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Topological Indices of ARMS-Product of Certain Graphs

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Abstract:
A mathematical parameter known as the topological graph index, or molecular descriptor, can be applied to any graph that represents a molecule structure. This index can be used to analyze mathematical numbers and look into specific physical and chemical characteristics of molecules in more detail. It is therefore a useful strategy for avoiding costly and time-consuming laboratory experiments. In this paper topological indices of a noval graph product called ARMS-Product of certain graphs are determined.

Keywords: ARMS-Product, first Zagreb index, second Zagreb index, Harmonic index, Geometric-arithmetic index, Bull graph, Path.

2020 AMS subject classifications: 05C07, 05C76, 05C92.

1. Introduction

Topological indices are graph invariant. A graph invariant is any function on a graph that does not depend on labelling of its vertices. In chemistry, graphs can represent different chemical objects such as molecules, crystals, polymers, etc. Molecular graphs are chemical graphs which represent the constitution of molecules. In these graphs, individual atoms represent vertices and edges are chemical bonds between them. A single number that can associate with chemical graphs is called topological index. All graphs under our consideration are simple, connected and undirected. Let $G = (V(G), E(G))$ be a graph with order $n = |V(G)|$ and size $m = |E(G)|$. The degree of a vertex v_i in G is the number of edges incident on v_i and is denoted by $d(v_i)$ or simply d_i. The corona $G_1 \odot G_2$ of two graphs G_1 and G_2 is defined as the graph G obtained by taking one copy of G_1(which has p_1 points) and p_1 copies of G_2, and then joining the i^{th} point of G_1 to every point in the i^{th} copy of G_2. We follow [2] for more terminologies and notations not mentioned here.

Definition 1. A molecular graph $G = (V, E)$ is a simple graph having $p = |V(G)|$ vertices and $q = |E(G)|$ edges. The vertices $v_i \in V$ represent non-hydrogen atoms and and the edges $(v_i, v_j) \in E$ represent covalent bonds between the corresponding atoms. In particular, hydrocarbons are formed only by carbon and hydrogen atoms and their molecular graphs represent the carbon skeleton of the molecule.

Definition 2. [3] Let G be a graph, then the first and second Zagreb indices of G are defined as

$$M_1(G) = \sum_{u \in V(G)} d(u) + d(v)$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v)\,.$$

Definition 3. [4] The Harmonic index of a graph *G* is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}\,.$$

Definition 4. [5] The Geometric-Arithmetic index of a graph *G* is defined as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}$$

A significant field of graph theory is graph operations, which involves creating new graphs from existing ones by carrying out a series of actions on the basis of some graph theoretical parameters. They comprise unary and binary operations. There are several operations on two graphs G_1 and G_2 which result in a graph *G* whose set of vertices is the cartesian product $V_1 \times V_2$, where V_k is the vertex set of G_k. These include the cartesian product, the composition, tensor product etc.

In 2024, [1] Akhil B., Roy John, Manju V.N. and G. Suresh Singh introduced a new graph product called ARMS-product of two graphs G_1 and G_2 as follows:

Definition 5. Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs with order *m* and *n* respectively. The ARMS-Product of G_1 and G_2 denoted by $G_1 \boxtimes G_2$ is a graph *G* with vertex set $V = V_1 \times V_2$ and two vertices $x = (u_i, v_j)$ and $y = (u_k, v_l)$ are adjacent in *G* if:

1. either $u_i = u_k$ *and* $\gcd\left(d_{G_2}(v_j), d_{G_2}(v_l)\right) = 1$ or
2. $\gcd\left(d_{G_1}(u_i), d_{G_1}(u_k)\right) = 1$ and $v_j = v_l$

$for\ all\ i, k = 1,2, \ldots, m\ with\ i \neq k\ and\ j, l = 1,2, \ldots, n\ with\ j \neq l.$

Keeping the importance of this newly introduced graph product, in this paper various topological indices of graphs obtained through ARMS-product is evaluated. In [1] it is shown that the ARMS-product of two connected graph need not be connected. Therefore, we are considering only those graphs which produce connected graphs as an outcome and hence compute their topological indices in detail.

2. Topological Indices of ARMS-Product of Graph

In this section topological indices namely first, second Zagreb indices, Harmonic index and Geometric-Arithmetic index of certain graphs obtained through the ARMS-Product of certain graphs are determined.

Theorem 2.1. Let *B* be the bull graph and P_2 be a path on two vertices. Then for the graph $B \boxtimes P_2$, first and second Zagreb indices, Harmonic index and Geometric-Arithmetic index are respectively given by:

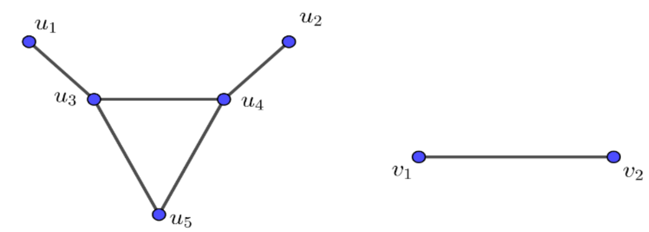
1. $M_1(B \boxtimes P_2) = 214.$

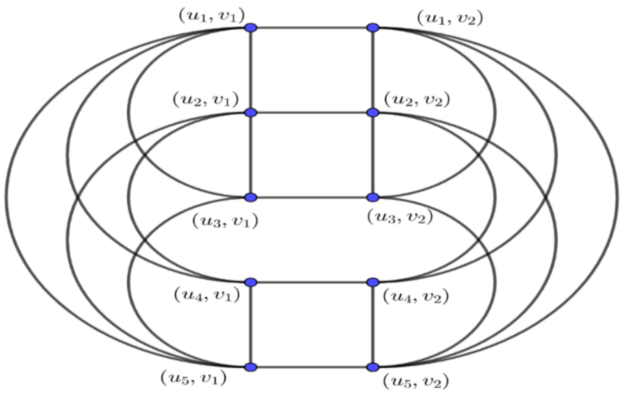
2. $M_2(B \boxtimes P_2) = 497.$

3. $H(\, B \boxtimes P_2) = \frac{149}{30}.$

4. $GA(B \boxtimes P_2) = 11 + \frac{16\sqrt{5}}{3}.$

Proof: The ARMS-product of the bull graph, *B* and the path graph, P_2 is a graph with 10 vertices.





$B \boxtimes P_2$

The edge set of $B \boxtimes P_2$ can be partitioned as follows:

$$E_1 = \{uv \mid d_u = 5, d_v = 5\}, \qquad |E_1| = 9.$$
$$E_2 = \{uv \mid d_u = 5, d_v = 4\}, \qquad |E_2| = 12.$$
$$E_3 = \{uv \mid d_u = 4, d_v = 4\}, \qquad |E_3| = 2.$$

$$M_1(B \boxtimes P_2) \quad = \sum_{uv \in E(B \boxtimes P_2)} d(u) + d(v)$$

$$= \sum_{uv \in E_1} d(u) + d(v) + \sum_{uv \in E_2} d(u) + d(v) + \sum_{uv \in E_3} d(u) + d(v)$$

$$= \sum_{uv \in E_1} 5 + 5 + \sum_{uv \in E_2} 5 + 4 + \sum_{uv \in E_3} 4 + 4$$

$$= 10 \sum_{uv\in E_1} 1 + 9 \sum_{uv\in E_2} 1 + 8 \sum_{uv\in E_3} 1$$

$$= 10 \times 9 + 9 \times 12 + 8 \times 2$$

$$= 214.$$

$$M_2(B \boxtimes P_2) \quad = \sum_{uv\in E(B\boxtimes P_2)} d(u)d(v)$$

$$= \sum_{uv\in E_1} d(u)d(v) + \sum_{uv\in E_2} d(u)d(v) + \sum_{uv\in E_3} d(u)d(v)$$

$$= \sum_{uv\in E_1} 25 + \sum_{uv\in E_2} 20 + \sum_{uv\in E_3} 16$$

$$= 25 \sum_{uv\in E_1} 1 + 20 \sum_{uv\in E_2} 1 + 16 \sum_{uv\in E_3} 1$$

$$= 25 \times 9 + 20 \times 12 + 16 \times 2$$

$$= 497.$$

$$H(B \boxtimes P_2) \quad = \sum_{uv\in E(B\boxtimes P_2)} \frac{2}{d(u) + d(v)}$$

$$= \sum_{uv\in E_1} \frac{2}{10} + \sum_{uv\in E_2} \frac{2}{9} + \sum_{uv\in E_3} \frac{2}{8}$$

$$= \frac{2}{10} \sum_{uv\in E_1} 1 + \frac{2}{9} \sum_{uv\in E_2} 1 + \frac{2}{8} \sum_{uv\in E_3} 1$$

$$= \frac{149}{30}.$$

$$GA\ (B \boxtimes P_2) \quad = \sum_{uv\in E(B\boxtimes P_2)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}$$

$$= \sum_{uv\in E_1} \frac{2\sqrt{25}}{10} + \sum_{uv\in E_2} \frac{2\sqrt{20}}{9} + \sum_{uv\in E_3} \frac{2\sqrt{16}}{8}$$

$$= \sum_{uv\in E_1} 1 + \frac{4\sqrt{5}}{9} \sum_{uv\in E_2} 1 + \sum_{uv\in E_3} 1$$

$$= 9 + 12 \frac{4\sqrt{5}}{9} + 2$$

$$= 11 + \frac{16\sqrt{5}}{3}.$$

This completes the proof.

Theorem 2.2. Let $K_{1,n}$ and $K_{1,m}$ be two bipartite graphs. Then for the graph $K_{1,n} \boxtimes K_{1,m}$ first and second Zagreb indices, Harmonic index and Geometric-Arithmetic index are respectively given by:

1. $M_1\left(K_{1,n} \boxtimes K_{1,m}\right) = (m+n)^2(m+1)(n+1)$.

2. $M_2\left(K_{1,n} \boxtimes K_{1,m}\right) = \dfrac{(m+n)^2(m+1)(n+1)}{2}$.

3. $H\left(K_{1,n} \boxtimes K_{1,m}\right) = \dfrac{(m+1)(n+1)}{2}$.

4. $GA\left(K_{1,n} \boxtimes K_{1,m}\right) = \dfrac{(m+n)(m+1)(n+1)}{2}$

Proof: The ARMS- product of $K_{1,n}$ and $K_{1,m}$ is a $(m + n)$ -regular graph on $(m + 1)(n + 1)$ vertices. The number of edges of $K_{1,n} \boxtimes K_{1,m}$ is $\frac{(m+n)(m+1)(n+1)}{2}$.

$$M_1\left(K_{1,n} \boxtimes K_{1,m}\right) = \sum_{uv\in E\left(K_{1,n}\boxtimes K_{1,m}\right)} d(u) + d(v)$$

$$= \sum_{uv\in E\left(K_{1,n}\boxtimes K_{1,m}\right)} d(u) + d(v)$$

$$= \sum_{uv\in E\left(K_{1,n}\boxtimes K_{1,m}\right)} 2(m+n)$$

$$= 2(m+n)\frac{(m+n)(m+1)(n+1)}{2}$$

$$= (m+n)^2(m+1)(n+1).$$

$$M_2\left(K_{1,n} \boxtimes K_{1,m}\right) = \sum_{uv\in E\left(K_{1,n}\boxtimes K_{1,m}\right)} d(u)d(v)$$

$$= \sum_{uv\in E\left(K_{1,n}\boxtimes K_{1,m}\right)} d(u)d(v)$$

$$= \sum_{uv\in E\left(K_{1,n}\boxtimes K_{1,m}\right)} (m+n)^2$$

$$= (m+n)^2 \times \frac{(m+n)(m+1)(n+1)}{2}$$

$$= \frac{(m+n)^2(m+1)(n+1)}{2}.$$

$$H(K_{1,n} \boxtimes K_{1,m}) = \sum_{uv\in E(K_{1,n}\boxtimes K_{1,m})} \frac{2}{d(u)+d(v)}$$

$$= \sum_{uv\in E(K_{1,n}\boxtimes K_{1,m})} \frac{2}{2(m+n)}$$

$$= \frac{1}{m+n} \sum_{uv\in E(K_{1,n}\boxtimes K_{1,m})} 1$$

$$= \frac{(m+1)(n+1)}{2}.$$

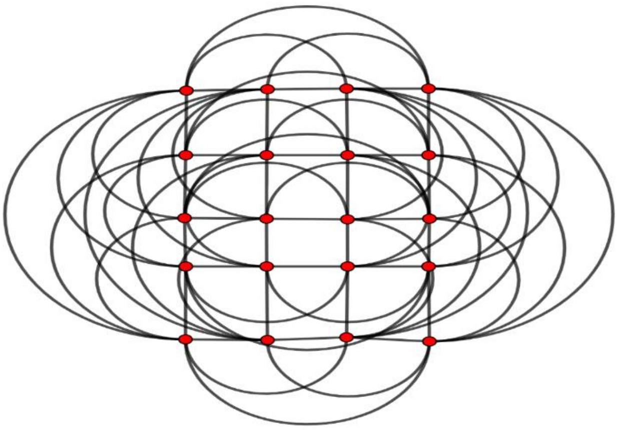
$$GA(K_{1,n} \boxtimes K_{1,m}) = \sum_{uv\in E(K_{1,n}\boxtimes K_{1,m})} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$$

$$= \sum_{uv\in E(K_{1,n}\boxtimes K_{1,m})} \frac{2\sqrt{(m+n)(m+n)}}{2(m+n)}$$

$$= \frac{(m+n)(m+1)(n+1)}{2}.$$

This completes the proof.

Note: For $n = 3$ and $n = 4$, the ARMS- product of $K_{1,3}$ and $K_{1,4}$ is the rook graph and it is given below:



$K_{1,3} \boxtimes K_{1,4}$

Theorem 2.3. Let $P_n \odot K_1$ be a given graph and P_2 be a path graph. Then for the graph $(P_n \odot K_1) \boxtimes P_2$, first and second Zagreb indices, Harmonic index and Geometric-Arithmetic index are respectively given by:

1. $M_1((P_n \odot K_1) \boxtimes P_2) = \begin{cases} 100, & for\ n = 2 \\ n(4n-1)^2, & for\ \ n > 3\,. \end{cases}$

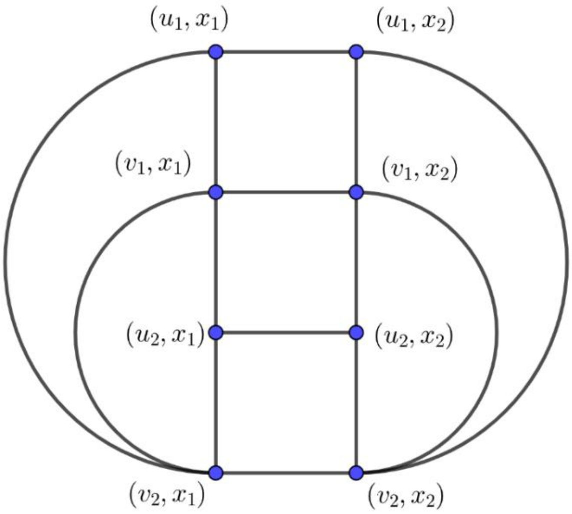
2. $M_2\big((P_n \odot K_1) \boxtimes P_2\big) = \begin{cases} 178, & for\ n = 2 \\ n^2(3(2n-1)^2 + 4n^2), & for\ \ n > 3\ . \end{cases}$

3. $H\big((P_n \odot K_1) \boxtimes P_2\big)\ = \begin{cases} \dfrac{83}{21}, & for\ n = 2 \\ \dfrac{2n^2}{4n-2} + \dfrac{2n(2n-1)}{4n-1} + \dfrac{n}{2}, & for\ \ n > 3. \end{cases}$

4. $GA\big((P_n \odot K_1) \boxtimes P_2\big) = \begin{cases} \dfrac{42 + (32\sqrt{3})}{7}, & for\ n = 2 \\ 2n^2 + \dfrac{2n(2n-1)\sqrt{(4n^2-2n)}}{(4n-1)}, & for\ \ n > 3. \end{cases}$

Proof: **Case 1**. $n\ =\ 2$

If $n\ =\ 2$, consider *(P_2 ⨀ K_1) ⊠ P_2*.



(P_2 ⨀ K_1) ⊠ P_2

The edge set of (P_2 ⨀ K_1) ⊠ P_2 can be partitioned as follows:

$$E_1 = \{uv \mid d_u = 3, d_v = 3\}, \qquad |E_1| = 2.$$

$$E_2 = \{uv \mid d_u = 3, d_v = 4\}, \qquad |E_2| = 8.$$

$$E_3 = \{uv \mid d_u = 4, d_v = 4\}, \qquad |E_3| = 4.$$

$$M_1\big((P_2 \odot K_1) \boxtimes P_2\big) = \sum_{uv \in E((P_2 \odot K_1) \boxtimes P_2)} d(u) + d(v)$$

$$= \sum_{uv \in E_1} 3 + 3 + \sum_{uv \in E_2} 3 + 4 + \sum_{uv \in E_3} 4 + 4$$

$$= 6 \sum_{uv \in E_1} 1 + 7 \sum_{uv \in E_2} 1 + 8 \sum_{uv \in E_3} 1$$

$= 6 \times 2 + 7 \times 8 + 8 \times 4$

$= 100.$

$$M_2\big((P_2 \odot K_1) \boxtimes P_2\big) = \sum_{uv \in E\left((P_2 \odot K_1) \boxtimes P_2\right)} d(u)\, d(v)$$

$$= \sum_{uv \in E_1} 9 + \sum_{uv \in E_2} 12 + \sum_{uv \in E_3} 16$$

$= 9 \times 2 + 12 \times 8 + 16 \times 4$

$= 178.$

$$H\big((P_2 \odot K_1) \boxtimes P_2\big) \;= \sum_{uv \in E\left((P_2 \odot K_1) \boxtimes P_2\right)} \frac{2}{d(u) + d(v)}$$

$$= \sum_{uv \in E_1} \frac{2}{6} + \sum_{uv \in E_2} \frac{2}{7} + \sum_{uv \in E_3} \frac{2}{8}$$

$$= \frac{2}{6} \times 2 + \frac{2}{7} \times 8 + \frac{2}{8} \times 4$$

$$= \frac{83}{21}.$$

$$GA\big((P_2 \odot K_1) \boxtimes P_2\big) = \sum_{uv \in E\left((P_2 \odot K_1) \boxtimes P_2\right)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}$$

$$= \sum_{uv \in E_1} \frac{2\sqrt{3 \times 3}}{6} + \sum_{uv \in E_2} \frac{2\sqrt{3 \times 4}}{7} + \sum_{uv \in E_3} \frac{2\sqrt{4 \times 4}}{8}$$

$$= \sum_{uv \in E_1} 1 + \frac{4\sqrt{3}}{7} \sum_{uv \in E_2} 1 + \sum_{uv \in E_3} 1$$

$$= 2 + \frac{4\sqrt{3}}{7} \times 8 + 4$$

$$= \frac{42 + 32\sqrt{3}}{7}.$$

Case 2. $n > 3$

If $n > 3$, the edge set of $(P_n \odot K_1) \boxtimes P_2$ can be partitioned as follows:

$$E_1 = \{uv \mid d_u = 2n - 1, d_v = 2n - 1\}, \qquad |E_1| = n^2.$$

$$E_2 = \{uv \mid d_u = 2n - 1, d_v = 2n\}, \qquad |E_2| = 2n^2 - n.$$

$E_3 = \{uv \mid d_u = 2n, d_v = 2n\}, \qquad |E_3| = n^2.$

$$M_1\big((P_n \odot K_1) \boxtimes P_2\big) = \sum_{uv\in E\left((P_n\odot K_1)\boxtimes P_2\right)} d(u) + d(v)$$

$$= \sum_{uv\in E_1} (2n-1) + (2n-1) + \sum_{uv\in E_2} (2n-1) + (2n) + \sum_{uv\in E_3} (2n) + (2n)$$

$$= (4n-2)\sum_{uv\in E_1} 1 + (4n-1)\sum_{uv\in E_2} 1 + (4n)\sum_{uv\in E_3} 1$$

$$= (4n-2) \times n^2 + (4n-1) \times (2n^2 - n) + (4n) \times n^2$$

$$= n(4n-1)^2.$$

$$M_2\big((P_n \odot K_1) \boxtimes P_2\big) = \sum_{uv\in E\left((P_n\odot K_1)\boxtimes P_2\right)} d(u)\, d(v)$$

$$= \sum_{uv\in E_1} (2n-1)(2n-1) + \sum_{uv\in E_2} (2n-1)\,(2n) + \sum_{uv\in E_3} (2n)\,(2n)$$

$$= (2n-1)^2\sum_{uv\in E_1} 1 + (4n^2-2n)\sum_{uv\in E_2} 1 + (4n^2)\sum_{uv\in E_3} 1$$

$$= (2n-1)^2 \times n^2 + (4n^2-2n) \times (2n^2-n) + (4n^2) \times n^2$$

$$= n^2(3(2n-1)^2 + \ 4n^2).$$

$$H\big((P_n \odot K_1) \boxtimes P_2\big) \ = \sum_{uv\in E\left((P_n\odot K_1)\boxtimes P_2\right)} \frac{2}{d(u)+d(v)}$$

$$= \sum_{uv\in E_1} \frac{2}{(4n-2)} + \sum_{uv\in E_2} \frac{2}{(4n-1)} + \sum_{uv\in E_3} \frac{2}{(4n)}$$

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

$$= \frac{n^2}{(2n-1)} + \frac{2n(2n-1)}{(4n-1)} + \frac{n}{2}.$$

$$GA\big((P_n \odot K_1) \boxtimes P_2\big) = \sum_{uv\in E\left((P_n\odot K_1)\boxtimes P_2\right)} \frac{2\sqrt{d(u)\,d(v)}}{d(u)+d(v)}$$

$$= \sum_{uv\in E_1} \frac{2\sqrt{2n-1 \times 2n-1}}{4n-2} + \sum_{uv\in E_2} \frac{2\sqrt{2n \times 2n-1}}{4n-1} + \sum_{uv\in E_3} \frac{2\sqrt{2n \times 2n}}{4n}$$

$$= \sum_{uv\in E_1} \frac{2(2n-1)}{(4n-2)} + \sum_{uv\in E_2} \frac{2\sqrt{(4n^2-2n)}}{(4n-1)} + \sum_{uv\in E_3} \frac{2 \times 2n}{4n}$$

$$= 2n^2 + \frac{2n(2n-1)\sqrt{(4n^2-2n)}}{(4n-1)}.$$

This completes the proof.

Note: For $n = 3$, first and second Zagreb indices, Harmonic index and Geometric-Arithmetic index of $(P_3 \odot K_1) \boxtimes P_2$ are 388, 1106, $\frac{986}{165}$ and $\frac{198+32\sqrt{30}}{11}$ respectively.

3. Conclusion

In this work, we determined various topological indices of ARMS-product of certain classes of graphs. Since the ARMS-product is a newly introduced graph product, it has great significance in the field of topological indices.

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Declarations

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