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On the entire ABC index of graphs

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Abstract

Topological indices are graph invariants computed usually by means of the distances or vertex degrees of molecular graphs. In chemical graph theory, topological indices have been successfully used in describing the structure and also predicting certain physico-chemical properties of chemical compounds. Atom-bond connectivity (ABC) index has been applied to the study of the stability of alkanes and to the strain the energy of cycloalkanes. The atom bond connectivity (ABC) index of a graph G is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{deg(u) + deg(v) - 2}{deg(u)deg(v)}},$$

where $E(G)$ denotes the set of edges of G and $deg(u)$ and $deg(v)$ are the degrees of the vertices u and v, respectively.

Recently, for several applications, the entire versions of the topological indices are defined and studied. In this versions of the topological indices, not only the vertices or the edges are considered in calculations. Both of them are used instead. In this research, we introduce and study the entire atom bond connectivity index of a graph. Exact values of this index for some families of graphs are obtained and some important properties of this new index are established.

Keywords: entire ABC index, ABC index, topological index
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1 Introduction

Let G be a finite connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $deg(v)$ denote the degree of a vertex $v \in V(G)$. In chemical graph theory, we usually make use of graphs to represent molecular structures. One of the most useful tools to study and predict various properties of molecular graphs is the topological indices which are used directly as simple numerical descriptors in quantitative structure property relationships (QSPR) and quantitative structure activity relationships (QSAR) [8].

In 1998, Estrada et al. [13] proposed a topological index based on the degrees of vertices of graphs, which is called the atom-bond connectivity index and denoted by ABC index for short. This index is defined in [13] for a graph G by

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{deg(u) + deg(v) - 2}{deg(u)deg(v)}}.$$

Initially, in the light of the existing close relationship between the ABC index and the heats of formation of alkanes, the ABC index became an efficient tool to study the thermodynamic properties of organic chemical compounds [13]. In 2008, Estrada [9] elaborated a novel quantum-theory-like justification of the ABC index and explained the stability of branched alkanes.

It has become a tradition to try to discover several modifications of some existing topological index for their new applications similar to the ones of the existing index. These trials usually end with a few papers discussing some purely mathematical properties instead of giving actual applications. Farahani [20] proposed the edge version of the ABC index as follows

$$ABC_e(G) = \sum_{ef \in E(L(G))} \sqrt{\frac{deg_{L(G)}(e) + deg_{L(G)}(f) - 2}{deg_{L(G)}(e)deg_{L(G)}(f)}}.$$

This recently introduced version of the ABC index has been applied up to now to the study of the stability of alkanes and to strain the energy of cycloalkanes.

Following this, in this paper, we introduce the entire version of the ABC index of a graph denoted by $ABC^{\mathcal{E}}(G)$. The motivation to do that is as follows. The classical topological indices defined by means of either vertex or edge degrees are useful to calculate only one type of a property. But for example, the intermolecular forces depend on the interactions not only between the atoms but also between the bonds and even between atoms and bonds. Therefore in recent years, people started to study entire versions of topological graph indices. Exact values of the entire ABC index for some families of graphs are obtained and some important properties of this new index are established. Some useful applications and recent results related to the entire topological graph indices can be found in [1] and [3].

2 Some general results on $ABC^{\mathcal{E}}(G)$

Definition 2.1. *Let $G = (V, E)$ be a simple graph and let*

$$B(G) = \{\{x, y\} : \{x, y\} \subseteq V(G) \cup E(G) \text{ and the elements } x \text{ and } y \text{ either adjacent or incident to each other}\}.$$

Then the entire atom bond connectivity index of G is defined by

$$ABC^{\mathcal{E}}(G) = \sum_{\{x,y\}\subseteq B(G)} \sqrt{\frac{deg(x) + deg(y) - 2}{deg(x)deg(y)}}.$$

Observation 2.2. *For any graph G with m edges, we have*

$$|B(G)| = 2m + \frac{M_1(G)}{2}$$

where $M_1(G)$ denotes the first Zagreb index of G.

The relation between the ABC, edge ABC and entire ABC indices is as follows:

Observation 2.3. *For any graph G,*

$$ABC^{\mathcal{E}}(G) = ABC(G) + ABC_e(G) + \sum_{v \text{ is incident to } e} \sqrt{\frac{deg(v) + deg(e) - 2}{deg(v)deg(e)}}.$$

Proposition 2.4. *For any k-regular graph G on n vertices with $k \geq 2$, we have*

$$ABC^{\mathcal{E}}(G) = \frac{n}{\sqrt{2}}\sqrt{k-1} + \frac{kn}{4}\sqrt{4k-6} + \frac{kn}{\sqrt{2}}\sqrt{\frac{3k-4}{k(k-1)}}.$$

Proof. Let G be a k-regular graph on n vertices with $k \geq 2$. Then G has $\frac{kn}{2}$ edges and $L(G)$ has

$$\frac{1}{2}\sum_{v\in V(G)} \big(deg(v)\big)^2 - q = \frac{nk^2}{2} - \frac{nk}{2} = \frac{kn(k-1)}{2}$$

edges. Therefore,

$$\begin{aligned} ABC^{\mathcal{E}}(G) =& \frac{kn}{2}\sqrt{\frac{2k-2}{k^2}} + \frac{kn(k-1)}{2}\sqrt{\frac{2k-2+2k-2-2}{(2k-2)^2}} + kn\sqrt{\frac{k+2k-2-2}{k(2k-2)}} \\ =& \frac{n}{\sqrt{2}}\sqrt{k-1} + \frac{kn}{4}\sqrt{4k-6} + \frac{kn}{\sqrt{2}}\sqrt{\frac{3k-4}{k(k-1)}}. \end{aligned}$$

Corollary 2.5. *For any complete graph K_n with $n \geq 3$ vertices,*

$$ABC^{\mathcal{E}}(K_n) = \frac{n}{\sqrt{2}}\sqrt{n-2} + \frac{n(n-1)}{4}\sqrt{4n-10} + \frac{n(n-1)}{\sqrt{2}}\sqrt{\frac{3n-7}{(n-1)(n-2)}}.$$

Corollary 2.6. *For any cycle graph C_n with $n \geq 3$ vertices,*

$$ABC^{\mathcal{E}}(C_n) = 2\sqrt{2}\,n.$$

Proposition 2.7. *For any path graph P_n with $n \geq 3$ vertices,*

$$ABC^{\mathcal{E}}(P_n) = 2\sqrt{2}\,n - \frac{7}{\sqrt{2}}.$$

Proof. Let P_n be a path graph with $n \geq 3$ vertices labeled by $v_1, v_2, \cdots, v_n$ and $n-1$ edges labeled by $e_1, e_2, \cdots, e_{n-1}$. The vertices v_1 and v_n are of degree one and the edges e_1 and e_{n-1} are of degree one. All other vertices and edges are of degree two. Therefore

$$\begin{aligned} ABC^{\mathcal{E}}(P_n) = & \sqrt{\frac{2+2-2}{4}}(n-3) + 2\sqrt{\frac{1+2-2}{2}} \\ & + \sqrt{\frac{2+2-2}{4}}(n-4) + 2\sqrt{\frac{1+2-2}{2}} \\ & + \sqrt{\frac{2+2-2}{4}}2(n-3) + 2\sqrt{\frac{1+2-2}{2}} + 2\sqrt{\frac{1+1-2}{1}} \\ = & \, 2\sqrt{2}n - \frac{7\sqrt{2}}{2}. \end{aligned}$$

Proposition 2.8. *For any complete bipartite graph $K_{a,b}$,*

$$ABC^{\mathcal{E}}(K_{a,b}) = \sqrt{ab(a+b-2)} + \frac{ab}{\sqrt{2}}\sqrt{a+b-3} + \sqrt{\frac{ab\big[(a+b)(a+b-4)+2ab\big]}{a+b-2}}.$$

Proof. Let the vertices of $K_{a,b}$ be labeled by $v_1, v_2, \cdots, v_a, v_{a+1}, v_{a+2}, \cdots, v_b$. Then

$$\begin{aligned} ABC^{\mathcal{E}}(K_{a,b}) = & ab\sqrt{\frac{b+a-2}{ab}} + \left(\frac{1}{2}(a^2b+b^2a) - ab\right)\sqrt{\frac{2(a+b-2)-2}{(a+b-2)^2}} \\ & + ab\sqrt{\frac{a+(a+b-2)-2}{a(a+b-2)}} + ab\sqrt{\frac{b+(a+b-2)-2}{b(a+b-2)}} \\ = & \sqrt{ab(a+b-2)} + \frac{ab}{\sqrt{2}}\sqrt{a+b-3} + \sqrt{\frac{ab\big[(a+b)(a+b-4)+2ab\big]}{a+b-2}}. \end{aligned}$$

Proposition 2.9. *Let G be the k-bridge graph $Q(a_1, a_2, \cdots, a_k)$. Then*

$$ABC^{\mathcal{E}}(G) = 2\sqrt{2}\sum_{i=1}^{k} a_i + \sqrt{2}(k+1)\sqrt{k-1} - 3k/\sqrt{2}.$$

Proposition 2.10. *Let G be the wheel graph W_n with $n+1$ vertices. Then*

$$\begin{aligned} ABC^{\mathcal{E}}(G) &= \left(\frac{2}{3} + \sqrt{\tfrac{5}{3}} + \sqrt{\tfrac{3}{8}}\right) n + n\sqrt{\frac{n+1}{3n}} \\ &\quad + n\sqrt{\frac{n+3}{n+1}} + \frac{n(n-1)}{n+1}\sqrt{\frac{n}{2}} \\ &\quad + 2n\sqrt{\frac{5}{12}} + n\sqrt{\frac{n+2}{3(n+1)}} + n\sqrt{\frac{2n-1}{n(n+1)}}. \end{aligned}$$

Proof. Let $G \cong W_n$ be the wheel graph of $n+1$ vertices. Then $|V_{3,3}| = n$, $|V_{3,n}| = n$, $|E_{4,4}| = n$, $|E_{4,n+1}| = 2n$, $|E_{n+1,n+1}| = \frac{n(n-1)}{2}$, $|A_{3,4}| = 2n$, $|A_{3,n+1}| = n$ and $|A_{n,n+1}| = n$. Then using Observation 2.3, we get

$$\begin{aligned} ABC^{\mathcal{E}}(G) &= \left(\frac{2}{3} + \sqrt{\tfrac{5}{3}} + \sqrt{\tfrac{3}{8}}\right) n + n\sqrt{\frac{n+1}{3n}} \\ &\quad + n\sqrt{\frac{n+3}{n+1}} + \frac{n(n-1)}{n+1}\sqrt{\frac{n}{2}} \\ &\quad + 2n\sqrt{\frac{5}{12}} + n\sqrt{\frac{n+2}{3(n+1)}} + n\sqrt{\frac{2n-1}{n(n+1)}}. \end{aligned}$$

Lemma 2.11. *Let s, t be arbitrary positive integers such that $s, t \geq 4$ and $G \cong P_t \Box P_s$. Then*

$$ABC(G) = 4\sqrt{2} + \frac{4s+4t-24}{3} + (s+t-4)\sqrt{\frac{5}{3}} + (2st-5t-5s+12)\sqrt{\frac{3}{8}}.$$

Proof. Let s, t be any positive integers such that $s, t \geq 4$ and $G \cong P_t \Box P_s$. Let $V_{a,b} = \{\{u.v\} : uv \in E(G) \text{ such that } deg(u) = a \text{ and } deg(v) = b\}$, so we have four partition sets of the vertices of G and it is not difficult to see that $|V_{2,3}| = 8, |V_{3,3}| = 2(s+t-6), |V_{3,4}| = s+t-4$ and $|V_{4,4}| = (s-3)(t-2) + (s-2)(t-3) = 2st - 5s - 5t + 12$. Then

$$\begin{aligned} ABC(G) = 8\sqrt{\frac{2+3-2}{6}} + 2(s+t-6)\sqrt{\frac{3+3-2}{9}} + (s+t-4)\sqrt{\frac{3+4-2}{12}} \\ + (2st-5s-5t+12)\sqrt{\frac{4+4-2}{16}}. \end{aligned}$$

Hence, $ABC(G) = 4\sqrt{2} + \dfrac{4s+4t-24}{3} + (s+t-4)\sqrt{\dfrac{5}{3}} + (2st-5t-5s+12)\sqrt{\dfrac{3}{8}}$.

Lemma 2.12. *[25] If $s, t \geq 4$, then*

$$ABC_e(G) = \frac{1}{2}\sqrt{\frac{3}{2}}(2t+2s-16) + \frac{1}{2}\sqrt{\frac{7}{5}}(st+4s-24) + \sqrt{\frac{3}{10}}(6t+6m-32) + \frac{\sqrt{10}}{6}(6ts-18t-18s+52) + \frac{8\sqrt{2}}{5} + 4\sqrt{\frac{5}{3}} + 8\sqrt{\frac{2}{5}} + \frac{8}{3}.$$

Theorem 2.13. *Let s, t be any positive integers such that $s, t \geq 4$ and $G \cong P_t \square P_s$. Then,*

$$\begin{aligned} ABC^{\mathcal{E}}(G) &= 4\sqrt{2} + \frac{4s+4t-24}{3} + (s+t-4)\sqrt{\frac{5}{3}} + (2st-5t-5s+12)\sqrt{\frac{3}{8}} \\ &+\tfrac{1}{2}\sqrt{\tfrac{3}{2}}(2t+2s-16) + \tfrac{1}{2}\sqrt{\tfrac{7}{5}}(st+4s-24) + \sqrt{\tfrac{3}{10}}(6t+6S-32) \\ &+\tfrac{\sqrt{10}}{6}(6ts-18t-18s+52) + \tfrac{8\sqrt{2}}{5} + 4\sqrt{\tfrac{5}{3}} + 8\sqrt{\tfrac{2}{5}} \\ &+\tfrac{8}{3} + 4\sqrt{2} + \tfrac{16}{3} + (4s+4t-24)\sqrt{\tfrac{5}{12}} + (2s+2t-8)(\sqrt{\tfrac{2}{5}} + \sqrt{\tfrac{7}{20}}). \end{aligned}$$

Proof. Let s, t be any positive integers such that $s, t \geq 4$ and $G \cong P_t \square P_s$. By using Observation 2.3, we have

$$ABC^{\mathcal{E}}(G) = ABC(G) + ABC_e(G) + \sum_{v \text{ is incident to } e} \sqrt{\frac{deg(v)+deg(e)-2}{deg(v)deg(e)}}.$$

To get $\sum_{v \text{ incident to } e} \sqrt{\frac{deg(v)+deg(e)-2}{deg(v)deg(e)}}$, let $A_{a,b}$ be the set of all subsets $\{x, y\}$ where x is an edge in G, y is a vertex in G and x is incident with y such that $deg(x) = a$ and $deg(y) = b$. Then we have $|A_{3,2}| = 8$, $|A_{3,3}| = 8$, $|A_{4,3}| = 4(s-3)+4(t-3) = 4s+4t-24$, $|A_{5,3}| = 2(s-2)+2(t-2) = 2s+2t-8$, $|A_{5,4}| = 2s+2t-8$ and $|A_{6,4}| = (s-3)(t-2)$. Then,

$$\begin{aligned} \sum_{v \text{ incident to } e} \sqrt{\frac{deg(v)+deg(e)-2}{deg(v)deg(e)}} &= 8\sqrt{\frac{3}{6}} + 8\sqrt{\frac{4}{9}} + (4s+4t-24)\sqrt{\frac{5}{12}} \\ &+ (2s+2t-8)\sqrt{\frac{6}{15}} + (2s+2t-8)\sqrt{\frac{7}{20}} + (s-3)(t-2)\sqrt{\frac{8}{24}} \\ &= 4\sqrt{2} + \frac{16}{2} + (4s+4t-24)\sqrt{\frac{5}{12}} \\ &+ (2s+2t-8)\sqrt{\frac{6}{15}} + (2s+2t-8)\sqrt{\frac{7}{20}} + (s-3)(t-2)\sqrt{\frac{1}{3}}. \quad (2.1) \end{aligned}$$

Then by Lemma 2.11 , Lemma 2.12 and Eqn. 2.1 we get:

$$ABC^{\mathcal{E}}(G) = 4\sqrt{2}+\frac{4s+4t-24}{3}+(s+t-4)\sqrt{\frac{5}{3}}+(2st-5t-5s+12)\sqrt{\frac{6}{16}}+\frac{1}{2}\sqrt{\frac{3}{2}}(2t+2s-16)$$
$$+\frac{1}{2}\sqrt{\frac{7}{5}}(st+4s-24)+\sqrt{\frac{3}{10}}(6t+6S-32)+\frac{\sqrt{10}}{6}(6ts-18t-18s+52)$$
$$+\frac{8\sqrt{2}}{5}+4\sqrt{\frac{5}{3}}+8\sqrt{\frac{2}{5}}+\frac{8}{3}+4\sqrt{2}+\frac{16}{3}+(4s+4t-24)\sqrt{\frac{5}{12}}$$
$$+(2s+2t-8)(\sqrt{\frac{2}{5}}+\sqrt{\frac{7}{20}}).$$

Lemma 2.14. *For any positive integers $s \geq 4$ and $t \geq 3$, if $G \cong P_s \square C_t$, then*

$$ABC(G) = (\frac{4}{3}+\sqrt{\frac{5}{3}})t+\sqrt{\frac{6}{16}}t(2s-5).$$

Proof. Let $s \geq 4$ and $t \geq 3$. Let $V_{a,b} = \{\{u.v\} : uv \in E(G)\, such\, that\, deg(u) = a\, and\, deg(v) = b\}$. We have three partitioning sets of the vertices of G and it is not difficult to see that $|V_{2,3}| = 8, |V_{3,3}| = 2t, |V_{3,4}| = 2t$ and $|V_{4,4}| = t(s-2)+t(s-3)$. Then, we get

$$ABC(G) = (\frac{4}{3}+\sqrt{\frac{5}{3}})t+\sqrt{\frac{6}{16}}t(2s-5).$$

Lemma 2.15. *[25] For any positive integers $s \geq 4$ and $t \geq 3$, if $G \cong P_s \square C_t$, then*

$$ABC_e(G) = \sqrt{10}st+(\frac{\sqrt{6}}{2}+2\sqrt{\frac{7}{5}}+3\frac{\sqrt{30}}{5}-9\frac{\sqrt{10}}{3})t.$$

Theorem 2.16. *For any positive integers $s \geq 4$ and $t \geq 3$, if $G \cong P_s \square C_t$, then,*

$$ABC^{\mathcal{E}}(G) = \left(\sqrt{\frac{3}{2}}+\sqrt{\frac{16}{3}}+\sqrt{10}\right)st$$
$$+\left(\frac{4}{3}+\sqrt{\frac{5}{3}}+\frac{5}{2}\sqrt{\frac{3}{2}}+\frac{\sqrt{6}}{2}+\frac{2\sqrt{7}}{5}+\frac{3\sqrt{30}}{5}-\frac{9\sqrt{10}}{3}+\sqrt{\frac{20}{3}}+\sqrt{\frac{8}{5}}+\sqrt{\frac{7}{5}}-\frac{10}{\sqrt{3}}\right)t.$$

Proof. Let s, t be any positive integers such that $s \geq 4$ and $t \geq 3$. If $G \cong P_s \square C_t$, then by Observation 2.3, we have

$$ABC^{\mathcal{E}}(G) = ABC(G)+ABC_e(G)+\sum_{v \text{ incident to } e}\sqrt{\frac{deg(v)+deg(e)-2}{deg(v)deg(e)}}.$$

To get $\displaystyle\sum_{v \text{ incident to } e}\sqrt{\frac{deg(v)+deg(e)-2}{deg(v)deg(e)}}$, let $B_{a,b}$ be the set of all subsets $\{x, y\}$

where x is a vertex in G, y is an edge in G and x is incident with y such that $deg(x) = a$ and $deg(y) = b$. Then we have $|B_{3,4}| = 4t$, $|B_{3,5}| = 2t$, $|B_{4,5}| = 2t$, and $|B_{4,6}| = 2t(s-2) + 2t(s-3)$. Hence

$$\begin{aligned}\sum_{v \text{ incident to } e} \sqrt{\frac{deg(v)+deg(e)-2}{deg(v)deg(e)}} &= 4t\sqrt{\frac{3+4-2}{12}} + 2t\sqrt{\frac{3+5-2}{15}} \\ &+ 2t\sqrt{\frac{4+5-2}{20}} + (2t(s-2)+2t(s-3))\sqrt{\frac{4+6-2}{24}} \\ &= \left(\sqrt{\frac{20}{3}} + \sqrt{\frac{8}{5}} + \sqrt{\frac{7}{5}} - \frac{10}{\sqrt{3}}\right) t + \frac{4}{\sqrt{3}} st. \quad (2.2)\end{aligned}$$

Then by Lemma 2.11, Lemma 2.12 and Eqn. 2.2, we get

$$\begin{aligned}ABC^{\mathcal{E}}(G) &= \left(\sqrt{\frac{3}{2}} + \sqrt{\frac{16}{3}} + \sqrt{10}\right) st \\ &+ \left(\frac{4}{3} + \sqrt{\frac{5}{3}} + \frac{5}{2}\sqrt{\frac{3}{2}} + \frac{\sqrt{6}}{2} + \frac{2\sqrt{7}}{5} + \frac{3\sqrt{30}}{5} - \frac{9\sqrt{10}}{3} + \sqrt{\frac{20}{3}} + \sqrt{\frac{8}{5}} + \sqrt{\frac{7}{5}} - \frac{10}{\sqrt{3}}\right) t.\end{aligned}$$

Graph operations of basic molecular structures are frequently found in new chemical compounds, nanomaterials and drugs in the fields of chemical and pharmaceutical engineering. The phenomenon provides us some hints on the significance and feasibility of the research on the chemical and pharmacological properties of these molecular structures. The definition of the join graph operation is given as follows: If we are given two graphs G and H and two vertices $v_i \in V(G)$, $u_j \in V(H)$, the join graph is obtained by merging v_i and u_j into one vertex [25]. Then we can show

Lemma 2.17. *Let P_n, C_m be path and cycle graphs of $n \geq 4$, $m \geq 3$ disjoint vertices, respectively. If $G \cong P_n + C_m$, then*

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

Proof. Let P_n, C_m be path and cycle graphs of $n \geq 4$, $m \geq 3$ disjoint vertices, respectively. If $G \cong P_n + C_m$, then it is easy to see that $|V_{1,2}| = 1$, $|V_{2,3}| = 3$ and $|V_{2,2}| = n - 3 + m - 2 = n + m - 5$. Hence

$$ABC(G) = \sqrt{\frac{1+2-2}{2}} + 3\sqrt{\frac{2+3-2}{6}} + (n+m-5)\sqrt{\frac{2+2-2}{4}} = \frac{\sqrt{2}}{2}(n+m-1).$$

Lemma 2.18. *[25] Let P_n, C_m be path and cycle graphs of $n \geq 4$, $m \geq 3$ disjoint vertices, respectively. If $G \cong P_n + C_m$, then*

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

Theorem 2.19. *Let P_n, C_m be path and cycle graphs of $n \geq 4$, $m \geq 3$ disjoint vertices, respectively. If $G \cong P_n + C_m$, then*

$$ABC^{\mathcal{E}}(G) = 2\sqrt{2}(n+m-5)+4.$$

Proof. Let P_n, C_m be path and cycle graphs of $n \geq 4$, $m \geq 3$ disjoint vertices, respectively. If $G \cong P_n + C_m$, then by Observation 2.3, we have

$$ABC^{\mathcal{E}}(G) = ABC(G) + ABC_e(G) + \sum_{v \text{ incident to } e} \sqrt{\frac{deg(v)+deg(e)-2}{deg(v)deg(e)}}.$$

To calculate $\sum_{v \text{ incident to } e} \sqrt{\frac{deg(v)+deg(e)-2}{deg(v)deg(e)}}$, it is easy to show that $|A_{1,1}| = 1$, $|A_{3,3}| = 3$, $|A_{2,1}| = 1$, $|A_{2,3}| = 3|$ and $|A_{2,2}| = 2(n-3)+2(m-2) = 2n+2m-10$. Then

$$\begin{aligned}\sum_{v \text{ incident to } e} \sqrt{\frac{deg(v)+deg(e)-2}{deg(v)deg(e)}} &= \sqrt{\frac{1+1-2}{2}} + 3\sqrt{\frac{4}{9}} + \sqrt{\frac{1}{2}} \\ &\quad + 3\sqrt{\frac{2+3-2}{6}} + (2n+2m-10)\sqrt{\frac{2+2-2}{4}}.\end{aligned}$$

Therefore,

$$\sum_{v \text{ incident to } e} \sqrt{\frac{deg(v)+deg(e)-2}{deg(v)deg(e)}} = \frac{2\sqrt{2}}{2}(n+m-3)+2. \tag{2.3}$$

Hence by Lemma 2.17, Lemma 2.18 and Eqn. 2.3, we get

$$ABC^{\mathcal{E}}(G) = 2\sqrt{2}(n+m-5)+4.$$

Lemma 2.20. *Let P_n, S_m be path and star graphs of $n \geq 4$, $m \geq 4$ disjoint vertices, respectively. If $G \cong P_n + S_m$, then*

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

Proof. Let P_n, S_m be path and star graphs of $n \geq 4$, $m \geq 4$ disjoint vertices, respectively. If $G \cong P_n + S_m$, then it is easy to see that $|V_{1,2}| = 1$, $|V_{1,m}| = m-1$, $|V_{2,m}| = 1$, and $|V_{2,2}| = n-3$. Then

$$\begin{aligned}ABC(G) &= \sqrt{\frac{1+2-2}{2}} + (m-1)\sqrt{\frac{1+m-2}{m}} + \sqrt{\frac{2+m-2}{2m}} + (n-3)\sqrt{\frac{2+2-2}{4}} \\ &= \frac{\sqrt{n-1}}{\sqrt{2}} + \sqrt{m(m-1)} - \sqrt{\frac{m-1}{m}}.\end{aligned}$$

Lemma 2.21. *[26] Let P_n, S_m be path and star graphs of $n \geq 4$, $m \geq 4$ disjoint vertices, respectively. If $G \cong P_n + S_m$, then*

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

Theorem 2.22. *Let P_n, S_m be path and star of $n \geq 4$, $m \geq 4$ disjoint vertices, respectively. If $G \cong P_n + S_m$, then*

$$\begin{aligned} ABC^{\mathcal{E}}(G) = {} & \sqrt{\frac{n-1}{2}} + \sqrt{m(m-1)} - \sqrt{\frac{m-1}{m}} + \frac{m-2}{2}\sqrt{2m-4} + \sqrt{2}n \\ & + (m-1)\left(\sqrt{\frac{m-2}{m-1}} + \sqrt{\frac{2m-3}{m(m-1)}}\right) + 2\frac{\sqrt{2(m-1)}}{m} + \frac{n-4}{\sqrt{2}}. \end{aligned}$$

Proof. Let P_n, S_m be path and star graphs of $n \geq 4$, $m \geq 4$ disjoint vertices, respectively. By Observation 2.3, we have

$$ABC^{\mathcal{E}}(G) = ABC(G) + ABC_e(G) + \sum_{v \text{ incident to } e} \sqrt{\frac{deg(v) + deg(e) - 2}{deg(v)deg(e)}}.$$

To get $\displaystyle\sum_{v \text{ incident to } e} \sqrt{\frac{deg(v) + deg(e) - 2}{deg(v)deg(e)}}$, it is easy to show that $|A_{1,1}| = 1$, $|A_{1,m-1}| = m-1$, $|A_{m,m-1}| = m-1$, $|A_{m,m}| = 1$ and $|A_{2,2}| = n-4$. Then

$$\begin{aligned} \sum_{v \text{ incident to } e} \sqrt{\frac{deg(v) + deg(e) - 2}{deg(v)deg(e)}} = {} & \sqrt{\frac{1+1-2}{1}} + (m-1)\sqrt{\frac{1+m-1-2}{m-1}} \\ & + (m-1)\sqrt{\frac{m+m-1-2}{m(m-1)}} + \sqrt{\frac{m+m-2}{m^2}} + (n-4)\sqrt{\frac{2+2-2}{4}}. \end{aligned}$$

Therefore,

$$\sum_{v \text{ incident to } e} \sqrt{\frac{deg(v) + deg(e) - 2}{deg(v)deg(e)}} = (m-1)\left(\sqrt{\frac{m-2}{m-1}} + \sqrt{\frac{2m-3}{m(m-1)}}\right) + \frac{\sqrt{2(m-1)}}{m} + \frac{n-4}{\sqrt{2}}. \tag{2.4}$$

Hence by Lemma 2.20, Lemma 2.21 and Eqn. 2.4, we get

$$\begin{aligned} ABC^{\mathcal{E}}(G) = {} & \sqrt{\frac{n-1}{2}} + \sqrt{m(m-1)} - \sqrt{\frac{m-1}{m}} + \frac{m-2}{2}\sqrt{2m-4} + \sqrt{2}n \\ & + (m-1)\left(\sqrt{\frac{m-2}{m-1}} + \sqrt{\frac{2m-3}{m(m-1)}}\right) + 2\frac{\sqrt{2(m-1)}}{m} + \frac{n-4}{\sqrt{2}}. \end{aligned}$$

In the next Theorem, we define some new concept regarding to the entire indices. The first and the second modified entire Zagreb indices are respectively denoted by $M_1^{\mathcal{E}*}$ and $M_2^{\mathcal{E}*}$ where

$$M_1^{\mathcal{E}*}(G) = \sum_{x\in V(G)\cup E(G)} \frac{1}{\big(deg(x)\big)^2},$$

and

$$M_2^{\mathcal{E}*}(G) = \sum_{\substack{\text{x is either adjacent} \\ \text{or incident to y}}} \frac{1}{deg(x)deg(y)}.$$

Theorem 2.23. *For any graph G with n vertices and m edges, we have*

$$ABC^{\mathcal{E}}(G) \leq \sqrt{(2m + \frac{M_1}{2})(n + 2m + In(L(G)) - 2M_2^{\mathcal{E}*})},$$

where $M_2^{\mathcal{E}*}$ is the second modified entire Zagreb index, $In(L(G))$ is the inverse sum degree of line graph of the graph G and $M_1(G)$ is the first Zagreb index of G.

Proof. Let G be a graph with n vertices and m edges. Then we have

$$ABC^{\mathcal{E}}(G) = \sum_{\{x,y\}\subseteq B(G)} \sqrt{\frac{deg(x)+deg(y)-2}{deg(x)deg(y)}}.$$

By using Cauchy-Schwarz inequality, we get

$$ABC^{\mathcal{E}}(G) = \sum_{\{x,y\}\subseteq B(G)} \sqrt{\frac{deg(x)+deg(y)-2}{deg(x)deg(y)}} \leq \sqrt{|B(G)| \sum_{\{x,y\}\subseteq B(G)} \frac{deg(x)+deg(y)-2}{deg(x)deg(y)}}.$$

$$= \sqrt{|B(G)| \sum_{\{x,y\}\subseteq B(G)} (\frac{1}{deg(x)} + \frac{1}{deg(y)} - \frac{2}{deg(x)deg(y)})}.$$

$$= \sqrt{|B(G)|(\sum_{x\in V(G)} \frac{1}{deg(x)}.deg(x) + \sum_{y\in E(G)} \frac{1}{deg(y)}.deg(y) + \sum_{x\in V(G)\, xy\in E(G)} \frac{1}{deg(x)} + \frac{1}{deg(y)} - \sum_{\{x,y\}\subseteq B(G)} \frac{2}{deg(x)deg(y)})}$$

$$= \sqrt{|B(G)|(n + m + \sum_{x\in V(G)\, xy\in E(G)} \frac{1}{deg(x)} + \frac{1}{deg(y)}) - 2M_2^{\mathcal{E}*}}$$

$$= \sqrt{|B(G)|(n + 2m + In(L(G)) - 2M_2^{\mathcal{E}*})}$$

$$= \sqrt{(2m + \frac{M_1}{2})(n + 2m + In(L(G)) - 2M_2^{\mathcal{E}*})}.$$

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