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ATOM-BOND-CONNECTIVITY INDEX OF CERTAIN GRAPHS

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ABSTRACT. The ABC index is one of the most applicable topological graph indices and several properties of it has been studied already due to its extensive chemical applications. Several variants of it have also been defined and used for several reasons. In this paper, we calculate the atom-bond connectivity index of some derived graphs such as double graphs, subdivision graphs and complements of some standard graphs.

Keywords: Atom-bond-connectivity index, double graphs, subdivision graphs, k-complement.

AMS Subject Classification: 05C07, 05C30, 05C50.

1. INTRODUCTION AND PRELIMINARIES

Let G be a graph with n vertices $v_1,\ v_2,\ \cdots,\ v_n$ and m edges. In this paper, we only consider simple, undirected and signless graphs.

The complement of a graph G is a graph $\overline{G}$ having the same vertex set such that two distinct vertices of $\overline{G}$ are adjacent if and only if they are not adjacent in G. The complement is a useful tool in many calculations, especially with the topological graph indices.

Let G be a graph and $P_k = \{V_1,\ V_2,\ \cdots,\ V_k\}$ be a partition of its vertex set V. Similarly to the complement of a graph, the k-complement of G is defined as follows: For all pairs of sets V_i and V_j in P_k for $i \neq j$, remove the edges between V_i and V_j and add the edges between the vertices of V_i and V_j which are not in G and this k-complement will be denoted by $\overline{G_k}$.

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Let G be a graph and again P_k be a partition of its vertex set V as above. Then the $k(i)$-complement of G, yet another type of the complement of a graph, is defined as follows: For each partition set V_r in P_k, remove the edges of G joining the vertices in V_r and add the edges of $\overline{G}$ (complement of G) joining the vertices of V_r, and it is denoted by $\overline{G_{k(i)}}$.

Topological graph indices are defined and used in many areas to study several properties of different objects such as atoms and molecules. These indices can be classified into several classes according to their way of definition: by means of matrices, by means of vertex degrees, by means of distances, etc. One of these topological indices is the atom bond-connectivity index (ABC index) which is defined in terms of the vertex degrees as follows:

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

In [6], the ABC index for some graphs is calculated together with GA, Randic and Zagreb indices. In [3], the first Zagreb index and multiplicative Zagreb coindices of graphs were calculated. There are many papers on the subject, see e.g. [1, 4].

A derived graph is the graph obtained from any given graph following some predefined rule. One of these derived graphs is the subdivision graph. The subdivision graph $S(G)$ of a simple graph G is defined as the new graph obtained by adding an extra vertex into each edge of G. The subdivision graph of the xcycle graph C_n is shown in Fig. 1. The subdivision graphs have been studied in literature, [2], [7], [8], [9], [10] and [14]. All versions of

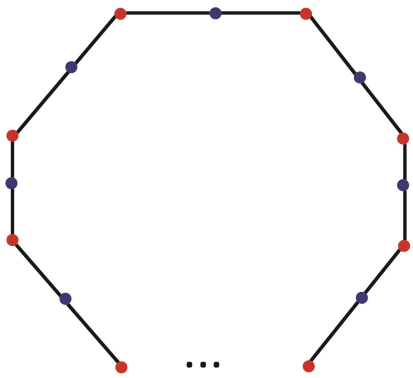

FIGURE 1. Subdivision graph of the cycle graph C_n

Zagreb indices and coindices of subdivision graphs of certain graph types were studied in [13]. The Zagreb indices and multiplicative Zagreb indices of subdivision graphs of double graphs were studied in [15].

In [11] and [12], a generalization of subdivision graphs were defined and studied: the r-subdivision graph of a graph G, which is denoted by $S^r(G)$, is the new graph obtained from G by replacing each of its edges by a path of length $r+1$; or equivalently by inserting r additional vertices into each edge of G. Clearly, in the case of $r = 1$, the obtained

1-subdivision graph is the subgraph.

In [5], topological indices of the derived graphs of subdivision graphs were studied.

For a graph G with vertex set $V(G) = \{v_1,\ v_2,\ \cdots,\ v_n\}$, we take another copy of G with vertices labelled by $\{v_1,\ v_2,\ \cdots,\ v_n\}$, this time, where v_i corresponds to v_i for each i. If we connect v_i to the neighbours of v_i for each i, we obtain a new graph called the double graph of G. It is denoted by $D(G)$. In Fig. 2 and 3, the double graphs of P_6 and C_4 are given: The Zagreb indices and multiplicative Zagreb indices of double graphs of

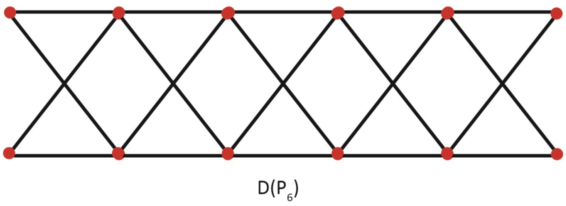

FIGURE 2. Double graph of P_6

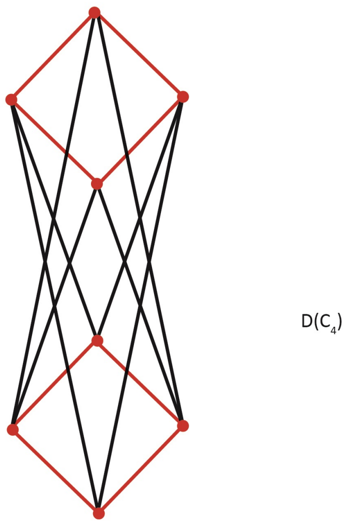

FIGURE 3. Double graph of C_4

subdivision graphs were studied in [10].

2. Atom-bond-connectivity index of double graphs

Several topological graph indices of some of the derived graphs have already been calculated. In this section, we calculate the atom-bond-connectivity indices of the double graphs of some classes of frequently-used graphs. In the proofs, we use some counting algorithm where each edge is named according to the vertex degrees of the edge: An edge e is called an (r, s)-edge if two end vertices of e has vertex degrees r and s. For example, all edges of a cycle graph are $(2, 2)$-edges and the edges of a path graph are either $(1, 2)$-edges or $(2, 2)$-edges.

Theorem 2.1.

$$ABC(D(G)) = \begin{cases} 4\sqrt{2}+(n-3)\sqrt{6} & \textit{if } G = P_n, \\ n\sqrt{6} & \textit{if } G = C_n, \\ n\sqrt{4n-6} & \textit{if } G = K_n, \\ 2n\sqrt{4n-2} & \textit{if } G = K_{n,n}, \\ 2\sqrt{2}(n-1) & \textit{if } G = K_{1,n-1}. \end{cases}$$

Proof. We shall give the proof for two of the graph types: For P_n and for C_n. Proofs of the other graph types can be done in a similar way by counting the edges and applying the formula.

Note that the double graph $D(P_n)$ of the path graph P_n has $4n-4$ edges. There are 8 $(2,4)$-edges and $4(n-3)$ $(4,4)$-edges. That is, the edge diagram of $D(P_n)$ is as follows:

(r,s)-edges	their number
$(2,4)$-edges	8
$(4,4)$-edges	$4(n-3)$

Therefore

$$\begin{aligned} ABC(D(P_n)) &= \textstyle\sum_{uv\in E(D(P_n))} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\ &= 8\sqrt{\tfrac{2+4-2}{2\cdot 4}} + 4(n-3)\sqrt{\tfrac{4+4-2}{4\cdot 4}} \\ &= 4\sqrt{2}+(n-3)\sqrt{6}. \end{aligned}$$

Secondly, consider $D(C_n)$. $D(C_n)$ has $4n$ $(4,4)$-edges. Therefore its edge diagram is simpler:

(r,s)-edges	their number
$(4,4)$-edges	$4n$

and using this information, we calculate the ABC index of the double graph of the cycle graph C_n as follows:

$$\begin{aligned} ABC(D(C_n)) &= \textstyle\sum_{uv\in E(D(C_n))} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\ &= 4n\sqrt{\tfrac{4+4-2}{4\cdot 4}} \\ &= n\sqrt{6}. \end{aligned}$$

□

3. Atom-bond-connectivity index of complements

In this section, we calculate the ABC indices of several complements of some graph classes. We first start with the ordinary complements:

Theorem 3.1.

$$ABC(\overline{G}) = \begin{cases} \frac{(n-1)\sqrt{2n-6}}{2} & \textit{if } \ G = K_{1,n-1}, \\ 0 & \textit{if } \ G = K_{n\times 2}, \\ \frac{n\sqrt{2}}{2}\sqrt{n-4} & \textit{if } \ G = C_n. \end{cases}$$

Proof. Let first $G = K_{1,n-1}$ be the star graph of order n. Then the complement of this graph is $\overline{K_{1,n-1}} = K_{n-1}$, that is, the complete graph of order $n-1$. The edge diagram of this complement graph is

(r, s)-edges	their number
$(n-2, n-2)$-edges	$\frac{(n-1)(n-2)}{2}$

This implies that the ABC index of this complement graph is

$$\begin{aligned} ABC(\overline{K_{1,n-1}}) &= \textstyle\sum_{uv\in E(\overline{K_{1,n-1}})} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\ &= \frac{(n-1)(n-2)}{2}\sqrt{\frac{n-2+n-2-2}{(n-2)\cdot(n-2)}} \\ &= \frac{(n-1)\sqrt{2n-6}}{2}. \end{aligned}$$

Secondly, consider the complement of the coctail party graph $K_{n\times 2}$. It is not difficult to see that this complement is the ladder rung graph LR_n consisting of n P_2's. The edge diagram of this complement graph is

(r, s)-edges	their number
$(1, 1)$-edges	n

This implies that the ABC index of this complement graph is

$$\begin{aligned} ABC(\overline{K_{1,n-1}}) &= \textstyle\sum_{uv\in E(\overline{K_{1,n-1}})} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\ &= \frac{(n-1)(n-2)}{2}\sqrt{\frac{n-2+n-2-2}{(n-2)\cdot(n-2)}} \\ &= \frac{(n-1)\sqrt{2n-6}}{2}. \end{aligned}$$

Finally, consider the complement of the cycle graph C_n. It is clear that in the complement, every vertex is connected to all the vertices except three: the vertex itself and its two neigbours. Therefore the edge diagram of this complement graph would be

(r, s)-edges	their number
$(n-3, n-3)$-edges	$\frac{n(n-3)}{2}$

This implies that the ABC index of the complement graph $ABC(\overline{C_n})$ is

$$\begin{aligned} ABC(\overline{C_n}) &= \textstyle\sum_{uv\in E(\overline{C_n})} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\ &= \frac{n(n-3)}{2}\sqrt{\frac{n-3+n-3-2}{(n-3)\cdot(n-3)}} \\ &= \frac{n}{2}\sqrt{2n-8} \end{aligned}$$

giving the result. □

The following results on other types of complements of some graphs can similarly be proven by constructing the edge diagram and using the index formula:

Theorem 3.2.

$$ABC(\overline{K_{(n\times 2)_2}}) = \frac{5n-6}{n}\sqrt{2n-2}.$$

Theorem 3.3.

$$ABC(\overline{(S_{n,n})_{2i}}) = (2n-2)\sqrt{\frac{3n-5}{2n^2-4n+2}} + (2n^2-5n+3)\frac{\sqrt{4n-6}}{2n-2}.$$

4. Atom-bond-connectivity index of subdivision graphs

Subdivision graphs are important tools in calculating several properties of larger graphs in terms of smaller graphs. Now we calculate the atom-bond-connectivity index of the subdivision graphs of some frequently-used graphs. First we give a useful result for regular graphs:

Lemma 4.1. *Let G be an r-regular graph of arder n and size m. Then the following are satisfied:*

(i) $ABC(G) = \frac{m}{r}\sqrt{2r-2}$;

(ii) $ABC(S(G)) = m\sqrt{2}$.

Proof. Both items can be proven by the definition. □

Theorem 4.1.

$$ABC(S(G)) = \begin{cases} \sqrt{2}(n-1) & \text{if } G = P_n, \\ \sqrt{2}n & \text{if } G = C_n, \\ \frac{n^2-n}{\sqrt{2}} & \text{if } G = K_n, \\ \sqrt{2}(n-1) & \text{if } G = K_{1,n-1} \end{cases}$$

Proof. We shall give the proof for two of the graph types: For P_n and for $K_{1,n-1}$. Proofs of the other graph types can be done in a similar way by counting the edges and applying the formula.

First, we consider the subdivision graph of the path graph P_n. It is known that this graph is $S(P_n) = P_{2n-1}$. The edge diagram of this complement graph would be

(r,s)-edges	their number
$(1,2)$-edges	2
$(2,2)$-edges	$2n-4$

.

This implies that the ABC index of the complement graph $ABC(\overline{C_n})$ is

$$\begin{aligned} ABC(S(P_n)) &= ABC(P_{2n-1}) \\ &= \sum_{uv\in E(S(P_n))}\sqrt{\frac{d_u+d_v-2}{d_ud_v}} \\ &= 2\sqrt{\frac{1+2-2}{1\cdot 2}} + (2n-4)\sqrt{\frac{2+2-2}{2\cdot 2}} \\ &= \sqrt{2}(n-1). \end{aligned}.$$

Secondly, we consider the subdivision graph of the star graph $K_{1,n-1}$. It is known that this graph is the double star graph. The edge diagram of this complement graph would be

(r,s)-edges	their number
$(1,2)$-edges	$n-1$
$(2,n-1)$-edges	$n-1$

.

This implies that the ABC index of the complement graph $ABC(S(K_{1,n-1}))$ is

$$\begin{aligned} ABC(S(K_{1,n-1})) &= \sum_{uv\in E(S(K_{1,n-1}))} \sqrt{\tfrac{d_u+d_v-2}{d_u d_v}} \\ &= (n-1)\sqrt{\tfrac{1+2-2}{1\cdot 2}} + (n-1)\sqrt{\tfrac{2+n-1-2}{2\cdot(n-1)}} \\ &= \sqrt{2}(n-1). \end{aligned}$$

□

5. Atom-bond-connectivity index of the friendship graph, its subdivision graph and its line graph

Theorem 5.1.

$$ABC(G) = \begin{cases} \frac{3n}{\sqrt{2}} & \text{if } G = F_n^3, \\ \frac{6n}{\sqrt{2}} & \text{if } G = S(F_n^3), \\ \sqrt{2}n + \frac{(2n-1)^{\frac{3}{2}}}{\sqrt{2}} & \text{if } G = L(F_n^3), \end{cases}$$

Proof. We shall prove only the last item as the other two are similar to the above proofs.

Line graph of a graph is an important tool as one of the derived graphs. Let $L(F_n^3)$ be the line graph of the friendship graph which is the graph consisting of n triangles which all have a common vertex. Then the line graph of it is a graph obtained by adding n triangles around a complete graph on $2n$ vertices. It has the following edge diagram:

(r,s)-edges	their number
$(2,2n)$-edges	$2n$
$(2n,2n)$-edges	$\frac{2n(2n-1)}{2}$

This implies that the ABC index of the complement graph $ABC(L(F_n^3))$ is

$$\begin{aligned} ABC(L(F_n^3)) &= \sum_{uv\in E(L(F_n^3))} \sqrt{\tfrac{d_u+d_v-2}{d_u d_v}} \\ &= 2n\sqrt{\tfrac{2+2n-2}{2\cdot 2n}} + \tfrac{2n(2n-1)}{2}\sqrt{\tfrac{2n+2n-2}{2n\cdot 2n}} \\ &= \sqrt{2}n + \tfrac{(2n-1)^{\frac{3}{2}}}{\sqrt{2}}. \end{aligned}$$

□

Finally we consider the ABC index of another interesting graph. First we recall the definition:

Definition 5.1. *Jahangir graphs $J_{n,m}$ for $m = 3$, is a graph on $nm+1$ vertices. i.e., it is a graph consisting of a cycle C_{nm} with one additional vertex which is adjacent to m vertices of C_{nm} at distance n to each other on C_{nm}.*

Theorem 5.2.

$$ABC(J_{2,m}) = \sqrt{2}m + m\sqrt{\tfrac{m+1}{3m}}$$

Proof. Similar to the above. □

6. Results and discussion

The fact that modelling a molecule by a graph gives us many required information on the physico-chemical properties of the molecule at the end of some mathematical calculations made on the graph has been used in the last seven decades. For this, we calculate the values of the so called topological graph index and also determine which values could be attained by this index.

Derived graphs are graphs produced from a given graph according to some rule. The relations between a graph and its derived graph help us to obtain information on one from the other. In this paper, three of the important derived graphs are studied and their atom-bond-connectivity indices are determined. The methods and calculations given here can be generalized to other graph thypes and also to other derived graphs. It is also possible to determine the ABC index of the graph operations.

Disclosure statement

No potential conflict of interest was reported by the authors.

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