
	2	16.6874	37.6767
	3	13.7517	30.7171
	4	9.5913	20.7576

Theorem 1: Consider the benzenoid system $T(n,m)$,

a) If $k \in \{1,2,3,\cdots\}$, $k' \in \{1,2,3,\cdots\}$ and $k > \frac{5k'-3}{3}$ then,

$$\chi(T(3k - 5k' + 3, 5k - 3k' + 3)) = \chi(T(4k', 4k + 2))$$

b) If $k \in \{0,1,2,3,\cdots\}$, $k' \in \{0,1,2,3,\cdots\}$ and $k > \frac{5k'-1}{3}$ then,

$$\chi(T(3k - 5k' + 1, 5k - 3k' + 1)) = \chi(T(4k' + 1, 4k + 1))$$

c) If $k \in \{1,2,3,\cdots\}$, $k' \in \{0,1,2,3,\cdots\}$ and $k > \frac{5k'+1}{3}$ then,

$$\chi(T(3k - 5k' - 1, 5k - 3k' - 1)) = \chi(T(4k' + 2, 4k))$$

d) If $k \in \{1,2,3,\cdots\}$, $k' \in \{1,2,3,\cdots\}$ and $k > \frac{5k'}{3}$ then,

$$\chi(T(3k - 5k', 5k - 3k' + 2)) = \chi(T(4k' + 3, 4k + 3))$$

Proof: Let r and s be the arbitrary integer numbers. Then

$$\chi(T(n+s, m+r)) - \chi(T(n,m)) = \frac{\sqrt{6}}{60}\begin{pmatrix} 12\sqrt{30}r - 4\sqrt{30}s + 30mr + 15r^2 \\ -30ns - 15s^2 - 15r + 25s \end{pmatrix} = 0.$$

Now, consider $s = 3r$. Then,

$$\chi(T(n+s, m+r)) - \chi(T(n,m)) = \frac{\sqrt{6}}{2} r(m - 4r - 3n + 2) = 0$$

Therefore,

$$m-4r-3n+2=0 \Rightarrow r=\frac{m-3n+2}{4}. \quad (1)$$

For the positive integer n four cases are taken into consideration:

Case 1: $n \equiv 0 \pmod 4$

In this case, by substituting $n=4k'$ in equation (1) we have,

$$\begin{cases} m=4k+2, \\ r=k-3k'+1, \\ s=3k-9k'+3. \end{cases}$$

Then we have,

$$\chi(T(n+s,m+r))=\chi(T(n,m)) \Rightarrow$$
$$\chi(T(3k-5k'+3,5k-3k'+3))=\chi(T(4k',4k+2))$$

For the benzenoid system $T(n,m)$, m and n are positive integer, also $m \geq n$. So, in this case, we obtain $k \geq k'$ from $4k+2 \geq 4k'$. Also, for any positive integer k and k', $5k-3k'+3 \geq 3k-5k'+3$ holds. On the other hand, for any positive integer numbers k and k', we must establish $3k-5k'+3>0$, and to do so we must have $k>\frac{5k'-3}{3}$. The proof of case 1 is now complete.

Case 2: $n \equiv 1 \pmod 4$

In this case, by substituting $n=4k'+1$ in equation (1) we have,

$$\begin{cases} m=4k+1, \\ r=k-3k', \\ s=3k-9k'. \end{cases}$$

Then, we have,

$$\chi(T(n+s,m+r))=\chi(T(n,m)) \Rightarrow$$
$$\chi(T(3k-5k'+1,5k-3k'+1))=\chi(T(4k'+1,4k+1))$$

For the benzenoid system $T(n,m)$, m and n are positive integer, also $m \geq n$. So, in this case we obtain $k \geq k'$ from $4k+1 \geq 4k'+1$. Also, for any positive integer k and k', the $5k-3k'+1 \geq 3k-5k'+1$ is true. On the other hand, for any positive integer numbers k and k' we must establish $3k-5k'+1>0$ and to do so we must have $k>\frac{5k'-1}{3}$. Then the proof of case 2 is now complete.

Case 3: $n \equiv 2 \pmod 4$

In this case, by substituting $n=4k'+2$ in equation (1) we have,

$$\begin{cases} m=4k, \\ r=k-3k'-1, \\ s=3k-9k'-3. \end{cases}$$

Then, we have,

$$\chi(T(n+s,m+r))=\chi(T(n,m)) \Rightarrow$$
$$\chi(T(3k-5k'-1,5k-3k'-1))=\chi(T(4k'+2,4k))$$

For the benzenoid system $T(n,m)$, m and n are positive integer numbers, also $m \geq n$. So, in this case we obtain $k>k'$ from $4k \geq 4k'+2$. Also $5k-3k'-1 \geq 3k-5k'-1$ holds for any positive integer numbers k and k'. On the other hand, for any positive integer numbers k and k' we must establish $3k-5k'-1>0$ and to do so it is necessary to have $k>\frac{5k'+1}{3}$. Then, the proof of case 3 is now complete.

Case 4: $n \equiv 3 \pmod 4$

In this case, by substituting $n=4k'+3$ in equation (1) we have,

$$\begin{cases} m=4k+3, \\ r=k-3k'-1, \\ s=3k-9k'-3. \end{cases}$$

Then, we have

$$\chi(T(n+s,m+r))=\chi(T(n,m)) \Rightarrow$$
$$\chi(T(3k-5k',5k-3k'+2))=\chi(T(4k'+3,4k+3))$$

For the benzenoid system $T(n,m)$, m and n are positive integer numbers, also $m \geq n$. So, in this case, we obtain $k \geq k'$ from $4k+3 \geq 4k'+3$. Also, for any positive integer number k and k', $5k-3k'+2 \geq 3k-5k'$ is true. On the other hand, for any positive integer numbers k and k', $3k-5k'>0$ must be established and for getting to it we must have $k>\frac{5k'}{3}$. Then the proof of case 4 is now complete.

Theorem 2: Consider the benzenoid system $T(n,m)$,

a) If $k \in \{1,2,3,\cdots\}$, $k' \in \{1,2,3,\cdots\}$ and

$$k > \frac{5k' - 3}{3}$$

then,

$$GA_1\left(T\left(3k - 5k' + 3, 5k - 3k' + 3\right)\right) = GA_1\left(T\left(4k', 4k + 2\right)\right)$$

b) If $k \in \{0,1,2,3,\cdots\}$, $k' \in \{0,1,2,3,\cdots\}$ and

$$k > \frac{5k' - 1}{3}$$

then,

$$GA_1\left(T\left(3k - 5k' + 1, 5k - 3k' + 1\right)\right) = GA_1\left(T\left(4k' + 1, 4k + 1\right)\right)$$

c) If $k \in \{1,2,3,\cdots\}$, $k' \in \{0,1,2,3,\cdots\}$ and

$$k > \frac{5k' + 1}{3}$$

then,

$$GA_1\left(T\left(3k - 5k' - 1, 5k - 3k' - 1\right)\right) = GA_1\left(T\left(4k' + 2, 4k\right)\right)$$

d) If $k \in \{1,2,3,\cdots\}$, $k' \in \{1,2,3,\cdots\}$ and

$$k > \frac{5k'}{3}$$

then,

$$GA_1\left(T\left(3k - 5k', 5k - 3k' + 2\right)\right) = GA_1\left(T\left(4k' + 3, 4k + 3\right)\right)$$

Proof: Let r and s be the arbitrary integer numbers. Then

$$GA_1\left(T(n+s, m+r)\right) - GA_1\left(T(n,m)\right) = \frac{12\sqrt{6}}{5}r - \frac{4\sqrt{6}}{5}s + 3mr + \frac{3}{2}r^2 - 3ns - \frac{3}{2}s^2 - \frac{3}{2}r + \frac{5}{2}s = 0.$$

Now, consider $s = 3r$. Then,

$$GA_1\left(T(n+s, m+r)\right) - GA_1\left(T(n,m)\right) = 3r\left(m - 4r - 3n + 2\right) = 0$$

Therefore,

$$m - 4r - 3n + 2 = 0 \Rightarrow r = \frac{m - 3n + 2}{4}. \quad (2)$$

For the positive integer n four cases are taken into consideration, and the rest of the proof is similar to Theorem 1.

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