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Benzenoid Systems: A Computational Study of Two Topological Indices

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***Abstract:** Different versions of Atom bond connectivity index and Randic' index are the most important topological indices defined in QSAR/QSPR. In this paper, the Atom bond connectivity index and Randic indices of one important class of Benzenoid systems are calculated.*

***Keywords:** Topological indices, Benzenoid systems, Randic' index, Atom bond connectivity index and Hexagonal system.*
***2000 Mathematics subject classification:** 05C12,05C75*

I. 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 $V = \{v_1, v_2, v_3, \dots . v_n\}$. If $u \in V$, 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, Randic index and Atom bond connectivity index.

In 1975, the chemist Milan Randić [19] proposed a topological index R under the name ''branching index'', suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. The branching index was renamed as the molecular connectivity index and is often referred to as the Randić index. There is a good correlation between the Randić index and several physico-chemical properties of alkanes: boiling points, enthalpies of formation, chromatographic retention times. The Randić index R(G) of a graph G = (V, E) is defined as follows:

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

In [1], the authors provided several basic properties for Randic' index, especially lower and upper bounds in terms of Randic' index and In [2] they determined upper bound for Randic index of trees. In [4], [5], [6] trees with the maximum Randic' index and trees with small Randic' index are discussed. In [3], Randic' index and diameter of chemical graphs were studied.

Estarda [7] defined a topological index and named it first Atom bond connectivity index. He abbreviated this topological index as ABC(G). The ABC(*G*) is defined as

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

The chemical applicability of the ABC index was examined and documented in detail in the paper [7] the ABC index of connected graphs and trees in [8], [9]. Some basic mathematical concepts and Extreme ABC index have been established in [10].

Benzenoid systems form one of the most important classes of chemical graphs. 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[11], [12], [13]. Bagheri and his colleagues have calculated the Edge-Szeged and vertex-indices of some benzenoid systems in [14]. For further studies on benzenoid systems the readers are referred to [15], [16], [17], [18].

In this article, a special kind of Benzenoid systems is studied and the Randic and ABC 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

II. 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 $i = 1,2, \dots, n - 1$ is denoted by n_i and

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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 $x_{i,j}$ $(x_{i,j} \ge 0)$ .Clearly, for every arbitrary graph *G*, we have $x_{i,j} = x_{j,i}$ and $n_0 = 0$. Then the Randic and ABC indices can be written as,

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

and,

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

For any graph *G*,

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

And,

$$2x_{1,1} + x_{1,2} + \cdots + x_{1,n-1} = n_1$$

$$x_{1,2} + 2x_{2,2} + \cdots + x_{2,n-1} = 2n_2$$

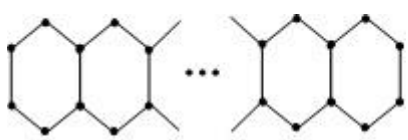
$$\vdots \qquad \vdots$$

$$x_{1,n-1} + x_{2,n-1} + \cdots + 2x_{n-1,n-1} = (n-1)x_{n-1}\ .$$

III. RESULTS

In this section, we investigate the Randic and Atom bond connectivity 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, Randic and Atom bond connectivity indices for $L(K)$.



k- times

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,

$$n = |V(L(K))\,| = 4K + 2.$$

$$m = |E(L(K))\,| = 5K + 1.$$

$$n_2 = 2K + 4.$$

$$n_3 = 2K - 2.$$

and,

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

The Randic and Atom bond connectivity indices are calculated as follows

$$R\big(L(K)\big) = \sum_{i,j} \frac{1}{\sqrt{i.j}} x_{i,j} = \sum_{2,3} \frac{1}{\sqrt{i.j}} x_{i,j}$$

$$R\big(L(K)\big) = \frac{1}{2} x_{2,2} + \frac{1}{\sqrt{6}} x_{2,3} + \frac{1}{3} x_{3,3}$$

and

$$ABC\big(L(K)\big) = \sum_{i,j} \sqrt{\frac{i+j-2}{i.j}} x_{i,j} = \sum_{2,3} \sqrt{\frac{i+j-2}{i.j}} x_{i,j}$$

$$ABC\big(L(K)\big) = \tfrac{1}{\sqrt{2}} x_{2,2} + \tfrac{1}{\sqrt{2}} x_{2,3} + \tfrac{2}{3} x_{3,3}$$

Therefore,

$$R\big(L(K)\big) = \tfrac{1}{2}(6) + \tfrac{4k-4}{\sqrt{6}} + \tfrac{k-1}{3}$$
$$= K\left(\tfrac{4}{\sqrt{6}} + \tfrac{1}{3}\right) + (\tfrac{8}{3} - \tfrac{4}{\sqrt{6}})$$
$$ABC\big(L(K)\big) = \tfrac{1}{\sqrt{2}}(6) + \tfrac{4k-4}{\sqrt{2}} + \tfrac{2}{3}(k-1)$$
$$= K\left(2\sqrt{2} + \tfrac{2}{3}\right) + \left(\sqrt{2} - \tfrac{2}{3}\right).$$

Hexagonal System $T(n, m)$

A hexagonal trapezoid $T(n, m)$, $(m \ge n)$ is a hexagonal system consisting of rows of $m - n + 1$ of Benzenoid chain in which every row has exactly one hexagon less than its immediate lower row. For $m = 4$ *and* $n = 1, 2, 3, 4$, hexagonal systems $T(n, m)$ is 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 $\big|V\big(T(n, m)\big)\big| = m^2 - n^2 + 4m + 2$ and the number of edges of $T(n, m)$ is equal to $\big|E\big(T(n, m)\big)\big| = \frac{3}{2}(m^2 - n^2) + \frac{9}{2}m + \frac{1}{2}n + 1.$ 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,

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

The Randic and Atom bond connectivity indices are calculated as follows,

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

$$ABC(T(n,m)) = \frac{1}{\sqrt{2}}x_{2,2} + \frac{1}{\sqrt{2}}x_{2,3} + \frac{2}{3}x_{3,3}$$

Therefore,

$R(T(n,m)) = 3 + \frac{1}{\sqrt{6}}(6m - 2n - 4) + \frac{1}{3}\left(\frac{3}{2}(m^2 - n^2) -\right.$
$32m+52n-1$

$$= \frac{1}{2}(m^2 - n^2) + \frac{m}{2}(2\sqrt{6} - 1) + \frac{n}{6}(5 - 2\sqrt{6}) + \left(\frac{8\sqrt{6}-12}{3\sqrt{6}}\right) \quad (1)$$

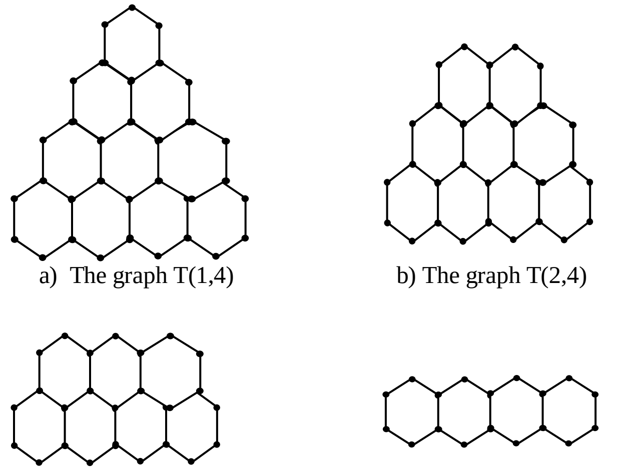
$$ABC(T(n,m)) = \frac{1}{\sqrt{2}}(6) + \frac{1}{\sqrt{2}}(6m - 2n - 4) + \frac{2}{3}\left(\frac{3}{2}(m^2 - n^2) - \frac{3}{2}m + \frac{5}{2}n - 1\right).$$

$$= m^2 + n^2 + \frac{m}{\sqrt{2}}(6 - \sqrt{2}) + \frac{n}{3\sqrt{2}}(5\sqrt{2} - 6) + \left(\frac{6 - 2\sqrt{2}}{3\sqrt{2}}\right) \quad (2)$$

Table 1 exhibits the amount of the Randic and Atom bond connectivity indices of the benzenoid system $T(n,m)$ for $m = 1,2,3,4, and\ n = 1, \dots . m$

Table 1.The R and ABC indices of T(n, m)

m	n	$R(T(n,m))$	$ABC(T(n,m))$
1	1	3	4.2426
2	1	6.4495	10.4853
	2	4.9663	7.7377
3	1	10.8989	18.7279
	2	9,4158	15.9803
	3	6.9327	11.2328
4	1	16.3485	37.9705
	2	16.1986	26.2230
	3	12.7155	18.6470
	4	8.8990	14.7279



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)

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

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

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

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

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

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

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

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

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

Proof:

Let r and s be the arbitrary integer numbers, then

$R(T(n + s, m + r)) - R(T(n,m))$

$= \frac{1}{6}(6\sqrt{6}r - 2\sqrt{6}s + 6mr + 3r^2 - 6ns - 3s^2 - 3r + 5s = 0$

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

$R(T(n+s, m+r)) - R(T(n,m)) =$

$r(m - 4r - 3n + 2) = 0$

Therefore,

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

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

Case 1: $n \equiv 0 \ (mod\ 4)$

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

$$m = 4k + 2,$$
$$r = k - 3k' + 1,$$
$$s = 3k - 9k' + 3.$$

Then we have,

$R(T(n+s, m+r)) = R(T(n,m)) \Rightarrow$

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

For the Benzenoid system $T(n,m), m\ and\ n$ *are positive* integers, also $m \geq n$. So, in this case, we obtain $k \geq k'$ from $4k + 2 \geq 4k'$.

Also, for any two positive integers $k\ and\ k'$, 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: $n \equiv 1 \ (mod\ 4)$

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

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

$R(T(n+s, m+r)) = R(T(n,m)) \Rightarrow$

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

$R\left(T(4k' + 1, 4k + 1)\right)$.

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 $k\ and\ k'$, we must establish $5k - 3k' + 1 \geq 3k - 5k' + 1$ 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 $k > \frac{5k'-1}{3}$

The proof of case 2 is now complete.

Case 3: $n \equiv 2 \ (mod\ 4)$

In this case, by substituting $n = 4k' + 2$ in equation (3) , we have

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

Then, we have

$R(T(n+s, m+r)) = R(T(n,m)) \Rightarrow$

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

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 $4k \geq 4k' + 2$. Also,

$5k - 3k' - 1$ holds for any positive integer $k\ and\ k'$. On the other hand, for any positive integer numbers $k\ and\ k'$ we must establish $3k - 5k' + 1 > 0$ and to do so we must have $k > \frac{5k'+1}{3}$.

The proof of case 3 is now complete.

Case 4: $n \equiv 3 \ (mod\ 4)$

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

$R(T(n+s, m+r)) = R(T(n,m)) \Rightarrow$

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

$R\left(T(4k' + 3, 4k + 3)\right)$.

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 $4k + 3 \geq 4k' + 3$. Also,

$5k - 3k' + 2 > 3k - 5k'$ holds for any positive integers $k\ and\ k'$. On the other hand, for any positive integer numbers $k\ and\ k'$ we must establish $3k - 5k' > 0$. For getting to it we must have $k > \frac{5k'}{3}$ .The proof of case 4 is now complete.

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

a) If $k \in \{1,2,3, \ldots\ldots\}$,$k' \in \{1,2,3, \ldots.\}$ and $k > \frac{5k'-3}{3}$, then ABC$\left(T(3k-5k'+3,5k-3k'+3)\right) = ABC\left(T(4k', 4k+2)\right)$

b) If $k \in \{0,1,2,3, \ldots\ldots\}$,$k' \in \{0,1,2,3, \ldots.\}$ and $k > \frac{5k'-1}{3}$, then ABC $(T(3k-5k'+1,5k-3k'+$ *1=ABCT4k'+1, 4k+1*

c) If $k \in \{1,2,3, \ldots\ldots\}$,$k' \in \{0,1,2,3, \ldots.\}$ and $k > \frac{5k'+1}{3}$, then ABC $\left(T(3k-5k'-1,5k-3k'-1)\right) = ABC\left(T(4k'+2, 4k)\right)$

d) If $k \in \{1,2,3, \ldots\ldots\}$,$k' \in \{1,2,3, \ldots.\}$ and $k > \frac{5k'}{3}$ ABC$\left(T(3k-5k', 5k-3k'+2)\right) = ABC\left(T(4k'+3, 4k+3)\right)$

Proof:

Let r and s be the arbitrary integer numbers, then ABC$\left(T(n+s\,, m+r)\right) - ABC\left(T(n,m)\right)$

$$= \frac{1}{6}\left(\frac{36}{\sqrt{2}}r - \frac{12}{\sqrt{2}}s + 12mr + 6r^2 - 12ns - 6s^2 - 6r + 10s\right) = 0$$

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

ABC$\left(T(n+s\,, m+r)\right) - ABC\left(T(n,m)\right)$

$= 2\,r(m-4r-3n+2) = 0$

Therefore,

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

IV. CONCLUSION

The future study can be made by comparing the topological indices on Benzenoid systems.

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