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On the ABC and GA indices of the corona products of some graphs

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In this research, we derived the formulae for the atom-bond connectivity (ABC) index and the geometric-arithmetic (GA) index of several corona products of graphs made by composing the path, the cycle and the complete graphs. Relevant mathematical results were presented with proofs, indicating the possibility of predicting physicochemical properties of several molecular graphs.

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Introduction

A molecular graph is a simple finite and connected graph of which the vertices represent the atoms and the edges represent the bonds between them. Graph invariants defined on molecular graphs, based on the degrees of vertices or the weights of the vertices or the edges are called topological indices. As an extensively studied area in chemical graph theory, these invariants generally help to predict certain physicochemical properties of molecular structures such as boiling point and stability in terms of molecular shapes. Wiener index, the pioneering topological index first appeared in literature in 1947 [10]. Since then, several topological indices including the Wiener index, the Randić index, the atom-bond connectivity (ABC) index, the Gutman index and the geometric-arithmetic (GA) index were studied by several researchers for extracting information of molecular structures mathematically [2,3,8,9].

On the other hand, composition of new compounds from the existing ones can be modeled by graph operations, where a new molecular graph is obtained by combining two molecular graphs. There are several graph operations such as the Cartesian product, the cluster product, the corona product and the Kronecker product, different compositions representing different chemical operations [4,5]. Therefore, it is useful to know the topological indices of these composite molecular graphs, in order to derive important information on their properties [1]. Accordingly, topological indices of product graphs have been an interesting research topic in the past few years and one may find many papers presenting formulae for different topological indices of different compositions of graphs [6,7,9,10]. This is the context based on which we were motivated to study the ABC index [2] and the GA index [9] of the corona products of several graph structures.

Preliminaries

The ABC index was proposed by Estrada et al in 1998 [2]. The index is based on the degree of vertices, which is used to describe the heats of formation of alkanes [2,12]. Consider a simple connected undirected graph H (V, E) with n vertices, then the ABC index is defined as follows:

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

where, d_u is the degree of vertex u.

Moreover, by considering the degrees of vertices in a graph, Vukičević and Furtula introduced GA index in 2009 [9]. The GA index is defined as follows:

$$GA(H) = \sum_{uv \in E(H)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \qquad (2)$$

According to the definition, GA index reflects the difference between the geometric and arithmetic means [3].

The corona product of H_1 and H_2 is defined as the graph obtained by taking one copy of graph H_1 and $|V(H_1)|$ copies of H_2, where each vertex of the ith copy of H_2 is connected with the ith vertex of H_1, and is denoted by $H_1 \odot H_2$ [11].

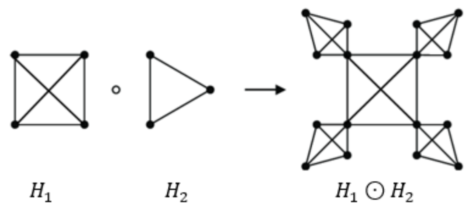

FIGURE 1 Corona product of complete graph on 4 vertices and cycle on 3 vertices

Main Results

Let P_n, C_n and K_n be path, cycle and complete graphs respectively on n vertices. In this section we discuss the ABC index and the GA index of $P_n \odot P_m$, $C_n \odot C_m$ and $K_n \odot K_m$.

Theorem 3.1. *The ABC index and the GA index of the corona product of two path graphs P_n and P_m are given by the following equations:*

$$ABC(P_n \odot P_m) = \begin{cases} 3\sqrt{2} + \frac{2}{3};\ n = 2, m = 2, \\ 4\sqrt{2} + \frac{4(m-3)}{3} + 2(m-2)\sqrt{\frac{m+2}{3(m+1)}} + \frac{\sqrt{2m}}{m+1};\ n = 2; m > 2, \\ \frac{3n}{\sqrt{2}} + \sqrt{\frac{5}{3}} + \frac{(n-3)\sqrt{6}}{4};\ n > 2; m = 2, \\ 2\sqrt{2}n + \frac{2n(m-3)}{3} + 2(m-2)\sqrt{\frac{m+2}{3(m+1)}} + \\ 2\sqrt{\frac{2m+1}{(m+1)(m+2)}} + \frac{(n-3)\sqrt{2m+2}}{m+2} + \\ (n-2)(m-2)\sqrt{\frac{m+3}{3(m+2)}};\ n > 2; m > 2. \end{cases} \quad (3)$$

$$GA(P_n \odot P_m) = \begin{cases} 3 + \frac{8\sqrt{6}}{5};\ n = 2, m = 2, \\ 1 + 2(m-3) + \frac{8\sqrt{6}}{5} + \frac{8\sqrt{2(m+1)}}{(m+3)} + \\ \frac{4(m-2)\sqrt{3(m+1)}}{m+4};\ n = 2; m > 2, \\ 2n - 3 + \frac{4\sqrt{2}(n-2)}{3} + 8\left(\frac{\sqrt{3}}{7} + \frac{\sqrt{6}}{5}\right);\ n > 2; m = 2, \\ 4\sqrt{m+1}\left(\frac{2\sqrt{2}}{m+3} + \frac{\sqrt{3}(m-2)}{m+4} + \frac{\sqrt{m+2}}{2m+3}\right) + \\ 2(n-2)\sqrt{m+2}\left(\frac{2\sqrt{2}}{m+4} + \frac{\sqrt{3}(m-2)}{m+5}\right) + \\ \frac{4\sqrt{6}n}{5} + n(m-3);\ n > 2; m > 2. \end{cases} \quad (4)$$

Proof. Consider the corona product of two path graphs $P_n \odot P_m$. If $n, m > 1$, four types of vertices can be seen by considering the degrees of them. The first type is vertices having degree 2; the second type is vertices having degree 3; the third type is vertices having degree $n+1$ and the fourth type is vertices having degree $n+2$. In this graph, $|V(P_n \odot P_m)| = n + nm$ and $|E(P_n \odot P_m)| = nm + (n-1) + n(m-1) = 2nm - 1$. Then by considering the degrees of the vertices, we can observe 10 types of edge partitions as in Table 1.

TABLE 1 Number of edges in each partition of $P_n \odot P_m$ on the basis of degree of end vertices of each edge

(d_u, d_v)	Number of edges
$(m+1, 2)$	4
$(m+1, 3)$	$2(m-2)$
$(m+1, m+1)$	$1; n = 2$ $0; n > 2$
$(m+2, m+2)$	$0; n = 2$ $n - 3\ n > 2$
$(m+1, m+2)$	$0; n = 2$ $2; n > 2$

$(m+2,2)$	$0;\, n=2$ $2(n-2);\ n>2$
$(m+2,3)$	$0;\, n=2$ $(n-2)(m-2)\ n>2$
$(2,2)$	n; $m=2$ $0;\, m>2$
$(2,3)$	$0;\, m=2$ 2n; $m>2$
$(3,3)$	$0;\, m=2$ $n(m-3);\, m>2$

Now substitute the values in Table 1 in Equation 1 for each case.

Case 1. $\boldsymbol{n=m=2}$

$$ABC(P_n \odot P_m) = 4\sqrt{\frac{(m+1)+2-2}{2(m+1)}} + 2(m-2)\sqrt{\frac{(m+1)+3-2}{3(m+1)}} + \sqrt{\frac{2(m+1)-2}{(m+1)(m+1)}} + 2(n-2)\sqrt{\frac{(m+2)+2-2}{2(m+2)}} + n\sqrt{\frac{2+2-2}{2^2}}$$

$$= 3\sqrt{2} + \frac{2}{3}.$$

Case 2. $\boldsymbol{n=2, m>2}$

$$ABC(P_n \odot P_m) = 4\sqrt{\frac{(m+1)+2-2}{2(m+1)}} + 2(m-2)\sqrt{\frac{(m+1)+3-2}{3(m+1)}} + \sqrt{\frac{2(m+1)-2}{(m+1)(m+1)}} + 2(n-2)\sqrt{\frac{(m+2)+2-2}{2(m+2)}} + 2n\sqrt{\frac{2+3-2}{6}} + n(m-3)\sqrt{\frac{3+3-2}{9}}$$

$$= 4\sqrt{2} + \frac{4(m-3)}{3} + 2(m-2)\sqrt{\frac{m+2}{3(m+1)}} + \frac{\sqrt{2m}}{(m+1)}.$$

Case 3. $\boldsymbol{n>2, m=2}$

$$ABC(P_n \odot P_m) = 4\sqrt{\frac{(m+1)+2-2}{2(m+1)}} + 2(m-2)\sqrt{\frac{(m+1)+3-2}{3(m+1)}} + 2\sqrt{\frac{(m+1)+(m+2)-2}{(m+1)(m+2)}} + (n-3)\sqrt{\frac{2(m+2)-2}{(m+2)(m+2)}} + 2(n-2)\sqrt{\frac{(m+2)+2-2}{2(m+2)}} + (n-2)(m-2)\sqrt{\frac{(m+2)+3-2}{3(m+2)}} + n\sqrt{\frac{2+2-2}{2^2}}$$

$$= \frac{3n}{\sqrt{2}} + \sqrt{\frac{5}{3}} + \frac{(n-3)\sqrt{6}}{4}.$$

Case 4: $\boldsymbol{n>2, m>2}$

$$ABC(P_n \odot P_m) = 4\sqrt{\frac{(m+1)+2-2}{2(m+1)}} + 2(m-2)\sqrt{\frac{(m+1)+3-2}{3(m+1)}} + 2\sqrt{\frac{(m+1)+(m+2)-2}{(m+1)(m+2)}} + (n-3)\sqrt{\frac{2(m+2)-2}{(m+2)(m+2)}} + 2(n-2)\sqrt{\frac{(m+2)+2-2}{2(m+2)}} + (n-2)(m-2)\sqrt{\frac{(m+2)+3-2}{3(m+2)}} + 2n\sqrt{\frac{2+3-2}{6}} + n(m-3)\sqrt{\frac{3+3-2}{3^2}}$$

$$= 2\sqrt{2}n + \frac{2n(m-3)}{3} + 2(m-2)\sqrt{\frac{m+2}{3(m+1)}} + 2\sqrt{\frac{2m+1}{(m+1)(m+2)}} + \frac{(n-3)\sqrt{2m+2}}{m+2} + (n-2)(m-2)\sqrt{\frac{m+3}{3(m+2)}}.$$

Similarly, using Equation 2 and the values in Table 1, we obtain the required result for $GA(P_n \odot P_m)$ and this completes the proof.

Theorem 3.2. *The ABC index and the GA index the corona product of two cycles C_n and C_m are given by the following equations:*

$$ABC(C_n \odot C_m) = \frac{2nm}{3} + \frac{n\sqrt{2m+2}}{m+2} + nm\sqrt{\frac{m+3}{3(m+2)}}. \quad (5)$$

$$GA(C_n \odot C_m) = n(m+1) + \frac{2nm\sqrt{3(m+2)}}{m+5}. \quad (6)$$

Proof. It is easily seen that $|V(C_n \odot C_m)| = n + nm$ and $|E(C_n \odot C_m)| = \text{n} + 2nm$, when, $n, m > 2$. Further, there are two types of vertices as considering the degrees of the vertices. One type of vertices has degree 3 and other type of vertices has degree m+2. The edge partitions, according to the degree of every vertex are shown in Table 2.

TABLE 2 Number of edges in each partition of $C_n \odot C_m$ on the basis of degree of end vertices of each edge

(d_u, d_v)	Number of edges
$(m+2, m+2)$	n
$(m+2, 3)$	nm
$(3, 3)$	nm

By substituting values in Table 2 in Equation 1 and simplifying the formula, we obtain,

$$ABC(C_n \odot C_m) = n\sqrt{\frac{(m+2)+(m+2)-2}{2(m+2)}} + nm\sqrt{\frac{(m+2)+3-2}{3(m+2)}} + nm\sqrt{\frac{3+3-2}{9}}$$

$$= \frac{2nm}{3} + \frac{n\sqrt{2m+2}}{m+2} + nm\sqrt{\frac{m+3}{3(m+2)}}.$$

Similarly, using Equation 2 and the values in Table 2, we obtain the required result for $GA(C_n \odot C_m)$.

Theorem 3.3. *For the corona product of two complete graphs K_n, K_m, ABC index and GA index are equal to the following equations, respectively:*

$$ABC(K_n \odot K_m) = n\sqrt{\frac{(m-1)^3}{2}} + \frac{n}{\sqrt{n+m-1}}\left(\sqrt{m(n+2m-3)} + (n-1)\sqrt{\frac{n+m-2}{2(n+m-1)}}\right). (7)$$

$$GA(K_n \odot K_m) = \frac{n((m-1)+n-1)}{2} + \frac{2nm\sqrt{m(n+m-1)}}{n+2m-1}. (8)$$

Proof. According to the definition of corona product, if $n, m > 1$, $|V(K_n \odot K_m)| = n + nm$ and $|E(K_n \odot K_m)| = nm + {}^nC_2 + n^mC_2$. Notice that, there are two types of vertices as considering the degrees of the vertices. One type of vertices has degree m and other type of vertices has degree $n+m-1$. Hence, there are three type of edge partitions as in Table 3.

TABLE 3 Number of edges in each partition of $K_n \odot K_m$ on the basis of degree of end vertices of each edge

(d_u, d_v)	Number of edges
(m, m)	n^mC_2
$(m, n+m-1)$	nm
$(n+m-1, n+m-1)$	${}^nC_2$

By substituting values in Table 3 in Equation 1 and simplifying the formula, we obtain,

$$ABC(K_n \odot K_m) = n\sqrt{\frac{(m-1)^3}{2}} + \frac{n}{\sqrt{n+m-1}}\left(\sqrt{m(n+2m-3)} + (n-1)\sqrt{\frac{n+m-2}{2(n+m-1)}}\right).$$

Similarly, by substituting values in Table 3 to Equation 2 and simplifying the formula, we have,

$$GA(K_n \odot K_m) = \frac{n((m-1)+n-1)}{2} + \frac{2nm\sqrt{m(n+m-1)}}{n+2m-1}.$$

This completes the proof.

Theorem 3.4. *For the corona product of complete graph and path graph K_n, P_m, ABC index and GA index are equal to the following equations, respectively:*

$$ABC(K_n \odot P_m) = \begin{cases} \dfrac{3n}{\sqrt{2}} + \dfrac{n(n-1)\sqrt{2n}}{2(n+1)} \ ; n \geq 2 \text{ and } m = 2, \\ \dfrac{n}{\sqrt{n+m-1}}\left((m-2)\sqrt{\dfrac{n+m}{3}} + \dfrac{n-1}{2}\sqrt{\dfrac{2n+2m-4}{n+m-1}}\right) \\ + \dfrac{4n}{\sqrt{2}} + \dfrac{2n(m-3)}{3} \ ; n \geq 2 \text{ and } m > 2. (9) \end{cases}$$

$$GA(K_n \odot P_m) = \begin{cases} \dfrac{n(n+1)}{2} + \dfrac{4n\sqrt{2(n+1)}}{n+3} \ ; n \geq 2 \text{ and } m = 2, \\ \dfrac{n(n-1)}{2} + \dfrac{4n\sqrt{2(n+m-1)}}{n+m+1} + n(m-3) + \\ \dfrac{2n(m-2)\sqrt{3(n+m-1)}}{n+m+2} + \dfrac{4n\sqrt{6}}{5} \ ; n \geq 2 \text{ and } m > 2. (10) \end{cases}$$

Proof. Consider the corona product of $K_n \odot P_m$. If $n, m > 1$, three type of vertices can be identified by considering the degrees of them. The first type is vertices having degree 2, the second type is vertices having degree 3 and the third type is vertices having degree $n+m-1$. In this graph, $|V(K_n \odot P_m)| = n + nm$ and $|E(K_n \odot P_m)| = nm + n(m-1) + {}^nC_2$. Then by reviewing the degree of the vertices, we can observe 6 type of edge partitions as in Table 4.

TABLE 4 Number of edges in each partition of $K_n \odot P_m$ on the basis of degree of end vertices of each edge

(d_u, d_v)	Number of edges
$(n+m-1, n+m-1)$	${}^nC_2$
$(n+m-1, 2)$	$2n$
$(n+m-1, 3)$	n(m-2)
$(2,2)$	n; $m=2$ 0; $m>2$
$(2,3)$	0; $m=2$ 2n; $m>2$
$(3,3)$	0; $m=2$ n(m-3); $m>2$

Now substitute the values in Table 4 in Equation 1 for both cases.

Case 1. $\boldsymbol{n \geq 2, m = 2}$

$$ABC(K_n \odot P_m) = {}^nC_2\sqrt{\frac{2(n+m-1)-2}{(n+m-1)^2}} + 2n\sqrt{\frac{2+(n+m-1)-2}{2(n+m-1)}} + n(m-2)\sqrt{\frac{3+(n+m-1)-2}{3(n+m-1)}} + n\sqrt{\frac{2+2-2}{2^2}}.$$

By simplifying the formula, we obtain,

$$ABC(K_n \odot P_m) = \frac{3n}{\sqrt{2}} + \frac{n(n-1)\sqrt{2n}}{2(n+1)}.$$

Case 2. $\boldsymbol{n \geq 2, m} > 2$

$$ABC(K_n \odot P_m) = {}^nC_2\sqrt{\frac{2(n+m-1)-2}{(n+m-1)^2}} + 2n\sqrt{\frac{2+(n+m-1)-2}{2(n+m-1)}} + n(m-2)\sqrt{\frac{3+(n+m-1)-2}{3(n+m-1)}} + 2n\sqrt{\frac{2+3-2}{2(3)}} + n(m-3)\sqrt{\frac{3+3-2}{3^2}}.$$

By simplifying the formula, we obtain the required result.

Similarly, by substituting values in Table 4 to Equation 2 and simplifying the formula, we obtained the required results for $GA(K_n \odot P_m)$.

Theorem 3.5. *The ABC index and the GA index of the corona product of path graph and complete graph P_m and K_n are given by the following equations:*

$$ABC(P_m \odot K_n) = \begin{cases} \frac{\sqrt{2n}}{n+1} + (n-1)\sqrt{2(n-1)} + 2n\sqrt{\frac{2n-1}{n(n+1)}} \; ; n \geq 2 \text{ and } m = 2, \\ \frac{m(n-1)\sqrt{2n-2}}{2} + 2n\sqrt{\frac{2n-1}{n(n+1)}} + 2\sqrt{\frac{2n+1}{(n+1)(n+2)}} + \frac{(m-3)\sqrt{2(n+1)}}{n+2} + n(m-2)\sqrt{\frac{2}{n+2}} \; ; n \geq 2 \text{ and } m > 2. \end{cases} \quad (11)$$

$$GA(P_m \odot K_n) = \begin{cases} 1 + n(n-1) + \frac{4n\sqrt{n(n+1)}}{2n+1} \; ; n \geq 2 \text{ and } m = 2, \\ \frac{nm(n-1)}{2} + \frac{4n\sqrt{n(n+1)}}{2n+1} + m - 3 + \frac{4\sqrt{(n+1)(n+2)}}{2n+3} + \frac{n(m-2)\sqrt{n(n+2)}}{n+1} \; ; n \geq 2 \text{ and } m > 2. \end{cases} \quad (12)$$

Proof. Consider the corona product of path graph and complete graph $P_m \odot K_n$. If $n, m > 1$, three types of vertices can be seen by considering the degree of them. The first type is vertices having degree n, the second type is vertices having degree $n+1$ and the third type is vertices having degree $n+2$. In this graph, $|V(P_m \odot K_n)| = m + nm$ and $|E(P_m \odot K_n)| = nm + (m-1) + m{}^nC_2$. Then by considering the degree of the vertices, we can identify 6 types of edge partitions as shown in Table 5.

TABLE 5 Number of edges in each partition of $P_m \odot K_n$ on the basis of degree of end vertices of each edge

(d_u, d_v)	Number of edges
$(n+1, n+1)$	1; $m=2$ 0; $m>2$
(n, n)	$m{}^nC_2$

$(n, n+1)$	$2n$
$(n+1, n+2)$	$0; m=2$ $2;\ m>2$
$(n+2, n+2)$	$0; m=2$ m-3; $m>2$
$(n+2, n)$	$0; m=2$ n(m-2); $m>2$

Now substitute the values in Table 5 in Equation 1 for both cases.

Case 1. $\boldsymbol{n \geq 2, m = 2}$

$$ABC(P_m \odot K_n) = \sqrt{\frac{2(n+1)-2}{(n+1)^2}} + m^nC_2\sqrt{\frac{2n-2}{n^2}} + 2n\sqrt{\frac{n+(n+1)-2}{n(n+1)}}.$$

By simplifying the formula, we obtain,

$$ABC(P_2 \odot K_n) = \frac{\sqrt{2n}}{n+1} + (n-1)\sqrt{2(n-1)} + 2n\sqrt{\frac{2n-1}{n(n+1)}}.$$

Case 2. $\boldsymbol{n \geq 2, m} > 2$

$$ABC(P_m \odot K_n) = m^nC_2\sqrt{\frac{2n-2}{n^2}} + 2n\sqrt{\frac{n+(n+1)-2}{n(n+1)}} + 2\sqrt{\frac{(n+1)+(n+2)-2}{(n+1)(n+2)}} + (m-3)\sqrt{\frac{2(n+2)-2}{(n+2)^2}} + n(m-2)\sqrt{\frac{n+(n+2)-2}{n(n+2)}}.$$

By simplifying the formula, we obtain the required result.

Similarly, by substituting values in Table 5 to Equation 2 and simplifying the formula, we obtained the required results for $GA(P_m \odot K_n)$.

Conclusion

In order to derive information of composite molecular graphs, it is helpful to generate formulae for the relevant topological indices of the graphs composed by the corresponding graph product. In this study, we formulated the ABC and GA indexes of the corona products of the path, the cycle and the complete graphs when composed with them.

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