The Eccentricity Version of Atom-Bond Connectivity Index of Linear Polycene Parallelogram Benzenoid

Wei Gao, Mohammad Reza Farahani and Muhammad Kamran Jamil

School of Information Science and Technology, Yunnan Normal University, Kunming 650500, China.

Department of Applied Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran.

Department of Mathematics, Riphah Institute of Computing and Applied Sciences (RICAS), Riphah International University, 14 Ali Road, Lahore, Pakistan.

*Corresponding author: E-mail: m.kamran.sms@gmail.com
Phone: +923464105447
Received: 23-02-2016

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

\[
ABC(G) = \sum_{v \in V(G)} \frac{d_v + d_{e(v)} - 2}{d_v d_{e(v)}},
\]

where \( d_v \) denotes the degree of vertex \( v \) of \( G \) and the eccentric connectivity index of the molecular graph \( G \) is defined as

\[
\xi(G) = \sum_{v \in V(G)} d_v \times e(v),
\]

where \( e(v) \) 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

\[
ABC_5(G) = \sum_{v \in V(G)} \frac{e(v) + e(e(v)) - 2}{e(v) e(e(v))}.
\]

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

\[
ABC(G) = \sum_{v \in V(G)} \sqrt{\frac{d_v + d_{e(v)} - 2}{d_v d_{e(v)}}},
\]

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

\[
\xi(G) = \sum_{v \in V(G)} d_v \times e(v),
\]

Gao et al.: The Eccentricity Version of Atom-Bond Connectivity ...
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 $G$.

$$\varepsilon(v) = \text{Max}\{d(v, u) | \forall v \in V(G)\}$$  \hspace{1cm} (3)

The Eccentric Connectivity polynomial of a graph $G$, was defined by Alaeiyan, Mojarrad and Asadpour as follows:\textsuperscript{8,9}

$$ECP(G;x) = \sum_{v \in V(G)} d_v x^{\varepsilon(v)}.$$  \hspace{1cm} (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:\textsuperscript{10}

$$ABC_5(G) = \sum_{e \in E(G)} \sqrt{\frac{\varepsilon(u) + \varepsilon(v) - 2}{\varepsilon(u)\varepsilon(v)}}.$$  \hspace{1cm} (5)

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

We denote this new index of a connected graph $G$ (Eccentric atom-bond connectivity index) by $ABC_5(G)$. For more details about the Atom-Bond Connectivity and Eccentricity connectivity indices see paper series.\textsuperscript{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,\textsuperscript{19} by continuing the results from.\textsuperscript{8,9,18,19} This Molecular graph has $2n^2 + 2$ vertices and $3n^2 + 4n - 1$ edges.

For further study and more detail representation of Linear Polycene Parallelogram of Benzenoid $P(n,n)$, see.\textsuperscript{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 Figure 1.

**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:

$$\text{Table 1. Eccentric connectivity index for all vertices of Linear Polycene Parallelogram Benzenoid graph } P(n,n).$$

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

**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.

Gao et al.: The Eccentricity Version of Atom-Bond Connectivity ...
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 \( \text{Max}_{\varepsilon(v)} = 4n - 1 \) and \( \text{Min}_{\varepsilon(v)} = 2n \).

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:

\[
ABC_s(P(n,n)) = \sum_{v \in V(P(n,n))} \frac{\varepsilon(u) + \varepsilon(v) - 2}{\varepsilon(u)\varepsilon(v)}
\]

\[
= \sum_{(u,v) \in E(P(n,n))} \frac{\varepsilon(u) + \varepsilon(v) - 2}{\varepsilon(u)\varepsilon(v)} + \sum_{v \in V(P(n,n))} \frac{\varepsilon(u) + \varepsilon(v) - 2}{\varepsilon(u)\varepsilon(v)} + \sum_{v \in V(P(n,n))} \frac{\varepsilon(u) + \varepsilon(v) - 2}{\varepsilon(u)\varepsilon(v)}
\]

\[
= 4\sum_{i=1}^{n-1} \left( \frac{(4n-2i)(4n-2i+1)}{4n-2i} - 2 \right) + 4\sum_{i=1}^{n-1} \left( \frac{(4n-2i)(4n-2i-1)}{4n-2i} - 2 \right) + 4\sum_{i=1}^{n-1} \left( \frac{(2n+1)(2n+1)}{2n+1} - 2 \right) + 2\sum_{i=1}^{n-1} \left( \frac{(4n-2i)(4n-2i-3)}{4n-2i} - 2 \right)
\]

\[
+ 2\sum_{i=1}^{n-1} \left( \frac{(4n-2i)(4n-2i-1)}{4n-2i} - 2 \right)
\]

\[
= 4\sum_{i=1}^{n-1} \left( \frac{(4n-2i)(4n-2i+1)}{4n-2i} - 2 \right) + 4\sum_{i=1}^{n-1} \left( \frac{(4n-2i)(4n-2i-1)}{4n-2i} - 2 \right) + 2\sum_{i=1}^{n-1} \left( \frac{(4n-2i)(4n-2i-3)}{4n-2i} - 2 \right) + 2\sum_{i=1}^{n-1} \left( \frac{(2n+1)(2n+1)}{2n+1} - 2 \right)
\]

\[
= 4\sum_{i=1}^{n-1} \left( \frac{8n-4i-1}{4i^2-2(4n+1)i+4n(4n+1)} \right) + 4\sum_{i=1}^{n-1} \left( \frac{8n-4i-5}{4i^2-2(8n-3)i+2(8n-6n+1)} \right) + 2\sum_{i=1}^{n-1} \left( \frac{8n-4i-7}{4i^2-2(8n+1)i+2(8n^2-10n+3)} \right) + \frac{4n-2}{n}.
\]
Finally, $\forall n \in \mathbb{N}$, the fifth ABC index of Linear Polycene Parallelogram Benzenoid $P(n,n)$ is equal to:

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

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 $ABC_5(G) = \sum_{v \in V(G)} \left( \frac{\epsilon(v) + e(v) - 2}{\epsilon(v)e(v)} \right)$, such that $\epsilon(v)$ (Max{$d(v,u) \forall v \in V(G)$}) is the largest distance between $v$ and any other vertex $u$ of $G$.

4. References

1. I. Gutman, N. Trinajstić, Chem. Phys. Lett. 1972, 17, 535–538. http://dx.doi.org/10.1016/0009-2614(72)85099-1
2. D. A. Klarner, Polyominoes, In: J. E. Goodman, J. O’Rourke, (eds.) Handbook of Discrete and Computational Geometry, CRC Press, Boca Raton, 1997, 12, 225–242.
3. M. Randić, J. Am. Chem. Soc. 1975, 97, 6609–6615. http://dx.doi.org/10.1021/ja00856a001
4. N. Trinajstić, Chemical Graph Theory. CRC Press, Boca Raton, FL., 1992. http://dx.doi.org/10.1007/s10910-009-9520-x

Povzetek

Med toplotoškimi deskriptorji so indeksi povezanosti izredno pomembni in imajo vidno vlogo v kemiji. Indeks atomske povezanosti grafa $G$ je definiran kot $ABC(G) = \sum_{v \in V(G)} \frac{\epsilon(v) + e(v) - 2}{\epsilon(v)e(v)}$, kjer je $d(v)$ stopnja vozlišča (točke) $v$ od $G$ ter je ecentrični indeks povezanosti grafa $G$ definiran kot $\xi(G) = \sum_{v \in V(G)} d(v)$, kjer je $\epsilon(v)$ najdaljša razdalja med $v$ in katerim koli vozliščem $u$ od $G$. Poleg tega je ecentrični indeks atomske povezanosti povezanega grafa $G$ enak $ABC_5(G) = \sum_{v \in V(G)} \left( \frac{\epsilon(v) + e(v) - 2}{\epsilon(v)e(v)} \right)$.

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

Gao et al.: The Eccentricity Version of Atom-Bond Connectivity ...