Research Article

Structural Analysis and Topological Characterization of Sudoku Nanosheet

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The physical and biological properties of chemical compounds are modelled using chemical graph theory. The geometric structure of chemical compounds can be modelled using a variety of topological indices derived from graph theory. The chemical structures, physicochemical characteristics, and biological activities are predicted by the topological indices using the real numbers derived from the molecular compound. The topological index’s first use was to identify the physical characteristics of alkenes. A topological index is a molecular structure descriptor calculated from a chemical compound’s molecular graph describing its topology. When applied to a chemical compound’s molecular structure, it tells the theoretical properties. The chemical structure is studied as a graph, where elements are denoted as vertices, and chemical bonds are called edges. In this study, we have computed some novel topological indices named as modified neighborhood version of the forgettrend topological index $F_N^*$, the neighborhood version of the first multiplicative Zagreb $M_1^*$, the neighborhood version of the second Zagreb index $M_2^*$, the neighborhood version of hyper-Zagreb index $HM_N$, the Sambor topological index $SO(G)$, and the Sambor reduced topological index $SO_{red}(G)$ for the Sudoku nanosheet and derived formulas for them. Based on the derived formulas, the numerical results of the understudy nanosheet’s physical and chemical properties are investigated. Our computed results are undoubtedly helpful in understanding the topology of the understudy nanosheet. These computed indices have the best correlation with acentric factor and entropy; therefore, they are effective in QSRRs and QSARs analysis with complete accuracy.

1. Introduction

The subject of intense research is the famous 2-dimensional nano-material graphene, the world’s [1–3] lightest 2D material with a hexagonal grid. Since their inventions, carbon nanotubes have gained a lot of attention [4, 5]. Carbon nanotubes (CNTs) are made of carbon using nanometer diameters. The one-wall carbon nanotubes are a bore in the variety of nanometers by Iijima and Ichihashi [4], and Bethune et al. [5] independently. The thickness of the 2D nanostructure varies from 1 to 100 nm [6]. These 2D nanosheets have interesting physical, electronic, biological, and chemical properties that are essential for various applications. Therefore, it is critical to predicting these nanostructures to attain discrimination and bring about the network topology, meliorate, and their physical characteristics. Chemical graph theory is used to represent better and characterise molecules to understand chemical compounds’ physical properties [7]. Graphs are mathematical structures that are used to model relationships. A Chemical graph is a basic calculable graph with atoms at the edge in an implicit system. In [8], Randić gives the concept of finding a suitable path to reach the desire vertex.

A TI describes a lot of prominent properties of some chemical compounds. These are essential in biological and chemical science and engineering. Physicochemical characteristics or theoretical molecular descriptors are used as forecasters in QSAR modelling [9–11], whilst the expression QSRR models as replication variables [12–15]. Wiener [16] introduced the TI concept while functioning on paraffin’s boiling point and set it as
a path number. From both a practical and theoretical standpoint, it is the first and maximum considered TI. It is described as the total distance of the distances between all pairs of vertices in graph $G$, with more information available in ref [17]. Degree-based TI is often used in chemical network graph theory, mainly in chemistry. Gutman et al. established the premature topological indices and the Zagreb indices [18–21], which have been used to investigate in molecular difficulty, boiling point, and chirality.

The discipline of graph theory is rapidly expanding and performing a vital function, cheminformatics, the investigation of various chemical formations and their physiochemical qualities that combine chemistry and mathematics, and information on technology. For example, Chemical network graph theory is the subsection of mathematics that deals with chemistry that uses the help of mathematicsthatdealswithchemistrythatusesthehelpofinformationontechnology. For example, Chemical network graph theory is the subsection of mathematics, and information on technology. For example, Chemical network graph theory is the subsection of mathematics, and information on technology. For example, Chemical network graph theory is the subsection of mathematics, and information on technology.

Let $M_1^r (G) = \sum_{mn \in E(G)} [\alpha_G (m) + \alpha_G (n)]$. (4)

Let $M_2^r$ denote the second Zagreb index, which is defined in [29] as follows:

$$M_2^r (G) = \sum_{mn \in E(G)} \alpha_G (m) \times \alpha_G (n).$$

The neighborhood form of the hyper-Zagreb index is expressed by $HM_N$, moreover, represented as follows [30]:

$$HM_N (G) = \sum_{mn \in E(G)} [\alpha_G (m) + \alpha_G (n)]^2.$$

The Sambor index $SO(G)$ and reduced Sambor index $SO_{red}(G)$ are introduced by Gutman in [31], which are defined as follows:

$$SO(G) = \sum_{mn \in E(G)} \sqrt{\alpha_G (m)^2 + \alpha_G (n)^2},$$

$$SO_{red}(G) = \sum_{mn \in E(G)} \sqrt{[(a_m - 1)^2 + (a_n - 1)^2]}.$$

Let $AI$ denote the Argumanted Zagreb topological index, which is defined by [32] as follows:

$$AI(G) = \sum_{mn \in E(G)} \left( \frac{\alpha_G (m) \times \alpha_G (n)}{\alpha_G (m) + \alpha_G (n) - 2} \right).$$

For a few essentials values $n \geq 2$, the Sudoku nanosheet $(SK_{n\times n})$ is a graphical description of the Sudoku puzzle in the form of a $n \times n$ grid chording of $n^2$ cells, where every single cell is a precise graph of nodes with four vertices of degree 5, 4 vertices of degree 7, and 1 vertex of degree 8. Besides, Sudoku graphs $[V(SK_{n\times n})] = 9n^2$, belong to the number of vertices and $|E(SK_{n\times n})| = n(34n - 6)$ are the number of edges, accordingly. For $n = 3$, the Sudoku nanosheet $SK_{3\times3}$ is demonstrated in Figure 1. In Table 1, we ciphered the consequence for the linked number-based partition of edges for $n \geq 3$ of the Sudoku graph $SK_{n\times n}$.

1.1. Main Results on Sudoku Nanosheet $SK_{(r\times r)}$

**Theorem 1.** Assume that $G$ denotes the Sudoku nanosheet, then the Modified neighborhood version of forgotten topological index of $G$ is

$$F_N^r (G) = 392r^4 + 3540r^3 + 1852r + 144.$$

**Proof.** By definition of $F_N^r (G)$ and Table 1, we have
Figure 1: The Sudoku nanosheet SK

Table 1: Edge partition of Sudoku nanosheet SK

<table>
<thead>
<tr>
<th>αᵣ</th>
<th>Edge partition</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>α₁</td>
<td>α₁(5,7)</td>
<td>8</td>
</tr>
<tr>
<td>α₂</td>
<td>α₅(5,8)</td>
<td>12</td>
</tr>
<tr>
<td>α₃</td>
<td>α₆(6,6)</td>
<td>4r - 4</td>
</tr>
<tr>
<td>α₄</td>
<td>α₄(4,7)</td>
<td>8r</td>
</tr>
<tr>
<td>α₅</td>
<td>α₆(6,8)</td>
<td>32r - 40</td>
</tr>
<tr>
<td>α₆</td>
<td>α₇(7,7)</td>
<td>4r²</td>
</tr>
<tr>
<td>α₇</td>
<td>α₇(7,8)</td>
<td>20r² - 36r + 20</td>
</tr>
<tr>
<td>α₈</td>
<td>α₈(8,8)</td>
<td>10r² - 14r + 4</td>
</tr>
</tbody>
</table>

\[
F_N^*(G) = \sum_{mn \in E(G)} [\alpha_G(m)² + \alpha_G(n)²] \\
= |α_{(5,7)}|(25 + 49) + |α_{(5,8)}|(25 + 64) + |α_{(6,6)}|(36 + 36) + |α_{(4,7)}|(16 + 49) + |α_{(6,8)}|(36 + 64) \\
+ |α_{(7,7)}|(49 + 49) + |α_{(7,8)}|(49 + 64) + |α_{(8,8)}|(64 + 64) \\
= (8)(74) + (12)(89) + (4r - 4)(72) + (8r)(65) + (32r - 40)(100) + 4r²(98) \\
+ (20r² - 36r + 20)(113) + 10r² - 14r + 4(128) \\
= 392r^4 + 3540r^3 + 1852r + 144.
\]

Theorem 2. Assume that G denotes the Sudoku nanosheet, then the Neighborhood version of first multiplicative Zagreb index is \( M₁^*(G) = 56r^4 + 460r^3 - 180r + 8 \)

Proof. By using the definition of \( M₁^* \) and Table 1, we can write as follows:

\[
M₁^*(G) = \sum_{mn \in E(G)} [\alpha_G(m) + \alpha_G(n)] \\
= \sum_{mn \in E(5,7)} [\alpha_G(u) + \alpha_G(v)] + \sum_{mn \in E(5,8)} [\alpha_G(u) + \alpha_G(v)] \\
+ \sum_{mn \in E(6,6)} [\alpha_G(u) + \alpha_G(v)] + \sum_{mn \in E(4,7)} [\alpha_G(u) + \alpha_G(v)] \\
+ \sum_{mn \in E(6,8)} [\alpha_G(u) + \alpha_G(v)] + \sum_{mn \in E(7,7)} [\alpha_G(u) + \alpha_G(v)] \\
+ \sum_{mn \in E(7,8)} [\alpha_G(u) + \alpha_G(v)] + \sum_{mn \in E(8,8)} [\alpha_G(u) + \alpha_G(v)]
\]
\[ M_1^*(G) = \sum_{mn \in E(G)} [a_G(m) \times a_G(n)] = \sum_{mn \in E(\{5,7\})} [a_G(m) \times a_G(n)] + \sum_{mn \in E(\{6,8\})} [a_G(m) \times a_G(n)] \]

\[ = 12(8) + 13(12) + 12(4r - 4) + 11(8r) + 14(32r - 40) + 14(4r^4) \]

\[ + 15(20r^2 - 36r + 20) + 16(10r^2 - 14r + 4) \]

\[ M_1^*(G) = 56r^4 + 460r^2 - 180r + 8. \]

**Theorem 3.** Assume that \( G \) denotes the Sudoku nanosheet, then the Neighborhood version of second Zagreb index is \( M_2^*(G) = 196r^4 + 1760r^2 - 1008r + 72 \)

**Proof.** According to the definition of \( M_2^* \) and Table 1, we can write as follows:

\[ M_2^*(G) = \sum_{mn \in E(G)} [a_G(m) \times a_G(n)] = \sum_{mn \in E(\{5,7\})} [a_G(m) \times a_G(n)] + \sum_{mn \in E(\{6,8\})} [a_G(m) \times a_G(n)] \]

\[ = 12(8) + 13(12) + 12(4r - 4) + 11(8r) + 14(32r - 40) + 14(4r^4) \]

\[ + 15(20r^2 - 36r + 20) + 16(10r^2 - 14r + 4) \]

\[ M_2^*(G) = 196r^4 + 1760r^2 - 1008r + 72. \]

**Theorem 4.** Assume that \( G \) denotes the Sudoku nanosheet, then the Neighborhood version of hyper-Zagreb index is \( HM_N(G) = 784r^4 + 7060r^2 - 3868r + 288. \)

**Proof.** According to the definition of \( HM_N \) and Table 1, we can write as follows:

\[ HM_N(G) = \sum_{mn \in E(G)} [a_G(m) + a_G(n)]^2 = \sum_{mn \in E(\{5,7\})} [a_G(m) + a_G(n)]^2 + \sum_{mn \in E(\{6,8\})} [a_G(m) + a_G(n)]^2 \]

\[ + \sum_{mn \in E(\{6,8\})} [a_G(m) + a_G(n)]^2 + \sum_{mn \in E(\{7,8\})} [a_G(m) + a_G(n)]^2 \]

\[ + \sum_{mn \in E(\{7,8\})} [a_G(m) + a_G(n)]^2 + \sum_{mn \in E(\{8,9\})} [a_G(m) + a_G(n)]^2. \]

\[ HM_N(G) = 784r^4 + 7060r^2 - 3868r + 288. \]
Theorem 5. Assume that $G$ denotes the Sudoku nanosheet, then the sambor index is

$$ S_0(G) = 39.59r^4 + 325.73r^2 - 122.631r + 5.919. \quad (14) $$

Proof. According to the definition of $S_0(G)$ and Table 1, we have

$$ S_0(G) = \sum_{m,n \in V(G)} \sqrt{\alpha_G(m)^2 + \alpha_G(n)^2} $$

$$ = \sqrt{25 + 49 \ (8) + \sqrt{25 + 64 \ (12) + \sqrt{36 + 36 \ (4r - 4) + \sqrt{16 + 49 \ (8r)}}} + \sqrt{36 + 64 \ (32r - 40) + \sqrt{49 + 49 \ (4r^4) + \sqrt{49 + 49 \ (20r^2 - 36r + 20) + \sqrt{64 + 64 \ (10r^2 - 14r + 4)}}}} \quad (15) $$

$$ = \sqrt{74 \ (8) + \sqrt{89 \ (12) + 6 \sqrt{2 \ (4r - 4) + \sqrt{65 \ (8r) + (10) (32r - 40) + 7 \sqrt{2 \ (4r^4)}}} + \sqrt{113 \ (20r^2 - 36r + 20) + 8 \sqrt{2} \ (10r^2 - 14r + 4)}} $$

$$ S_0(G) = 39.59r^4 + 325.73r^2 - 122.631r + 5.919. $$

Theorem 6. Assume that $G$ denotes the Sudoku nanosheet, then the reduced sambor index is $S_{0 \text{ red}}(G) = 33.941r^4 + 218.331r^2 - 113.275r + 6.049.$

Proof. Through analysis of the definition of $S_{0 \text{ red}}(G)$ as well as Table 1, we can write as follows:

$$ S_{0 \text{ red}}(G) = \sum_{m,n \in V(G)} \sqrt{\left(\alpha_m - 1\right)^2 + \left(\alpha_n - 1\right)^2} $$

$$ + \sqrt{16 + 36 \ (8) + \sqrt{16 + 49 \ (12) + \sqrt{25 + 25 \ (4r - 4) + \sqrt{9 + 36 \ (8r)}}} + \sqrt{25 + 49 \ (32r - 40) + \sqrt{36 + 36 \ (4r^4) + \sqrt{36 + 49 \ (20r^2 - 36r + 20) + \sqrt{49 + 49 \ (10r^2 - 14r + 4)}}}} \quad (16) $$

$$ = \sqrt{52 \ (8) + \sqrt{65 \ (12) + 50 \ (4r - 4) + \sqrt{45 \ (8r) + \sqrt{74 \ (32r - 40) + \sqrt{72 \ (4r^4)}}} + \sqrt{85 \ (20r^2 - 36r + 20) + \sqrt{98 \ (10r^2 - 14r + 4)}} $$

$$ = 33.941r^4 + 218.331r^2 - 113.275r + 6.049. $$

Theorem 7. Assume that $G$ denotes the Sudoku nanosheet, then the Argumented Zagreb Index is $AZI(G) = 272.33r^4 + 2553.6r^2 - 1738.966r + 153.955.$

Proof. Through analysis of the definition of $AZI(G)$ as well as Table 1, we have

$$ \left(\frac{5 \times 7}{5 + 7 - 2}\right)^3 \ (8) + \left(\frac{5 \times 8}{5 + 8 - 2}\right)^3 \ (12) + \left(\frac{6 \times 6}{6 + 6 - 2}\right)^3 \ (4r - 4) + \left(\frac{4 \times 7}{4 + 7 - 2}\right)^3 \ (8r) + \left(\frac{6 \times 8}{6 + 8 - 2}\right)^3 $$

$$ = (32r - 40) + \left(\frac{7 \times 7}{7 + 7 - 2}\right)^3 \ (4r^4) + \left(\frac{7 \times 8}{7 + 8 - 2}\right)^3 \ (20r^2 - 36r + 20) + \left(\frac{8 \times 8}{8 + 8 - 2}\right)^3 \ (10r^2 - 14r + 4) \quad (17) $$

$$ = 343 + 576.979 + 186.624r - 186.624 + 240.89r + 2048r - 2560 + 272.33r^4 $$

$$ + 1598.6r^2 - 2877.48 + 1598.6 + 955r^2 - 1337r + 382 $$

$$ = 272.33r^4 + 2553.6r^2 - 1738.966r + 153.955. $$

2. Comparison and Concluding Remarks

This study ciphered a few novel topological indices for $SK_{(8x8)}$ and their formulas. The knowing topological indices are the modified neighborhood version of Forgotten topological index $F_N^*$, the neighborhood version of the first multiplicative Zagreb $M_1^*$, the neighborhood version of the second Zagreb index $M_2^*$, the neighborhood version of
Our ciphered consequence is really beneficial in the apprehension of the topology and ameliorates the material characteristics of reserve SK_{r×r}. As previously stated, the beyond-ciphered indices F^*_N, M^*_1, M^*_2, HM_N, SO and SO_{red} have the best tie-up with entropy and acentric factor; therefore, the particular dynamic in QSAR and QSPR anatomy with robust precision. Their ability to distinguish between isomer momentous as opposed to other degree-based indices is extraneous. Meanwhile, Table 2 and Figures 2–8 indicate that all the considered indices also increase when we increase. This implies that there is a direct proportion between r the considered indices. In Figure 9, we

![Table 2: Numerical table corresponding with the structure of the Sudoku graph.](image)

<table>
<thead>
<tr>
<th>r</th>
<th>$F^*_N(G)$</th>
<th>$M^*_1(G)$</th>
<th>$M^*_2(G)$</th>
<th>HM_N(G)</th>
<th>SO(G)</th>
<th>SO_{red}(G)</th>
<th>AZI(G)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[1]</td>
<td>2134</td>
<td>344</td>
<td>1020</td>
<td>4264</td>
<td>248.608</td>
<td>145.046</td>
<td>1240.919</td>
</tr>
<tr>
<td>[2]</td>
<td>16872</td>
<td>2384</td>
<td>8232</td>
<td>33336</td>
<td>1697.017</td>
<td>1195.879</td>
<td>11247.703</td>
</tr>
<tr>
<td>[6]</td>
<td>624504</td>
<td>88064</td>
<td>311400</td>
<td>1247304</td>
<td>62305.053</td>
<td>51173.851</td>
<td>434589.43</td>
</tr>
<tr>
<td>[7]</td>
<td>1101832</td>
<td>155744</td>
<td>549852</td>
<td>2201536</td>
<td>110163.862</td>
<td>91403.684</td>
<td>766971.923</td>
</tr>
<tr>
<td>[8]</td>
<td>1817520</td>
<td>257384</td>
<td>907464</td>
<td>3632448</td>
<td>182032.231</td>
<td>152095.369</td>
<td>1265136.307</td>
</tr>
<tr>
<td>[9]</td>
<td>2842128</td>
<td>403064</td>
<td>1419516</td>
<td>5681160</td>
<td>285036.36</td>
<td>239358.286</td>
<td>1978101.991</td>
</tr>
<tr>
<td>[10]</td>
<td>4255624</td>
<td>604208</td>
<td>2125992</td>
<td>8507608</td>
<td>427252.609</td>
<td>360116.39</td>
<td>2961424.295</td>
</tr>
</tbody>
</table>

![Figure 2: The correlation of r and FN*.](image)

![Figure 3: The correlation of r and M^*_1.](image)
Figure 4: The correlation of $r$ and $M_2^\ast$.

Figure 5: The correlation of $r$ and $HM_N$.

Figure 6: The correlation of $r$ and $SO(G)$.
Figure 7: The correlation of $r$ and $SO_{red}(G)$.

Figure 8: The correlation of $r$ and AZI.

Figure 9: Correlation of $r$ with obtained indices.
collate all the indices together, reflecting that H_{M} it increases more speedily than other indices. Similarly, S_{O} (G) it increases slower than other indices.

Data Availability

There are no data associated with this article.

Additional Points

There is no code available for this article.

Conflicts of Interest

The authors declare that there are no conflicts of interest.

Authors’ Contributions

All authors have equally contributed to this manuscript in all stages, from conceptualization to the write up of final draft.

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