Study of The Paraline Graphs of Certain Benzenoid Structures Using Topological Indices

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Abstract: Topological indices are valuable in the study of QSAR/QSPR. There are numerous applications of graph theory in the field of structural chemistry. In this paper, we computed generalized Randic, general Zagreb, general sum-connectivity, \( ABC, GA, ABC^*, \) and \( GA_y \) indices of the paraline graphs of triangular and linear parallelogram Benzenoid structures.

Keywords: Topological indices, Paraline graph, Triangular Benzenoid, Parallelogram Benzenoid.

1. Introduction

Consider \( G \) is simple graph having vertex set \( V(G) \) and edge set \( E(G) \). For any vertex \( u \), \( N_u \) represents its neighbours set in \( G \). \( |N_u| \) is the degree \( d_u \) of vertex \( u \), \( S_u = \sum_{v \in N_u} d_v \) and \( K(u) \) is the complete graph on vertex set \( N_u \). If we replace each edge of a graph \( G \) by a path of length 2 then the resulting graph is known as subdivision graph \( S(G) \). The line graph \( L(G) \) is the graph whose vertices are the edges of \( G \), two vertices \( e \) and \( f \) are incident if and only if they have a common end vertex in \( G \). The paraline graph of \( G \) is the line graph of subdivision graph of \( G \) which will be denoted by \( G^* \). There is another way to build \( G^* \) from \( G \) as follows:

1. Substitute every vertex \( u \in V(G) \) by \( K(u) \);
2. Join by edge all vertices of \( K(u) \) with all vertices of \( K(u) \) in \( G^* \) if and only if there is an edge between \( u \) and \( u_i \) in \( G \);
3. For each vertex \( v \) of \( K(u) \), degree of \( v \) in \( G^* \) is same as the degree of \( u \) in \( G \).

Paraline graphs are very important in structural chemistry, but still in the last few decades they were considered very little in chemical graph theory. A molecular graph is a collection of points indicating the atoms in the molecule and set of lines indicating the covalent bonds. For example, consider the Hydrocarbon \( C_3H_8 \), its molecular structure and molecular graph is shown in Fig. 1 (a) and (b). However, there are other ways to attach graph with molecules, for instance a smallest collection of localized orbitals each represented by a vertex, with edges described the stronger connections among pairs of orbitals. In fact, such graphs were understood in some early quantum chemical mechanisms. The vertices of Paraline graphs of a molecular graph correspond to its atomic hybrid orbitals, and their edges corresponds to stronger interactions among pairs of these orbitals. Paraline graph of a molecular graph of Hydrocarbon \( C_3H_8 \) is shown in Fig. 1. In structural chemistry and biology, molecular structure descriptors are utilized for modeling information of molecules, which are known as topological indices. Many topological indices are introduced to explain the physical and chemical properties of molecules [1, 2]. Topological indices are generally divided into three categories: degree-based indices [3, 4, 5, 6], distance-based indices [7, 8, 9, 10, 11, 12], and spectrum-based indices [13, 14, 15]. There are also some topological indices based on both degrees and distances (see [16, 17, 18]). For further study on degree based topological indices see [31, 32, 33, 34].

The general Randić index of \( G \) is introduced in [19].
\[ R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha. \quad (1) \]

where \( \alpha \) is a real number. Then \( R_{1/2}(G) \) is known as Randic index of \( G \).

The first general Zagreb index is introduced by Li and Zhao in [20]:
\[ M_\alpha(G) = \sum_{uv \in V(G)} (d_u)^\alpha. \quad (2) \]

In 2010, general sum-connectivity index \( \chi_\alpha(G) \) has been introduced in [21]:
\[ \chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha. \quad (3) \]

Estrada et al. initiated the atom-bond connectivity (ABC) index in [22] which is defined as
\[ ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \quad (4) \]

D. Vukicevic and B. Furtula introduced the geometric arithmetic (GA) index in [23] which is defined as
\[ GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \quad (5) \]

The fourth member of the class of ABC index was given by M. Ghorbani et al. in [24] as:
\[ ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}. \quad (6) \]

Graovac et al. Introduced the 5th GA index in [25] as
\[ GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}. \quad (7) \]

In this paper, we computed generalized Randic, general Zagreb, general sum-connectivity, ABC, GA, \( ABC_4 \) and \( GA_5 \) indices of the paraline graphs of 2D-lattice, nanotube and nanotorus \( TUC_{C_p}\) [p, q] in [30].

In this paper, we computed generalized Randic, general Zagreb, general sum-connectivity, ABC, GA, \( ABC_4 \) and \( GA_5 \) indices of the paraline graphs of triangular and linear parallelogram benzenoid structures.

In order to calculate the number of edges of the line graph, the following lemma is important for us.

**Lemma 2.1.** Let \( G \) be a graph. Then
\[ |E(L(G))| = \sum_{uv \in V(G)} d_u^2 - |E(G)| \]
where \( L(G) \) is the line graph of \( G \).
3. Results and discussion.

3.1 Topological Indices Of The Paraline Graph Of Triangular Benzenoid.

The molecular graph of triangular benzenoid is shown in Fig. 2 and is denoted by $T_n$. There are $n^2 + 4n + 1$ vertices and $\frac{3(n^2 + 3n)}{2}$ edges in $T_n$.

![Figure 2. Triangular Benzenoid](image)

**Theorem 3.1.** Let $G^*$ be the Paraline graph of $T_n$. Then

$$M_a(G^*) = 2^{n+1}(3n + 3) + 3^{n+1}(n^2 + n - 2).$$

**Proof** The graph $G^*$ is shown in Fig. 3.

![Figure 3. Paraline graph of Triangular Benzenoid](image)

**Theorem 3.2.** Let $G^*$ be the Paraline graph of $T_n$. Then

1. $R_a(G^*) = 4^n(3n + 9) + 6^{n+1}(n - 1) + \frac{3}{2}9^n(3n + 4)(n - 1)$

2. $\chi_a(G^*) = 4^n(3n + 9) + 5^n(6n - 6) + \frac{3}{2}6^n(3n + 4)(n - 1)$

3. $ABC(G^*) = 3n^2 + \left(\frac{3n^2}{2} + 1\right)n + \frac{3n^2}{2} - 4$

4. $GA(G^*) = \frac{9}{2}n^2 + \left(\frac{15n^2}{2} + \frac{9}{2}\right)n + 3 - \frac{15n^2}{2}$

**Proof:** The subdivision graph $S(T_n)$ contains $3n^2 + 9n$ edges and $\frac{1}{2}(5n^2 + 17n + 2)$ vertices among which $\frac{1}{2}(3n^2 + 15n + 6)$ vertices

are of degree 2 and remaining \( n^2 + n - 2 \) vertices are of degree 3. Hence, by Lemma 2.1 the total number of edges of \( G^* \) are \( \frac{1}{2}(9n^2 + 21n - 6) \). The edge set \( E(G^*) \) divides into three edge partitions based on degrees of the end vertices, i.e.,

\[ E(G^*) = E_1(G^*) \cup E_2(G^*) \cup E_3(G^*) \]

The edge partition \( E_1(G^*) \) contains \( 3n + 9 \) edges \( uv \), where \( d_u = d_v = 2 \), the edge partition \( E_2(G^*) \) contains \( 6n - 6 \) edges \( uv \), where \( d_u = 2 \) and \( d_v = 3 \), and the edge partition \( E_3(G^*) \) contains \( \frac{1}{2}(3n + 4)(n - 1) \) edges \( uv \), where \( d_u = d_v = 3 \). From Formulas (1), (3), (4) and (5), we obtain the required results.

**Theorem 3.3.** Let \( G^* \) be the Paraline graph of \( T_n \). Then

1. \( ABC_4(G^*) = 2n^2 + \left( \frac{6\sqrt{2}}{5} + \frac{3\sqrt{10}}{10} + \frac{3\sqrt{14}}{8} + \frac{\sqrt{20}}{2} - \frac{10}{3} \right)n + \frac{9\sqrt{2}}{4} + \frac{3\sqrt{10}}{5} - \frac{12\sqrt{2}}{5} - \frac{3\sqrt{10}}{10} - \frac{3\sqrt{14}}{8} - \frac{\sqrt{20}}{2} + \frac{4}{3} \),

2. \( GA_4(G^*) = \frac{9}{2}n^2 + \left( \frac{24\sqrt{10}}{13} - \frac{1}{2} + \frac{72\sqrt{2}}{13} \right)n + \frac{4\sqrt{3}}{3} - \frac{24\sqrt{10}}{13} - \frac{24\sqrt{2}}{13} + 3 \).

**Proof** The edge set \( E(G^*) \) can be divided into seven edge partitions \( E_i(G^*) \), \( i = 4, 5, \ldots, 10 \), i.e., \( E(G^*) = \bigcup_{i=4}^{10} E_i(G^*) \) depending on the degree sum of neighbors of end vertices. The edge partition \( E_4(G^*) \) contains \( 9 \) edges \( uv \), where \( S_u = S_v = 4 \), the edge partition \( E_5(G^*) \) contains \( 6 \) edges \( uv \), where \( S_u = 4 \) and \( S_v = 5 \), the edge partition \( E_6(G^*) \) contains \( 3n - 6 \) edges \( uv \), where \( S_u = S_v = 5 \), the edge partition \( E_7(G^*) \) contains \( 6n - 6 \) edges \( uv \), where \( S_u = 5 \) and \( S_v = 6 \), the edge partition \( E_8(G^*) \) contains \( 3n - 3 \) edges \( uv \), where \( S_u = S_v = 8 \), the edge partition \( E_9(G^*) \) contains \( 6n - 6 \) edges \( uv \), where \( S_u = 8 \) and \( S_v = 9 \), and the edge partition \( E_{10}(G^*) \) contains \( \frac{1}{2}(n - 1)(3n - 2) \) edges \( uv \), where \( S_u = S_v = 9 \).

From Formulas (6) and (7), we obtain the required results.

**4. Topological Indices Of The Paraline Graph Of Linear Parallelogram Benzenoid.**

The molecular graph of linear parallelogram benzenoid is shown in Fig. 4 and is denoted by \( P_{m,n} \). There are \( 2mn + 2m + 2n \) vertices and \( 3mn + 2n + 2m - 1 \) edges in \( P_{m,n} \).

![Figure 4. Linear parallelogram Benzenoid](doi:1444-8939.2017/4-3/MRR.14)
Theorem 4.1. Let $G'$ be the Paraline graph of $P_{m,n}$ Then
$$M_a(G') = 2^a + 2(m + n + 1) + 3^{a+1}(2mn - 2).$$

Proof The graph $G'$ is shown in Fig. 5.

![Figure 5. Paraline graph of Linear parallelogram Benzenoid](image)

Theorem 4.2. Let $G'$ be the Paraline graph of $P_{m,n}$. Then
\begin{align*}
1) R_a(G') &= 4a(2m + 2n + 8) + 6a(4m + 4n - 8) + 9a(9mn - 2m - 2n - 5) \\
2) \chi_a(G') &= 4a(2m + 2n + 8) + 5a(4m + 4n - 8) + 6a(9mn - 2m - 2n - 5) \\
3) ABC(G') &= (6m + 3\sqrt{2} - \frac{a}{5})n + \left(3\sqrt{2} - \frac{a}{3}\right)m - \frac{10a}{5} \\
4) GA(G') &= \left(9m + \frac{8\sqrt{6}}{3}\right)n + \frac{8\sqrt{6}}{3}m + 3 - \frac{16\sqrt{6}}{5}.
\end{align*}

Proof The subdivision graph $S(P_{m,n})$ contains $6mn + 4m + 4n - 2$ edges and $5mn + 4m + 4n - 1$ vertices among which $3mn + 4m + 4n + 1$ vertices are of degree 2 and remaining $2mn - 2$ vertices are of degree 3. Hence, by Lemma the total number of edges of $G'$ are $9mn + 4m + 4n - 5$. The edge set $E(G')$ divides into three edge partitions based on degrees of the end vertices. i.e.

$$E(G') = E_1(G') \cup E_2(G') \cup E_3(G').$$

The edge partition $E_1(G')$ contains $2m + 2n + 8$ edges $uv$, where $d_u = d_v = 2$, the edge partition $E_2(G')$ contains $4m + 4n - 8$ edges $uv$, where $d_u = 2$ and $d_v = 3$, and the edge partition $E_3(G')$ contains $9mn - 2m - 2n - 5$ edges $uv$, where $d_u = d_v = 3$.

From Formulas (1), (3), (4) and (5), we obtain the required results.

Theorem 4.3. Let $G'$ be the Paraline graph of $P_{m,n}$ Then
\begin{align*}
1. ABC(G') &= \left(4m + \frac{4\sqrt{6}}{5} + \frac{4\sqrt{6}}{3} + \frac{4\sqrt{6}}{3} + \frac{4\sqrt{6}}{3} - \frac{32}{9}\right)n + \\
&\left(4m + \frac{4\sqrt{6}}{5} + \frac{4\sqrt{6}}{3} - \frac{32}{9} + \frac{4\sqrt{6}}{3}\right)m \\
&- \frac{4\sqrt{6}}{2} + 2\sqrt{6} + \frac{4\sqrt{6}}{3} - \frac{16\sqrt{6}}{5} - \frac{2\sqrt{6}}{3} - 2\sqrt{3} + 28; \\
2. \end{align*}

2. $GA_i(G') = \left(9m + \frac{48\sqrt{3}}{17} - 4 + \frac{16\sqrt{15}}{13}\right)n + \left(\frac{16\sqrt{15}}{13} - 4 + \frac{48\sqrt{3}}{17}\right)m + 3 + \frac{33\sqrt{3}}{9} - \frac{96\sqrt{17}}{17} - \frac{32\sqrt{15}}{13}.$

**Proof** The edge set $E(G')$ can be divided into seven edge partitions $E_i(G')$, $i = 4, 5, ..., 10$, i.e. $E(G') = \bigcup_{i=4}^{10} E_i(G')$ depending on the degree sum of neighbors of end vertices. The edge partition $E_4(G')$ contains 8 edges $uv$, where $S_u = S_v = 4$, the edge partition $E_5(G')$ contains 8 edges $uv$, where $S_u = 4$ and $S_v = 5$, the edge partition $E_6(G')$ contains $2m + 2n - 8$ edges $uv$, where $S_u = S_v = 5$, the edge partition $E_7(G')$ contains $4m + 4n - 8$ edges $uv$, where $S_u = 5$ and $S_v = 8$, the edge partition $E_8(G')$ contains $2m + 2n - 4$ edges $uv$, where $S_u = S_v = 8$, the edge partition $E_9(G')$ contains $4m + 4n - 8$ edges $uv$, where $S_u = 8$ and $S_v = 9$, and the edge partition $E_{10}(G')$ contains $9m - 8m - 8n + 7$ edges $uv$, where $S_u = S_v = 9$. From Formulas (6) and (7), we obtain the required results.

5. **Conclusion**

In this paper, generalized Randic, general Zagreb, general sum-connectivity, $ABC$, $GA$, $ABC_4$ and $GA_4$ indices for paraline graphs of triangular and linear parallelogram benzenoid structures were studied.

**References**


