Research Article

The Degree-Based Topological Indices for Two Special Families of Graphs of Diameter Three

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In this research article, we determine some vertex degree-based topological indices or descriptors of two families of graphs, i.e.,

\[ G = C_4(K_n) \] and \[ G = C_4(K_n) + v_1v_3 \],

where \( C_4(K_n) \) is a graph obtained by identifying one of the vertices of \( K_n \) with one vertex of \( C_4 \). Similarly, a graph formed by joining one of the vertices of \( K_n \) with one vertex of \( C_4 + v_1v_3 \) is known as the \( C_4(K_n) + v_1v_3 \) graph.

1. Introduction

Around the center of a century ago, theoretical experts found some interesting relationships between different properties of organic substances and those of molecular structure by analyzing a few invariants of the underlying molecular graph. These graph invariants are useful for molecular objects and are named as topological indices or topological descriptors. These are numerical parameters of graphs which can be used to describe the physiochemical properties like boiling point, molecular weight, density and refractive index of a molecule [1, 2]. The three main categories of topological indices are distance-based topological indices, degree-based indices and spectrum-based topological indices. Among these, degree-based topological indices are of great significance [1, 3, 4]. Some vertex degree-based topological indices are Randic or connectivity index, first and second Zagreb indices, Narumi Katayama and multiplicative Zagreb indices, atom bond connectivity index, augmented Zagreb index, geometric arithmetic index, harmonic index, and sum connectivity index [5]. The topological descriptors are beneficial tools to chemists that are provided by graph theory. The use of these theoretical invariants in QSAR/QSPR modeling has been a popular work in the past years [4, 6].

The first most widely used topological index in chemistry is the Wiener index. Initially, it was presented by the American Chemist Harold Wiener in 1947 and is denoted by \( W(G) \). After its success, many other topological indices have been introduced that are based on Wiener’s work [3, 7].
Milan Randić introduced the Randić index in 1975. It was the most popular index among all topological indices [2, 8]. The mathematical form of this descriptor is

\[ R(G) = \sum_{\mu \sim \nu} \frac{1}{\sqrt{d_{\mu}(G)d_{\nu}(G)}}, \]  

with a summation going with overall pairs of adjacent vertices of the graph \( G \).

Later, mathematicians did not pay any attention to this index for almost two decades. However, Erdős together with Bollobas worked on this index and discovered the mathematical hidden in it. In 1998, they published their first paper on this index. When the mathematical community began to understand the importance of this descriptor, they started to do researches on it. There have been hundreds of articles and several books dedicated to this structural descriptor [9]. The chemists [1] found out some expressions during the study of molecular structure dependency of total pi-electron energy which includes the terms of the form

\[ M_1(G) = \sum_{\mu} d_{\mu}(G)^2, \]
\[ M_2(G) = \sum_{\mu \sim \nu} d_{\mu}(G)d_{\nu}(G). \]

Immediately, it was identified that these two terms provide quantitative measures of the branching of the molecular carbon atom skeleton. In chemical theory, \( M_1 \) and \( M_2 \) are called first and second Zagreb indices. These two indices have been introduced by Gutman and Trinajstić in 1972. Initially, the first Zagreb index was also known as the Gutman index. But, Balaban et al. did not want to introduce these indices by the names of the discovers. After 1982, Balaban et al. included these two terms in the topological indices and named them as Zagreb indices. In 2012, multiplicative versions of multiplicative Zagreb indices have been proposed by Todoshene et al. and are known as Narumi Katayama indices. They were the first topological index defined by the product of some graph theoretical quantities. In 1984, Narumi and Katayama determined the term \( \prod_{\mu} d_{\mu}(G)^2 \) and named it as the first multiplicative Zagreb index. It is denoted by \( \prod_1(G) \). The second multiplicative Zagreb index and modified first multiplicative Zagreb index are defined, respectively, by

\[ \prod_2(G) = \prod_{\mu \sim \nu} d_{\mu}(G)d_{\nu}(G), \]
\[ \prod_3(G) = \prod_{\mu \sim \nu} [d_{\mu}(G) + d_{\nu}(G)], \]

with a product going with overall adjacent vertices of a graph \( G \) [10, 11]. The first, second, and modified multiplicative Zagreb indices are known as Narumi Katayama multiplicative Zagreb indices. The geometric arithmetic index is the modified form of the Randić index. This topological descriptor was introduced by Vukicevic and Furtula in 2009. The mathematical form [12] of this index is

\[ GA(G) = \sum_{\mu \sim \nu} \sqrt{d_{\mu}(G)d_{\nu}(G)} / (d_{\mu}(G) + d_{\nu}(G)). \]

Another vertex degree-based topological index that keeps the spirit of Randić index is the atom bond connectivity index. This topological descriptor was introduced by Estrada et al. in 1998. This index has turned out to be an important index for the stability of Alkanes. The mathematical form [8, 13] of this index is

\[ ABC(G) = \sum_{\mu \sim \nu} \frac{d_{\mu}(G) + d_{\nu}(G) - 2}{d_{\mu}(G)d_{\nu}(G)}. \]

Furtula et al. introduced the modified form of atom bond connectivity index in 2009 and named it as the augmented Zagreb index. The mathematical form [8, 14] of this descriptor is

\[ AZI(G) = \sum_{\mu \sim \nu} \left[ \frac{d_{\mu}(G)d_{\nu}(G)}{d_{\mu}(G) + d_{\nu}(G) - 2} \right]^3. \]

In the investigation of heat creation in heptanes and octanes, the prediction capability of the augmented Zagreb index outperforms that of the atom bond connectivity index. Ali et al. investigated the correlation abilities of 20 vertex degree-based topological descriptors for the case of normal heats of formation and ordinary boiling factor of octane isomers, finding that the \( AZI \) produces the best results [15].

In 1980, Fajtlowicz introduced another topological index. In 2012, Zhang worked on this index and named it as the harmonic index. This index is defined as

\[ H(G) = \sum_{\mu \sim \nu} \frac{2}{d_{\mu}(G) + d_{\nu}(G)}. \]

No chemical applications of this index have been found so far, but in the last few years, this index has attracted the great attention of theoreticians [16, 17]. Another vertex degree-based topological index was proposed by Zhou and Trinajstić and was named as the sum connectivity index. They observed in the definition of Randić index that the term \( d_{\mu} \times d_{\nu} \) can be replaced by \( d_{\mu} + d_{\nu} \) which is defined by ([2, 18, 19]).

\[ SCI(G) = \sum_{\mu \sim \nu} \frac{1}{d_{\mu}(G) + d_{\nu}(G)}. \]

Many topological indices are bond-additive, i.e., they can be presented as a sum of edge contributions and have the following form:
\[
\sum_{\mu \nu \in E(G)} f(g(\mu), g(\nu)),
\]

where \(g(\mu)\) are usually degrees or the sum of distances from \(\mu\) to all other vertices of \(G\). Inspired by the most successful indices of this type, such as the Randić index, the second Zagreb index and others, a whole family of Adriatic indices [20] was defined. A particularly intriguing subclass of these descriptors is made up of 148 discrete Adriatic indices. They were examined on the testing sets provided by the International Academy of Mathematical Chemistry, and it had been shown that they have good predictive properties in many cases and it was found that they have good predictive properties in many cases. One of these useful discrete Adriatic indices is the symmetric division deg (SDD) index, which is defined as

\[
\text{SDD}(G) = \sum_{\mu \nu \in E(G)} \left( \frac{d_{\mu}}{d_{\nu}} + \frac{d_{\nu}}{d_{\mu}} \right),
\]

where \(E(G)\) is the edge set of a molecular graph \(G\) (a graph in which vertices correspond to atoms of a (hydrogen-suppressed) molecule and edges correspond to bonds between the atoms) and \(d_{\mu}\) and \(d_{\nu}\) denote the degrees of the vertices \(\mu, \nu \in V(G)\), respectively [21].

In this paper, we compute the degree-based topological indices, namely, Randić or connectivity index, Zagreb indices, Narumi-Katayama and multiplicative Zagreb indices, atom bond connectivity index, augmented Zagreb index, geometric arithmetic index, harmonic index, and sum connectivity index for two special families of graphs of diameter three. These graphs are undirected having no loops and multiple edges. In Section 2, the topological indices of families of graphs \(C_4(K_n)\) are determined, while in Section 3, the topological indices of families of graphs \(C_4(K_n) + v_1v_3\) are computed.

2. Topological Indices of Families of Graphs \(C_4(K_n)\)

In this section, we have determined and computed the closed formulas of degree-based topological indices for families of graphs \(C_4(K_n)\). The results are analyzed, and the general formulas are derived for these families of graphs.

**Theorem 1.** The Randić and sum connectivity indices of families of graphs \(C_4(K_n)\) are

\[
R(G) = \frac{n-1}{\sqrt{n^2-1}} + \frac{1}{n-1} \left( \frac{n^2 - 3n + 2}{2} \right) + \frac{2}{\sqrt{2n+2}} + 1,
\]

\[
\text{SCI}(G) = \frac{n-1}{\sqrt{2n}} + \frac{2}{\sqrt{n+3}} + \frac{1}{\sqrt{2n-2}} \left( \frac{n^2 - 3n + 2}{2} \right) + 1.
\]

**Proof.** To find the Randić or connectivity index of \(C_4(K_n)\) as shown in Figure 1, we first select a vertex \(u_1\) on \(C_4(K_n)\) of degree \(n+1\). There are \((n-1)\) vertices \(u_2, u_3, \ldots, u_n\) of degree \(n-1\), which are adjacent to \(u_1\). For the vertices \(u_1\) and \(u_i\), where \(i = 2, 3, 4, \cdots, n\), the sum is obtained as

\[
\sum_{u_i \neq u_1} \frac{1}{\sqrt{d_{u_1}(G)d_{u_i}(G)}} = \frac{n-1}{\sqrt{(n+1)(n-1)}} i = 2, 3, \cdots, n = \frac{n-1}{\sqrt{n^2-1}}.
\]

Since the degree of \(u_1\) is \(n+1\), the other two vertices which are adjacent to \(u_1\), are \(v_1\) and \(v_3\) of degree two. For the vertices \(u_1\) and \(v_1\), we have

\[
\frac{1}{\sqrt{d_{u_1}(G)d_{v_1}(G)}} = \frac{1}{\sqrt{2n+2}}.
\]

Similarly, for the vertices \(u_1\) are \(v_3\), we have

\[
\frac{1}{\sqrt{d_{u_1}(G)d_{v_3}(G)}} = \frac{1}{\sqrt{2n+2}}.
\]

Now, we select a vertex \(u_2\) in \(C_4(K_n)\). Since the degree of \(u_2\) is \(n-1\), the other \((n-2)\) vertices which are adjacent to \(u_2\), are \(u_3, u_4, \cdots, u_n\). For the vertices \(u_2\) and \(u_j\), where \(j = 3, 4, 5, \cdots, n\), the sum is obtained as

\[
\sum_{u_i \neq u_2} \frac{1}{\sqrt{d_{u_2}(G)d_{u_i}(G)}} = \frac{n-2}{n-1}.
\]

Since \(K_n\) is symmetric, the same result is obtained for the remaining \((n-2)\) vertices \(u_3, u_4, \cdots, u_n\). So combining the result for all \((n-1)\) vertices \(u_2, u_3, \cdots, u_n\) we have

\[
\frac{n-2}{n-1} + \frac{n-3}{n-1} + \frac{n-4}{n-1} + \cdots + \frac{n-(n-1)}{n-1} = \frac{1}{n-1} \left( \frac{n^2 - 3n + 2}{2} \right).
\]

Now, we select \(v_1\) on \(C_4(K_n)\). The degree of \(v_1\) is two, the other vertex which is adjacent to \(v_1\) is \(v_2\) of degree two. For the vertices \(v_1\) and \(v_2\), we have
Theorem 3. The geometric arithmetic index and harmonic index of families of graphs $C_4(K_n)$ are defined, respectively, by

\[
\begin{align*}
G_A(G) &= \frac{(n-1)\sqrt{n^2-1}}{n} + \frac{4\sqrt{2n+2}}{n+3} + \frac{n^2-3n+2}{2} + 2, \\
H(G) &= \frac{n-1}{n} + \frac{4}{n+3} + \frac{1}{n-1} \left(\frac{n^2-3n+2}{2}\right) + 1.
\end{align*}
\]

The proof is similar to the proof of Theorem 1.
Table 1: Topological indices of \( G = C_4(K_6) \).

<table>
<thead>
<tr>
<th>( t_i(G) )</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( H(G) )</td>
<td>4.278</td>
</tr>
<tr>
<td>( R(G) )</td>
<td>4.380</td>
</tr>
<tr>
<td>( SCI(G) )</td>
<td>6.272</td>
</tr>
<tr>
<td>( ACG(G) )</td>
<td>11.158</td>
</tr>
<tr>
<td>( GA(G) )</td>
<td>18.593</td>
</tr>
<tr>
<td>( M_1(G) )</td>
<td>186</td>
</tr>
</tbody>
</table>

For the vertex \( u_i \), we have

\[
\deg(u_i) = (n + 1)^2.
\]  
(31)

Similarly, for the vertices \( v_1, v_2, \) and \( v_3 \), we have

\[
\deg(v_1) \cdot \deg(v_2) \cdot \deg(v_3) = (2)^2 \cdot (2)^2 = 64.
\]  
(32)

Multiplying equations (30) to (32), \( \prod_1(G) \) = first multiplicative Zagreb index of \( C_4(K_6) \) is

\[
\prod_1(G) = 64(n + 1)^2(n^2 - 2n + 1)^{n-1}.
\]  
(33)

Similarly, second multiplicative and modified first multiplicative Zagreb indices of \( C_4(K_6) \) are defined, respectively, by

\[
\prod_2(G) = 16(n^2 - 1)(2n + 2)(n - 1)^{(n^2 - 3n + 2)},
\]

\[
\prod_3(G) = 16(2n)^{(n-1)}(3 + n)^2(2n - 2)^{(n^2 - 3n + 2)/2}.
\]  
(34)

Example 6. Topological indices of graph \( C_4(K_6) \) are shown in Table 1.

3. Topological Indices of Families of Graphs \( C_4(K_n) + v_1v_3 \)

By looking at the earlier results for computing the topological indices for different families of graphs, here, we introduce new degree-based topological indices to compute their values for families of graphs \( C_4(K_n) + v_1v_3 \).

Theorem 7. The Randic and sum connectivity indices of families of graphs \( C_4(K_n) + v_1v_3 \) are defined, respectively, by

\[
R(G) = \frac{n - 1}{\sqrt{n^2 - 1}} + \frac{1}{n - 1} \left( \frac{n - 3n + 2}{2} \right) + \frac{2}{\sqrt{3n + 3}} + \frac{2}{\sqrt{6}} + \frac{1}{3}.
\]

\[
SCI(G) = \frac{n - 1}{\sqrt{2n}} + \frac{2}{\sqrt{n + 4}} + \frac{1}{\sqrt{2n - 2}} \left( \frac{n - 3n + 2}{2} \right) + \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}}.
\]  
(35)

Proof. To find the Randic or connectivity index of \( C_4(K_n) + v_1v_3 \) as presented in Figure 2, we first select a vertex \( u_i \) on \( C_4(K_n) + v_1v_3 \) of degree \( n + 1 \). There are \((n - 1)\) vertices \( u_2, u_3, \ldots, u_n \) of degree \( n - 1 \), which are adjacent to \( u_i \). For the vertices \( u_i \) and \( u_j \) where \( i = 2, 3, 4, \ldots, n \), the sum

\[
\sum_{u_i \sim u_j} \frac{1}{\sqrt{d_{u_i}(G)d_{u_j}(G)}}, i = 2, 3, 4, \ldots, n
\]  
(36)

is obtained as

\[
= \frac{n - 1}{\sqrt{(n + 1)(n - 1)}} = \frac{n - 1}{\sqrt{n^2 - 1}}.
\]  
(37)

Since the degree of \( u_i \) is \( n + 1 \), the other two vertices which are adjacent to \( u_i \), are \( v_1 \) and \( v_3 \) of degree 3. For the vertices \( u_i \) and \( v_1 \), we have

\[
\frac{1}{\sqrt{d_{u_i}(G)d_{v_1}(G)}} = \frac{1}{\sqrt{3n + 3}}.
\]  
(38)

Similarly, for the vertices \( u_i \) are \( v_3 \), we have

\[
\frac{1}{\sqrt{d_{u_i}(G)d_{v_3}(G)}} = \frac{1}{\sqrt{3n + 3}}.
\]  
(39)

Now, we select a vertex \( u_2 \) on \( C_4(K_n) \). Since the degree of \( u_2 \) is \( n - 1 \), the other \((n - 2)\) vertices which are adjacent to \( u_2 \), are \( u_3, u_4, \ldots, u_n \). For the vertices \( u_2 \) and \( u_j \) where \( j = 3, 4, 5, \ldots, n \), the sum is obtained as

\[
\sum_{u_2 \sim u_j} \frac{1}{\sqrt{d_{u_2}(G)d_{u_j}(G)}} = \frac{n - 2}{n - 1}.
\]  
(40)

Since \( K_n \) is symmetric, the same result is obtained for the remaining \( n - 2 \) vertices \( u_3, u_4, \ldots, u_n \). By using equation (16), the above equation can be written as

\[
= \frac{1}{n - 1} \left( \frac{n - 3n + 2}{2} \right).
\]  
(41)
Now, we select $v_1$ on $C_4(K_n)$. Since the degree of $v_1$ is three, the other two vertices which are adjacent to $v_1$, are $v_2$ and $v_3$. For vertices $v_1$ and $v_2$, we have
\[
\frac{1}{\sqrt{d_{v_1(G)} d_{v_2(G)}}} = \frac{1}{\sqrt{6}}. \tag{42}
\]

Similarly, for the vertices $v_1$ and $v_3$, we have
\[
\frac{1}{\sqrt{d_{v_1(G)} d_{v_3(G)}}} = \frac{1}{3}. \tag{43}
\]

Now, we select $v_2$ on $C_4(K_n)$. The degree of $v_2$ is two, the other vertex which is adjacent to $v_2$, is $v_3$ of degree three. For vertices $v_2$ and $v_3$, we have
\[
\frac{1}{\sqrt{d_{v_2(G)} d_{v_3(G)}}} = \frac{1}{\sqrt{6}}. \tag{44}
\]

Adding equations (37) to (44) $R(G) =$ Randić or connectivity index of $C_4(K_n) + v_1v_3$ is $R(G) = (n-1)/\sqrt{n^2 - 1} + (1/((n-1)(n^2 - 3n + 2)/2) + (2/\sqrt{2n+2}) + 1$.

Similarly, $SCI(G) =$ sum connectivity index of $C_4(K_n) + v_1v_3$ is
\[
SCI(G) = \frac{n-1}{\sqrt{3n}} + \frac{2}{\sqrt{n+4}} + \frac{1}{\sqrt{2n-2}} = \frac{(n^2-3n+2)}{2} + \frac{2}{\sqrt{5}} + \frac{1}{\sqrt{6}} \tag{45}
\]

Using the same arguments as in Theorem 6, we determine some other topological indices of $C_4(K_n) + v_1v_3$. \hfill \square

**Theorem 8.** The atom bond connectivity index and augmented Zagreb index of families of graphs $C_4(K_n) + v_1v_3$ are defined, respectively, by

\[
ABC(G) = (n-1)\sqrt{\frac{2}{n+1} + \frac{\sqrt{2n-4}}{n-1} - \frac{n^2-3n+2}{2} + 2\sqrt{\frac{n+2}{3n+3}} + \sqrt{\frac{2}{3}}},
\]

\[
AZI(G) = (n-1)\left(\frac{n+1}{2}\right)^3 + (n-1)^6 \left(\frac{n^2-3n+2}{2}\right) + 2\left(\frac{3n+3}{n+2}\right)^3 + \frac{1753}{64}.
\]

**Theorem 9.** The geometric arithmetic index and harmonic index of families of graphs $C_4(K_n) + v_1v_3$ are defined, respectively, by

\[
GA(G) = \frac{(n-1)\sqrt{n^2-1}}{n} + \frac{4\sqrt{3n+3}}{n+4} + \frac{n^2-3n+2}{2} + \frac{4\sqrt{6}+1}{5},
\]

\[
H(G) = \frac{n-1}{n} + \frac{4}{n+4} + \frac{1}{n-1} \left(\frac{n^2-3n+2}{2}\right) + \frac{17}{15}.
\]

**Theorem 10.** The Zagreb indices of the families of graphs $C_4(K_n) + v_1v_3$ are

\[
M_1(G) = n^3 - 2n^2 + 5n + 22,
\]

\[
M_2(G) = n^3 - n^2 + 5n + 28 + \left(\frac{(n^2-3n+2)(n-1)^2}{2}\right).
\]

**Proof.** For the families of graphs $C_4(K_n) + v_1v_3$ there are $n - 1$ vertices $v_2, v_3, \ldots, v_n$ of degree $n - 1$, one vertex $v_i$ of degree $n+1$ and two vertices $v_1$ and $v_3$ of degree three and one vertex $v_2$ of degree two, respectively.

\[
\text{deg} (v_1)^2 = (n+1)^2.
\]

For vertices $v_1$ and $v_3$, the first Zagreb index is

\[
\text{deg} (v_1)^2 + \text{deg} (v_3)^2 = (3)^2 + (3)^2 = 18.
\]

For vertices $v_2, v_3, \ldots, v_n$, we have

\[
\text{deg} (v_2)^2 + \text{deg} (v_3)^2 + \cdots + \text{deg} (v_n)^2
\]

\[
= (n-1)^2 + (n-1)^2 + \cdots + (n-1)^2 \text{ times}
\]

\[
= (n-1)(n-1)^2 = (n-1)^3.
\]

Similarly, for vertex $v_2$ we have

\[
\text{deg} (v_2)^2 = 2^2 = 4.
\]

Adding equations (49) to (52), we have $M_1(G) =$ first Zagreb index of $C_4(K_n) + v_1v_3$

\[
M_1(G) = (n+1)^2 + (n-1)^2 + 22 = n^3 - 2n^2 + 5n + 22.
\]

Similarly, $M_2(G) =$ second Zagreb index of $C_4(K_n) + v_1v_3$

\[
M_2(G) = n^3 - n^2 + 5n + 28 + \left(\frac{(n^2-3n+2)(n-1)^2}{2}\right).
\]

\hfill \square
Theorem 11. The Katayama and multiplicative Zagreb indices of families of graphs $C_4(K_n) + v_1v_3$ are

$$\prod_1(G) = 324 (n+1)^2 (n^2 - 2n + 1)^{n-1},$$

$$\prod_2(G) = 324 (n^2 - 1)^{(n-1)(3n+3)^2} (n-1)^{(n^2-3n+2)},$$

$$\prod^*(G) = 150(2n)^{(n-1)(n+4)^2} (2n-2)^{(n^2-3n+2)/2}.$$ (55)

Proof. Since there are $n - 1$ vertices $u_2, u_3, \ldots, u_n$ of degree $n - 1$, one vertex of degree $n + 1$ and three vertices of degree two in $C_4(K_n) + v_1v_3$ graph. Thus, we have

$$\text{deg} (u_2) \cdot \text{deg} (u_3) \cdot \cdots \cdot \text{deg} (u_n) \cdot \text{deg} (u_1) \cdot \text{deg} (v_1) \cdot \text{deg} (v_3) = (n-1)^2(n-1)\ldots(n-1)(n-1)\text{times}$$

$$= (n^2 - 2n + 1)^{n-1}. \quad (56)$$

For vertex $u_1$, we have

$$\text{deg} (u_1) = (n+1)^2. \quad (57)$$

Similarly, for vertices $v_1$ and $v_3$, we have

$$\text{deg} (v_1) \cdot \text{deg} (v_3) = (3)^2. (3)^2 = 81. \quad (58)$$

Also, for vertex $v_2$, we have

$$\text{deg} (v_2) = (2)^2 = 4. \quad (59)$$

Multiplying equations (56) to (59), we have $\prod_1(G) = \text{first multiplicative Zagreb index of } C_4(K_n) + v_1v_3$.

$$\prod_1(G) = 324 (n+1)^2 (n^2 - 2n + 1)^{n-1}. \quad (60)$$

Similarly, second multiplicative Zagreb index and modified first multiplicative Zagreb index of $C_4(K_n) + v_1v_3$ are

$$\prod_2(G) = 324 (n^2 - 1)^{(n-1)(3n+3)^2} (n-1)^{(n^2-3n+2)}$$

$$\prod^*(G) = 150(2n)^{(n-1)(n+4)^2} (2n-2)^{(n^2-3n+2)/2}.$$ (61)

Example 12. Topological indices of graph $C_4(K_n) + v_1v_3$ are shown in Table 2.


