On Topological Indices of Sudoku Graphs and Titania TiO$_2$ Nanotubes

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Abstract— In this paper, we obtain the exact formulae for some topological indices such as the general sum-connectivity index, atom-bond connectivity index, geometric arithmetic index, inverse sum indeg index, symmetric division deg index and harmonic polynomial of titania TiO$_2$ Nanotubes and Sudoku graphs.

Keywords— sum-connectivity index, Sudoku graph, TiO$_2$ Nanotubes.

MSC: Primary: 05C35; Secondary: 05C07, 05C40

I. INTRODUCTION

A topological index is a mathematical measure which correlates to the chemical structures of any simple finite graph. They are invariant under the graph isomorphism. They play an important role in the study of QS AR / QS PR. In theoretical chemistry, molecular structure descriptors (also called topological indices) are used for modeling physicochemical, pharmacologic, toxicologic, nanoscience, biological and other properties of chemical compounds. Among these topological descriptors the degree-based topological indices are of great importance. The first degree-based topological indices that were defined by Gutman and Trinajstić in [8] 1972, are the first and second Zagreb indices. These indices were originally defined as $M_1(G) = \sum_{u \in V(G)} (d_G(u))^2$ and $M_2(G) = \sum_{u \in V(G)} (d_G(u)+d_G(v))^2$, where $M_1(G)$ and $M_2(G)$ denote the first and second Zagreb indices, respectively.

The sum-connectivity index was proposed by Zhou and Trinajstić [15] in 2009, which is defined as the sum over all the edges of the graph of the terms $(d_G(u)+d_G(v))^\alpha$. This concept was extended to the general sum-connectivity index in 2010 [16], which is defined as $\chi_\alpha(G) = \sum_{u \in V(G)} (d_G(u)+d_G(v))^\alpha$, where $\alpha$ is a real number. If $\alpha = 1, -\frac{1}{2}$ and 2, then $\chi_1(G) = M_1(G)$, $\chi_{-\frac{1}{2}}(G) = H(G)$ and $\chi_2(G) = HM(G)$ (hyper Zagreb index). The sum-connectivity index and product-connectivity index correlate well with the π-electron energy of benzenoid hydrocarbons [12]. Another variant of the Randić index of $G$ is the harmonic index, denoted by $H(G)$ and define as $H(G) = \sum_{u,v \in E(G)} \frac{2}{d_G(u)+d_G(v)} = 2\chi - 1(G)$.

Motivated by definition of the Randić connectivity index, Vukičević and Furtula [14] proposed another degree-based topological index, named the geometric-arithmetic index. The geometric-arithmetic index of a graph $G$ is denoted by $GA(G)$ and defined as $GA(G) = \sum_{u,v \in E(G)} \frac{2d_G(u)d_G(v)}{d_G(u)+d_G(v)}$.

One of the well-know degree based topological index is the atom-bond connectivity (ABC) index of $G$, proposed by Estrada et al. in [4], and defined as $ABC(G) = \sum_{u,v \in E(G)} \sqrt{d_G(u)+d_G(v)}$. The inverse sum indeg index IS I $(G)$ of a simple graph $G$ is defined [5] in as $IS I (G) = \sum_{u,v \in E(G)} \frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)}$. The symmetric division deg index of a connected graph $G$, (S DD) is defined in [7] as $S DD \ (G) = \sum_{u,v \in E(G)} \frac{d_G(u)^2+d_G(v)^2}{d_G(u)d_G(v)}$. The harmonic polynomial is defined in [9] as $H \ (G, x) = \sum_{u,v \in E(G)} 2x^{d_G(u)+d_G(v)-1}$. Note that $\int_0^1 H(G, x)dx = H(G)$.
In this paper, we obtain the exact formulae for some topological indices such as the general sum-connectivity index, atom-bond connectivity index, geometric arithmetic index, inverse sum indeg index, symmetric division deg index and harmonic polynomial of titania TiO$_2$ nanotubes and Sudoku graphs.

II. $n \times n$ SUDOKU GRAPHS

Sudoku is a popular puzzle game. An $n \times n$ sudoku puzzle is a grid of cells partitioned into $n$ smaller block of $n$ element. Sudoku can also be viewed as a bipartite graph. From the structure of $n \times n$ sudoku graph, the edge set can be partitioned into eight sets show in Table 1

**Theorem 2.1.** Consider $G = (SK)_{n \times n}$ is a sudoku graph for $n \geq 2$. Then its general sum connectivity index is $\chi_\alpha (G) = (12)\alpha 8 + (13)\alpha 12+ (13)\alpha 8n + (12)\alpha (4n - 4) + (14)\alpha (32n - 40) + (14)\alpha 4n^2 + (15)\alpha (20n^2 - 36n + 20) + (16)\alpha (10n^2 - 14n + 4)$.

**Proof:** Now we compute the sum connectivity index of $n \times n$ sudoku graph and by the definition of $\chi_\alpha$, we have

$$\chi_\alpha (G) = \sum_{u,v \in E(G)} (d_G(u) + d_G(v))^\alpha$$

$$= (12)\alpha |E_1| + (13)\alpha |E_2| + (12)\alpha |E_3| + (14)\alpha |E_4| + (14)\alpha |E_5| + (15)\alpha |E_6| + (16)\alpha |E_7|$$

Hence $\chi_\alpha (G) = (12)\alpha 8 + (13)\alpha 12 + (13)\alpha 8n + (12)\alpha (4n - 4) + (14)\alpha (32n - 40)$

$$+ (14)\alpha 4n^2 + (15)\alpha (20n^2 - 36n + 20) + (16)\alpha (10n^2 - 14n + 4)$$

<table>
<thead>
<tr>
<th>$(d_G(u), d_G(v))$ where $uv \in E(G)$</th>
<th>Number of edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(5, 7)$</td>
<td>8</td>
</tr>
<tr>
<td>$(5, 8)$</td>
<td>12</td>
</tr>
<tr>
<td>$(6, 6)$</td>
<td>$4n - 4$</td>
</tr>
<tr>
<td>$(6, 7)$</td>
<td>$8n$</td>
</tr>
<tr>
<td>$(6, 8)$</td>
<td>$32n - 40$</td>
</tr>
<tr>
<td>$(7, 7)$</td>
<td>$4n^2$</td>
</tr>
<tr>
<td>$(7, 8)$</td>
<td>$20n^2 - 36n + 20$</td>
</tr>
<tr>
<td>$(8, 8)$</td>
<td>$10n^2 - 14n + 4$</td>
</tr>
</tbody>
</table>

Table 1. Edge partition of sudoku $(SK)_{1 \times 1}$ based on degrees of end vertices of each edge.

**Theorem 2.2.** Using the above theorem, we obtain the following result Let $G = (SK)_{n \times n}$ sudoku graph for $n \geq 2$, Then

$$\chi_\alpha (G) = \begin{cases} 
4(129n^2 - 41n + 2), & \text{if } \alpha = 1; \\
\frac{3055n^2 - 362n + 6380}{1560}, & \text{if } \alpha = -1; \\
1385n^2 - 87n + 72, & \text{if } \alpha = 2; \\
\frac{2n + 2}{\sqrt{3}} + \frac{12 + 8n}{\sqrt{13}} + \frac{20n^2 - 36n + 20}{\sqrt{15}} + \frac{5n^2 - 7n + 2}{\sqrt{2}}, & \text{if } \alpha = -\frac{1}{2}; 
\end{cases}$$

**Proof:** Putting $\alpha = 1$ in Theorem 2.1, we get

$$\chi (G) = (12)\alpha 8 + (13)\alpha 12 + (13)\alpha 8n + (12)\alpha (4n - 4) + (14)\alpha (32n - 40) + (14)\alpha 4n^2 + (15)\alpha (20n^2 - 36n + 20) + (16)\alpha (10n^2 - 14n + 4)$$

Putting $\alpha = -1$ in Theorem 2.1, we get

$$\chi_{-1} (G) = (12)^{-1} 8 + (13)^{-1} 12 + (13)^{-1} 8n + (12)^{-1} (4n - 4) + (14)^{-1} (32n - 40) + (14)^{-1} 4n^2 + (15)^{-1} (20n^2 - 36n + 20) + (16)^{-1} (10n^2 - 14n + 4)$$

Putting $\alpha = 2$ in Theorem 2.1, we get

$$\chi_2 (G) = (12)^2 8 + (13)^2 12 + (13)^2 8n + (12)^2 (4n - 4)$$
Putting $\alpha = -\frac{1}{2}$ in Theorem 2.1, we get

$$\chi(G) = (12)^{-\frac{1}{2}} 8 + (13)^{-\frac{1}{2}} 12 + (13)^{-\frac{1}{2}} 8n + (12)^{-\frac{1}{2}} (4n-4) + (14)^{-\frac{1}{2}} (32n-40)$$

$$+ (14)^{-\frac{1}{2}} 4n^2 + (15)^{-\frac{1}{2}} (20n^2 - 36n + 20) + (16)^{-\frac{1}{2}} (10n^2 - 14n + 4)$$

$$= 2n + 2 + \frac{12 + 8n}{\sqrt{3}} + \frac{2(20n^2 - 36n + 20)}{\sqrt{15}} + \frac{5n^2 - 7n + 2}{\sqrt{2}}. \blacksquare$$

**Theorem 2.3.** Let $G = ((SK)n \times n)$ then the $SD$ $D(G)$ index and $IS$ $I(G)$ index are

(i) $SD$ $D(G) = \frac{845}{14} n^2 - \frac{7777}{294} n - \frac{2533}{70}$

and (ii) $IS$ $I(G) = \frac{386}{3} n^2 - \frac{1949}{455} n - \frac{40797}{546}$.

**Proof:** By the definition of $SD$ $D(G)$,

$$SDD(G) = \sum_{uv \in E(G)} \frac{d_G(u)^2 + d_G(v)^2}{d_G(u)d_G(v)}$$

From Table 1, $SDD(G) = \frac{74}{35} |E_1| + \frac{89}{40} |E_2| + 2|E_3| + \frac{85}{42} |E_4| + \frac{25}{12} |E_5| + 2|E_6| + 1\frac{13}{56} |E_7| + 2|E_8|$

$$= \frac{5}{2} 2^{r+2} + 2 \times 2^{r+1} (r - 2)$$

$$SDD(G) = \frac{845}{14} n^2 - \frac{7777}{294} n - \frac{2533}{70}.$$ By the definition of $IS$ $I(G)$,

$$IS(G) = \sum_{uv \in E(G)} \frac{d_G(u)d_G(v)}{d_G(u) + d_G(v)}$$

From Table 1, $IS(G) = \frac{35}{12} |E_1| + \frac{40}{13} |E_2| + 3|E_3| + \frac{42}{13} |E_4| + \frac{24}{7} |E_5| + \frac{49}{14} |E_6| + \frac{56}{15} |E_7| + 4|E_8|

$$= \frac{35}{12} 8 + \frac{40}{13} 12 + 3(4n - 4) + \frac{42}{13} 8n + \frac{24}{7} (32n - 40)$$

$$+ 4|E_2| + \frac{56}{15} (20n^2 - 36n + 20) + 4(10n^2 - 14n + 4)$$

$$IS(G) = \frac{386}{3} n^2 - \frac{1949}{455} n - \frac{40797}{546}. \blacksquare$$

**Theorem 2.4.** The Harmonic polynomial for $(SK)_{n \times n}$ is given by, $H(G, x) = 2^x x^1(4 + 6x + 4(n-1)) + 2nx + 4x^2(4n - 5) + 2n^2 x^2 + 2x^3(5n^2 - 9n + 5) + 2x^4(5n^2 - 7n + 2)$.  

**Proof:** By the definition of Harmonic polynomial

$$H(G, x) = \sum_{uv \in E(G)} 2^x d_G(u)^{d_G(v) - 1}$$

$$= 2x^1 |E_1| + 2x^1 2 |E_2| + 2x^1 1 |E_3| + 2x^1 2 |E_4| + 2x^1 1 |E_5| + 2x^1 3 |E_6| + 2x^1 1 |E_6| + 2x^1 4 |E_7| + 2x^1 6 |E_8|$$

$$= 2^2 x^1 (4 + 6x + 4(n-1)) + 2nx + 4x^2(4n - 5) + 2n^2 x^2 + 2x^3(5n^2 - 9n + 5) + 2x^4(5n^2 - 7n + 2). \blacksquare$$

From the structure of 1 X 1 sudoku graph, the edge set can be patitiand into four sets show in Table 2

<table>
<thead>
<tr>
<th>$(d_G(u), d_G(v))$ where $uv \in E(G)$</th>
<th>Number of edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>(5, 7)</td>
<td>16</td>
</tr>
<tr>
<td>(5, 8)</td>
<td>4</td>
</tr>
<tr>
<td>(7, 7)</td>
<td>4</td>
</tr>
<tr>
<td>(7, 8)</td>
<td>4</td>
</tr>
</tbody>
</table>

**Table 2** Edge partition of sudoku $(SK)_{1 \times 1}$ based on degrees of end vertices of each edge.
Now we compute the general sum connectivity index of 1 x 1 sudoku graph.

**Theorem 2.5.** Consider a Sudoku graph $G = (S K)_{1x1}$. Then its general sum connectivity index is $\chi_{\alpha}(G) = (12)^{\alpha}16 + (13)^{\alpha}4 + (14)^{\alpha}4 + (15)^{\alpha}4$.

**Proof:** By the definition of $X_{\alpha}$ and Table 2, we have

$$\chi_{\alpha}(G) = \sum_{\nu, u \in E(G)} (d_G(\nu) + d_G(u))^{\alpha}$$

$$= (12)^{\alpha}|E_1| + (13)^{\alpha}|E_2| + (14)^{\alpha}|E_3| + (15)^{\alpha}|E_4|$$

Hence $\chi_{\alpha}(G) = (12)^{\alpha}16 + (13)^{\alpha}4 + (14)^{\alpha}4 + (15)^{\alpha}4$. $\blacksquare$

**Theorem 2.6.** Using the above theorem, we obtain the following result, consider a Sudoku graph $G = (S K)_{1x1}$, Then

$$\chi_{\alpha}(G) = \begin{cases} 360, & \text{if } \alpha = 1; \\ 1286, & \text{if } \alpha = -1; \\ 4664, & \text{if } \alpha = 2; \\ \frac{8}{\sqrt{2}} + \frac{4}{\sqrt{13}} + \frac{4}{\sqrt{14}} + \frac{4}{\sqrt{15}}, & \text{if } \alpha = -\frac{1}{2}; \end{cases}$$

**Proof:** Putting $\alpha = 1$ in Theorem 2.5, we get

$$\chi(G) = (12)16 + (13)4 + (14)4 + (15)4 = 360.$$  

Putting $\alpha = -1$ in Theorem 2.5, we get

$$\chi(-1)(G) = (12)^{-1}16 + (13)^{-1}4 + (14)^{-1}4 + (15)^{-1}4 = 1286.$$ 

Putting $\alpha = 2$ in Theorem 2.5, we get

$$\chi_2(G) = (12)^216 + (13)^24 + (14)^24 + (15)^24 = 4664.$$ 

Putting $\alpha = -\frac{1}{2}$ in Theorem 2.5, we get

$$\chi(-\frac{1}{2})(G) = (12)^{-\frac{1}{2}}16 + (13)^{-\frac{1}{2}}4 + (14)^{-\frac{1}{2}}4 + (15)^{-\frac{1}{2}}4 = \frac{8}{\sqrt{2}} + \frac{4}{\sqrt{13}} + \frac{4}{\sqrt{14}} + \frac{4}{\sqrt{15}}.$$  

$\blacksquare$

**Theorem 2.7.** For sudoku graph $G = (S K)_{1x1}$ then S DD(G) index and IS I(G) index are (i) $S \text{ DD}(G) = \frac{294}{5}$ and (ii) $I(S) = \frac{51426}{586}$.

**Proof:** by the definition of $S \text{ DD}(G)$ we have

$$S \text{ DD}(G) = \sum_{\nu, u \in E(G)} \frac{d_G(\nu)^2 + d_G(u)^2}{d_G(\nu) + d_G(u)}$$

From Table 2, $S \text{ DD}(G) = \frac{74}{35}|E_1| + \frac{89}{40}|E_2| + 2|E_3| + \frac{113}{56}|E_4|$  

$$S \text{ DD}(G) = \frac{294}{5}. $$

$$I(S) = \sum_{\nu, u \in E(G)} \frac{d_G(\nu)d_G(u)}{d_G(\nu) + d_G(u)}$$

From Table 2,  

$$I(S) = \frac{35}{12}|E_1| + \frac{40}{13}|E_2| + \frac{49}{14}|E_3| + \frac{56}{15}|E_4|$$

$$I(S) = \frac{51426}{586}. $$

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Theorem 2.8. The Harmonic polynomial for $G = (S, K)_{x \times 1}$ is given by $H(G, x) = 2^3x^7(4 + x^8)$.

Proof: By the definition of Harmonic polynomial

$$H(G, x) = \sum_{uv \in E(G)} 2^3x^7(4 + x^8) = 2^3x^7(4 + x^8).$$

III. $\text{TiO}_2$ NANOTUBES

The molecular graph of $\text{TiO}_2[6, n]$ has total $2n + 2$ rows and $mn$ columns. For $\text{TiO}_2$ nanotubes $2 \leq d(v) \leq 5$, for all $v \in V(\text{TiO}_2)$. We denote the partitions of the vertex set of $\text{TiO}_2$ by $V_i(\text{TiO}_2)$, where $v \in V(\text{TiO}_2)$ if $d(v) = i$. Thus we have the following partitions of the vertex set.

<table>
<thead>
<tr>
<th>Vertex Partition</th>
<th>$V_2$</th>
<th>$V_3$</th>
<th>$V_4$</th>
<th>$V_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cardinality</td>
<td>$2mn + 4n$</td>
<td>$2mn$</td>
<td>$2n$</td>
<td>$2mn$</td>
</tr>
</tbody>
</table>

Table 3. The vertex partition of $\text{TiO}_2$ nanotubes

where, $V_2(\text{TiO}_2) = \{v \in V(\text{TiO}_2) : d(u) = 2\}$, $V_3(\text{TiO}_2) = \{v \in V(\text{TiO}_2) : d(u) = 3\}$, $V_4(\text{TiO}_2) = \{v \in V(\text{TiO}_2) : d(u) = 4\}$, and $V_5(\text{TiO}_2) = \{v \in V(\text{TiO}_2) : d(u) = 5\}$.

The direct calculation we get, $|V_2(\text{TiO}_2)| = 2mn + 4n$, $|V_3(\text{TiO}_2)| = 2mn$, $|V_4(\text{TiO}_2)| = 2n$, and $|V_5(\text{TiO}_2)| = 2mn$. The partitions of the vertex set of $\text{TiO}_2$ nanotubes is given in Table 3.

Again the edge set of $\text{TiO}_2$ is divided into three edge partitions based on the sum of degrees of the end vertices and denote it by $E_j(\text{TiO}_2)$ so that if $e = uv \in E_j(\text{TiO}_2)$ then $d(u) + d(v) = j$ for $\delta(G) \leq j \leq \Delta(G)$. Thus we write,

$$E(\text{TiO}_2) = \bigcup_{j=\delta}^{\Delta} E_j(\text{TiO}_2),$$

where $E_j = \{e = uv \in E(\text{TiO}_2) : d(u) = 2d(v) = j\}$ and $E_j = \{e = uv \in E(\text{TiO}_2) : d(u) = 3d(v) = j\}$.

$E_6(\text{TiO}_2) = \{e = uv \in E(\text{TiO}_2) : d(u) = 2d(v) = 4\}$ and $E_7 = \{e = uv \in E(\text{TiO}_2) : d(u) = 3d(v) = 4\}$. From direct calculation, we get $|E_6(\text{TiO}_2)| = 6n$, $|E_7| = 4mn + 4n$, $|E_8(\text{TiO}_2)| = 2mn$, and $|E_9(\text{TiO}_2)| = 6mn - 2n$.

Similarly, the edge set of $\text{TiO}_2$ is also divided into four edge partitions based on the product of degrees of the end vertices and denote it by $E_j(\text{TiO}_2)$ so that if $d(u)d(v) = k$ for $\delta(G)^2 \leq k \leq \Delta(G)^2$. Thus we have the following partitions of the edge set.

$E_8(\text{TiO}_2) = \{e = uv \in E(\text{TiO}_2) : d(u) = 2d(v) = 4\}$, $E_9(\text{TiO}_2) = \{e = uv \in E(\text{TiO}_2) : d(u) = 2d(v) = 5\}$, $E_{10}(\text{TiO}_2) = \{e = uv \in E(\text{TiO}_2) : d(u) = 3d(v) = 4\}$ and $E_{11}(\text{TiO}_2) = \{e = uv \in E(\text{TiO}_2) : d(u) = 3d(v) = 5\}$.

Table 4. The edge partition of $\text{TiO}_2$ nanotubes

From the structure of $\text{TiO}_2$ nanotubes, we get $|E_8(\text{TiO}_2)| = 6n$, $|E_9(\text{TiO}_2)| = 4mn + 2n$, $|E_{10}(\text{TiO}_2)| = 2mn$, and $|E_{11}(\text{TiO}_2)| = 6mn - 2n$. Clearly, $E_7 = E_8 \cup E_9, E_6 = E_8 \cup E_9, E_6 = E_8 \cup E_9$. The partitions of the edge set of $\text{TiO}_2$ nanotubes is given in Table 4. In the following we calculate the general sum-connectivity index, atom-bond connectivity index, geometric arithmetic index, inverse sum indeg index, symmetric division deg index and harmonic polynomial $\text{TiO}_2[6, n]$ nanotube as defined in the previous section.

Theorem 3.1. General sum connectivity index of $\text{TiO}_2$ is given by $X_{sc}(G) = (6)^7 6n + (7)^n (4mn + 12n) + (7)^8 2n + (8)^9 6mn - 2n$.

Proof. Now we compute the sum connectivity index of $\text{TiO}_2$ and by the definition of $X_{sc}$ we have

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\[
\chi_a(G) = \sum_{v, u \in E(G)} (d_G(u) + d_G(v))^{\alpha} \\
= (6)^{\alpha} E_0^v + (7)^{\alpha} E_1^v + (8)^{\alpha} E_2^v + (8)^{\alpha} E_3^v \\
Hence \chi_a(G) = (6)^{\alpha} 6n + (7)^{\alpha} (4mn + 12n) + (7)^{\alpha} 2n + (8)^{\alpha} 6mn - 2n.
\]

**Theorem 3.2.** Using the above theorem, we obtain the following result, consider \( G = \text{TiO}_2 \), then

\[
\chi_a(G) = \begin{cases} 
4(19mn + 12n) & \text{if } \alpha = 1; \\
37mn - 37n & \text{if } \alpha = -1; \\
28 & \text{if } \alpha = 2; \\
6n + 4mn + 4n & \frac{3mn - n}{\sqrt{2}} & \text{if } \alpha = -\frac{1}{2}; 
\end{cases}
\]

**Proof:** Putting \( \alpha = 1 \) in Theorem 2.9, we get

\[
\chi(G) = (6)^{\alpha} 6n + (7)^{\alpha} (4mn + 12n) + (7)^{\alpha} 2n + (8)^{\alpha} 6mn - 2n \\
= 4(19mn + 12n).
\]

Putting \( \alpha = -1 \) in Theorem 2.9, we get

\[
\chi_{-1}(G) = (6)^{-1} 6n + (7)^{-1} (4mn + 12n) + (7)^{-1} 2n + (8)^{-1} 6mn - 2n \\
= \frac{37mn - 37n}{28}.
\]

Putting \( \alpha = 2 \) in Theorem 2.9, we get

\[
\chi_2(G) = (6)^{\alpha} 6n + (7)^{\alpha} (4mn + 12n) + (7)^{\alpha} 2n + (8)^{\alpha} 6mn - 2n \\
= 580mn + 284n.
\]

Putting \( \alpha = -\frac{1}{2} \) in Theorem 2.9, we get

\[
\chi_{-\frac{1}{2}}(G) = (6)^{-\frac{1}{2}} 6n + (7)^{-\frac{1}{2}} (4mn + 12n) + (7)^{-\frac{1}{2}} 2n + (8)^{-\frac{1}{2}} 6mn - 2n \\
= \frac{6n}{\sqrt{6}} + \frac{4mn + 4n}{\sqrt{7}} + \frac{3mn - n}{\sqrt{2}}.
\]

**Theorem 3.3.** For \( G = \text{TiO}_2 \), we have

(i) \( ABC(G) = \frac{8n + 4mn}{\sqrt{2}} + \frac{5n}{\sqrt{3}} + \frac{6mn - 2n}{\sqrt{5}}. \)

(ii) \( GA(G) = 4n\sqrt{7} + \frac{2}{7} \sqrt{10(4mn + 2n)} + \sqrt{12(2n)} + \frac{\sqrt{15}}{2} 3mn - n. \)

(iii) \( SDD(G) = \frac{756mn + 613n}{30}. \)

(iv) \( ISI(G) = \frac{475mn + 295n}{28}. \)

**Proof.** By the definition of atom-bond connectivity index,

\[
ABC(G) = \sum_{u \in V(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}} \\
= \sum_{u \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}} + \sum_{u \in E_G} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}} \\
+ \sum_{u \in E_2(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}} + \sum_{u \in E_3(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}} \\
= \frac{8n + 4mn}{\sqrt{2}} + \frac{5n}{\sqrt{3}} + \frac{6mn - 2n}{\sqrt{5}}.
\]
By the definition of Geometric Arithmetic index,

\[ GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)} \]

\[ = \sum_{uv \in E_6} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)} + \sum_{uv \in E_0} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)} + \sum_{uv \in E_5} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)} \]

\[ = 4n\sqrt{2} + \frac{2}{7}(\sqrt{10}(4mn + 2n) + \sqrt{122}n + \frac{\sqrt{15}}{2}3mn - n). \]

Similarly we can prove (iii) and (vi). \[\Box\]

**Theorem 3.4.** The Harmonic polynomial for \( G = TiO_2 \) is given by \( H(G, x) = 2^2x^5(3n + x(2mn + n) + xn + x^2(3mn - n)). \)

**Proof:** By the definition of Harmonic polynomial

\[ H(G, x) = \sum_{uv \in E(G)} 2x^{d_G(u)+d_G(v)-1} \]

\[ = 2x^3|E_6^*| + 2x^6|E_{10}^*| + 2x^6|E_{12}^*| + 2x^7|E_{15}^*| \]

\[ = 2^2x^5(3n + x(2mn + n) + xn + x^2(3mn - n)). \] \[\Box\]

**Table 4**

<table>
<thead>
<tr>
<th>Edge Partition</th>
<th>( E_6 )</th>
<th>( E_7 )</th>
<th>( E_8 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cardinality</td>
<td>6n</td>
<td>4mn + 4n</td>
<td>6mn - 2n</td>
</tr>
</tbody>
</table>

**Theorem 3.5.** For \( G = TiO_2 \), we have

(i) \( ABC(G) = \frac{2(5n + 2mn)}{\sqrt{2}} + \frac{56mn - 2n}{\sqrt{2}} \).

(ii) \( GA(G) = \frac{2\sqrt{2}}{3} + \frac{8\sqrt{10}}{7}(\sqrt{10}(mn + n) + \frac{\sqrt{15}}{2}2n + \frac{\sqrt{15}}{2}3mn - n). \)

(iii) \( SDD(G) = \frac{276mn + 365n}{15} \).

(iv) \( ISI(G) = \frac{475mn + 279n}{28} \).

**Proof:** By the definition of atom-bond connectivity index,

\[ ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}} \]

\[ = \sum_{uv \in E_6} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}} + \sum_{uv \in E_0} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}} + \sum_{uv \in E_5} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u)d_G(v)}} \]

\[ = \frac{2(5n + 2mn)}{\sqrt{2}} + \frac{56mn - 2n}{\sqrt{2}}. \]

By the definition of Geometric Arithmetic index,

\[ GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)} \]

\[ = \sum_{uv \in E_6} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)} + \sum_{uv \in E_0} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)} + \sum_{uv \in E_5} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u) + d_G(v)} \]

\[ = \frac{2\sqrt{2}}{3} + \frac{8\sqrt{10}}{7}(\sqrt{10}(mn + n) + \frac{\sqrt{15}}{2}2n + \frac{\sqrt{15}}{2}3mn - n). \] \[\Box\]
Similarly we can prove (iii) and (vi).

**Theorem 3.6.** The Harmonic polynomial for $G = \text{TiO}_2$ is given by $H(G, x) = 2^3 x^5 (3n + 2x(mn + n) + x^2 (3mn - n))$.  

**Proof:** By the definition of Harmonic polynomial

$$H(G, x) = \sum_{uv \in E(G)} 2x^{d(u) + d(v) - 1}$$

$$= 2x^5 |E_6| + 2x^6 |E_7| + 2x^7 |E_8|$$

$$= 2^2 x^5 (3n + 2x(mn + n) + x^2 (3mn - n)).$$  

IV. CONCLUSION

The study of the degree based topological indices for important classes of graphs is an essential problem in Chemical graph theory. In this view, we obtain the same topological indices of Titania $\text{TiO}_2$ Nanotubes and Sudoku graphs.

REFERENCES


