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Scientific paper

The Eccentricity Version of Atom-Bond Connectivity Index of Linear Polycene Parallelogram Benzenoid $ABC_5(P(n,n))$

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Abstract

Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry. The atom-bond connectivity index of a connected graph G is defined as $ABC(G) = \sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$, where d_v denotes the degree of vertex v of G and the eccentric connectivity index of the molecular graph G is defined as $\xi(G) = \sum_{v\in V} d_v \times \varepsilon(v)$, where $\varepsilon(v)$ is the largest distance between v and any other vertex u of G. Also, the eccentric atom-bond connectivity index of a connected graph G is equal to $ABC_5(G) = \sum_{uv\in E(G)}\sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)\varepsilon(v)}}$.

In this present paper, we compute this new Eccentric Connectivity index for an infinite family of *Linear Polycene Parallelogram Benzenoid.*

Keywords: Molecular graph, Atom-bond connectivity index; Eccentricity connectivity index, Linear Polycene Parallelogram Benzenoid

1. Introduction

Let $G = (V, E)$ be a graph, where $V(G)$ is a non-empty set of vertices and $E(G)$ is a set of edges. In chemical graph theory, there are many molecular descriptors (or *Topological Index*) for a connected graph, that have very useful properties to study of chemical molecules.[1–4] This theory had an important effect on the development of the chemical sciences.

A topological index of a graph is a number related to a graph which is invariant under graph automorphisms. Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry.

One of them is *Atom-Bond Connectivity* (*ABC*) index of a connected graph $G = (V,E)$ and defined as

$$ABC(G) = \sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}, \quad (1)$$

where d_v denotes the degree of vertex v of G, that introduced by *Furtula* et.al. [5,6]

On the other hands, Sharma, Goswami and Madan[7] (in 1997) introduced the eccentric connectivity index of the molecular graph G as

$$\xi(G) = \sum_{v\in V} d_v \times \varepsilon(v), \quad (2)$$

where $\varepsilon(u)$ is the largest distance between u and any other vertex v of G. If $x,y \in V(G)$, then the distance $d(x,y)$ between x and y is defined as the length of any shortest path in G connecting x and y. In other words, is maximum distance with first-point v in G.

$$\varepsilon(v) = Max\{d(v, u) \mid \forall v \in V(G)\} \tag{3}$$

The *Eccentric Connectivity polynomial* of a graph G, was defined by *Alaeiyan, Mojarad* and *Asadpour* as follows:[8,9]

$$ECP(G,x) = \sum_{v \in V(G)} d_v x^{ecc(v)}. \tag{4}$$

Alternatively, the eccentric connectivity index is the first derivative of $ECP(G;x)$ evaluated at $x = 1$. Now, by combine these above topological indexes, we now define a new version of ABC index as:[10]

$$ABC_5(G) = \sum_{uv \in E(G)} \sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)\varepsilon(v)}}. \tag{5}$$

We denote this new index of a connected graph G (*Eccentric atom-bond connectivity index*) by $ABC_5(G)$ (Since it is fifth definition of ABC index). For more details about the Atom-Bond Connectivity and Eccentricity connectivity indices see paper series.[11–18]

The aim of this paper is to exhibit this new topological index for an infinite family of Linear Polycene Parallelogram *Benzenoid*.

2. Main Results and Discussion

In this section, we computed the Eccentric atom-bond connectivity index ABC_5 of an infinite family of Linear Polycene Parallelogram of Benzenoid graph,[19] by continuing the results from.[8,9,18,19] This Molecular graph has $2n(n + 2)$ vertices and $3n^2 + 4n - 1$ edges.

For further study and more detail representation of Linear Polycene Parallelogram of Benzenoid $P(n,n)$, see.[8,9,18,19] Also, reader can see the general case of this Benzenoid molecular graph in Figure 1.

The general representation of Linear Polycene Parallelogram of Benzenoid $P(n,n)$ is shown in Figure1.

Theorem 1. Let $P(n,n)$ $(\forall n \in \mathbb{N})$ be the Linear Polycene Parallelogram of benzenoid. Then the Eccentric atom-bond Connectivity index ABC_5 of $P(n,n)$ is equal to:

$$ABC_5(P(n,n)) = 4\sum_{i=1}^{n-1}\left[\sqrt{\frac{8n-4i-1}{4i^2-2(4n+1)i+4n(4n+1)}} + \sqrt{\frac{8n-4i-3}{4i^2-2(4n-1)i+4n(4n-1)}} + (i)\sqrt{\frac{8n-4i-5}{4i^2-2(8n-3)i+2(8n^2-6n+1)}} + \frac{i}{2}\sqrt{\frac{8n-4i-7}{4i^2-2(8n+1)i+2(8n^2-10n+3)}}\right] + \left[\frac{8\sqrt{n}}{(2n+1)} + (n-1)\frac{\sqrt{4n-2}}{n} - 2(n-1)\sqrt{\frac{4n+1}{4n^2-8n+5}}\right]. \tag{6}$$

Proof: Let $(\forall n \geq 1)$ $P(n,n)$ depicted in Figure 1 be the general representation of Linear Polycene Parallelogram Benzenoid graph with $2n(n+2)$ vertices, such that $4n + 2$ of them have degree two and $2n^2$-2 have degree three $(V(P(n,n) = V_2 \cup V_3)$. Thus there are $3n^2+4n-1$ $(=\frac{1}{2}[2(4n+2) + 3(4n^2-2)])$ edges.

Table 1. Eccentric connectivity index for all vertices of Linear Polycene Parallelogram Benzenoid graph $P(n,n)$.[8,9]

2n+1	2n+1	2n+2	...	4n-5	4n-4	4n-3	4n-2	4n-1
2n	2n+1	2n+2	...	4n-5	4n-4	4n-3	4n-2	
2n	2n+1	2n+2	...	4n-5	4n-4			
2n	2n+1	2n+2	...					
...	...	...						
...	...	...						
...	...	...						
2n	2n+1	2n+2						
	2n+1							

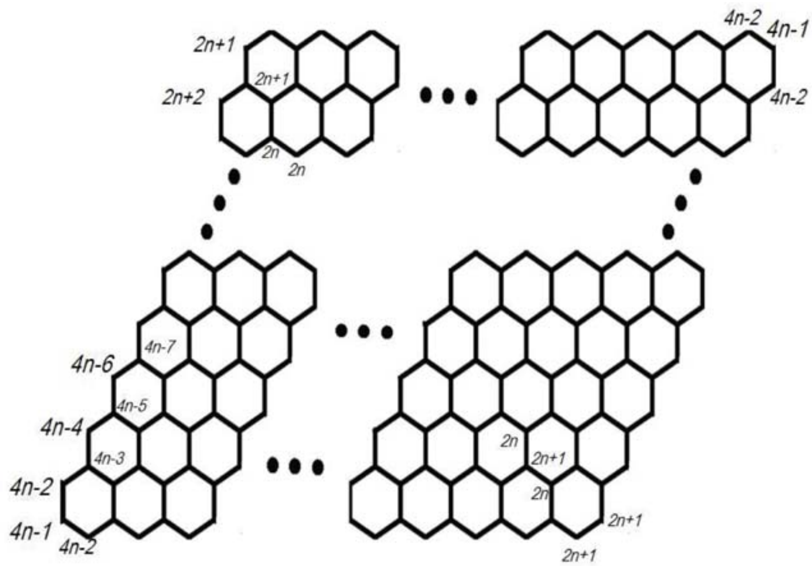

Figure 1. $\forall n\in\mathbb{N}$ the general representation of Linear Polycene Parallelogram of Benzenoid *P(n,n)* and the eccentric connectivity of its vertices.

Now by refer to,[8,9,16] we have the maximum eccentric connectivity and minimum eccentric connectivity for a $v\in V(P(n,n))$ as $Max_{\varepsilon(v)} = 4n-1$ and $Min_{\varepsilon(v)}=2n$.

Now by according to Figure 1 and Table 1, it is easy see that:

- For all vertices with degree two in *P(n,n)*, the eccentricity are equal to $4n–1$, $4n–2$, $4n–4$, $4n–6,\ldots,$ $2n + 2$, $2n + 1$.
- For all other vertices with degree three *P(n,n)* ($d_v = 3$), the eccentricity are equal to $4n–3$ until $2n$.

Thus, we have following computations by using Figure 1 and results in Table 1 as:

$$
\begin{aligned}
ABC_5(P(n,n)) &= \sum_{e=uv\in E(P(n,n))}\sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)\varepsilon(v)}}\\
&= \sum_{\substack{uv\in E(P(n,n))\\ u,v\in V_2}}\sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)\varepsilon(v)}}+\sum_{\substack{uv\in E(P(n,n))\\ u\in V_3 \& v\in V_2}}\sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)\varepsilon(v)}}+\sum_{\substack{uv\in E(P(n,n))\\ u,v\in V_3}}\sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)\varepsilon(v)}}\\
&= \underbrace{4\sum_{i=1}^{n-1}\sqrt{\frac{(4n-2i)+(4n-2i+1)-2}{(4n-2i)(4n-2i+1)}}}_{u\in V_3 \& v\in V_2}+\underbrace{4\sum_{i=1}^{n-1}\sqrt{\frac{(4n-2i)+(4n-2i-1)-2}{(4n-2i)(4n-2i-1)}}}_{u\in V_3 \& v\in V_2}+\underbrace{4\sqrt{\frac{(2n+1)+(2n+1)-2}{(2n+1)(2n+1)}}}_{u,v\in V_2}\\
&+\underbrace{2\sum_{i=1}^{n-1}(i)\sqrt{\frac{(4n-2i-2)+(4n-2i-1)-2}{(4n-2i-2)(4n-2i-1)}}}_{u,v\in V_3}+\underbrace{2\sum_{i=1}^{n-2}(i)\sqrt{\frac{(4n-2i-2)+(4n-2i-3)-2}{(4n-2i-2)(4n-2i-3)}}}_{u,v\in V_3}+\underbrace{2\sum_{i=1}^{n-1}\sqrt{\frac{(2n)+(2n)-2}{(2n)(2n)}}}_{u,v\in V_3}\\
&+\underbrace{2\sum_{i=1}^{n-1}(i)\sqrt{\frac{(4n-2i-2)+(4n-2i-1)-2}{(4n-2i-2)(4n-2i-1)}}}_{u,v\in V_3}\\
&=4\sum_{i=1}^{n-1}\sqrt{\frac{(4n-2i)+(4n-2i+1)-2}{(4n-2i)(4n-2i+1)}}+4\sum_{i=1}^{n-1}\sqrt{\frac{(4n-2i)+(4n-2i-1)-2}{(4n-2i)(4n-2i-1)}}++\frac{8\sqrt{n}}{(2n+1)}\\
&+4\sum_{i=1}^{n-1}(i)\sqrt{\frac{(4n-2i-2)+(4n-2i-1)-2}{(4n-2i-2)(4n-2i-1)}}+2\sum_{i=0}^{n-3}(i+1)\sqrt{\frac{(4n-2i)+(4n-2i-1)-2}{(4n-2i)(4n-2i-1)}}+(n-1)\frac{\sqrt{4n-2}}{n}\\
&=4\sum_{i=1}^{n-1}\sqrt{\frac{8n-4i-1}{4i^2-2(4n+1)i+4n(4n+1)}}+4\sum_{i=1}^{n-1}\sqrt{\frac{8n-4i-3}{4i^2-2(4n-1)i+4n(4n-1)}}+\frac{8\sqrt{n}}{(2n+1)}\\
&+4\sum_{i=1}^{n-1}(i)\sqrt{\frac{8n-4i-5}{4i^2-2(8n-3)i+2(8n^2-6n+1)}}+2\sum_{i=1}^{n-2}(i)\sqrt{\frac{8n-4i-7}{4i^2-2(8n+1)i+2(8n^2-10n+3)}}+(n-1)\frac{\sqrt{4n-2}}{n}.
\end{aligned}
\tag{7}
$$

Finally, $\forall n\in\mathbb{N}$, the fifth ABC index of Linear Polycene Parallelogram Benzenoid *P(n,n)* is equal to:

$$ABC_5(P(n,n))=4\sum_{i=1}^{n-1}\left[\sqrt{\frac{8n-4i-1}{4i^2-2(4n+1)i+4n(4n+1)}}+\sqrt{\frac{8n-4i-3}{4i^2-2(4n-1)i+4n(4n-1)}}+(i)\sqrt{\frac{8n-4i-5}{4i^2-2(8n-3)i+2(8n^2-6n+1)}}+\frac{i}{2}\sqrt{\frac{8n-4i-7}{4i^2-2(8n+1)i+2(8n^2-10n+3)}}\right]$$
$$+\left[\frac{8\sqrt{n}}{(2n+1)}+(n-1)\frac{\sqrt{4n-2}}{n}-2(n-1)\sqrt{\frac{4n+1}{4n^2-8n+5}}\right]. \quad (8)$$

Here, we complete the proof of Theorem 1. ■

3. Conclusions

In this paper, we consider a family of Linear Polycene Parallelogram Benzenoid and compute the Eccentric atom-bond Connectivity index ABC_5. The Eccentric atom-bond Connectivity index ABC_5 was defined as $ABC_5(G) = \sum_{uv\in E(G)}\sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)\varepsilon(v)}}$, such that $\varepsilon(v)$ (*Max{d(v, u)*$\mathbb{N}$ $\forall v\in V(G)\}$) is the largest distance between *v* and any other vertex *u* of *G*.

4. References

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Povzetek

Med topološkimi deskriptorji so indeksi povezanosti izredno pomembni in imajo vidno vlogo v kemiji. Indeks atomske povezanosti grafa G je definiran kot $ABC(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}$, kjer je d_v stopnja vozlišča (točke) *v* od *G* ter je ecentrični indeks povezanosti grafa *G* definiran kot $\xi(G)=\sum_{v\in V}d_v\times\varepsilon(v)$, kjer je $\varepsilon(v)$ najdaljša razdalja med *v* in katerim koli vozliščem *u* od *G*. Poleg tega je ecentrični indeks atomske povezanosti povezanega grafa *G* enak $ABC_5(G) = \sum_{uv\in E(G)}\sqrt{\frac{\varepsilon(u)+\varepsilon(v)-2}{\varepsilon(u)\varepsilon(v)}}$.

V tem članku smo izračunali novi ecentrični indeks povezanosti za neskončno družino linearnih policenskih paralelogramskih benzenoidov.