

Schultz and Modified Schultz Polynomials of two operations Gutman's

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ABSTRACT

In this paper, we given the some properties of Schultz and modified Schultz polynomials and indices. Also, we find Schultz and modified Schultz polynomials of two operations Gutman's (Formulas for Schultz and modified Schultz polynomials of compound graphs $G_1 \bullet G_2$ and $G_1 : G_2$) for vertex- disjoint connected graphs G_1 and G_2 . The Schultz index and modified Schultz index of two operations Gutman's are obtained in this paper and some results.

Keywords: Two operations Gutman's, Schultz and modified Schultz polynomials, Topological indices.

1. INTRODUCTION

We follow the terminology of ([1],[2]). Suppose that $G = (V(G), E(G))$ is a simple undirected connected graph of order $p = |V(G)|$ and size $q = |E(G)|$. Then the distance $d(u, v)$ between two vertices $u, v \in V(G)$ is the length of the shortest path joining u and v . For $u \in V(G)$, we use δ_u to denoted the degree of a vertex u . Topological indices based on the distance between the vertices of a connected graph are widely used in theoretical chemistry to establish relation between the structure and the properties of molecules [3]. The Wiener index of G is defined as:

$$W(G) = \sum_{u, v \in V(G)} d(u, v).$$

Hosoya polynomial (also called Wiener polynomial [4]) of G is defined as:

$$H(G; x) = \sum_{\substack{u, v \in V(G) \\ u \neq v}} x^{d(u, v)}.$$

Hosoya polynomial of a vertex u of G is defined as:

$$H(u, G; x) = \sum_{\substack{v \in V(G) \\ u \neq v}} x^{d(u, v)}.$$

Another based structure descriptors is Schultz index (or Schultz molecular topological index [5]), the Schultz index of a graph G was introduced by Schultz [6]. The Schultz index is defined by:

$$Sc(G) = \sum_{\substack{u, v \in V(G) \\ u \neq v}} (\delta_u + \delta_v) d(u, v).$$

On based the Schultz index Klavžar and Gutman are introduced the Modified Schultz index (or Gutman index) [7] and it is defined as:

$$Sc^*(G) = \sum_{\substack{u, v \in V(G) \\ u \neq v}} (\delta_u \delta_v) d(u, v).$$

In chemical graph theory, there are two important polynomials for these structure descriptors are Schultz polynomial and modified Schultz polynomial of a graph G [5] are defined respectively as:

$$Sc(G; x) = \sum_{\substack{u, v \in V(G) \\ u \neq v}} (\delta_u + \delta_v) x^{d(u,v)},$$

$$Sc^*(G; x) = \sum_{\substack{u, v \in V(G) \\ u \neq v}} (\delta_u \delta_v) x^{d(u,v)}.$$

Schultz and modified Schultz polynomials of a vertex u of G are defined respectively as:

$$Sc(u, G; x) = \sum_{\substack{v \in V(G) \\ u \neq v}} (\delta_u + \delta_v) x^{d(u,v)},$$

$$Sc^*(u, G; x) = \sum_{\substack{v \in V(G) \\ u \neq v}} (\delta_u \delta_v) x^{d(u,v)},$$

where the summation for all above are taken over all unordered pairs of distinct vertices in $V(G)$.

In 2005, Gutman [8], find many relations between Hosoya, Schultz and modified Schultz polynomials of a tree graph and some properties. Bo Zhou [9], find some lower and upper bounds for the Schultz index of a graph G . In 2013, Hassani et al. computed the Schultz and modified Schultz polynomials of isomers of C100 fullerene by GAP program [10]. The Schultz index and modified Schultz index can be obtained by the derivative of Schultz and modified Schultz polynomials with respect to x at $x = 1$, i.e. :

$$Sc(G) = \frac{d}{dx} Sc(G; x) \Big|_{x=1},$$

and

$$Sc^*(G) = \frac{d}{dx} Sc^*(G; x) \Big|_{x=1} \text{ respectively.}$$

Also, the Schultz index and modified Schultz index of a vertex $u \in V(G)$ can be obtained by the derivative of Schultz and modified Schultz polynomials of a vertex u of G with respect to x at $x = 1$, i.e. :

$$Sc(u, G) = \frac{d}{dx} Sc(u, G; x) \Big|_{x=1},$$

and

$$Sc^*(u, G) = \frac{d}{dx} Sc^*(u, G; x) \Big|_{x=1} \text{ respectively.}$$

His paper [11] contains number of results on Schultz and modified Schultz polynomials of compound graphs obtained from two binary operations of graphs. In [12], Behmaram et. al. obtained The Schultz polynomial of some graph operations, therefore in this paper, we find the Schultz and modified Schultz polynomials of two Gutman's, also we given many results auxiliary and completely.

Gutman [4] defined the compound graphs $G_1 \bullet G_2$ and $G_1 : G_2$ as follows :

If G_1 and G_2 are vertex - disjoint connected graphs and $w \in V(G_1)$ and $z \in V(G_2)$, then $G_1 \bullet G_2$ is the graph obtained by identifying the vertices w and z . The compound graph $G_1 : G_2$ is the graph obtained from G_1 and G_2 by introduced a new edge joining the two vertices w and z .

Remark: In this paper we consider the distance " $d(u, v)$ " between any two vertices u and v of G are distinct vertices.

2. AUXILIARY RESULTS

Lemma 2.1: If G is a connected graph of order p and size q and u is any vertex of G , then:

1. $Sc(G;1) = 2(p-1)q$.
2. $Sc^*(G;1) = \{4q^2 - \sum_{u \in V(G)} (\delta_u)^2\} / 2$.
3. $Sc(u, G;1) = (p-2)\delta_u + 2q$.
4. $Sc^*(u, G;1) = \delta_u(2q - \delta_u)$.

Proof: Obvious.

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Lemma 2.2 [4] : If G is a connected graph of order p and u is any vertex of G then:

1. $H(G;1) = p(p-1)/2$.
2. $H(u, G;1) = p-1$.
3. $\frac{d}{dx} H(G; x) \Big|_{x=1} = W(G)$.
4. $\frac{d}{dx} H(u, G; x) \Big|_{x=1} = W(u, G)$, where $W(u, G)$ is Wiener index of a vertex u of G .

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Lemma 2.3: If v is any vertex of a connected graph G , then

1. $\sum_{\substack{v \in V(G) \\ u \neq v}} \delta_v x^{d(u,v)} = Sc(u, G; x) - \delta_u H(u, G; x)$.
2. $\sum_{\substack{v \in V(G) \\ u \neq v}} \delta_v x^{d(u,v)} = \frac{1}{\delta_u} Sc^*(u, G; x)$.
3. $Sc^*(v, G; x) = \delta_v (Sc(v, G; x) - \delta_v H(v, G; x))$.

Proof: Obvious.

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3. SCHULTZ POLYNOMIALS

Theorem 3.1: Let G_1 and G_2 be two disjoint connected graphs and let w be a vertex of G_1 and z of G_2 , then

1. $Sc(G_1 \bullet G_2; x) = Sc(G_1; x) + Sc(G_2; x) - (\delta_z + \delta_w)H(w, G_1; x)H(z, G_2; x) + H(z, G_2; x)\{\delta_w + Sc(w, G_1; x)\} + H(w, G_1; x)\{\delta_z + Sc(z, G_2; x)\}$.
2. $Sc(G_1 : G_2; x) = Sc(G_1; x) + Sc(G_2; x) - x(\delta_w + \delta_z)H(z, G_2; x)H(w, G_1; x) + \{1 + x(1 + \delta_z - \delta_w)\}H(w, G_1; x) + \{1 + x(1 + \delta_w - \delta_z)\}H(z, G_2; x) + x\{1 + H(z, G_2; x)\}Sc(w, G_1; x) + x\{1 + H(w, G_1; x)\}Sc(z, G_2; x) + (2 + \delta_w + \delta_z)x$.

Proof:

$$\begin{aligned}
 1. Sc(G_1 \bullet G_2; x) &= \sum_{u, v \in V(G_1 \bullet G_2)} (\delta_u + \delta_v) x^{d(u,v)} \\
 &= \sum_{u', u'' \in V(G_1) - \{w\}} (\delta_{u'} + \delta_{u''}) x^{d(u', u'')} + \sum_{v', v'' \in V(G_2) - \{z\}} (\delta_{v'} + \delta_{v''}) x^{d(v', v'')} \\
 &\quad + \sum_{u' \in V(G_1) - \{w\}} (\delta_w + \delta_z + \delta_{u'}) x^{d(w, u')} + \sum_{v' \in V(G_2) - \{z\}} (\delta_w + \delta_z + \delta_{v'}) x^{d(z, v')} \\
 &\quad + \sum_{\substack{u' \in V(G_1) - \{w\} \\ v' \in V(G_2) - \{z\}}} (\delta_{u'} + \delta_{v'}) x^{d(u', v')} \\
 &= \sum_{u', u'' \in V(G_1)} (\delta_{u'} + \delta_{u''}) x^{d(u', u'')} + \sum_{u' \in V(G_1) - \{w\}} \delta_z x^{d(w, u')} \\
 &\quad + \sum_{v', v'' \in V(G_2)} (\delta_{v'} + \delta_{v''}) x^{d(v', v'')} + \sum_{v' \in V(G_2) - \{z\}} \delta_w x^{d(z, v')} \\
 &\quad + (2 + \delta_w + \delta_z)x
 \end{aligned}$$

$$\begin{aligned}
& + \sum_{v', v'' \in V(G_2)} (\delta_{v'} + \delta_{v''}) x^{d(v', v'')} + \sum_{v' \in V(G_2) - \{z\}} \delta_w x^{d(z, v')} \\
& + \sum_{\substack{u' \in V(G_1) - \{w\} \\ v' \in V(G_2) - \{z\}}} (\delta_{u'} + \delta_{v'}) x^{d(u', w) + d(z, v')} \\
& = Sc(G_1; x) + \delta_z H(w, G_1; x) + Sc(G_2; x) + \delta_w H(z, G_2; x) \\
& + \sum_{u' \in V(G_1) - \{w\}} \sum_{v' \in V(G_2) - \{z\}} \delta_{u'} x^{d(u', w)} x^{d(z, v')} \\
& + \sum_{u' \in V(G_1) - \{w\}} \sum_{v' \in V(G_2) - \{z\}} \delta_{v'} x^{d(u', w)} x^{d(z, v')} \\
& = Sc(G_1; x) + \delta_z H(w, G_1; x) + Sc(G_2; x) + \delta_w H(z, G_2; x) \\
& + \sum_{v' \in V(G_2) - \{z\}} x^{d(z, v')} \left\{ \sum_{u' \in V(G_1) - \{w\}} \delta_{u'} x^{d(u', w)} \right\} + \sum_{u' \in V(G_1) - \{w\}} x^{d(u', w)} \left\{ \sum_{v' \in V(G_2) - \{z\}} \delta_{v'} x^{d(z, v')} \right\} .
\end{aligned}$$

Since $\sum_{g \in V(G)} \delta_g x^{d(y, g)} = Sc(y, G; x) - \delta_y H(y, G; x)$ by Lemma 2.3 (1). Then

$$\begin{aligned}
Sc(G_1 \bullet G_2; x) &= Sc(G_1; x) + \delta_z H(w, G_1; x) + Sc(G_2; x) + \delta_w H(z, G_2; x) \\
&+ H(z, G_2; x) \{Sc(w, G_1; x) - \delta_w H(w, G_1; x)\} \\
&+ H(w, G_1; x) \{Sc(z, G_2; x) - \delta_z H(z, G_2; x)\} . \\
\therefore Sc(G_1 \bullet G_2; x) &= Sc(G_1; x) + Sc(G_2; x) - (\delta_z + \delta_w) H(w, G_1; x) H(z, G_2; x) \\
&+ H(z, G_2; x) \{\delta_w + Sc(w, G_1; x)\} + H(w, G_1; x) \{\delta_z + Sc(z, G_2; x)\} .
\end{aligned}$$

$$\begin{aligned}
2. Sc(G_1 : G_2; x) &= \sum_{u, v \in V(G_1; G_2)} (\delta_u + \delta_v) x^{d(u, v)} \\
&= \sum_{u', u'' \in V(G_1) - \{w\}} (\delta_{u'} + \delta_{u''}) x^{d(u', u'')} + \sum_{v', v'' \in V(G_2) - \{z\}} (\delta_{v'} + \delta_{v''}) x^{d(v', v'')} \\
&+ \sum_{u' \in V(G_1) - \{w\}} (1 + \delta_w + \delta_{u'}) x^{d(u', w)} + \sum_{v' \in V(G_2) - \{z\}} (1 + \delta_z + \delta_{v'}) x^{d(v', z)} \\
&+ \sum_{u' \in V(G_1) - \{w\}} (1 + \delta_z + \delta_{u'}) x^{1+d(u', w)} + \sum_{v' \in V(G_2) - \{z\}} (1 + \delta_w + \delta_{v'}) x^{1+d(v', z)} \\
&+ \sum_{\substack{u' \in V(G_1) - \{w\} \\ v' \in V(G_2) - \{z\}}} (\delta_{u'} + \delta_{v'}) x^{d(u', v')} + (2 + \delta_w + \delta_z) x . \\
&= \sum_{u', u'' \in V(G_1)} (\delta_{u'} + \delta_{u''}) x^{d(u', u'')} + \sum_{v', v'' \in V(G_2)} (\delta_{v'} + \delta_{v''}) x^{d(v', v'')} \\
&+ \sum_{u' \in V(G_1) - \{w\}} x^{d(u', w)} + \sum_{v' \in V(G_2) - \{z\}} x^{d(v', z)} \\
&+ x(1 + \delta_z) \sum_{u' \in V(G_1) - \{w\}} x^{d(u', w)} + x \sum_{u' \in V(G_1) - \{w\}} \delta_{u'} x^{d(u', w)} \\
&+ x(1 + \delta_w) \sum_{v' \in V(G_2) - \{z\}} x^{d(v', z)} + x \sum_{v' \in V(G_2) - \{z\}} \delta_{v'} x^{d(v', z)} \\
&+ x \sum_{u' \in V(G_1) - \{w\}} \sum_{v' \in V(G_2) - \{z\}} \delta_{u'} x^{d(u', w)} x^{d(z, v')} \\
&+ x \sum_{u' \in V(G_1) - \{w\}} \sum_{v' \in V(G_2) - \{z\}} \delta_{v'} x^{d(u', w)} x^{d(z, v')} + (2 + \delta_w + \delta_z) x \\
&= Sc(G_1; x) + Sc(G_2; x) + H(w, G_1; x) + H(z, G_2; x) \\
&+ x(1 + \delta_z) H(w, G_1; x) + x \{Sc(w, G_1; x) - \delta_w H(w, G_1; x)\} \\
&+ x(1 + \delta_w) H(z, G_2; x) + x \{Sc(z, G_2; x) - \delta_z H(z, G_2; x)\} \\
&+ x \sum_{v' \in V(G_2) - \{z\}} x^{d(v', z)} \left\{ \sum_{u' \in V(G_1) - \{w\}} \delta_{u'} x^{d(u', w)} \right\} + x \sum_{u' \in V(G_1) - \{w\}} x^{d(u', w)} \left\{ \sum_{v' \in V(G_2) - \{z\}} \delta_{v'} x^{d(v', z)} \right\} \\
&+ (2 + \delta_w + \delta_z) x
\end{aligned}$$

$$\begin{aligned}
 &= Sc(G_1; x) + Sc(G_2; x) + H(w, G_1; x) + H(z, G_2; x) \\
 &+ x(1 + \delta_z)H(w, G_1; x) + x\{Sc(w, G_1; x) - \delta_w H(w, G_1; x)\} \\
 &+ x(1 + \delta_w)H(z, G_2; x) + x\{Sc(z, G_2; x) - \delta_z H(z, G_2; x)\} \\
 &+ xH(z, G_2; x)\{Sc(w, G_1; x) - \delta_w H(w, G_1; x)\} \\
 &+ xH(w, G_1; x)\{Sc(z, G_2; x) - \delta_z H(z, G_2; x)\} + (2 + \delta_w + \delta_z)x. \\
 \therefore Sc(G_1 : G_2; x) &= Sc(G_1; x) + Sc(G_2; x) - x(\delta_w + \delta_z)H(z, G_2; x)H(w, G_1; x) \\
 &+ \{1 + x(1 + \delta_z - \delta_w)\}H(w, G_1; x) + \{1 + x(1 + \delta_w - \delta_z)\}H(z, G_2; x) \\
 &+ x\{1 + H(z, G_2; x)\}Sc(w, G_1; x) + x\{1 + H(w, G_1; x)\}Sc(z, G_2; x) \\
 &+ (2 + \delta_w + \delta_z)x. \quad \#
 \end{aligned}$$

Corollary 3.2: If $G_1(p_1, q_1) \equiv G_2(p_2, q_2) \equiv G(p, q)$, and the identical vertices w and z of G_1 and G_2 respectively are identical (let $w \equiv z \equiv y$), then

$$\begin{aligned}
 1. Sc(G \bullet G; x) &= 2Sc(G; x) + 2H(y, G; x)\{\delta_y + Sc(y, G; x) - \delta_y H(y, G; x)\}. \\
 2. Sc(G : G; x) &= 2Sc(G; x) + 2xH(y, G; x)\{1 + Sc(y, G; x) - \delta_y H(y, G; x)\} \\
 &+ 2x\{1 + Sc(y, G; x) + \delta_y\} + 2H(y, G; x). \quad \#
 \end{aligned}$$

Corollary 3.3: The Schultz indices of $G_1 \bullet G_2$, $G_1 : G_2$, $G \bullet G$ and $G : G$ are:

$$\begin{aligned}
 1. Sc(G_1 \bullet G_2) &= Sc(G_1) + Sc(G_2) + (p_2 - 1)Sc(w, G_1) + (p_1 - 1)Sc(z, G_2) \\
 &+ \{2q_1 - \delta_z(p_1 - 1)\}W(z, G_2) + \{2q_2 - \delta_w(p_2 - 1)\}W(w, G_1). \\
 2. Sc(G_1 : G_2) &= Sc(G_1) + Sc(G_2) + p_2Sc(w, G_1) + p_1Sc(z, G_2) + p_1(2q_2 + 1) + p_2(2q_1 + 1) \\
 &+ \{2(q_2 + 1) - \delta_w p_2\}W(w, G_1) + \{2(q_1 + 1) - \delta_z p_1\}W(z, G_2). \\
 3. Sc(G \bullet G) &= 2Sc(G) + 2(p - 1)Sc(y, G) + 2\{2q - \delta_y(p - 1)\}W(y, G). \\
 4. Sc(G : G) &= 2Sc(G) + 2pSc(y, G) + 2\{2(q + 1) - \delta_y p\}W(y, G) + 2p(2q + 1). \quad \#
 \end{aligned}$$

4. MODIFIED SCHULTZ POLYNOMIALS

Theorem 4.1: Let G_1 and G_2 be two disjoint connected graphs and let w be a vertex of G_1 and z of G_2 , then

$$\begin{aligned}
 1. Sc(G_1 \bullet G_2; x) &= Sc(G_1; x) + Sc(G_2; x) + (\delta_w / \delta_z)Sc(z, G_2; x) + (\delta_z / \delta_w)Sc(w, G_1; x) \\
 &+ (1 / \delta_w \delta_z)Sc(w, G_1; x)Sc(z, G_2; x). \\
 2. Sc(G_1 : G_2; x) &= Sc(G_1; x) + Sc(G_2; x) + \frac{x}{\delta_w \delta_z}Sc(w, G_1; x)Sc(z, G_2; x) \\
 &+ \frac{1 + (1 + \delta_w)x}{\delta_z}Sc(z, G_2; x) + \frac{1 + (1 + \delta_z)x}{\delta_w}Sc(w, G_1; x) \\
 &+ (1 + \delta_w)(1 + \delta_z)x.
 \end{aligned}$$

Proof:

$$\begin{aligned}
 1. Sc(G_1 \bullet G_2; x) &= \sum_{\substack{u, v \in V(G_1 \bullet G_2) \\ u \neq v}} (\delta_u \delta_v) x^{d(u, v)} \\
 &= \sum_{u', u'' \in V(G_1) - \{w\}} (\delta_{u'} \delta_{u''}) x^{d(u', u'')} + \sum_{v', v'' \in V(G_2) - \{z\}} (\delta_{v'} \delta_{v''}) x^{d(v', v'')} \\
 &+ \sum_{u' \in V(G_1) - \{w\}} \{(\delta_w + \delta_z) \delta_{u'}\} x^{d(u', w)} + \sum_{v' \in V(G_2) - \{z\}} \{(\delta_w + \delta_z) \delta_{v'}\} x^{d(v', z)} \\
 &+ \sum_{\substack{u' \in V(G_1) - \{w\} \\ v' \in V(G_2) - \{z\}}} (\delta_{u'} \delta_{v'}) x^{d(u', v')}.
 \end{aligned}$$

$$\begin{aligned}
 &= \sum_{u', u'' \in V(G_1)} (\delta_u \delta_{u''}) x^{d(u', u'')} + \sum_{u' \in V(G_1) - \{w\}} (\delta_z \delta_{u'}) x^{d(u', w)} \\
 &+ \sum_{v', v'' \in V(G_2)} (\delta_v \delta_{v''}) x^{d(v', v'')} + \sum_{v' \in V(G_2) - \{z\}} (\delta_w \delta_{v'}) x^{d(v', z)} \\
 &+ \sum_{u' \in V(G_1) - \{w\}} \sum_{v' \in V(G_2) - \{z\}} (\delta_u \delta_{v'}) x^{d(u', w) + d(v', z)} . \\
 &= Sc(G_1; x) + (\delta_z / \delta_w) Sc(w, G_1; x) + Sc(G_2; x) + (\delta_w / \delta_z) Sc(z, G_2; x) \\
 &+ \sum_{u' \in V(G_1) - \{w\}} \delta_u x^{d(u', w)} \sum_{v' \in V(G_2) - \{z\}} \delta_v x^{d(v', z)} . \\
 &= Sc(G_1; x) + Sc(G_2; x) + (\delta_z / \delta_w) Sc(w, G_1; x) + (\delta_w / \delta_z) Sc(z, G_2; x) \\
 &+ (1 / \delta_w \delta_z) Sc(w, G_1; x) Sc(z, G_2; x) .
 \end{aligned}$$

Corollary 4.2: If $G_1(p_1, q_1) \equiv G_2(p_2, q_2) \equiv G(p, q)$, and the identical vertices w and z of G_1 and G_2 respectively are identical (let $w \equiv z \equiv y$), then

1. $Sc(G \bullet G; x) = 2 Sc(G; x) + Sc(y, G; x) \{ 2 + \frac{1}{(\delta_y)^2} Sc(y, G; x) \}$.
2. $Sc(G : G; x) = 2 Sc(G; x) + \frac{1}{\delta_y} Sc(y, G; x) \{ \frac{x}{\delta_y} Sc(y, G; x) + 2(1 + (1 + \delta_y)x) \} + (1 + \delta_y)^2 x$.

Corollary 4.3: The modified Schultz indices of $G_1 \bullet G_2$, $G_1 : G_2$, $G \bullet G$ and $G : G$ are:

1. $Sc(G_1 \bullet G_2) = Sc(G_1) + Sc(G_2) + (2q_2 / \delta_w) Sc(w, G_1) + (2q_1 / \delta_z) Sc(z, G_2)$.
2. $Sc(G_1 : G_2) = Sc(G_1) + Sc(G_2) + \frac{2(1 + q_1)}{\delta_z} Sc(z, G_2) + \frac{2(1 + q_2)}{\delta_w} Sc(w, G_1) + \frac{2q_1 - \delta_w}{\delta_z} + 2q_2(1 + \delta_w) + 2q_1(1 + \delta_z) + 1 - \delta_w \delta_z$.
3. $Sc(G \bullet G) = 2 Sc(G) + (4 / \delta_y) q Sc(y, G)$.
4. $Sc(G : G) = 2 Sc(G) + \frac{4(1 + q)}{\delta_y} Sc(y, G) + \frac{2q}{\delta_y} + 4q(1 + \delta_y) - \delta_y^2$.

#

CONCLUSION

Finally, in this paper we managed to find the Schultz and Modified Schultz polynomials and Schultz and Modified Schultz indices of compound graphs from G_1 and G_2 of two operation Gutman's ($G_1 \bullet G_2$ and $G_1 : G_2$), where G_1 and G_2 are vertex - disjoint connected graphs. Also we obtain some result with respect to the Schultz and Modified Schultz polynomials and Schultz and Modified Schultz indices when $(G_1 \cong G_2) = G$.

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