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TWO GENERALIZED TOPOLOGICAL INDICES OF SOME GRAPH STRUCTURES

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Abstract. A topological index (TI) can capture many information of a chemical structure into a real number. The topological indices have an important role in theoretical chemistry. A topological index is a graph based molecular descriptor, which is graph theoretic invariant characterizing some physicochemical properties of chemical compounds. There are several topological indices that have been introduced in theoretical chemistry to measure the properties of chemical compounds, based on various parameters such as distance-based topological indices, degree-based topological indices etc. In recent times, unified approaches are also being adopted to study these topological indices in groups. In this work, we study the generalized ISI index and generalized Zagreb index with which we can obtain some other topological indices as special cases of conical graph, polyomino chains, trianglar benzenoid and lattice graph. These generalized indices surely reduce the work for calculating some topological indices differently.

Keywords: topological index; generalized isi index; generalized zagreb index.

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1. INTRODUCTION

In chemical graph theory, a topological index or a molecular descriptor [13] is a mathematical formula that gives a numerical value which can be applied to any molecular graph while modelling molecular structures. It gives us vital information about the physical, chemical and biological properties of chemical compounds of graphs. Also it is potentially used to study the various properties of molecular structures such as boiling point, acentric factor, total surface area, isomer discrimination, structural-activity relationships(SAR), structural-property relationships, chemical documentation and pharmaceutical drug designing etc.

In 2020, Buragohain et al.[6] introduced a novel generalized topological index for some chemical structures and is defined as

$$ISI_{(\alpha,\,\beta)}(G) = \sum_{uv \in E(G)} (d(u)d(v))^{\alpha}(d(u)+d(v))^{\beta},$$

Some standard topological indices can be find for some particular values of α and β as a special case of this index. For more details of these topological indices see [10, 11, 12, 14, 15, 19, 21, 24, 25, 26, 27].

Table 1 shows that the relationships between $ISI_{(\alpha,\,\beta)}$-index with some other topological indices.

A generalized version of degree based topological index introduced by Azari et al.[4] in 2011, named as generalized Zagreb index or $(\alpha,\ \beta)$-Zagreb index and is defined as

$$Z_{\alpha,\,\beta}(G) = \sum_{uv \in E(G)} [d_G(u)^{\alpha} d_G(v)^{\beta} + d_G(u)^{\beta} d_G(v)^{\alpha}],$$

For some particular values of α & β gives some other degree based topological indices. More details of these TI's can be found in[2, 5, 9, 11, 16, 17, 18, 21]. Table 2 represents the relationships between $(\alpha,\ \beta)$-Zagreb index and other degree based topological indices. Some recent works on this index may be found in [7, 22, 23]

Topological index	**Corresponding** (α,β) **ISI-index**
First Zagreb index, $M_1(G)$	$ISI_{0,1}(G)$
Second Zagreb index, $M_2(G)$	$ISI_{1,0}(G)$
Randić index, $R(G)$	$ISI_{-\frac{1}{2},0}(G)$
Sum connectivity index, $SCI(G)$	$ISI_{0,-\frac{1}{2}}(G)$
Inverse sum indeg index, $ISI(G)$	$ISI_{1,-1}(G)$
Harmonic index, $H(G)$	$2ISI_{0,-1}(G)$
Geometric-Arithmetric Mean index, $GA(G)$	$2ISI_{\frac{1}{2},-1}(G)$
Hyper-Zagreb index, $HM(G)$	$ISI_{0,2}(G)$
First Generalized Randić index, $R_\alpha(G)$	$ISI_{\alpha,0}(G)$
General sum-connectivity index, $\chi_\alpha(G)$	$ISI_{0,\alpha}(G)$

TABLE 1. Relationships between (α,β) ISI-index and some other topological indices.

Topological index	**corresponding** $Z_{(\alpha,\,\beta)}$**-index**
First Zagreb index, $M_1(G)$	$Z_{1,0}(G)$
Second Zagreb index, $M_2(G)$	$\frac{1}{2}Z_{1,1}(G)$
F-index, $F(G)$	$Z_{2,0}(G)$
Redefined Zagreb index, $ReZM(G)$	$Z_{2,1}(G)$
Symmetric division deg index, $SDD(G)$	$Z_{1,-1}(G)$
General first Zagreb index, $M^\alpha(G)$	$Z_{\alpha-1,0}(G)$
First General Randić index, $R_\alpha(G)$	$\frac{1}{2}Z_{\alpha,\alpha}(G)$

TABLE 2. Relationships between $Z_{(\alpha,\,\beta)}$-index and some other topological indices.

2. Graphs and Their Generalized Indices

2.1. Conical Graph.

In 2020, Ayache et al. [3] studied the Conical Graphs $G(m,n)$, The graph consists of a center and mn cycles say $C_n^1, C_n^2, C_n^3, C_n^4, \ldots, C_n^m$

The cardinalities of vertices and edges of the $G(m,n)$ are $mn+1$, and $2mn$ respectively. Consider

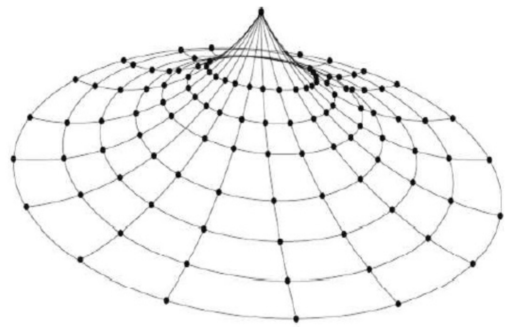

FIGURE 1. $G_{19}(7)$

the vertex set be $V(G(m,n)) = \{u_0, u_1^1, u_2^1, \ldots, u_n^1, u_1^2, u_2^2, \ldots, u_n^2, \ldots, u_1^m, u_2^m, \ldots, u_n^m\}$ and

$$deg(V(G)) = n : u = u_0; 3 : u = u_i^m; 4 : otherwise.$$

The edge sets of $G(m,n)$ can be written as $E(G) = \cup_{k=0}^{3} E_k : \cap E_k = \phi$ such that

$$\begin{aligned}
E_0 =& \{u_0 u_i^1 \in E(G) : d(u_0) = n \text{ and } d(u_i^1) = 4\}\\
& \text{where } i = 1, 2, ..., n\\
E_1 =& \{u_i^{m-1} u_i^m \in E(G) : d(u_i^{m-1}) = 4 \text{ and } d(u_i^m) = 3\}\\
E_2 =& \{u_i^m u_{i+1}^m \text{ and } u_n^m u_1^m \in E(G) : d(u_i^m) = 3 \text{ and } d(u_{i+1}^m) = 3\}\\
& \text{where } i = 1, 2, ..., n-1\\
E_3 =& E_+ \cup E_* \ \text{ such that } \ \forall j = 1, 2, ..., m-1
\end{aligned}$$

where

$$\begin{aligned}
E_+ =& \{u_i^j u_{i+1}^j \text{ and } u_n^j u_1^j \in E(G) : d(u_i^j) = 4 = d(u_{i+1}^j)\}\\
E_* =& \{u_i^{j-1} u_i^m \in E(G) : d(u_i^{j-1}) = 4 = d(u_i^m)\}
\end{aligned}$$

then the cardinalities are

$$\begin{aligned}
|E_0(G)| =& n,\\
|E_1(G)| =& n,\\
|E_2(G)| =& n,\\
|E_3(G)| =& |E_+| + |E_*|\\
=& n(m-1) + n(m-2)\\
=& n(2m-3).
\end{aligned}$$

Theorem 2.1. *The $ISI_{(\alpha,\,\beta)}$-index of Conical graph $G(m,n)$ is given by*

$$ISI_{(\alpha,\,\beta)}(G(m,n)) = n[4n]^{\alpha}[4+n]^{\beta} + n[12]^{\alpha}[7]^{\beta} + n[9]^{\alpha}[6]^{\beta} + n(2m-3)[16]^{\alpha}[8]^{\beta}.$$

Proof.

$$\begin{aligned}
ISI_{(\alpha,\,\beta)}(G(m,n)) =& \sum_{uv\in E(G(m,n))} [d(u)d(v)]^{\alpha}[d(u)+d(v)]^{\beta}\\
=& \sum_{uv\in E_0(G(m,n))} [4n]^{\alpha}[4+n]^{\beta} + \sum_{uv\in E_1(G(m,n))} [12]^{\alpha}[7]^{\beta}\\
+& \sum_{uv\in E_2(G(m,n))} [9]^{\alpha}[6]^{\beta} + \sum_{uv\in E_3(G(m,n))} [16]^{\alpha}[8]^{\beta}\\
=& |E_0(G(m,n)|[4n]^{\alpha}[4+n]^{\beta} + |E_1(G(m,n))|[12]^{\alpha}[7]^{\beta}\\
+& |E_2(G(m,n))|[9]^{\alpha}[6]^{\beta} + |E_3(G(m,n))|[16]^{\alpha}[8]^{\beta}\\
=& n[4n]^{\alpha}[4+n]^{\beta} + n[12]^{\alpha}[7]^{\beta} + n[9]^{\alpha}[6]^{\beta} + n(2m-3)[16]^{\alpha}[8]^{\beta}
\end{aligned}$$

□

Theorem 2.2. *The generalized Zagreb index of of conical graph $G(m,n)$ is given by*

$$Z_{(\alpha,\beta)}(G) = n[n^{\alpha}4^{\beta} + n^{\beta}4^{\alpha}] + n[4^{\alpha}3^{\beta} + 4^{\beta}3^{\beta}] + 2n3^{\alpha+\beta} + 2n(2m-3)4^{\alpha+\beta}$$

Proof.

$$\begin{aligned}
Z_{(\alpha,\beta)}(G) &= \sum_{uv\in E(G(m,n))} [d(u)^{\alpha}d(v)^{\beta}+d(u)^{\beta}d(v)^{\alpha}] \\
&= \sum_{uv\in E_0(G(m,n))} [n^{\alpha}4^{\beta}+n^{\beta}4^{\alpha}] + \sum_{uv\in E_1(G(m,n))} [4^{\alpha}3^{\beta} \\
&+4^{\beta}3^{\alpha}] + \sum_{uv\in E_2(G(m,n))} [3^{\alpha}3^{\beta}+3^{\beta}3^{\alpha}] \\
&+ \sum_{uv\in E_3(G(m,n))} [4^{\alpha}4^{\beta}+4^{\beta}4^{\alpha}] \\
&= n[n^{\alpha}4^{\beta}+n^{\beta}4^{\alpha}]+n[4^{\alpha}3^{\beta}+4^{\beta}3^{\alpha}]+2n3^{\alpha+\beta} \\
&+2n(2m-3)4^{\alpha+\beta}
\end{aligned}$$

□

2.2. A 2-dimensional zig-zag polyomino chain. A polyomino system is a nite 2-connected plane graph. A regular square of length one surrounds each interior face(cell). In either words, it is an edge-connected union of cells in the plane square lattice[20]. For more about the rich history of polynomino see [8]. We consider a 2-dimensional zig-zag polyomino chain, Z_n. Clearly from the Fig. 2 $|V(Z_n)| = 12n+2$ and $|E(Z_n)| = 14n+2$.

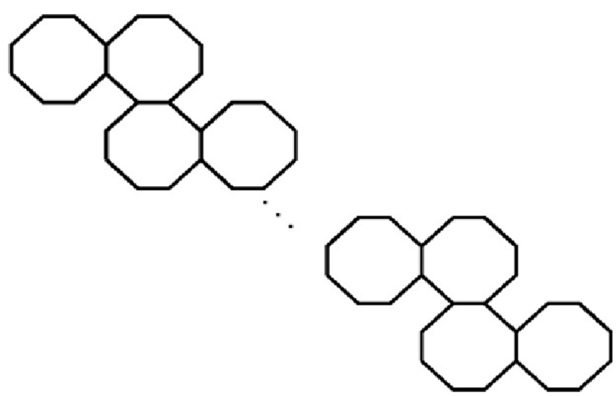

FIGURE 2. 2-dimensional zig-zag polyomino chain

The edge set of Z_n can be partitioned as follows:

$$E_1(Z_n) =\{uv \in E(Z_n) : d(u) = 2 \text{ and } d(v) = 2\},$$
$$E_2(Z_n) =\{uv \in E(Z_n) : d(u) = 2 \text{ and } d(v) = 3\},$$
$$E_3(Z_n) =\{uv \in E(Z_n) : d(u) = 3 \text{ and } d(v) = 3\}.$$

such that,

$$|E_1(Z_n)| =6n+4,$$
$$|E_2(Z_n)| =4n,$$
$$|E_3(Z_n)| =4n-3.$$

Theorem 2.3. *For a molecular graph $Z_n, n \geq 1$, of zig-zag polyomino chain the generalized ISI index is*

$$(6n+4)4^{\alpha+\beta} + 4n6^{\alpha}5^{\beta} + (4n-3)9^{\alpha}6^{\beta}$$

Proof.

$$\begin{aligned} ISI_{(\alpha,\beta)}(Z_n) &= \sum_{uv\in E(Z_n)} [d(u)d(v)]^{\alpha}[d(u)+d(v)]^{\beta} \\ &= \sum_{uv\in E_1(Z_n)} (2.2)^{\alpha}(2+2)^{\beta} + \sum_{uv\in E_2(Z_n)} (2.3)^{\alpha}(2+3)^{\beta} + \sum_{uv\in E_3(Z_n)} (3.3)^{\alpha}(3+3)^{\beta} \\ &=(6n+4)4^{\alpha+\beta} + 4n6^{\alpha}5^{\beta} + (4n-3)9^{\alpha}6^{\beta} \end{aligned}$$

□

Theorem 2.4. *For a molecular graph $Z_n, n \geq 1$, of zig zag polyomino chain the generalized Zagreb index is*

$$(12n+8)2^{\alpha+\beta} + 4n(2^{\alpha}3^{\beta} + 2^{\beta}3^{\alpha}) + (8n-6)3^{\alpha+\beta}$$

Proof.

$$
\begin{aligned}
Z_{\alpha,\beta}(Z_n) &= \sum_{uv\in E(Z_n)} \left[d(u)^\alpha d(v)^\beta + d(u)^\beta d(v)^\alpha\right] \\
&= \sum_{uv\in E_1(Z_n)} (2^\alpha 2^\beta + 2^\beta 2^\alpha) + \sum_{uv\in E_2(Z_n)} (2^\alpha 3^\beta + 2^\beta 3^\alpha) + \sum_{uv\in E_3(Z_n)} (3^\alpha 3^\beta + 3^\beta 3^\alpha) \\
&= (12n+8)2^{\alpha+\beta} + 4n(2^\alpha 3^\beta + 2^\beta 3^\alpha) + (8n-6)3^{\alpha+\beta}
\end{aligned}
$$

□

2.3. A linear polyomino chain. A linear polyomino chain denoted by L_n is shown in Fig. 3. From the figure we have $|V(L_n)|$=2(n+1) and $|E(L_n)|$=3n+1.

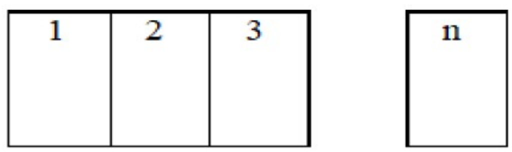

FIGURE 3. A linear polyomino chain

The edge set of L_n can be partitioned as follows:

$$
\begin{aligned}
E_1(L_n) =& \{uv \in E(L_n) : d(u) = 2 \text{ and } d(v) = 2\}, \\
E_2(L_n) =& \{uv \in E(L_n) : d(u) = 2 \text{ and } d(v) = 3\}, \\
E_3(L_n) =& \{uv \in E(L_n) : d(u) = 3 \text{ and } d(v) = 3\}.
\end{aligned}
$$

such that,

$$
\begin{aligned}
|E_1(L_n)| =& 2, \\
|E_2(L_n)| =& 4, \\
|E_3(L_n)| =& 3n-5.
\end{aligned}
$$

Theorem 2.5. *For a molecular graph $L_n, n \geq 2$, of linear polyomino chain the generalized ISI index is*

$$2 \times 4^{\alpha+\beta} + 4 \times 6^{\alpha} 5^{\beta} + (3n-5) 9^{\alpha} 6^{\beta}$$

Proof.

$$\begin{aligned} ISI_{(\alpha,\beta)}(L_n) &= \sum_{uv \in E(L_n)} [d(u)d(v)]^{\alpha} [d(u)+d(v)]^{\beta} \\ &= \sum_{uv \in E_1(L_n)} (2.2)^{\alpha}(2+2)^{\beta} + \sum_{uv \in E_2(L_n)} (2.3)^{\alpha}(2+3)^{\beta} + \sum_{uv \in E_3(L_n)} (3.3)^{\alpha}(3+3)^{\beta} \end{aligned}$$

$$= 2 \times 4^{\alpha+\beta} + 4 \times 6^{\alpha} 5^{\beta} + (3n-5) 9^{\alpha} 6^{\beta}$$

□

Theorem 2.6. *For a molecular graph $L_n, n \geq 2$, of linear polyomino chain the generalized Zagreb index is*

$$2^{\alpha+\beta+2} + 4(2^{\alpha}3^{\beta} + 2^{\beta}3^{\alpha}) + (6n-10)3^{\alpha+\beta}$$

Proof.

$$\begin{aligned} Z_{\alpha,\beta}(L_n) &= \sum_{uv \in E(L_n)} \left[d(u)^{\alpha} d(v)^{\beta} + d(u)^{\beta} d(v)^{\alpha} \right] \\ &= \sum_{uv \in E_1(L_n)} (2^{\alpha}2^{\beta} + 2^{\beta}2^{\alpha}) + \sum_{uv \in E_2(L_n)} (2^{\alpha}3^{\beta} + 2^{\beta}3^{\alpha}) + \sum_{uv \in E_3(L_n)} (3^{\alpha}3^{\beta} + 3^{\beta}3^{\alpha}) \\ &= 2^{\alpha+\beta+2} + 4(2^{\alpha}3^{\beta} + 2^{\beta}3^{\alpha}) + (6n-10)3^{\alpha+\beta} \end{aligned}$$

□

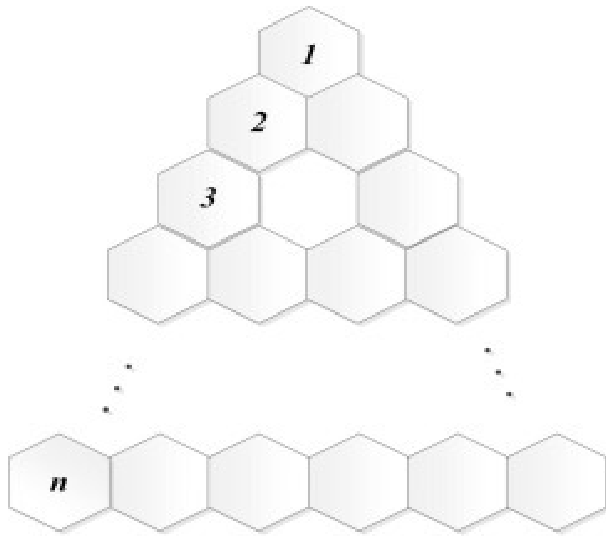

FIGURE 4. Triangular benzenoid

2.4. Triangular benzenoid. The triangular benzenoid system denoted by T_n, where n denotes the number of hexagons is shown in Fig. 4.

From the figure we have $|V(T_n)|$=n^2+4n+1 and $|E(T_n)|$=$\frac{3}{2}$n(n+3).

The edge set of T_n can be partitioned as follows:

$$E_1(T_n) =\{uv \in E(T_n) : d(u) = 2 \textit{ and } d(v) = 2\},$$

$$E_2(T_n) =\{uv \in E(T_n) : d(u) = 2 \textit{ and } d(v) = 3\},$$

$$E_3(T_n) =\{uv \in E(T_n) : d(u) = 3 \textit{ and } d(v) = 3\}.$$

such that,

$$|E_1(L_n)| =6,$$

$$|E_2(L_n)| =6(n-1),$$

$$|E_3(L_n)| =\frac{3}{2}n(n-1).$$

Theorem 2.7. *For a molecular graph triangular benzenoid $T_n, n \geq 1$, the generalized ISI index is*

$$6 \times 4^{\alpha+\beta} + (n-1)6^{\alpha+1}5^{\beta} + \frac{3}{2}n(n-1)9^{\alpha}6^{\beta}$$

Proof.

$$\begin{aligned}
ISI_{(\alpha,\beta)}(T_n) &= \sum_{uv\in E(T_n)} [d(u)d(v)]^{\alpha}[d(u)+d(v)]^{\beta} \\
&= \sum_{uv\in E_1(T_n)} (2.2)^{\alpha}(2+2)^{\beta} + \sum_{uv\in E_2(T_n)} (2.3)^{\alpha}(2+3)^{\beta} + \sum_{uv\in E_3(T_n)} (3.3)^{\alpha}(3+3)^{\beta}
\end{aligned}$$

$$= 6 \times 4^{\alpha+\beta} + (n-1)6^{\alpha+1}5^{\beta} + \frac{3}{2}n(n-1)9^{\alpha}6^{\beta}$$

□

Theorem 2.8. *For a molecular graph triangular benzenoid $T_n, n \geq 1$, the generalized Zagreb index is*

$$6 \times 2^{\alpha+\beta+1} + 6(n-1)(2^{\alpha}3^{\beta} + 2^{\beta}3^{\alpha}) + n(n-1)3^{\alpha+\beta+1}$$

Proof.

$$\begin{aligned}
Z_{\alpha,\beta}(T_n) &= \sum_{uv\in E(T_n)} \left[d(u)^{\alpha}d(v)^{\beta} + d(u)^{\beta}d(v)^{\alpha}\right] \\
&= \sum_{uv\in E_1(T_n)} (2^{\alpha}2^{\beta} + 2^{\beta}2^{\alpha}) + \sum_{uv\in E_2(T_n)} (2^{\alpha}3^{\beta} + 2^{\beta}3^{\alpha}) + \sum_{uv\in E_3(T_n)} (3^{\alpha}3^{\beta} + 3^{\beta}3^{\alpha}) \\
&= 6 \times 2^{\alpha+\beta+1} + 6(n-1)(2^{\alpha}3^{\beta} + 2^{\beta}3^{\alpha}) + n(n-1)3^{\alpha+\beta+1}
\end{aligned}$$

□

2.5. The Square Lattice Graph. Lattice network has a wide range of application such as in distributing parallel computation, wired circuits, distributing control etc. They are also called mesh or grid networks. Here for theoretical analysis we choose a square lattice [1].

we consider a square lattice graph $SL_n(V,E)$ of size $n \times n$ vertices. From the Fig. 5 we get the number of vertices, $|V| = n^2$ and the number of edges, $|E| = 2n(n-1)$.

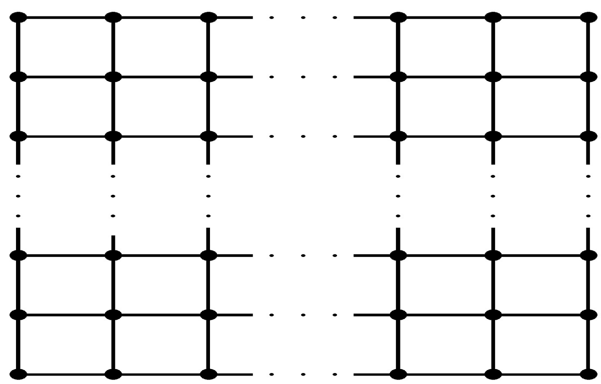

FIGURE 5. Square lattice, SL_n with $n \geq 1$

The edge set of SL_n can be partitioned as follows:

$$E_1(SL_n) = \{uv \in E(SL_n) : d(u) = 2 \text{ and } d(v) = 3\},$$

$$E_2(SL_n) = \{uv \in E(SL_n) : d(u) = 3 \text{ and } d(v) = 3\},$$

$$E_3(SL_n) = \{uv \in E(SL_n) : d(u) = 3 \text{ and } d(v) = 4\},$$

$$E_4(SL_n) = \{uv \in E(SL_n) : d(u) = 4 \text{ and } d(v) = 4\}$$

such that,

$$
\begin{aligned}
|E_1(SL_n)| =& 8,\\
|E_2(SL_n)| =& 4(n-3),\\
|E_3(SL_n)| =& 4(n-2),\\
|E_4(SL_n)| =& 2n^2-10n+12.
\end{aligned}
$$

Theorem 2.9. *For the square lattice graph SL_n the generalized ISI index is*

$$8.6^{\alpha}5^{\beta}+4(n-3)9^{\alpha}6^{\beta}+4(n-2)12^{\alpha}7^{\beta}+(2n^2-10n+12)16^{\alpha}8^{\beta}$$

Proof.

$$
\begin{aligned}
ISI(SL_n) &= \sum_{uv\in E(SL_n)} [d(u)d(v)]^{\alpha}[d(u)+d(v)]^{\beta}\\
&= \sum_{uv\in E_1(SL_n)} (2.3)^{\alpha}(2+3)^{\beta} + \sum_{uv\in E_2(SL_n)} (3.3)^{\alpha}(3+3)^{\beta} + \sum_{uv\in E_3(SL_n)} (3.4)^{\alpha}(3+4)^{\beta}\\
&+ \sum_{uv\in E_4(SL_n)} (4.4)^{\alpha}(4+4)^{\beta}
\end{aligned}
$$

$$=8.6^{\alpha}5^{\beta}+4(n-3)9^{\alpha}6^{\beta}+4(n-2)12^{\alpha}7^{\beta}+(2n^2-10n+12)16^{\alpha}8^{\beta}$$

□

Theorem 2.10. *For the Square lattice SL_n, the generalized Zagreb index is*

$$8(2^{\alpha}3^{\beta}+2^{\beta}3^{\alpha})+8(n-3)3^{\alpha+\beta}+4(n-3)(3^{\alpha}4^{\beta}+3^{\beta}4^{\alpha})+(4n^2-20n+24)4^{\alpha+\beta}$$

Proof.

$$
\begin{aligned}
Z_{\alpha,\beta}(SL_n) &= \sum_{uv\in E(SL_n)} \left[d(u)^{\alpha}d(v)^{\beta}+d(u)^{\beta}d(v)^{\alpha}\right] \\
&= \sum_{uv\in E_1(SL_n)} \left[2^{\alpha}3^{\beta}+2^{\beta}3^{\alpha}\right]+\sum_{uv\in E_2(SL_n)} \left[3^{\alpha}3^{\beta}+3^{\beta}3^{\alpha}\right]+\sum_{uv\in E_3(SL_n)} \left[3^{\alpha}4^{\beta}+3^{\beta}4^{\alpha}\right] \\
&+ \sum_{uv\in E_4(SL_n)} \left[4^{\alpha}4^{\beta}+4^{\beta}4^{\alpha}\right]
\end{aligned}
$$

$$
= 8(2^{\alpha}3^{\beta}+2^{\beta}3^{\alpha})+8(n-3)3^{\alpha+\beta}+4(n-3)(3^{\alpha}4^{\beta}+3^{\beta}4^{\alpha})+(4n^2-20n+24)4^{\alpha+\beta}
$$

□

3. CONCLUSION

In this study, we obtain the Generalized ISI and Zagreb index and some popular degree based topological indices as special cases of some standard graphs. It also reduces the work for calculating some indices separately.

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CONFLICT OF INTERESTS

The author(s) declare that there is no conflict of interests.

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