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# SOME INVARIANTS OF SPECIAL GRAPHS

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**Abstract:** The topological invariants are very important role in mathematical chemistry, especially, they are used in the studies of QSAR/QSPR. In this paper, we study the some topological invariants of special types of graphs.

**Keywords and Phrases:** Graph invariant, Degree, Topological descriptor.

**2010 Mathematics Subject Classification:** 05C12, 05C76.

## 1. Introduction and Preliminaries

Chemical graph theory is the topological branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena. A topological descriptor is a map $f$ from $G$ to $R$ in which $G$ is a set of simple finite graphs. The Zagreb invariants have been introduced more than thirty years ago by Gutman and Trinajestić [1]. They are defined as $M_1(G) = \sum\limits_{u\in V(G)} d_G(u)^2$ and $M_2(G) = \sum\limits_{uv\in E(G)} d_G(u)d_G(v)$, where $d_G(u)$ is the degree of $u$ in $G$.

Furtula and Gutman in [4] recently investigated this invariant and named this invariant as $F$-invariant and showed that the predictive ability of this invariant is almost similar to that of first Zagreb invariant and for the entropy and acetic factor, both of them yield correlation coefficients greater than 0.95. The $F$-invariant of a graph $G$ is defined as $F(G) = \sum\limits_{u\in V(G)} d_G^3(u) = \sum\limits_{uv\in E(G)} (d_G^2(u) + d_G^2(v))$. The inverse degree invariant of a connected graph $G$ is defined as $ID(G) = \sum\limits_{u\in V(G)} \frac{1}{d_G(u)}$.

Recently, Shirdel et al. [3] introduced a variant of the first Zagreb invariant called $H$-invariant which defined as $HZ(G) = \sum_{uv\in E(G)} (d(u) + d(v))^2$. Feng et al. [2] have given a sharp bounds for the Zagreb invariants of graphs with a given matching number. Some upper and lower bounds on $H$-invariant for a connected graph are obtained by Falahati-Nezhad and Azari [5]. In this paper, we study the some graph invariants of special graphs.

## 2. Vertex-edge Corona Product Graph

Let $G_1$ be a graph with vertex set $V(G_1) = \{x_1, x_2, \ldots, x_{n_1}\}$ and edge set $E(G_1) = \{e_1, e_2, \ldots, e_{m_1}\}$. Let $G_2$ be a graph with vertex set $V(G_2) = \{y_1, y_2, \ldots, y_{n_2}\}$ and edge set $E(G_1) = \{e'_1, e'_2, \ldots, e'_{m_2}\}$. The vertex-edge corona of $G_1$ and $G_2$, denoted by $G_1 \circ G_2$, is the graph obtained by taking one copy of $G_1$, $|V(G_1)|$ copies of $G_2$ and $|E(G_1)|$ copies of $G_2$, then joining $i^{th}$ vertex of $G_1$ to every vertex in the $i^{th}$ vertex copy of $G_2$ and also joining end vertices of $j^{th}$ edge of $G_1$ to every vertex in $j^{th}$ edge copy of $G_2$, where $1 \le i \le n_1$ and $1 \le j \le m_1$. One can see that $|V(G_1 \circ G_2)| = n_1 + n_2(m_1 + n_1)$ and $|E(G_1 \circ G_2)| = m_1 + m_1(m_2 + 2n_2) + n_1(m_2 + n_2)$. We denote the vertex set of the $j^{th}$ edge copy of $G_2$ by $V_{je}(G_2) = \{x_{j1}, x_{j2}, \ldots, x_{jn_2}\}$ and the vertex set of the $i^{th}$ vertex copy of $G_2$ by $V_{iv}(G_2) = \{w_{i1}, w_{i2}, \ldots, w_{in_2}\}$. Also, we denote by $E_{je}(G_2)$ and $E_{iv}(G_2)$, the set of the $j^{th}$ edge $i^{th}$ vertex copy of $G_2$, respectively.

**Lemma 2.1.** *Let $G_i$ be a graph with $n_i$ vertices, $i = 1, 2$. Then*
*(i) $d_{G_1\circ G_2}(x_i) = (n_2 + 1)d_{G_1}(x_i) + n_2$, for all $x_i \in V(G_1)$.*
*(ii)$d_{G_1\circ G_2}(x_{ij}) = d_{G_2}(y_j) + 2$, for all $x_{ij} \in V(G_2)$.*
*(iii)$d_{G_1\circ G_2}(w_{ij}) = d_{G_2}(w_j) + 1$, for all $w_{ij} \in V(G_2)$.*

**Theorem 2.2.** *Let $G_i$ be a $(n_i, m_i)$ graph, $i = 1, 2$. Then $F(G_1 \circ G_2) = (n_2 + 1)^2\Big(F(G_1)(n_2 + 1) + 3n_2M_1(G_1)\Big) + m_1\Big(F(G_2) + 6M_1(G_2) + 24m_2 + 6n_2^2(n_2 + 1)^2 + 8n_2\Big) + n_1\Big(F(G_2) + 3M_1(G_2) + 6m_2 + n_2^4\Big)$.*

**Proof.** From the definition of $F$-invariant and Lemma 2.1, we have
$F(G_1\circ G_2) = \sum_{v\in V(G_1\circ G_2)} d^3_{G_1\circ G_2}(v) = \sum_{x_i\in V(G_1)} d^3_{G_1\circ G_2}(x_i) + \sum_{e_i\in E(G_1)} \sum_{x_{ij}\in V(G_2)} d^3_{G_1\circ G_2}(x_{ij}) + \sum_{x_k\in V(G_1)} \sum_{w_{ij}\in V(G_2)} d^3_{G_1\circ G_2}(w_{ij}) = I_1 + I_2 + I_3$, where

$I_1 = \sum_{x_i\in V(G_1\circ G_2)} d^3_{G_1\circ G_2}(x_i) = \sum_{x_i\in V(G_1)} \Big((n_2 + 1)d_{G_1}(x_i) + n_2\Big)^3 = (n_2 + 1)^3F(G_1) + n_1n_2^3 + 3(n_2 + 1)^2n_2M_1(G_1) + 6(n_2 + 1)n_2^2m_1$.

$I_2 = \sum_{e_i \in E(G_1)} \sum_{x_{ij} \in V(G_2)} d^3_{G_1 \circ G_2}(x_{ij}) = \sum_{e_i \in E(G_1)} \sum_{x_{ij} \in V_{ie}(G_2)} \Big(d_{G_2}(y_j) + 2\Big)^3 = m_1(F(G_2) + 6M_1(G_2) + 24m_2 + 8n_2)$.

$I_3 \sum_{x_k \in V(G_1)} \sum_{w_{ij} \in V_{iv}(G_2)} d^3_{G_1 \circ G_2}(w_{ij}) = \sum_{x_k \in V(G_1)} \sum_{w_{ij} \in V_{iv}(G_2)} \Big(d_{G_2}(w_{ij}) + 1\Big)^3 = n_1(F(G_2) + 3M_1(G_2) + 6m_2 + n_2)$.

Adding the sums $I_1$ to $I_3$, we obtain the required results.

**Theorem 2.3.** *Let $G_i$ be a $(n_i, m_i)$ graph, $i = 1, 2$. Then* $HZ(G_1 \circ G_2) = M_1(G_1)(n_2+1)\Big(n_2(4m_2 + 5(n_2+1) + 4)\Big) + M_1(G_2)(9m_1 + 5n_1) + HZ(G_1)(n_2+1)^3 + HZ(G_2)(m_1+n_1) + (n_2+1)^2(8m_1m_2 + n_1(n_2+4m_1)) + 4m_2(4m_1 + n_1(n_2+2)) + 4n_2^2m_1 + m_1(2n_1+2)((2n_2+2)n_2 + 4m_2)$.

**Proof.** From the definition of $H$-invariant and Lemma 2.1, we have $HZ(G_1 \circ G_2) = \sum_{uv \in E(G_1 \circ G_2)} \Big(d_{G_1 \circ G_2}(u) + d_{G_1 \circ G_2}(v)\Big)^2 = I_1 + I_2 + I_3 + I_4 + I_5$, where

$I_1 = \sum_{x_ix_j \in E(G_1 \circ G_2)} \Big(d_{G_1 \circ G_2}(x_i) + d_{G_1 \circ G_2}(x_j)\Big)^2 = \sum_{x_ix_j \in E(G_1)} \Big((n_2+1)d_{G_1}(x_i) + n_2 + (n_2+1)d_{G_1}(x_j) + n_2\Big)^2 = (n_2+1)^2 HZ(G_1) + 4n_2^2 m_1 + 4n_2(n_2+1)M_1(G_1)$.

$$I_2 = \sum_{e_i \in E(G_1)} \sum_{x_{ij}, x_{ik} \in E_{ie}(G_2)} \Big(d_{G_1 \circ G_2}(x_{ij}) + d_{G_1 \circ G_2}(x_{ik})\Big)^2$$
$$= \sum_{e_i \in E(G_1)} \sum_{y_j, y_k \in E(G_2)} \Big(d_{G_2}(y_j) + d_{G_2}(y_k) + 4\Big)^2 = m_1\Big(HZ(G_2) + 8M_1(G_2) + 16m_2\Big).$$

$$I_3 = \sum_{e = x_lx_m \in E(G_1)} \sum_{x_{ij} \in V_{ie}(G_2)} \Big(d_{G_1 \circ G_2}(x_l) + d_{G_1 \circ G_2}(x_m) + d_{G_1 \circ G_2}(x_{ij})\Big)^2$$
$$= \sum_{x_lx_m \in E(G_1)} \sum_{y_j \in V(G_2)} \Big((n_2+1)d_{G_1}(x_l) + n_2 + (n_2+1)d_{G_1}(x_m) + n_2 + d_{G_2}(y_j) + 2\Big)^2$$
$= n_2(n_2+1)^2 HZ(G_1) + m_1M_1(G_2) + M_1(G_1)\Big(4(n_2+1)^2n_2 + 4(n_2+1)m_2\Big) + (2n_2+2)^2m_1n_2 + 4m_2m_1(2n_2+2)$.

$$I_4 = \sum_{x_i \in V(G_1)} \sum_{w_{ij}w_{ik} \in E_{iv}(G_2)} \Big(d_{G_1 \circ G_2}(w_{ij}) + d_{G_1 \circ G_2}(w_{ik})\Big)^2$$
$$= \sum_{x_i \in V(G_1)} \sum_{w_jw_k \in E(G_2)} (d_{G_2}(w_j) + d_{G_2}(w_k) + 2)^2 = n_1HZ(G_2) + 4n_1M_1(G_2) + 4n_1m_2.$$

$I_5 = \sum_{x_i \in V(G_1)} \sum_{w_{ij} \in V_{iv}(G_2)} \Big(d_{G_1 \circ G_2}(x_i) + d_{G_1 \circ G_2}(w_{ij})\Big)^2 = \sum_{x_i \in V(G_1)} \sum_{w_{ij} \in V_{iv}(G_2)} \Big((n_2+1)d_{G_1}(v_i) + d_{G_2}(w_j) + (n_2+1)\Big)^2 = n_2(n_2+1)^2M_1(G_1) + n_1M_1(G_2) + (n_2+1)^2n_1n_2 +$

$8m_1m_2(n_2+1)+4m_1n_2(n_2+1)^2+4(n_2+1)m_2n_1$.

Adding the sums $I_1$ to $I_5$, we get the desired result.

## 3. Inverse Degree of Graphs

The subdivision graph $S(G)$ is the graph obtained from $G$ by replacing each edge of $G$ by a path of length two. The edge $S$-join graph of two graphs $G_1$ and $G_2$ denoted by $G_1 \vee_s G_2$ and is obtained from $S(G_1)$ and $G_2$ by joining each vertex of $I(G_1)$ with every vertex of $G_2$.

**Lemma 3.1.** [6] *Let $f$ be a convex function on the interval $I$ and $x_1, x_2, \ldots, x_n \in I$. Then $f\Big(\frac{x_1+x_2+\ldots+x_n}{n}\Big) \leq \frac{f(x_1)+f(x_2)+\ldots f(x_n)}{n}$, with equality if and only if $x_1 = x_2 = \ldots = x_n$.*

**Theorem 3.2.** *Let $G_i$ be $(n_i, m_i)$ graph, $i = 1, 2$. Then $ID(G_1 \vee_S G_2) \leq \frac{1}{4}\Big(4ID(G_1) + ID(G_2)\Big) + \Big(\frac{m_1}{n_2+2} + \frac{n_2}{4m_1}\Big)$.*

**Proof.** From the definition of edge version of $S$-join graph, the degree of a vertex $v \in G_1 \vee_S G_2$ is given by $d_{G_1 \vee_S G_2}(v) = \begin{cases} d_{G_1}(v), \text{if} \quad v \in V(G_1) \\ 2+n_2, \text{if} \quad v \in I(G_1) \\ d_{G_2}(v)+m_2, \text{if} \quad v \in V(G_2). \end{cases}$

Hence

$ID(G_1 \vee_S G_2) = \sum\limits_{x \in V(G_1 \vee_S G_2)} \frac{1}{d_{G_1 \vee_S G_2}(x)} = \Big(\sum\limits_{x \in V(G_1)} + \sum\limits_{x \in I(G_1)} + \sum\limits_{x \in V(G_2)}\Big) \frac{1}{d_{G_1 \vee_S G_2}(x)} = \sum\limits_{x \in V(G_1)} \frac{1}{d_{G_1}(x)} + \sum\limits_{x \in I(G_1)} \frac{1}{n_2+2} + \sum\limits_{x \in V(G_2)} \frac{1}{d_{G_2}(x)+m_1}$.

Jensen's inequality is used for the convex function $f : \mathcal{R}_+ \to \mathcal{R}_+, f(x) = \frac{1}{x}$ according to Lemma 3.1, we have $\frac{1}{d_{G_2}(x)+m_1} \leq \frac{1}{4d_{G_2}(x)} + \frac{1}{4m_1}$ with equality if and only if $d_{G_2}(x) = m_1$. Thus $ID(G_1 \vee_S G_2) \leq ID(G_1) + \frac{m_1}{n_2+2} + \frac{1}{4} \sum\limits_{x \in V(G_2)} \Big(\frac{1}{d_{G_2}(x)} + \frac{1}{m_1}\Big) = \frac{1}{4}\Big(4ID(G_1) + ID(G_2)\Big) + \Big(\frac{m_1}{n_2+2} + \frac{n_2}{4m_1}\Big)$.

The graph $R(G)$ is obtained from $G$ by adding a new vertex corresponding to each edge of $G$, then joining each new vertex to the end vertices of the corresponding edge. The edge $R$-join graph of two graphs $G_1$ and $G_2$ denoted by $G_1 \vee_R G_2$ and is obtained from $R(G_1)$ and $G_2$ by joining each vertex of $I(G_1)$ with every vertex of $G_2$. Note that $d_{G_1 \vee_R G_2}(y) = \begin{cases} 2d_{G_1}(y), \text{if} \quad y \in V(G_1) \\ 2+n_2, \text{if} \quad y \in I(G_1) \\ d_{G_2}(y)+m_1, \text{if} \quad y \in V(G_2) \end{cases}$

A similar argument of Theorem 3.2, we obtain the following theorem.

**Theorem 3.3.** *Let $G_i$ be $(n_i, m_i)$ graph, $i = 1, 2$. Then $ID(G_1 \vee_R G_2) \leq \frac{1}{4}(2ID(G_1) +$*

$ID(G_2)) + \left(\frac{m_1}{n_2+2} + \frac{n_2}{4m_1}\right)$.

The graph $Q(G)$ is obtained from $G$ by inserting a new vertex into each edge of $G$, then joining with edges those pairs of new vertices on adjacent edges of $G$. The edge $Q$-join graph of two graphs $G_1$ and $G_2$ denoted by $G_1 \vee_Q G_2$ and is obtained from $Q(G_1)$ and $G_2$ by joining each vertex of $I(G_1)$ with every vertex of $G_2$.

**Theorem 3.4.** *Let $G_i$ be $(n_i, m_i)$ graph, $i = 1, 2$. Then* $ID(G_1 \vee_Q G_2) \le \frac{1}{4}(4ID(G_1) + ID(G_2)) + \frac{H(G_1)}{8} + \frac{1}{4}\left(\frac{n_2}{m_1} + \frac{m_1}{n_2}\right)$.

**Proof.** By the definition of edge version of $Q$-join graph, the degree of a vertex $v \in G_1 \vee_Q G_2$ is given by $d_{G_1 \vee_Q G_2}(y) = \begin{cases} d_{G_1}(y), \text{if} \quad y \in V(G_1) \\ d_{G_2}(y) + m_1, \text{if} \quad y \in V(G_2) \\ d_{G_1}(u) + d_{G_1}(v) + n_2, \text{if} \quad e = uv, e \in I(G_1). \end{cases}$

Thus

$$ID(G_1 \vee_Q G_2) = \sum_{x \in V(G_1 \vee_S G_2)} \frac{1}{d_{G_1 \vee_S G_2}(x)} = \left(\sum_{x \in V(G_1)} + \sum_{x \in V(G_2)} + \sum_{x \in I(G_1)}\right) \frac{1}{d_{G_1 \vee_Q G_2}(x)}$$
$$= \sum_{x \in V(G_1)} \frac{1}{d_{G_1}(x)} + \sum_{x \in V(G_2)} \frac{1}{d_{G_2}(x) + m_1} + \sum_{xy \in E(G_1)} \frac{1}{d_{G_1}(x) + d_{G_1}(x) + n_2}.$$

Jensen's inequality is used for the convex function $f : \mathcal{R}_+ \to \mathcal{R}_+, f(x) = \frac{1}{x}$ according to Lemma 3.1, we have $\frac{1}{d_{G_1}(x) + d_{G_1}(x) + n_2} \le \frac{1}{4(d_{G_1}(x) + d_{G_1}(x))} + \frac{1}{4n_2}$ with equality if and only if $d_{G_1}(x) + d_{G_1}(x) = n_2$. Hence $ID(G_1 \vee_Q G_2) \le ID(G_1) + \frac{1}{4}\sum_{x \in V(G_2)}\left(\frac{1}{d_{G_2}(x)} + \frac{1}{m_1}\right) + \frac{1}{4}\sum_{xy \in E(G_1)}\left(\frac{1}{d_{G_1}(x) + d_{G_1}(y)} + \frac{1}{n_2}\right) = ID(G_1) + \frac{1}{4}ID(G_2) + \frac{1}{4}\frac{n_2}{m_1} + \frac{1}{8}H(G_1) + \frac{m_1}{4n_2} = \frac{1}{4}(4ID(G_1) + ID(G_2)) + \frac{H(G_1)}{8} + \frac{1}{4}\left(\frac{n_2}{m_1} + \frac{m_1}{n_2}\right)$.

The total graph $T(G)$ has as its vertices the edges and vertices of $G$. Adjacency in $T(G)$ is defined as adjacency or incidence for the corresponding elements of $G$. The edge $T$-join graph of two graphs $G_1$ and $G_2$ denoted by $G_1 \vee_T G_2$ and is obtained from $T(G_1)$ and $G_2$ by joining each vertex of $I(G_1)$ with every vertex of $G_2$.

One can see that $d_{G_1 \vee_T G_2}(y) = \begin{cases} 2d_{G_1}(y), \text{if} \quad y \in V(G_1) \\ d_{G_2}(y) + m_1, \text{if} \quad y \in V(G_2) \\ d_{G_1}(u) + d_{G_1}(v) + n_2, \text{if } e \in I(G_1). \end{cases}$

A similar argument of Theorem 3.7, we obtain the following theorem.

**Theorem 3.5.** *Let $G_i$ be $(n_i, m_i)$ graph, $i = 1, 2$. Then* $ID(G_1 \vee_T G_2) \le \frac{1}{4}(2ID(G_1) + ID(G_2)) + \frac{H(G_1)}{8} + \frac{1}{4}\left(\frac{n_2}{m_1} + \frac{m_1}{n_2}\right)$.

Now we compute the upper bound for inverse degree invariant of vertex-edge corona product of two graphs.

**Theorem 3.6.** *Let $G_i$ be a $(n_i, m_i)$ graph, $i = 1, 2$. Then* $ID(G_1 \circ G_2) \le \frac{1}{4}\left(\frac{ID(G_1)}{(n_2+1)} + \right.$

$\frac{n_1}{n_2} + ID(G_2)(m_1 + n_1) + n_2(\frac{m_1}{2} + n_1)\Big)$.

**Proof.** By the Lemma 2.1, we obtain;

$ID(G_1 \circ G_2) = \sum\limits_{v \in V(G_1 \circ G_2)} \frac{1}{d_{G_1 \circ G_2}(v)} = \sum\limits_{x_i \in V(G_1)} \frac{1}{d_{G_1 \circ G_2}(x_i)} + \sum\limits_{e_i \in E(G_1)} \sum\limits_{x_{ij} \in V(G_2)} \frac{1}{d_{G_1 \circ G_2}(x_{ij})} + \sum\limits_{x_i \in V(G_1)} \sum\limits_{w_{ij} \in V(G_2)} \frac{1}{d_{G_1 \circ G_2}(w_{ij})} = I_1 + I_2 + I_3$, where

$I_1 = \sum\limits_{x_i \in V(G_1)} \frac{1}{d_{G_1 \circ G_2}(x_i)} = \sum\limits_{x_i \in V(G_1)} \frac{1}{(n_2+1)d_{G_1}(x_i) + n_2} \leq \frac{1}{4} \sum\limits_{x_i \in V(G_1)} \Big(\frac{1}{(n_2+1)d_{G_1}(x_i)} + \frac{1}{n_2}\Big)$with equality $\Leftrightarrow (n_2+1)d_{G_1}(x_i) = n_2 = \frac{1}{4}\Big(\frac{ID(G_1)}{(n_2+1)} + \frac{n_1}{n_2}\Big)$.

$I_2 = \sum\limits_{e_i \in E(G_1)} \sum\limits_{x_{ij} \in V(G_2)} \frac{1}{d_{G_1 \circ G_2}(x_{ij})} = \sum\limits_{e_i \in E(G_1)} \sum\limits_{x_{ij} \in V_{ie}(G_2)} \frac{1}{d_{G_2}(x_{ij}) + 2}$

$\leq \frac{1}{4} \sum\limits_{e_i \in E(G_1)} \sum\limits_{y_j \in V(G_2)} \Big(\frac{1}{d_{G_2}(y_j)} + \frac{1}{2}\Big)$with equality $\Leftrightarrow d_{G_2}(y_j) = 2 = \frac{m_1}{4}\Big(ID(G_2) + \frac{n_2}{2}\Big)$.

$I_3 = \sum\limits_{x_i \in V(G_1)} \sum\limits_{w_{ij} \in V(G_2)} \frac{1}{d_{G_1 \circ G_2}(w_{ij})} = \sum\limits_{x_i \in V(G_1)} \sum\limits_{w_{ij} \in V(G_2)} \frac{1}{d_{G_2}(w_{ij}) + 1}$

$\leq \frac{1}{4} \sum\limits_{x_i \in V(G_1)} \sum\limits_{w_{ij} \in V(G_2)} \Big(\frac{1}{d_{G_2}(w_{ij})} + 1\Big)$with equality $\Leftrightarrow d_{G_2}(w_{i_j}) = 1 = \frac{n_1}{4}(ID(G_2) + n_2)$. Summing $I_1$ to $I_3$, we get the required result.

**3. Conclusion:** The topological invariants are play an important role in mathematical chemistry. In this paper, we have obtained the some topological invariants of various derived graphs.

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