Valency based topological indices of organosilicon dendrimers and cactus chains

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Topological indices are the global parameters defined for the simple graphs such that they give the same numerical value if the graphs are isomorphic. These numbers are of much importance because of their chemical importance, they correlate certain physico-chemical properties of certain organic compounds such hydrocarbons etc. A chemical graph is a graph which is created from some molecular structure by applying some graphical operations. Valency is a local graph parameter, which is defined for every vertex as the number of connections with other vertices in a graph, just like for an atom in a molecule. Dendrimers are recognized as one of the major commercially available nanoscale building blocks, large and complex molecules with well defined chemical structure. Cactus chains are simple linear polymers which were first known as Husimi trees. A cactus graph is a connected graph in which no edge lies in more than one cycle. In this article, we study general Randić, harmonic, atom-bond connectivity (ABC), and geometric arithmetic (GA) indices for organosilicon dendrimers and cactus chains of three types.

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1. Introduction and preliminary results

Nanobiotechnology is a rapidly advancing area of scientific and technological opportunity that applies the tools and processes of nanofabrication to build devices for studying biosystems. *Dendrimers* are one of the main objects of this new area of science. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers using a nanoscale fabrication process. Dendrimers are recognized as one of the major commercially available nanoscale building blocks, large and complex molecules with very well defined chemical structure. From a polymer chemistry point of view, dendrimers are nearly perfect monodisperse macromolecules with a regular and highly branched three dimensional architecture. They consist of three major architectural components: core, branches and end groups. New branches emitting from a central core are added in steps until a tree-like structure is created. The nanostar dendrimer is a part of a new group of macroparticles that appear to be photon funnels just like artificial antennas. These macromolecules and more precisely those containing phosphorus are used in the formation of nanotubes, micro and macrocapsules, nanolatex, coloured glasses, chemical sensors, modified electrodes and so on [3].

In this paper, we consider a class of simple linear polymers called *cactus chains*. Cactus graphs were first known as *Husimi trees*; they appeared in the scientific literature some sixty years ago in papers by Husimi and Riddell concerned with cluster integrals in the theory of condensation in statistical mechanics [12, 15, 20].

In this article, H is considered to be simple connected graph with vertex set $V(H)$ and edge set $E(H)$ and degree of vertex $a \in V(H)$ is d_a. The notations used in this article are mainly taken from the books [6, 11, 22].

The very first and oldest degree based topological index is *Randić* index [23] denoted by $\chi(H)$ and introduced by *Milan Randić* in 1975.

Definition. The Randić index of graph H is defined as

$$R_{-\frac{1}{2}}(H) = \sum_{ab \in E(H)} \frac{1}{\sqrt{d_a d_b}}$$

The general Randić index was proposed by Bollobás and Erdös [4] and Amic et al. [2] independently, in 1998. Then it has been extensively studied by both mathematicians and theoretical chemists [16]. Many important mathematical properties have been established [5]. For a survey of results, we refer to the new book by Li and Gutman [18].

Definition. The general *Randić* index $R_\alpha(H)$ is the sum of $(d_u d_v)^\alpha$ over all edges $e = ab \in E(H)$ defined as

$$R_\alpha(H) = \sum_{ab\in E(H)} (d_a d_b)^\alpha$$

Obviously $R_{-\frac{1}{2}}(H)$ is the particular case of $R_\alpha(H)$ when $\alpha = -\frac{1}{2}$.

Another variant of the Randić index named the harmonic index which first appeared in [8].

Definition. For a graph G, the harmonic index $\mathrm{H}(G)$ is defined as

$$\mathrm{H}(G) = \sum_{ab\in E(H)} \frac{1}{\sqrt{d_a d_b}}$$

One of the well-known connectivity topological index is *atom-bond connectivity* (ABC) index introduced by *Estrada* et al. in [7].

Definition. For a graph H, the ABC index is defined as

$$ABC(H) = \sum_{ab\in E(H)} \sqrt{\frac{d_a + d_b - 2}{d_a d_b}}$$

Another well-known connectivity topological descriptor is *geometric-arithmetic* (GA) index which was introduced by *Vukičević* et al. in [21].

Definition. Consider a graph H, then its GA index is defined as

$$GA(H) = \sum_{ab\in E(H)} \frac{2\sqrt{d_a d_b}}{(d_a + d_b)}$$

In this paper, we compute general Randić R_α for $\alpha = 1, \frac{1}{2}, -1, -\frac{1}{2}$, harmonic, ABC and GA indices for an important type of dendrimer and cactus triangular and square chains. In the following section, we compute these topological indices for organosilicon dendrimer. We encourage readers to review these papers [13, 14, 17] to further study these topological indices for nanostructures and networks.

2. Topological indices of organosilicon dendrimer

Nakayama and Lin in [19] prepared the organosilicon dendrimer composed of 16 thiophene rings, $C_{64}H_{44}S_{16}Si_5$. The aim of this section is to compute the valency based topological indices of organosilicon dendrimer $G[n]$, $n \geq 1$. The first two members of this dendrimer class is depicted in Fig. 1. See [24] for further study of this class of dendrimers.

Lemma 2.1. Let $G = G[n]$ be the molecular graph of organosilicon dendrimer for $n \geq 1$, then $|V(G)| = 32\times 3^{n-1} - 11$.

Proof. This graph is constructed from four isomorphic branches sharing the common vertex. Let g_n be one of the four isomorphic branches. This graph g_n contains $\sum_{j=1}^{n} 3^j$ vertices, which is a geometric series having sequence of its partial sums is $\frac{1}{2}(3^n - 1)$. Then $G[n]$ contains $4\sum_{j=1}^{n} 3^j = 2(3^n - 1)$ pentagons, which clearly shows that $G[n]$ is non-bipartite graph. The graph G_n also has $4\sum_{j=1}^{n-1} 3^j + 1 = 2\times 3^{n-1} - 1$ vertices outside pentagons. So total number of vertices in $G[n]$ are

$$|V(G[n])| = 4\sum_{j=1}^{n}(6\times 3^j - 3^{n-1}) + 1 = 32\times 3^{n-1} - 11.$$

Lemma 2.2. Let $G = G[n]$ be the molecular graph of organosilicon dendrimer for $n \geq 1$, then $|E(G)| = 38\times 3^{n-1} - 14$.

Proof. This graph is constructed from four isomorphic branches sharing the common vertex. Let g_n be one of the four isomorphic branches. This graph g_n contains $4\sum_{j=1}^{n} 3^{j-1} = 2\times 3^{n-1} - 1$ edges outside pentagons. Then $G[n]$, of course contains $4\{4\sum_{j=1}^{n} 3^{j-1}\} = 8\times 3^n - 4$ edges outside pentagons. Also $G[n]$ contains $4\sum_{j=1}^{n} 3^j = 2(3^n - 1)$ pentagons. So cardinality of edge set of $G[n]$ becomes,

$$|E(G[n])| = 4\{4\sum_{j=1}^{n} 3^{j-1} + 5\sum_{j=1}^{n} 3^j\} = 38\times 3^{n-1} - 14.$$

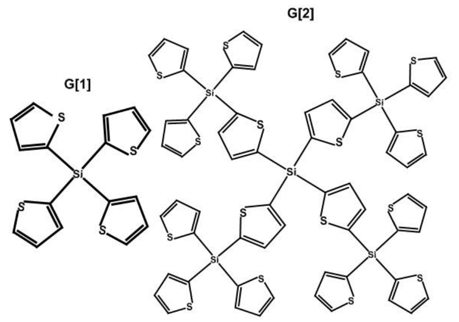

Fig. 1. The first two members of $G[n]$ *with* $n = 1,2$.

Now we compute certain degree based topological indices for these dendrimers. We can clearly see that, there are three type of edges in graph of this dendrimer based on degrees of end vertices of each edge. Table 1shows such a partition for $G[n]$ for $n \geq 1$.

Table 1. Edge partition of organosilicon dendrimer $G[n]$, $n \geq 1$ *based on degrees of end vertices of each edge.*

(d_a, d_b) where $ab \in E(H)$	(2,2)	(2,3)	(3,4)
Cardinality of partite set	$6(3^n - 1)$	$4(3^n - 1)$	$8 \times 3^{n-1} - 4$

In the following theorem, we compute general Randi c′ R_α for $\alpha = 1, \frac{1}{2}, -1, -\frac{1}{2}$ for $G[n]$, $n \geq 1$.

Theorem 2.1. Consider $G[n]$, $n \geq 1$, then its general Randi c′ index is equal to

$$R_\alpha(G[n]) = \begin{cases} 240 \times 3^{n-1} - 96, & \alpha = 1; \\ (12\sqrt{6} + 16\sqrt{3} + 36)3^{n-1} - 8\sqrt{3} - 4\sqrt{6} - 12, & \alpha = \frac{1}{2}; \\ \frac{43}{6} \times 3^{n-1} - \frac{5}{2}, & \alpha = -1; \\ (\frac{4\sqrt{3}}{3} + 2\sqrt{6} + 9)3^{n-1} - \frac{2\sqrt{6}}{3} - \frac{2\sqrt{3}}{3} - 3, & \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Consider the organosilicon dendrimer $G[n]$, $n \geq 1$ with n as defining parameter. There are three types of edges in H based on degrees of end vertices of each edge. Table 1 shows such an edge partition of H.

For $\alpha = 1$

Now we apply the formula of $R_\alpha(H)$ for $\alpha = 1$.

$$R_1(H) = \sum_{ab \in E(H)} (d_a \times d_b)$$

By using edge partition given in Table 1, we get a non-linear expression,

$$R_1(G[n]) = 6(3^n - 1)(2 \times 2) + 4(3^n - 1)(2 \times 3) + (8 \times 3^{n-1} - 4)(3 \times 4)$$

After simplifying, we get

$$R_1(G[n]) = 240 \times 3^{n-1} - 96$$

For $\alpha = \frac{1}{2}$

We apply the formula of $R_\alpha(H)$ for $\alpha = \frac{1}{2}$.

$$R_{\frac{1}{2}}(H) = \sum_{ab \in E(H)} \sqrt{(d_a \times d_b)}$$

By using edge partition given in Table 1, we get this exponential expression in parameters n,

$$R_{\frac{1}{2}}(G[n]) = 6(3^n - 1)\sqrt{2 \times 2} + 4(3^n - 1)\sqrt{2 \times 3} + (8 \times 3^{n-1} - 4)\sqrt{3 \times 4}$$

$$R_{\frac{1}{2}}(G[n]) = (12\sqrt{6} + 16\sqrt{3} + 36)3^{n-1} - 8\sqrt{3} - 4\sqrt{6} - 12$$

For $\alpha = -1$

We apply the formula of $R_\alpha(H)$ for $\alpha = -1$.

$$R_{-1}(H) = \sum_{ab \in E(H)} \frac{1}{(d_a \times d_b)}$$

$$R_{-1}(G[n]) = 6(3^n - 1)(\frac{1}{2 \times 2}) + 4(3^n - 1)(\frac{1}{2 \times 3}) + (8 \times 3^{n-1} - 4)(\frac{1}{3 \times 4})$$

$$R_{-1}(G[n]) = \frac{43}{6} \times 3^{n-1} - \frac{5}{2}$$

For $\alpha = -\frac{1}{2}$

We apply the formula of $R_\alpha(H)$ for $\alpha = -\frac{1}{2}$.

$$R_{-\frac{1}{2}}(H) = \sum_{ab\in E(H)} \frac{1}{\sqrt{(d_a \times d_b)}}$$

$$R_{-\frac{1}{2}}(G[n]) = 6(3^n - 1)(\frac{1}{\sqrt{2\times 2}}) + 4(3^n - 1)(\frac{1}{\sqrt{2\times 3}}) +$$

$$(8\times 3^{n-1} - 4)(\frac{1}{\sqrt{3\times 4}})$$

$$R_{-\frac{1}{2}}(G[n]) = (\frac{4\sqrt{3}}{3} + 2\sqrt{6} + 9)3^{n-1} - \frac{2\sqrt{6}}{3} - \frac{2\sqrt{3}}{3} - 3$$

In the following theorem, we compute harmonic index for these dendrimers.

Theroem 2.2. For $G[n]$, $n \geq 1$, the harmonic index is equal to

$$\mathrm{H}(G[n]) = \frac{43}{6} \times 3^{n-1} - \frac{5}{2}$$

Proof. Let $G[n]$ be the chemical graph of organosilicon dendrimer. By using edge partition from Table1, we easily prove it. We know

$$\mathrm{H}(H) = \sum_{ab\in E(H)} \frac{2}{d_a + d_b}$$

$$\mathrm{H}(G[n]) = 6(3^n - 1)(\frac{2}{2+2}) + 4(3^n - 1)(\frac{2}{2+3}) + (8\times 3^{n-1} - 4)(\frac{2}{3+4})$$

By doing some calculation, we get our required result

$$\mathrm{H}(G[n]) = \frac{43}{6} \times 3^{n-1} - \frac{5}{2}$$

In the following theorem, we compute the ABC index of organosilicon dendrimer $G[n]$.

Theroem 2.3. Consider $G[n]$ be the graph of organosilicon dendrimer, then its ABC index is equal to

$$ABC(G[n]) = (\frac{4\sqrt{15}}{3} + 15\sqrt{2})3^{n-1} - \frac{2\sqrt{15}}{3} - 5\sqrt{2}$$

Proof. Consider the graph of organosilicon dendrimer. By using the edge partition based on the degrees of end vertices of each edge given in Table 1, we compute the ABC index of $G[n]$.Since

$$ABC(H) = \sum_{ab\in E(H)} \sqrt{\frac{d_a + d_b - 2}{d_a d_b}}$$

This gives that

$$ABC(G[n]) = 6(3^n - 1)\sqrt{\frac{2+2-2}{2\times 2}} + 4(3^n - 1)\sqrt{\frac{2+3-2}{2\times 3}} + (8\times 3^{n-1} - 4)\sqrt{\frac{3+4-2}{3\times 4}}$$

After simplification, we get

$$ABC(G[n]) = (\frac{4\sqrt{15}}{3} + 15\sqrt{2})3^{n-1} - \frac{2\sqrt{15}}{3} - 5\sqrt{2}$$

The GA index for $G[n]$ is computed in the following theorem.

Theroem 2.4. Consider the graph of organosilicon dendrimer $G[n]$, $n \geq 1$, then its GA index is equal to

$$GA(G[n]) = (\frac{32\sqrt{3}}{7} + \frac{24\sqrt{6}}{5} + 18)3^{n-1} - \frac{16\sqrt{3}}{7} - \frac{8\sqrt{6}}{5} - 6$$

Proof. Consider the graph of organosilicon dendrimer $G[n]$, $n \geq 1$. Since

$$GA(H) = \sum_{ab\in E(H)} \frac{2\sqrt{d_a d_b}}{d_a + d_b}$$

This directly implies from table 1 that

$$GA(G[n]) = 6(3^n - 1)\frac{2\sqrt{2\times 2}}{2+2} + 4(3^n - 1)\frac{2\sqrt{2\times 3}}{2+3} + (8\times 3^{n-1} - 4)\frac{2\sqrt{3\times 4}}{3+4}$$

After simplification, we get

$$GA(G[n]) = (\frac{32\sqrt{3}}{7} + \frac{24\sqrt{6}}{5} + 18)3^{n-1} - \frac{16\sqrt{3}}{7} - \frac{8\sqrt{6}}{5} - 6$$

3. Cactus chains

A cactus graph is a connected graph in which no edge lies in more than one cycle. Consequently, each block of a cactus graph is either an edge or a cycle. If all blocks of a cactus G are cycles of the same size i, the cactus is i-uniform. A triangular cactus is a graph whose blocks are triangles, i.e., a 3-uniform cactus. A vertex shared by two or more triangles is called a cut-vertex. If each triangle of a triangular cactus G has at most two cut-vertices, and each cut-vertex is shared by exactly two triangles, we say that G is a chain triangular cactus. By replacing triangles in this definitions by cycles of length 4 we obtain cacti whose every block is C_4. We call such cacti "square cacti". Note that the internal squares may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-square; if the cut-vertices are not adjacent, we call the square a para-square.

In Section 3.1 we study the topological indices of the chain triangular cactus. In subsection 3.2 we study the topological indices of chains of squares (see [1]).

3.1 Topological indices of chain triangular cactus

We call the number of triangles in G, the length of the chain. An example of a chain triangular cactus is shown in Fig. 2. Obviously, all chain triangular cacti of the same length are isomorphic. Hence, we denote the chain triangular cactus of length n by T_n.

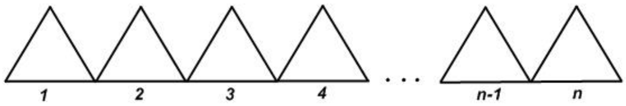

Fig. 2. An n-dimensional triangular chain cactus.

There are three types of edges in the T_n based on the degree of end vertices of each edge showed in Table 2.

Table 2. Edge partition of triangular cactus T_n, $n \geq 1$ based on degrees of end vertices of each edge.

(d_a, d_b) where $ab \in E(H)$	(2,2)	(2,4)	(4,4)
Cardinality of partite set	2	$2n$	$n-2$

Following theorem presents the analytically closed formula of general Randić index $R_\alpha(G)$ with $\alpha = 1,-1,\frac{1}{2},-\frac{1}{2}$ for this cactus graph.

Theroem 3.1.1. Consider the T_n cactus, then its general Randić index is equal to

$$R_\alpha(T_n) = \begin{cases} 32n-24, & \alpha = 1; \\ (4\sqrt{2}+4)n-4, & \alpha = \frac{1}{2}; \\ \frac{5}{16}n+\frac{3}{8}, & \alpha = -1; \\ (\frac{\sqrt{2}}{2}+\frac{1}{4})n+\frac{3}{4}, & \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Consider H be the triangular cactus T_n with defining parameter n. There are three types of edges in H based on degrees of end vertices of each edge. Table 2 shows such an edge partition of H.

For $\alpha = 1$

Now we apply the formula of $R_\alpha(H)$ for $\alpha = 1$.

$$R_1(H) = \sum_{ab \in E(H)} (d_a \times d_b)$$

By using edge partition given in Table 2, we get,

$$R_1(T_n) = 2(2\times 2) + 2n(2\times 4) + (n-2)(4\times 4)$$

After simplifying, we get

$$R_1(T_n) = 32n - 24$$

For $\alpha = \frac{1}{2}$

We apply the formula of $R_\alpha(H)$ for $\alpha = \frac{1}{2}$.

$$R_{\frac{1}{2}}(H) = \sum_{ab \in E(H)} \sqrt{(d_a \times d_b)}$$

By using edge partition given in Table 2, we get,

$$R_{\frac{1}{2}}(T_n) = 2\sqrt{2\times 2} + 2n\sqrt{2\times 4} + (n-2)\sqrt{4\times 4}$$

$$R_{\frac{1}{2}}(T_n) = (4\sqrt{2}+4)n - 4$$

For $\alpha = -1$

We apply the formula of $R_\alpha(H)$ for $\alpha = -1$.

$$R_{-1}(H) = \sum_{ab \in E(H)} \frac{1}{(d_a \times d_b)}$$

$$R_{-1}(T_n) = 2(\frac{1}{2\times 2}) + 2n(\frac{1}{2\times 4}) + (n-2)(\frac{1}{4\times 4})$$

$$R_{-1}(T_n) = \frac{5}{16}n + \frac{3}{8}$$

For $\alpha = -\frac{1}{2}$

We apply the formula of $R_\alpha(H)$ for $\alpha = -\frac{1}{2}$.

$$R_{-\frac{1}{2}}(H) = \sum_{ab \in E(H)} \frac{1}{\sqrt{(d_a \times d_b)}}$$

$$R_{-\frac{1}{2}}(T_n) = 2(\frac{1}{\sqrt{2\times 2}}) + 2n(\frac{1}{\sqrt{2\times 4}}) + (n-2)(\frac{1}{\sqrt{4\times 4}})$$

$$R_{-\frac{1}{2}}(T_n) = (\frac{\sqrt{2}}{2} + \frac{1}{4})n + \frac{3}{4}$$

In the following theorem, we compute harmonic index for this dendrimer.

Theroem 3.1.2. For T_n, $n \geq 1$, the harmonic index is equal to

$$H(T_n) = \frac{11}{12}n - \frac{1}{2}$$

Proof. Let T_n be the chemical graph of triangular cactus chain graph. By using edge partition from Table 2, we easily prove it. We know

$$H(H) = \sum_{ab \in E(H)} \frac{2}{d_a + d_b}$$

$$H(T_n) = 2(\frac{2}{2+2}) + 2n(\frac{2}{2+4}) + (n-2)(\frac{2}{4+4})$$

By doing some calculation, we get our required result

$$H(T_n) = \frac{11}{12}n - \frac{1}{2}$$

Now we compute ABC index of T_n.

Theroem 3.1.3. Consider the triangular cactus chain T_n, then its ABC index is,

$$ABC(T_n) = (\frac{\sqrt{6}}{4} + \sqrt{2})n - \frac{\sqrt{6}}{2} + \sqrt{2}$$

Proof. Let T_n be the n-dimensional triangular cactus chain. By using edge partition given in Table 2, we easily prove it. We know

$$ABC(H) = \sum_{ab \in E(H)} \sqrt{\frac{d_a + d_b - 2}{d_a d_b}}$$

$$ABC(T_n) = 2\sqrt{\frac{2+2-2}{2 \times 2}} + 2n\sqrt{\frac{2+4-2}{2 \times 4}} + (n-2)\sqrt{\frac{4+4-2}{4 \times 4}}$$

By doing some calculation, we get,

$$ABC(T_n) = (\frac{\sqrt{6}}{4} + \sqrt{2})n - \frac{\sqrt{6}}{2} + \sqrt{2}$$

In the following theorem, we compute GA index of triangular cactus T_n.

Theroem 3.1.4. Consider the T_n triangular cactus, the its GA index is,

$$GA(T_n) = (\frac{4\sqrt{2}}{3} + 1)n$$

Proof. Let T_n be the n-dimensional triangular cactus chain. We easily prove it by using edge partition given in Table 2. We know

$$GA(H) = \sum_{ab \in E(H)} \frac{2\sqrt{d_a d_b}}{(d_a + d_b)}$$

$$GA(T_n) = 2(\frac{2\sqrt{2 \times 2}}{2+2}) + 2n(\frac{2\sqrt{2 \times 4}}{2+4}) + (n-2)(\frac{2\sqrt{4 \times 4}}{4+4})$$

By doing some calculation, we get

$$GA(T_n) = (\frac{4\sqrt{2}}{3} + 1)n$$

3.2 Topological indices of chain square cacti

By replacing triangles in the definitions of triangular cactus, by cycles of length 4 we obtain cacti whose every block is C_4. We call such cacti, square cacti. An example of a square cactus chain is shown in Fig. 3. We see that the internal squares may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an ortho-square; if the cut-vertices are not adjacent, we call the square a para-square.

We denote the para-chain square cactus graph of length n as Q_n, and ortho-chain square cactus graph of length n as O_n. We first study topological indices of Q_n. An n-dimensional para-chain square cactus graph is depicted in Fig. 3.

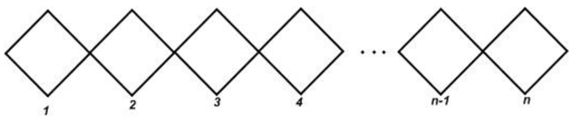

Fig. 3. An n-dimensional para-chain square cactus.

There are two types of edges in this graph based on degrees of end vertices of each edge showed in Table 3.

Table 3. Edge partition of para-square chain cactus Q_n, $n \geq 1$ based on degrees of end vertices of each edge.

(d_a, d_b) where $ab \in E(H)$	(2,2)	(2,4)
Cardinality of partite set	4	$4n-4$

Following theorem presents the analytically closed formula of general Randić index $R_\alpha(G)$ with $\alpha = 1, -1, \frac{1}{2}, -\frac{1}{2}$ for this cactus graph.

Theroem 3.2.1. Consider the Q_n cactus, then its general Randić index is equal to

$$R_\alpha(Q_n) = \begin{cases} 32n-16, & \alpha = 1; \\ 8\sqrt{2}n - 8\sqrt{2} + 8, & \alpha = \frac{1}{2}; \\ \frac{1}{2}(n+1), & \alpha = -1; \\ \sqrt{2}(n-1)+2, & \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Consider Q_n be the para-chain square cactus with defining parameter n. There are two types of edges in Q_n based on degrees of end vertices of each edge. Table 3 shows such an edge partition of Q_n.

For $\alpha = 1$

Now we apply the formula of $R_\alpha(H)$ for $\alpha = 1$.

$$R_1(H) = \sum_{ab \in E(H)} (d_a \times d_b)$$

By using edge partition given in Table 3, we get,

$$R_1(Q_n) = 4(2 \times 2) + (4n-4)(2 \times 4)$$

After simplifying, we get

$$R_1(Q_n) = 32n - 16$$

For $\alpha = \frac{1}{2}$

We apply the formula of $R_\alpha(H)$ for $\alpha = \frac{1}{2}$.

$$R_{\frac{1}{2}}(H) = \sum_{ab \in E(H)} \sqrt{(d_a \times d_b)}$$

By using edge partition given in Table 3, we get,

$$R_{\frac{1}{2}}(Q_n) = 4\sqrt{2 \times 2} + (4n-4)\sqrt{2 \times 4}$$

$$R_{\frac{1}{2}}(Q_n) = 8\sqrt{2}n - 8\sqrt{2} + 8$$

For $\alpha = -1$

We apply the formula of $R_\alpha(H)$ for $\alpha = -1$.

$$R_{-1}(H) = \sum_{ab \in E(H)} \frac{1}{(d_a \times d_b)}$$

$$R_{-1}(Q_n) = 4(\frac{1}{2 \times 2}) + (4n-4)(\frac{1}{2 \times 4})$$

$$R_{-1}(Q_n) = \frac{1}{2}(n+1)$$

For $\alpha = -\frac{1}{2}$

We apply the formula of $R_\alpha(H)$ for $\alpha = -\frac{1}{2}$.

$$R_{-\frac{1}{2}}(H) = \sum_{ab \in E(H)} \frac{1}{\sqrt{(d_a \times d_b)}}$$

$$R_{-\frac{1}{2}}(Q_n) = 4(\frac{1}{\sqrt{2 \times 2}}) + (4n-4)(\frac{1}{\sqrt{2 \times 4}})$$

$$R_{-\frac{1}{2}}(Q_n) = \sqrt{2}(n-1) + 2$$

In the following theorem, we compute harmonic index for this dendrimer.

Theroem 3.2.2. For Q_n, $n \geq 1$, the harmonic index is equal to

$$\mathrm{H}(Q_n) = n - 1$$

Proof. Let Q_n be the chemical graph of para-chain square cactus. By using edge partition from Table 3, we easily prove it. We know

$$\mathrm{H}(H) = \sum_{ab \in E(H)} \frac{2}{d_a + d_b}$$

$$\mathrm{H}(Q_n) = 2(\frac{2}{2+2}) + (4n-4)(\frac{2}{2+4})$$

By doing some calculation, we get our required result

$$\mathrm{H}(Q_n) = n - 1$$

Now we compute ABC index of Q_n.

Theroem 3.2.3. Consider the para-chain square cactus Q_n, then its ABC index is,

$$ABC(Q_n) = 2\sqrt{2}n$$

Proof. Let H be the para-chain square cactus Q_n. By using edge partition given in Table 3, we easily prove it. We know

$$ABC(H) = \sum_{ab \in E(H)} \sqrt{\frac{d_a + d_b - 2}{d_a d_b}}$$

$$ABC(Q_n) = 4\sqrt{\frac{2+2-2}{2\times 2}} + (4n-4)\sqrt{\frac{2+4-2}{2\times 4}}$$

By doing some calculation, we get,

$$ABC(Q_n) = 2\sqrt{2}n$$

In the following theorem, we compute GA index of para-chain square cactus Q_n.

Theroem 3.2.4. Consider the para-chain square cactus Q_n, the its GA index is,

$$GA(Q_n) = \frac{8\sqrt{2}}{3}(n-1)+4$$

Proof. Let H be the para-chain square cactus Q_n. We easily prove it by using edge partition given in Table 3. We know

$$GA(H) = \sum_{ab\in E(H)} \frac{2\sqrt{d_a d_b}}{(d_a+d_b)}$$

$$GA(Q_n) = 4(\frac{2\sqrt{2\times 2}}{2+2}) + (4n-4)(\frac{2\sqrt{2\times 4}}{2+4})$$

By doing some calculation, we get

$$GA(Q_n) = \frac{8\sqrt{2}}{3}(n-1)+4$$

Now we study topological indices of ortho-chain square O_n. An n-dimensional ortho-chain square cactus graph is depicted in Fig. 4.

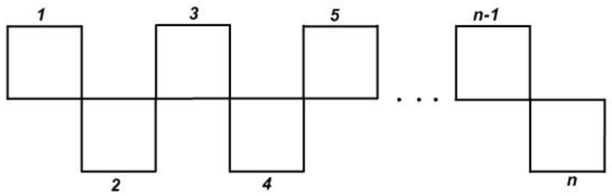

Fig. 4. An n-dimensional ortho-chain square cactus.

There are three types of edges in this graph based on degrees of end vertices of each edge showed in Table 4.

Table 4. Edge partition of ortho-chain square cactus O_n, $n\geq 1$ based on degrees of end vertices of each edge.

(d_a, d_b) where $ab\in E(H)$	(2,2)	(2,4)	(4,4)
Cardinality of partite set	$n+2$	$2n$	$n-2$

Following theorem presents the analytically closed formula of general Randić index $R_\alpha(G)$ with $\alpha = 1, -1, \frac{1}{2}, -\frac{1}{2}$ for this cactus graph.

Theroem 3.3.1. Consider the O_n cactus, then its general Randić index is equal to

$$R_\alpha(O_n) = \begin{cases} 36n-24, & \alpha = 1; \\ (4\sqrt{2}+6)n-4, & \alpha = \frac{1}{2}; \\ \frac{9}{16}n+\frac{3}{8}, & \alpha = -1; \\ (\frac{\sqrt{6}}{3}+\frac{3}{4})n+\frac{1}{2}, & \alpha = -\frac{1}{2}. \end{cases}$$

Proof. Consider O_n be the ortho-chain square cactus with defining parameter n. There are three types of edges in H based on degrees of end vertices of each edge. Table 4 shows such an edge partition of H.

For $\alpha = 1$

Now we apply the formula of $R_\alpha(H)$ for $\alpha = 1$.

$$R_1(H) = \sum_{ab\in E(H)} (d_a \times d_b)$$

By using edge partition given in Table 4, we get,

$$R_1(O_n) = (n+2)(2\times 2) + 2n(2\times 4) + (n-2)(4\times 4)$$

After simplifying, we get

$$R_1(O_n) = 36n-24$$

For $\alpha = \frac{1}{2}$

We apply the formula of $R_\alpha(H)$ for $\alpha = \frac{1}{2}$.

$$R_{\frac{1}{2}}(H) = \sum_{ab\in E(H)} \sqrt{(d_a \times d_b)}$$

By using edge partition given in Table 4, we get,

$$R_{\frac{1}{2}}(O_n) = (n+2)\sqrt{2\times 2} + 2n\sqrt{2\times 4} + (n-2)\sqrt{4\times 4}$$

$$R_{\frac{1}{2}}(O_n) = (4\sqrt{2}+6)n - 4$$

For $\alpha = -1$

We apply the formula of $R_\alpha(H)$ for $\alpha = -1$.

$$R_{-1}(H) = \sum_{ab\in E(H)} \frac{1}{(d_a \times d_b)}$$

$$R_{-1}(O_n) = (n+2)(\frac{1}{2\times 2}) + 2n(\frac{1}{2\times 4}) + (n-2)(\frac{1}{4\times 4})$$

$$R_{-1}(O_n) = \frac{9}{16}n + \frac{3}{8}$$

For $\alpha = -\frac{1}{2}$

We apply the formula of $R_\alpha(H)$ for $\alpha = -\frac{1}{2}$.

$$R_{-\frac{1}{2}}(H) = \sum_{ab\in E(H)} \frac{1}{\sqrt{(d_a \times d_b)}}$$

$$R_{-\frac{1}{2}}(O_n) = (n+2)(\frac{1}{\sqrt{2\times 2}}) + 2n(\frac{1}{\sqrt{2\times 4}}) + (n-2)(\frac{1}{\sqrt{4\times 4}})$$

$$R_{-\frac{1}{2}}(O_n) = (\frac{\sqrt{2}}{2} + \frac{1}{4})n + \frac{3}{4}$$

In the following theorem, we compute harmonic index for this dendrimer.

Theroem 3.3.2. For O_n, $n \ge 1$, the harmonic index is equal to

$$\mathrm{H}(O_n) = \frac{17}{21}n + \frac{1}{2}$$

Proof. Let O_n be the chemical graph of ortho-chain square cactus graph. By using edge partition from Table 4, we easily prove it. We know

$$\mathrm{H}(H) = \sum_{ab\in E(H)} \frac{2}{d_a + d_b}$$

$$\mathrm{H}(O_n) = (n+2)(\frac{2}{2+2}) + 2n(\frac{2}{2+4}) + (n-2)(\frac{2}{4+4})$$

By doing some calculation, we get our required result

$$\mathrm{H}(O_n) = \frac{11}{12}n - \frac{1}{2}$$

Now we compute ABC index of O_n.

Theroem 3.3.3. Consider the ortho-chain square cactus O_n, then its ABC index is,

$$ABC(O_n) = (\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \sqrt{2})n - \frac{\sqrt{6}}{2} + \sqrt{2}$$

Proof. Let O_n be the ortho-chain square cactus. By using edge partition given in Table 4, we get it. We know

$$ABC(H) = \sum_{ab\in E(H)} \sqrt{\frac{d_a + d_b - 2}{d_a d_b}}$$

$$ABC(O_n) = (n+2)\sqrt{\frac{2+2-2}{2\times 2}} + 2n\sqrt{\frac{2+4-2}{2\times 4}} + (n-2)\sqrt{\frac{4+4-2}{4\times 4}}$$

By doing some calculation, we get,

$$ABC(O_n) = (\frac{\sqrt{2}}{2} + \frac{\sqrt{6}}{4} + \sqrt{2})n - \frac{\sqrt{6}}{2} + \sqrt{2}$$

In the following theorem, we compute GA index of ortho-chain square cactus O_n.

Theroem 3.3.4. Consider the ortho-chain square cactus O_n, the its GA index is,

$$GA(O_n) = (\frac{4\sqrt{2}}{3} + 2)n$$

Proof. Let H be the ortho-chain square cactus O_n. We prove it by using edge partition given in Table 4. We know

$$GA(H) = \sum_{ab\in E(H)} \frac{2\sqrt{d_a d_b}}{(d_a + d_b)}$$

$$GA(O_n) = (n+2)(\frac{2\sqrt{2\times 2}}{2+2}) + 2n(\frac{2\sqrt{2\times 4}}{2+4}) + (n-2)(\frac{2\sqrt{4\times 4}}{4+4})$$

By doing some calculation, we get

$$GA(O_n) = (\frac{4\sqrt{2}}{3} + 2)n$$

4. Conclusion

In this paper, certain valency based topological indices, namely general Randić index, harmonic index, atomic-bond connectivity index *(ABC)* and geometric-arithmetic index *(GA)* for organosilicon dendrimer were studied for the first time. We also studied the cactus chain graphs having triangle and square as a unit of the chain. These results are very helpful in understanding and predicting the physico-chemical properties for these chemical structures. The study of distance related graph indices for these important chemical graphs are still open to work on.

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