FULL PAPER

Degree-based topological descriptors of Star of David and Hexagonal Cage networks

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Topological indices are numerical parameters of a graph that characterize its molecular topology. In theoretical chemistry, the numerical parameters which are used to depict the molecular topology of graphs are called topological indices. Several physical and chemical properties like boiling point, entropy, heat-formation and vaporization enthalpy of chemical compounds can be determined through these topological indices. Graph theory has a considerable use in evaluating the relation for various topological indices of some derived graphs. In this paper, we studied the general Randić, first Zagreb, ABC, GA, ABC 4 and GA 5, indices for the Star of David and Hexagonal Cage networks and provided closed formulas of these indices.

KEYWORDS
General Randić index; atom-bond connectivity (ABC) index; geometric-arithmetic (GA) index; Star of David network (SD(n)); Hexagonal Cage network (HXCa(n)).

Introduction

A branch of numerical science, Graph theory, in which we use tools of graph parameters to reveal the compound phenomenon precisely. Graph theory, for instance, when used in the study of Molecular structures, characterizes a field among various disciplines of science known as Molecular topology or chemical graph theory. Chemical graph theory has provided a considerable part of study to chemist through which they can execute graph theory to mathematical demonstrating of chemical marvel. We are usually interested in estimating the structural characters to elaborate in quantitative structure-activity relationships using apparatuses taken from Graph theory. Physico-chemical properties and topological indices such as the Wiener Index, the Szeged Index, the Randić Index, the Zagreb Indices and the ABC Index are used in the QSAR/QSPR analysis to estimate chemical compound bioactivity [33]. A polynomial, a numeric number and a sequence of numbers or a matrix will define a graph. A numeric quantity interrelated with a graph which remains invariant under the graph automorphism and differentiate the topology of graph is called Molecular descriptor. A graph theoretical characteristic which is sustained by an isomorphism is called topological descriptor [11]. There are some major types of topological indices, such as topological indices based on distance, topological indices based on degrees, and associated polynomials and graph indices classified. In chemical graph theory and especially in chemistry, degree-based topological indices are of great significance among these groups, and play a vital role. A topological index \(Top(Q)\) of a graph, in a more detailed way, is a number with the property that isomorphic to \(Q\) for any graph \(H\), \(Top(H)=Top(Q)\). While working on the boiling point of paraffin, the topological index concept...
of topological indices originated from Wiener [33], and this index is Wiener index [8].

1.1. Higher dimension SD(n) Drawing Algorithm for Star of David Network

**Step-1:** Draw David’s Star graph $Q$, which is one and two dimensional, as seen in Figure 1.

**Step-2:** Divide each edge by inserting $2n - 2$ vertices at each edge of $H$ into $2n - 1$ edges.

**Step-3:** Connect all vertices which line all three directions in the same odd number line.

**Step-4:** At each new crossing of the edge, insert a new vertex.

This is going to be an SD(n) Star of David network of dimensions $n$ [29].

![FIGURE 1 Star of David network (SD(1)) and (SD(2))](image1)

**Hexagonal Cage network HXCa(n) drawing algorithm**

**Step-1:** Find two hexagonal $n$-dimensional networks, which denoted as $HX_{1}(n)$ and $HX_{2}(n)$.

**Step-2:** In $HX_{2}(n)$, each $HX_{1}(n)$ boundary vertex is connected to its mirror image vertex by an edge. The graph is called the Hexagonal cage network of two layers, as shown in Figure 2.

In this paper $E(Q)$ is used for the edge of graph and the $V(Q)$ use for the vertex of the graph. $d_r$ is the degree of vertex $r \in V(Q)$ and $S_r = \sum_{r \in N(r)} d_r$ where $N(r) = \{s \in V(Q)|rs \in E(Q)\}$.

The notations used in this article are mainly taken from books [9,15]. The wiener index for a graph $Q$ is written as:

$$W(Q) = \frac{1}{2} \sum_{(r,s)} d(r,s),$$

(1)

The first and oldest topological index based on degree is the Randić index [28] denoted by $R_{\sqrt{2}}(Q)$ and defined as:

$$R_{\sqrt{2}}(Q) = \sum_{r \in E(Q)} \frac{1}{d_r d_s}$$

(2)

The general Randić index $R(Q)$ is the sum of $(d_r d_s)^{\alpha}$ over all edges $e=uv \in E(Q)$ defined as:

$$R_{\alpha}(Q) = \sum_{r \in E(Q)} (d_r d_s)^{\alpha}, \text{ for } \alpha = 1, \frac{1}{2}, -1, -\frac{1}{2}$$

(3)

The Zagreb index denoted by $M_1(Q)$ is very valuable topological index and this index introduced by Ivan Gutman and Trinajstić, defined as:

$$M_1(Q) = \sum_{r \in E(Q)} (d_r + d_s).$$

(4)

The atom-bond connectivity (ABC) index introduced by Estrada et al. in [10] is one of the well-known topological indices based on degrees and defined as:

$$ABC(Q) = \sum_{r \in E(Q)} \sqrt[\alpha]{d_r d_s}$$

(5)

The geometric-arithmetic (GA) index, proposed by Vukičević et al, in [32] is another well-known topological description of connectivity and defined as:

$$GA(Q) = \sum_{r \in E(Q)} \frac{2 \sqrt[\alpha]{d_r d_s}}{d_r + d_s}$$

(6)

If we can find the edge partition of these interconnection networks on the basis of the sum of the degrees of the end vertices of each edge of these graphs, only ABC4 and GA5 indices can be computed. Ghorbani et al. [13] were also introduced the fourth version of the ABC index and defined as:
The 5th edition of the GA index was recently introduced by Graovac et al. [14] and mathematically it can be written as:

$$GA_{5}(Q) = \sum_{v \in V(G)} \frac{\sqrt{s_{v} + s_{w}}}{s_{v} + s_{w}}$$  \hspace{1cm} (8)

Main results

In this research paper, we compute the general Randić, ABC, first Zagreb, ABC4, GA and GA5 indices for Star of David and Hexagonal Cage networks, Provide these indices with closed formulas. There is now an extensive research activity for further study of topological indices of different graph families on ABC and GA indices and their variants see, [1-7, 12, 17-27, 30, 34].

Results for Star of David network

We calculate some degree-based topological indexes of the SD(n) in this section. We calculated the Randić index $R_{\alpha}(Q)$ for $\alpha=-\frac{1}{2}, 1, \frac{1}{2}$ and the first Zagreb, ABC, $ABC_{d}$, GA and $ABC_{4}$ for the Star David network.

**Theorem 2.1.1.** Let $Q_{1} \cong SD(n)$ and the Randić index is

$$R_{\alpha}(SD(n)) = \begin{cases} \frac{3(94-216n+192n^2)}{2(16+44+48n+2n^2)}, & \alpha = 1; \\ \frac{6(17-8\sqrt{3}+2\sqrt{5}+4(-9+2\sqrt{3})n+24n^2)}{1(-4+2n+27n^2)}, & \alpha = -1; \\ 2-4\sqrt{3}+2\sqrt{5}-10n+4\sqrt{5}n+9n^2, & \alpha = \frac{1}{2}. \end{cases}$$

**Proof.** Let $Q_{1} \cong SD(n)$ with condition $n \geq 2$. Using the edge partition from Table 1, from Equation 3, $R_{\alpha}(Q) = \sum_{uv \in E(G)} (d_{u}d_{v})^{\alpha}$

Using formula $R_{\alpha}(Q)$ for $\alpha=1$.

$$R_{1}(Q) = \sum_{j=1}^{4} \sum_{r \in E_{j}(Q)} d_{r}d_{j}$$

**TABLE 1** Edge partition of Star of David network SD(n) based on degrees of end vertices of each edge

<table>
<thead>
<tr>
<th>((d_{u},d_{v})) where (uv \in E(G))</th>
<th>Number of edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2;3)</td>
<td>12</td>
</tr>
<tr>
<td>(3;3)</td>
<td>24n-30</td>
</tr>
<tr>
<td>(3;4)</td>
<td>24n-24</td>
</tr>
<tr>
<td>(4;4)</td>
<td>36n^2-72n+48</td>
</tr>
</tbody>
</table>

Using the edge Table 1,

$$R_{1}(G) = (3 \times 2) \cdot | E_{1}(SD(n)) | + (3 \times 3) \cdot | E_{2}(SD(n)) | + (4 \times 3) \cdot | E_{3}(SD(n)) | + (4 \times 4) \cdot | E_{4}(SD(n)) |$$

$$\Rightarrow R_{1}(G) = 3(94-216n+192n^2).$$

For $\alpha=\frac{1}{2}$.

$$R_{1/2}(Q) = \sum_{j=1}^{4} \sum_{r \in E_{j}(Q)} d_{r}d_{j}$$

Using Table 1, we have

$$R_{1/2}(G) = \frac{3}{2} \cdot | E_{1}(SD(n)) | + \frac{1}{3} \cdot | E_{2}(SD(n)) | + \frac{1}{5} \cdot | E_{3}(SD(n)) | + \frac{1}{7} \cdot | E_{4}(SD(n)) |$$

$$\Rightarrow R_{1/2}(G) = 6(17-8\sqrt{3}+2\sqrt{5}+4(-9+2\sqrt{3})n+24n^2).$$

For $\alpha=-1$.

$$R_{-1}(Q) = \sum_{j=1}^{4} \sum_{r \in E_{j}(Q)} d_{r}d_{j}$$

$$R_{-1}(G) = \frac{5}{6} \cdot | E_{1}(SD(n)) | + \frac{1}{5} \cdot | E_{2}(SD(n)) | + \frac{1}{15} \cdot | E_{3}(SD(n)) | + \frac{1}{21} \cdot | E_{4}(SD(n)) |$$

$$\Rightarrow R_{-1}(G) = 2-4\sqrt{3}+2\sqrt{5}-10n+4\sqrt{5}n+9n^2.$$  

We evaluate the first Zagreb index of the SD(n) as per the following theorem.

**Theorem 2.1.2.** The first Zagreb index is equal for Star of David network:

$$M_{1}(SD(n)) = 6(16-44n+48n^2).$$

**Proof.** Let $Q_{1} \cong SD(n)$ and using Equation 4,

$$M_{1}(Q) = \sum_{uv \in E(G)} (d_{u} + d_{v}) = \sum_{j=1}^{4} \sum_{r \in E_{j}(Q)} (d_{r} + d_{j})$$

$$M_{1}(Q) = (3+2) \cdot | E_{1}(SD(n)) | + (3+3) \cdot | E_{2}(SD(n)) | + (3+4) \cdot | E_{3}(SD(n)) |$$

After calculations, we get the results

$$\Rightarrow M_{1}(Q) = 6(16-44n+48n^2).$$

**Theorem 2.1.3.** Let $Q_{1} \cong SD(n)$ be the Star of David network, then
After some calculations,

\[ GA(Q) = 2 \left( \sqrt{\frac{1}{5}} \right) |E(SD(n))| + \sqrt{\frac{1}{7}} |E_1(SD(n))| + \sqrt{\frac{1}{7}} |E_2(SD(n))| \]

\[ + \frac{4}{7} \sqrt{\frac{1}{5}} |E_3(SD(n))| \]

From (7), we obtain:

\[ ABC_s(Q) = \sum_{\text{resE}(Q)} \frac{S_r + S_s - 2}{S_r S_s} \]

Using Table 2, we have

\[ ABC_s(Q) = \sum_{\text{resE}(Q)} \frac{S_r + S_s - 2}{S_r S_s} \]

Proof. For the ABC index, using Table 1, we have

\[ ABC(Q) = \sum_{\text{resE}(Q)} \frac{d_i + d_j - 2}{d_i d_j} \]

After some calculations,

\[ ABC(Q) = 9 \left( \sqrt{\frac{1}{5}} \right) |E(SD(n))| + \sqrt{\frac{1}{7}} |E_1(SD(n))| + \sqrt{\frac{1}{7}} |E_2(SD(n))| \]

\[ + \frac{4}{7} \sqrt{\frac{1}{5}} |E_3(SD(n))| \]

from (6), we get

\[ GA(Q) = \sum_{\text{resE}(Q)} \frac{d_i + d_j}{d_i d_j} = \sum_{j=1}^{n} \sum_{\text{resE}(Q)} \frac{\sqrt{d_i d_j}}{d_i d_j} \]

Using Table 2, we have

| Table 2 | Edge partition of Star of David network SD(n) based on sum of degrees of end vertices of each edge |
| --- | --- | --- | --- |
| (S_rS_s) where uv∈E(G) | Number of edges | (S_rS_s) where uv∈E(G) | Number of edges |
| (6;8) | 12 | (11;15) | 12 |
| (8;8) | 6 | (14;14) | 6 |
| (8;10) | 12 | (14;15) | 12 |
| (10;10) | 24n-60 | (14;16) | 24n-60 |
| (10;11) | 12 | (15;16) | 24 |
| (10;14) | 24n-48 | (16;16) | 36n^2-96n+66 |
| (11;14) | 12 | - | - |
Results for Hexagonal Cage network

We calculate some degree-based topological indices and compute general Randić $R_\alpha(Q)$ with $\alpha = 1, -1, \frac{1}{2}, \frac{1}{2}$. M1, ABC, GA, ABC4 and GA5 indices of the Hexagonal Cage network in this section.

**Theorem 2.2.1.** Let $Q_2 \cong \text{HXCa}(n)$, then its general Randić index is equal to:

$$R_\alpha(\text{HXCa}(n)) = \begin{cases} 
\frac{3}{10} (128 - 402n + 216n^2), & \alpha = 1; \\
\frac{4}{23} (6(46 + 2\sqrt{5} + \sqrt{6} - 2\sqrt{30}) + 51 + 4\sqrt{30}) + 18n^2, & \alpha = \frac{1}{2}; \\
\frac{19}{10} \sqrt{\frac{3}{5} + 12 \sqrt{3} - 4\sqrt{30}}, & \alpha = -1; \\
\frac{3\sqrt{5}}{5} - \frac{12}{5} \sqrt{3} - 8(37 + 4\sqrt{30}) + 3n^2, & \alpha = \frac{1}{2}.
\end{cases}$$

**Proof.** Let $Q_2 \cong \text{HXCa}(n)$ where $n > 2$. Using Table 3

$$R_\alpha(Q) = \sum_{r \in \mathbb{E}(Q)} (d_r^a + d_r^b)^\alpha.$$

Using above formula for $\alpha = 1$.

**TABLE 3** Edge partition of Hexagonal Cage network HXCa(n) based on degrees of end vertices of each edge

<table>
<thead>
<tr>
<th>(d_u, d_v) where uv ∈ E(G)</th>
<th>Number of edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>(4, 4)</td>
<td>6</td>
</tr>
<tr>
<td>(4, 5)</td>
<td>24</td>
</tr>
<tr>
<td>(4, 6)</td>
<td>12</td>
</tr>
<tr>
<td>(5, 5)</td>
<td>18n - 48</td>
</tr>
<tr>
<td>(5, 6)</td>
<td>24n - 48</td>
</tr>
<tr>
<td>(6, 6)</td>
<td>18n^2 - 66n + 60</td>
</tr>
</tbody>
</table>

Using Table 3,

$$R_\alpha(Q) = \sum_{j=1}^{6} \sum_{r \in \mathbb{E}(Q)} (d_r^a + d_r^b)^\alpha = (4 \times 4) [E_1(\text{HXCa}(n))] + (4 \times 5) [E_1(\text{HXCa}(n))] + (4 \times 6) [E_1(\text{HXCa}(n))] + (5 \times 5) [E_1(\text{HXCa}(n))] + (5 \times 6) [E_1(\text{HXCa}(n))] + (6 \times 6) [E_1(\text{HXCa}(n))].$$

For $\alpha = \frac{1}{2}$, using Table 3

$$R_\frac{1}{2}(Q) = \sum_{j=1}^{6} \sum_{r \in \mathbb{E}(Q)} \frac{1}{2} (d_r^a + d_r^b)^\frac{1}{2} = \frac{1}{2} [E_1(\text{HXCa}(n))] + \frac{1}{2} [E_1(\text{HXCa}(n))] + \frac{1}{2} [E_1(\text{HXCa}(n))] + \frac{1}{2} [E_1(\text{HXCa}(n))] + \frac{1}{2} [E_1(\text{HXCa}(n))] + \frac{1}{2} [E_1(\text{HXCa}(n))].$$

In the following theorem, we compute the first Zagreb index of Hexagonal Cage network.

**Theorem 2.2.2.** The first Zagreb index is equal to for Hexagonal Cage network

$$M_1(\text{HXCa}(n)) = 6(16 - 58n + 36n^2).$$

**Proof.** Let $Q_2 \cong \text{HXCa}(n)$, by using Tables 3 and 4 and Equation 4

$$M_1(Q) = \sum_{r \in \mathbb{E}(Q)} (d_r^a + d_r^b) = \sum_{j=1}^{6} \sum_{r \in \mathbb{E}(Q)} (d_r^a + d_r^b) = 9 [E_1(\text{HXCa}(n))] + 10 [E_1(\text{HXCa}(n))] + 10 [E_1(\text{HXCa}(n))] + 11 [E_1(\text{HXCa}(n))] + 12 [E_1(\text{HXCa}(n))].$$

After some calculations

$$M_1(Q) = 6(16 - 58n + 36n^2).$$

**Theorem 2.2.3.** Let $Q_2 \cong \text{HXCa}(n)$ be the Hexagonal Cage network, then
for \( n > 2 \),
\[
ABC(Q) = 12\sqrt[3]{\frac{7}{5}} + 3\sqrt[3]{\frac{7}{2}} + 4\sqrt[3]{3} + 12\sqrt[3]{\frac{2}{5}} + (n - 2) + \frac{12}{5}\sqrt[3]{(8 + 3n) + \sqrt[3]{10(10 - 11n + 3n^2)}}.
\]

for \( n > 4 \),
\[
GA(Q) = 18 + \frac{48}{\sqrt[3]{212}} + 24\sqrt[3]{\frac{6}{25}} + 18n^2
\]
\[
= 2(38 + 3) + 25
\]
using Equation 6 we get,
\[
GA(Q) = 18 + \frac{48}{\sqrt[3]{212}} + 24\sqrt[3]{\frac{6}{25}} + 18n^2 - 48n + \frac{48}{\sqrt[3]{212}} + 24\sqrt[3]{\frac{6}{25}} + 18n^2
\]

Using Table 4, and Equation 7
\[
ABC(Q) = \sum_{\substack{\sigma, \tau + \nu \neq 0 \\sigma, \tau, \nu \neq 0}} S_\sigma + S_\tau - S_\nu
\]
\[
= \frac{\sqrt[3]{38}}{20} | E_1(HXCa(n)) | + \frac{11}{130} | E_2(HXCa(n)) | + \frac{\sqrt[3]{8}}{5} | E_2(HXCa(n)) | + \frac{5}{26} | E_1(HXCa(n)) | + \frac{\sqrt[3]{142}}{78} | E_1(HXCa(n)) | + \frac{182}{52} | E_1(HXCa(n)) | + \frac{\sqrt[3]{58}}{24} | E_1(HXCa(n)) | + \frac{66}{34} | E_1(HXCa(n)) | + \frac{\sqrt[3]{25}}{6} | E_1(HXCa(n)) | + \frac{70}{36} | E_1(HXCa(n)) |
\]
\[
ABC(Q) = 12\sqrt[3]{\frac{7}{5}} + 3\sqrt[3]{\frac{7}{2}} + 4\sqrt[3]{3} + 12\sqrt[3]{\frac{2}{5}} + (n - 2) + \frac{12}{5}\sqrt[3]{(8 + 3n) + \sqrt[3]{10(10 - 11n + 3n^2)}}.
\]

Proof. Using the Table 3, and Equation 5
\[
AB(C) = \sum_{\sigma = 0} (d_\sigma + d_\delta - 2) = \frac{4}{3} \sum_{\sigma = 0} (S_\sigma + S_\delta)
\]
\[
= \frac{\sqrt[3]{3}}{3} | E_1(HXCa(n)) | + \frac{\sqrt[3]{7}}{10} | E_1(HXCa(n)) | + \frac{\sqrt[3]{10}}{6} | E_1(HXCa(n)) |
\]
\[
AB(C) = 12\sqrt[3]{\frac{7}{5}} + 3\sqrt[3]{\frac{7}{2}} + 4\sqrt[3]{3} + 12\sqrt[3]{\frac{2}{5}} + (n - 2) + \frac{12}{5}\sqrt[3]{(8 + 3n) + \sqrt[3]{10(10 - 11n + 3n^2)}}.
\]

After some calculations
\[
\Rightarrow ABC(Q) = 12\sqrt[3]{\frac{7}{5}} + 3\sqrt[3]{\frac{7}{2}} + 4\sqrt[3]{3} + 12\sqrt[3]{\frac{2}{5}} + (n - 2) + \frac{12}{5}\sqrt[3]{(8 + 3n) + \sqrt[3]{10(10 - 11n + 3n^2)}}.
\]
TABLE 4 Edge partition of Hexagonal Cage network HXCa(n) based on sum of degrees of end vertices of each edge

<table>
<thead>
<tr>
<th>$(S_u;S_v)$ where $uv \in E(G)$</th>
<th>Number of edges</th>
<th>$(S_w;S_v)$ where $uv \in E(G)$</th>
<th>Number of edges</th>
</tr>
</thead>
<tbody>
<tr>
<td>(20;20)</td>
<td>6</td>
<td>(27;27)</td>
<td>18n-84</td>
</tr>
<tr>
<td>(20;26)</td>
<td>24</td>
<td>(27;34)</td>
<td>24n-96</td>
</tr>
<tr>
<td>(20;32)</td>
<td>12</td>
<td>(32;34)</td>
<td>24</td>
</tr>
<tr>
<td>(26;26)</td>
<td>12</td>
<td>(32;36)</td>
<td>12</td>
</tr>
<tr>
<td>(26;27)</td>
<td>24</td>
<td>(34;34)</td>
<td>12n-48</td>
</tr>
<tr>
<td>(26;32)</td>
<td>24</td>
<td>(34;36)</td>
<td>24n-72</td>
</tr>
<tr>
<td>(26;34)</td>
<td>24</td>
<td>(36;36)</td>
<td>18n^2-102n+144</td>
</tr>
</tbody>
</table>

Conclusion

The topological indices for the Star of David and Hexagonal Cage networks and the analytical closed formulas evaluated and defined for these networks are computed in this paper, namely the general Randić index, atomic-bond connectivity index, geometric-arithmetic index, and the first Zagreb index. These results may be helpful for people working in computer science and chemistry who encounter hex-derived networks. There exist many open problems for calculating the expressions of similar derived networks.

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