The Augmented Zagreb Index Of Graph Operations^{*}

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Abstract

The augmented Zagreb index of a graph G, which is proven to be a valuable predictive index in the study of the heat of formation of octanes and heptanes, is the sum of $\left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$ for all edges uv of G, where d(u) denotes the degree of the vertex u in G. In this paper, tight lower and upper bounds on augmented Zagreb index of graphs obtained by using graph operations such as the Cartesian product, composition, join and corona product of graphs are presented. We also apply our results to compute the augmented Zagreb index of regular graph operations.

1 Introduction

Throughout this paper we consider only simple connected graphs. Such a graph will be denoted by G = (V(G), E(G)), where V(G) and E(G) are the vertex set and edge set of G, respectively. The degree of a vertex u is denoted by $d_G(u)$ (d(u) for short). Suppose *Graph* is the collection of all graphs. A mapping $Top : Graph \to$ R is called a topological index, if $G \cong H$ implies that Top(G) = Top(H). Many topological indices are closely correlated with some physico-chemical characteristics of the underlying compounds. The augmented Zagreb index (AZI for short) is a valuable predictive index in the study of the heat of formation in octanes and heptanes (see [3]), whose prediction power is better than atom-bond connectivity index (please refer to [1,2,6,8,9] for its research background). It is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d(u)d(v)}{d(u) + d(v) - 2}\right)^3.$$
 (1)

The join $G = G_1 + G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2 .

The Cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and (a, x) (b, y) is an edge of $G \times H$ if a = b and $xy \in E(H)$, or $ab \in E(G)$ and x = y.

The composition $G = G_1[G_2]$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph with vertex set $V_1 \times V_2$ and $u = (u_1, v_1)$ is

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adjacent with $v = (u_2, v_2)$ whenever $(u_1 \text{ is adjacent with } u_2)$ or $(u_1 = u_2 \text{ and } v_1 \text{ is adjacent with } v_2)$, see [20, p. 185].

The corona product $G \circ H$ of two graphs G and H is defined to be the graph Γ obtained by taking one copy of G (which has n_1 vertices) and n_1 copies of H, and then joining the *i*th vertex of G to every vertex in the *i*th copy of H. If G is a graph of order n_1 with m_1 edges and H is a graph of order n_2 with m_2 edges, then it follows from the definition of the corona that $G \circ H$ has $n_1(1 + n_2)$ vertices and $m_1 + n_1m_2 + n_1n_2$ edges. It is clear that if G is connected, then $G \circ H$ is connected, and in general $G \circ H$ is not isomorphic to $H \circ G$.

The Wiener index of the Cartesian product of graphs was studied in [13]. In [14,15], Klavžar et al. computed the Szeged index and PI index of Cartesian product graphs. In some papers [10,17,18], the Zagreb group indices of some graph operations are considered. Fath-Tabar et al. studied the ABC index of some graph operations in [11]. Here, we investigate the AZI of some graph operations. Our other notations are standard and taken mainly from [19].

2 Bounds on Augmented Zagreb Index of Graph Operations

LEMMA 1. Let $f(x, y) = \frac{(x+a)(y+b)}{x+a+y+b-2}$, where x, y, a, b are positive integers with $a, b \ge 2$. If x (resp. y) is fixed, then f(x, y) is increasing with respect to y (resp. x).

PROOF. If x is fixed, then $f(x, y) = \frac{x+a}{1+\frac{x+a-2}{y+b}}$ is increasing with respect to y.

THEOREM 1. Let G be a connected graph of order $n_1 \geq 2$ with m_1 edges, maximum degree Δ_G and minimum degree δ_G . Let H be a connected graph of order $n_2 \geq 2$ with m_2 edges, maximum degree Δ_H and minimum degree δ_H . Then

(i)
$$AZI(G+H) \ge \frac{m_1(\delta_G + n_2)^6}{8(\delta_G + n_2 - 1)^3} + \frac{m_2(\delta_H + n_1)^6}{8(\delta_H + n_1 - 1)^3} + \frac{n_1n_2(\delta_G + n_2)^3(\delta_H + n_1)^3}{(\delta_G + \delta_H + n_1 + n_2 - 2)^3}$$

with equality if and only if G and H are regular graphs.

(ii)
$$AZI(G+H) \leq \frac{m_1(\Delta_G+n_2)^6}{8(\Delta_G+n_2-1)^3} + \frac{m_2(\Delta_H+n_1)^6}{8(\Delta_H+n_1-1)^3} + \frac{n_1n_2(\Delta_G+n_2)^3(\Delta_H+n_1)^3}{(\Delta_G+\Delta_H+n_1+n_2-2)^3}$$

with equality if and only if G and H are regular graphs.

PROOF. From (1), we have

$$\begin{split} AZI(G+H) &= \sum_{uv \in E(G+H)} (\frac{d(u)d(v)}{d(u) + d(v) - 2})^3 \\ &= \sum_{\substack{uv \in E(G+H)\\ u, v \in V(G)}} (\frac{d(u)d(v)}{d(u) + d(v) - 2})^3 + \sum_{\substack{uv \in E(G+H)\\ u, v \in V(H)}} (\frac{d(u)d(v)}{d(u) + d(v) - 2})^3 \\ &+ \sum_{\substack{uv \in E(G+H)\\ u \in V(G), v \in V(H)}} (\frac{d(u)d(v)}{d(u) + d(v) - 2})^3. \end{split}$$

If $u \in V(G)$, then $d(u) = d_G(u) + n_2$. So

$$\sum_{\substack{uv \in E(G+H)\\u,v \in V(G)}} \left(\frac{d(u)d(v)}{d(u) + d(v) - 2}\right)^3 = \sum_{\substack{uv \in E(G+H)\\u,v \in V(G)}} \left(\frac{(d_G(u) + n_2)(d_G(v) + n_2)}{d_G(u) + d_G(v) + 2n_2 - 2}\right)^3.$$

By Lemma 1, we have

$$\frac{(\delta_G + n_2)^6}{8(\delta_G + n_2 - 1)^3} \le \left(\frac{(d_G(u) + n_2)(d_G(v) + n_2)}{d_G(u) + d_G(v) + 2n_2 - 2}\right)^3 \le \frac{(\Delta_G + n_2)^6}{8(\Delta_G + n_2 - 1)^3},$$

 thus

$$\frac{m_1(\delta_G + n_2)^6}{8(\delta_G + n_2 - 1)^3} \le \sum_{\substack{uv \in E(G+H)\\u, v \in V(G)}} (\frac{d(u)d(v)}{d(u) + d(v) - 2})^3 \le \frac{m_1(\Delta_G + n_2)^6}{8(\Delta_G + n_2 - 1)^3}.$$
 (2)

The left equality holds if and only if $d_G(u) = d_G(v) = \delta_G$ and the right equality holds if and only if $d_G(u) = d_G(v) = \Delta_G$. In a similar way,

$$\frac{m_2(\delta_H + n_1)^6}{8(\delta_H + n_1 - 1)^3} \le \sum_{\substack{uv \in E(G+H)\\u,v \in V(H)}} (\frac{d(u)d(v)}{d(u) + d(v) - 2})^3 \le \frac{m_2(\Delta_H + n_1)^6}{8(\Delta_H + n_1 - 1)^3}$$
(3)

where the equality on the left side holds if and only if $d_H(u) = d_H(v) = \delta_H$ and right equality holds if and only if $d_H(u) = d_H(v) = \Delta_H$.

If $u \in V(G)$, $v \in V(H)$, then

$$\sum_{\substack{uv \in E(G+H)\\u \in V(G), v \in V(H)}} \left(\frac{d(u)d(v)}{d(u) + d(v) - 2}\right)^3 = \sum_{\substack{uv \in E(G+H)\\u \in V(G), v \in V(H)}} \left(\frac{(d_G(u) + n_2)(d_H(v) + n_1)}{d_G(u) + d_H(v) + n_1 + n_2 - 2}\right)^3$$

By Lemma 1, we have

$$\frac{(\delta_G + n_2)^3 (\delta_H + n_1)^3}{(\delta_G + \delta_H + n_1 + n_2 - 2)^3} \le \left(\frac{(d_G(u) + n_2)(d_H(v) + n_1)}{d_G(u) + d_H(v) + n_1 + n_2 - 2}\right)^3 \le \frac{(\Delta_G + n_2)^3 (\Delta_H + n_1)^3}{(\Delta_G + \Delta_H + n_1 + n_2 - 2)^3},$$

thus

$$\sum_{\substack{uv \in E(G+H)\\u \in V(G), v \in V(H)}} \left(\frac{d(u)d(v)}{d(u) + d(v) - 2}\right)^3 \ge \frac{n_1 n_2 (\delta_G + n_2)^3 (\delta_H + n_1)^3}{(\delta_G + \delta_H + n_1 + n_2 - 2)^3} \tag{4}$$

with equality holds if and only if $d_G(u) = \delta_G$, $d_H(v) = \delta_H$, and

$$\sum_{\substack{uv \in E(G+H)\\u \in V(G), v \in V(H)}} \left(\frac{d(u)d(v)}{d(u) + d(v) - 2}\right)^3 \le \frac{n_1 n_2 (\Delta_G + n_2)^3 (\Delta_H + n_1)^3}{(\Delta_G + \Delta_H + n_1 + n_2 - 2)^3}.$$
(5)

with equality holding if and only if $d_G(u) = \Delta_G$, $d_H(v) = \Delta_H$.

Combining (2)-(5), we get the results of Theorem 1.

For $G \circ H$, from (1), we can get

$$\begin{split} AZI(G \circ H) &= \sum_{uv \in E(G \circ H)} (\frac{d(u)d(v)}{d(u) + d(v) - 2})^3 \\ &= \sum_{\substack{uv \in E(G \circ H)\\ u, v \in V(G)}} (\frac{(d_G(u) + n_2)(d_G(v) + n_2)}{d_G(u) + d_G(v) + 2n_2 - 2})^3 \\ &+ \sum_{\substack{uv \in E(G \circ H)\\ u, v \in V(H)}} (\frac{(d_H(u) + 1)(d_H(v) + 1)}{d_H(u) + d_H(v)})^3 \\ &+ \sum_{\substack{uv \in E(G \circ H)\\ u \in V(G), v \in V(H)}} (\frac{(d_G(u) + n_2)(d_H(v) + 1)}{d_G(u) + d_H(v) + n_2 - 1})^3 \end{split}$$

Similarly as Theorem 1, we have the following theorem.

THEOREM 2. Let G be a connected graph of order $n_1 \geq 2$ with m_1 edges, maximum degree Δ_G and minimum degree δ_G . Let H be a connected graph of order $n_2 \geq 2$ with m_2 edges, maximum degree Δ_H and minimum degree δ_H . Then

(i)
$$AZI(G \circ H) \ge \frac{m_1(\delta_G + n_2)^6}{8(\delta_G + n_2 - 1)^3} + \frac{n_1m_2(\delta_H + 1)^6}{8\delta_H^3} + \frac{n_1n_2(\delta_G + n_2)^3(\delta_H + 1)^3}{(\delta_G + \delta_H + n_2 - 1)^3}$$

with equality if and only if G and H are regular graphs.

(ii)
$$AZI(G \circ H) \le \frac{m_1(\Delta_G + n_2)^6}{8(\Delta_G + n_2 - 1)^3} + \frac{n_1m_2(\Delta_H + 1)^6}{8\Delta_H^3} + \frac{n_1n_2(\Delta_G + n_2)^3(\Delta_H + 1)^3}{(\Delta_G + \Delta_H + n_2 - 1)^3}$$

with equality if and only if G and H are regular graphs.

Next, we give tight lower and upper bounds on augmented Zagreb index of graphs obtained by using graph operations of the Cartesian product.

510

J. Du and X. Sun

THEOREM 3. Let G be a connected graph of order n_1 with m_1 edges, maximum degree Δ_G and minimum degree δ_G . Let H be a connected graph of order n_2 with m_2 edges, maximum degree Δ_H and minimum degree δ_H . Then

$$\frac{(n_1m_2 + n_2m_1)(\delta_G + \delta_H)^6}{8(\Delta_G + \Delta_H - 1)^3} \le AZI(G \times H) \le \frac{(n_1m_2 + n_2m_1)(\Delta_G + \Delta_H)^6}{8(\delta_G + \delta_H - 1)^3}$$

where left or right equality holds if and only if G and H are regular graphs.

PROOF. Suppose u = (a, b) and v = (c, d) are vertices of $G \times H$. Then we have

$$\begin{split} AZI(G \times H) &= \sum_{\substack{uv \in E(G \times H) \\ a=c, bd \in E(H)}} (\frac{d(u)d(v)}{d(u) + d(v) - 2})^3 \\ &= \sum_{\substack{uv \in E(G \times H) \\ a=c, bd \in E(H)}} (\frac{(d_G(a) + d_H(b))(d_G(c) + d_H(d))}{d_G(a) + d_H(b) + d_G(c) + d_H(d) - 2})^3 \\ &+ \sum_{\substack{uv \in E(G \times H) \\ b=d, ac \in E(G)}} (\frac{(d_G(a) + d_H(b))(d_G(c) + d_H(d))}{d_G(a) + d_H(b) + d_G(c) + d_H(d) - 2})^3. \end{split}$$

Since

$$\frac{(\delta_G + \delta_H)^6}{8(\Delta_G + \Delta_H - 1)^3} \le \left(\frac{(d_G(a) + d_H(b))(d_G(c) + d_H(d))}{d_G(a) + d_H(b) + d_G(c) + d_H(d) - 2}\right)^3 \le \frac{(\Delta_G + \Delta_H)^6}{8(\delta_G + \delta_H - 1)^3},$$

we have

$$\frac{(n_1m_2 + n_2m_1)(\delta_G + \delta_H)^6}{8(\Delta_G + \Delta_H - 1)^3} \le AZI(G \times H) \le \frac{(n_1m_2 + n_2m_1)(\Delta_G + \Delta_H)^6}{8(\delta_G + \delta_H - 1)^3}$$

with left or right equality if and only if $d_G(a) = d_G(c) = \Delta_G = \delta_G$ for any $a, c \in V(G)$ and $d_H(b) = d_H(d) = \Delta_H = \delta_H$ for any $b, d \in V(H)$, that is, G and H are regular graphs.

Suppose u = (a, b) and v = (c, d) are vertices of G[H]. It follows that

$$\begin{split} AZI(G[H]) &= \sum_{uv \in E(G[H])} (\frac{d(u)d(v)}{d(u) + d(v) - 2})^3 \\ &= \sum_{\substack{uv \in E(G[H])\\a=c,bd \in E(H)}} (\frac{(n_2d_G(a) + d_H(b))(n_2d_G(c) + d_H(d))}{n_2d_G(a) + d_H(b) + n_2d_G(c) + d_H(d) - 2})^3 \\ &+ \sum_{\substack{uv \in E(G[H])\\ac \in E(G)}} (\frac{(n_2d_G(a) + d_H(b))(n_2d_G(c) + d_H(d))}{n_2d_G(a) + d_H(b) + n_2d_G(c) + d_H(d) - 2})^3. \end{split}$$

Similarly as Theorem 3, we have the following theorem.

THEOREM 4. Let G be a connected graph of order n_1 with m_1 edges, maximum degree Δ_G and minimum degree δ_G . Let H be a connected graph of order n_2 with m_2 edges, maximum degree Δ_H and minimum degree δ_H . Then

$$\frac{(n_1^2 m_2 + n_1 m_2)(n_2 \delta_G + \delta_H)^6}{8(n_2 \Delta_G + \Delta_H - 1)^3} \le AZI(G[H]) \le \frac{(n_1^2 m_2 + n_1 m_2)(n_2 \Delta_G + \Delta_H)^6}{8(n_2 \delta_G + \delta_H - 1)^3}$$

with left or right equality if and only if G and H are regular graphs.

3 The Augmented Zagreb Index of Operations on Regular Graphs

Suppose G is a r-regular graph of order n with m edges. Then $m = \frac{nr}{2}$. From the cases of equality holding in Theorem 1-4, we can easily get the following theorem.

THEOREM 5. Let G be a r_1 -regular graph of order n_1 and H be a r_2 -regular graph of order n_2 . Then

 $\begin{array}{l} \text{(i)} \ AZI(G+H) = \frac{n_1 r_1 (r_1 + n_2)^6}{16 (r_1 + n_2 - 1)^3} + \frac{n_2 r_2 (r_2 + n_1)^6}{16 (r_2 + n_1 - 1)^3} + \frac{n_1 n_2 (r_1 + n_2)^3 (r_2 + n_1)^3}{(r_1 + r_2 + n_1 + n_2 - 2)^3}, \\ \text{(ii)} \ AZI(G \circ H) = \frac{n_1 r_1 (r_1 + n_2)^6}{16 (r_1 + n_2 - 1)^3} + \frac{n_1 n_2 r_2 (r_2 + 1)^6}{16 r_2^3} + \frac{n_1 n_2 (r_1 + n_2)^3 (r_2 + 1)^3}{(r_1 + r_2 + n_2 - 1)^3}, \\ \text{(iii)} \ AZI(G \times H) = \frac{n_1 n_2 (r_1 + r_2)^7}{16 (r_1 + r_2 - 1)^3}, \end{array}$

(iv)
$$AZI(G[H]) = \frac{n_1 n_2 (n_2 r_1 + r_2)^7}{16(n_2 r_1 + r_2 - 1)^3}.$$

This theorem can be used to compute the augmented Zagreb index of the Cartesian product, composition, join and corona product of regular graphs. It is easy to check that the theorem is right for the cases when one of G and H is a trivial graph with one vertex.

EXAMPLE 1. In the papers [10-12], the authors computed the PI index, first Zagreb index, second Zagreb index, ABC index of C_4 nanotubes and nanotori. In this example, we compute the augmented Zagreb index of C_4 nanotori and one type of C_4 nanotubes. Let $S = C_n \times C_m$ and $R = P_2 \times C_m$. Then S is C_4 nanotori and R is one type of C_4 nanotubes. By (*iii*) of Theorem 5, we have $AZI(S) = \frac{1024mn}{27}$ and $AZI(R) = \frac{2187m}{64}$.

Furthermore, if a graph G' is isomorphic to the Cartesian product, composition, join and corona product of regular graph G_1 and G_2 , we can compute the augmented Zagreb index of G'. Here is a simple example.

EXAMPLE 2. Let G be a trivial graph with one vertex and $H \cong C_n$. Suppose W_{n+1} is a wheel graph of order n+1. Then $W_{n+1} \cong G + H$. By (i) of Theorem 5, we have

$$AZI(W_{n+1}) = \frac{729n}{64} + \frac{27n^4}{(n+1)^3}.$$

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