

COMPUTATION OF TOPOLOGICAL INDICES OF INTERSECTION GRAPHS AND CONCENTRIC WHEELS GRAPH

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Let $G = (V, E)$ be a graph with vertex set V and edge set E . In this paper we compute the some topological indices for various graphs. Here we use different methods for calculating these indices. One method using the group of automorphisms of G . This is an efficient method of finding these indices especially when the automorphism group of G has a few orbits on V or E . Alternatively, using a recursion method that is used to calculate the Wiener index.

Key words: Wiener, Hyper-Wiener, Szeged and PI index, intersection graphs, wheel graph.

1. INTRODUCTION

A topological index is a real number related to a graph. It must be a structural invariant, i.e., it preserves by every graph automorphisms. Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffins. In a graph theoretical language, the Wiener index is equal to the count of all shortest distances in a graph. The hyper-Wiener index of acyclic graphs was introduced by Milan Randic in 1993. Then Klein et al.[11], generalized Randic's definition for all connected graphs, as a generalization of the Wiener index. We encourage the reader to consult [11] for the mathematical properties of hyper-Wiener index and its application in chemistry.

The Szeged index [7, 8, 15] is a topological index closely related to the Wiener index and is a summation of vertex–multiplicative type and coincides with the Wiener index in the case that the graph G is a tree. Since the Szeged index takes into account how the vertices of the graph G are distributed, it is natural to define an index that takes into account the distribution of the edges of G . The Padmakar–Ivan (PI) index, [14, 16], is an additive index which takes into account the distribution of edges of the graph and therefore complements the Szeged index in a certain sense.

All the indices mentioned above, when applied to chemical graphs have many chemical applications and it was shown that the PI index is related to the Szeged and the Wiener index of a graph, and all of them have connections with the physicochemical properties of many complex compounds.

In this paper we will develop different methods to calculate these indices. One method is to use group theory and in particular the automorphism group of the graph in question and another use recursion method to obtain a difference equation concerning for this indices. Throughout this paper all the graphs are simple and connected.

2. PRELIMINARIES

Let $G = (V, E)$ be a graph with vertex set V and edge set E . We will deal with finite graph, i.e. both $|V|$ and $|E|$ are finite sets. The distance between the vertices u and v is denoted by $d(u, v)$ and it is defined as the number of edges in a shortest path from u to v . The degree of v , denoted by $d_G(v)$, ($d(v)$ for short), is the

number of edges incident with v in G . The Wiener index $W(G)$ is defined as $W(G) = \sum_{\{u,v\} \in E(G)} d(u,v)$ and if

for $v \in V$ we define $d(v) = \sum_{x \in V} d(v,x)$ then $W(G) = \frac{1}{2} \sum_{v \in V} d(v)$.

The hyper-Wiener index of acyclic graphs was introduced by Milan Randic in 1993. Then Klein et al. [11], generalized Randic's definition for all connected graphs, as a generalization of the Wiener index. We encourage the reader to consult [11] for the mathematical properties of hyper-Wiener index and its application in chemistry. The hyper-Wiener index $WW(G)$ is defined by:

$$WW(G) = \frac{1}{2} W(G) + \frac{1}{2} \sum_{\{u,v\} \in E(G)} d^2(u,v),$$

where $d^2(u,v) = (d(u,v))^2$.

The Szeged index [7, 8] is a topological index closely related to the Wiener index and is a summation of vertex multiplicative type and coincides with the Wiener index in the case that the graph G is a tree. To define the Szeged and revised Szeged indices of the graph we need some terminology. For $e = uv \in E(G)$ we define the following sets:

$$N_u(e | G) = \{x \in V \mid d(u,x) < d(v,x)\},$$

$$N_v(e | G) = \{x \in V \mid d(u,x) > d(v,x)\}.$$

The sizes of $N_u(e | G)$ and $N_v(e | G)$ and are denoted by $n_u(e | G)$ and $n_v(e | G)$ respectively. Hence $n_u(e | G)$ is the number of vertices of G lying closer to vertex u than to vertex v and $n_v(e | G)$ is the number of vertices of G lying closer to vertex v than to vertex u . The Szeged index of G is defined by the following formula:

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e | G) n_v(e | G),$$

Considering contributions from vertices not considered in the definition of Sz, Randi [14] conceived a modified version of the Szeged index, which is named the revised Szeged index in [13,12], by dividing equally the count vertices at the same distance from both end vertices of an edge. The revised Szeged index of the graph G is defined as [14]

$$Sz^*(G) = \sum_{e=uv \in E(G)} [n_u(e | G) + \frac{1}{2} n_0(e | G)][n_v(e | G) + \frac{1}{2} n_0(e | G)],$$

where for the edge $e = uv \in E(G)$, $n_0(e | G)$ is the number of vertices with equal distances from both end vertices of the edge e .

Finally we define the PI-index of the graph $G = (V, E)$ as follows:

Given an edge $e = uv \in E(G)$, we defined the distance of e to a vertex $w \in V(G)$ as minimum of distance of its ends to w , i.e., $d(w,e) = \min\{d(w,u), d(w,v)\}$. For $e = uv \in E(G)$, $m_u(e | G)$ is the number of edges lying closer to u than v , and also $m_v(e | G)$ is defined analogously. The Padmakar-Ivan index of G is defined by

$$PI(G) = \sum_{e=uv \in E(G)} [m_u(e | G) + m_v(e | G)].$$

A permutation σ of V is called an automorphism of G if it preserve the edges of G , i.e., $e = uv$ is an edge of G if and only if $e^\sigma = u^\sigma v^\sigma$ is an edge of G . The set of all automorphisms of G forms a group under the composition of mapping and it is denoted by $A = \text{Aut}(G)$. We say that A acts transitively on V (or E) if for any vertices u and v (or edges e and f) there is an element $\sigma \in A$ such that $u^\sigma = v$ (or $e^\sigma = f$). If A acts transitively on V (or E), then G is called a vertex-transitive (or an edge-transitive) graph.

Result 2.1 [1]. Let $G = (V, E)$ be a simple connected graph. If $Aut(G)$ on E has orbits $\Delta_i = E_i(e_i)$, $1 \leq i \leq s$ where $e_i = u_i v_i$ is an edge of G , then $Sz(G) = \sum_{i=1}^s |\Delta_i| n_{u_i}(e_i | G) n_{v_i}(e_i | G)$.

Result 2.2 [1]. Let $G = (V, E)$ be a simple connected graph. If $Aut(G)$ on E has orbits E_1, E_2, \dots, E_r , with representatives e_1, e_2, \dots, e_r , respectively, where $e_i = u_i v_i$ then

$$PI(G) = \sum_{i=1}^r |E_i| [m_{u_i}(e_i | G) + m_{v_i}(e_i | G)]$$

We can have the following similar result for the revised index $Sz(G)$.

Result 2.3. Let $G = (V, E)$ be a simple connected graph. If $Aut(G)$ on E has orbits E_1, E_2, \dots, E_r , with representatives e_1, e_2, \dots, e_r , respectively, where $e_i = u_i v_i$ then

$$Sz^*(G) = \sum_{i=1}^r |E_i| [n_{u_i}(e_i | G) + \frac{1}{2} n_o(e_i | G)] [m_{v_i}(e_i | G) + \frac{1}{2} n_o(e_i | G)].$$

3. INTERSECTION GRAPHS

This type of graph is defined in [6] as follows. Let S be a set and $F = \{S_1, S_2, \dots, S_p\}$ be a non-empty family of distinct non-empty subsets of S such that $S = \bigcup_{i=1}^p S_i$. The intersection graph of S which is denoted by $\Omega(F)$ has F as its set of vertices and two distinct vertices S_i and S_j , $i \neq j$ are joint by an edge if and only if $S_i \cap S_j \neq \emptyset$.

Here we will consider a set S of cardinality n and let F be the set of all subsets of S of cardinality k , $1 < k < n$, which is denoted by $S^{\{k\}}$. Upon convenience we may set $S = \{1, 2, \dots, n\}$. Let the intersection graph $\Omega(S^{\{k\}})$ be denoted by $\Gamma^{\{k\}} = (V, E)$. The number of vertices of this graph is $\binom{n}{k}$, the degree of each vertex is $d = \binom{n}{k} - \binom{n-k}{k} - 1$, if $n \geq 2k$ and it is $d = \binom{n}{k} - 1$, if $n < 2k$ and the number of its edges is $|E| = \frac{1}{2} \binom{n}{k} \left[\binom{n}{k} - \binom{n-k}{k} - 1 \right]$ or $|E| = \frac{1}{2} \binom{n}{k} \left[\binom{n}{k} - 1 \right]$, in the respective cases $n \geq 2k$ or $n < 2k$.

In this section we will compute the indicated indices of this graph. The Wiener index of $\Gamma^{\{k\}}$ in [1] computed and we here obtain a formula for Wiener index of this graph.

THEOREM 3.1. The hyper-Wiener index of $\Gamma^{\{k\}}$ is

$$WW(\Gamma^{\{k\}}) = \begin{cases} \frac{1}{2} \binom{n}{k} \left[\binom{n}{k} + 2 \binom{n-k}{k} - 1 \right] & n \geq 2k \\ \frac{1}{2} \binom{n}{k} \left[\binom{n}{k} - 1 \right] & n < 2k. \end{cases}$$

Proof. By definition,

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \in V(G)} [d(u,v) + d^2(u,v)] = \frac{1}{2} \sum_{uv \in E(G)} [d(u,v) + d^2(u,v)] = \frac{1}{2} \sum_{uv \notin E(G)} [d(u,v) + d^2(u,v)].$$

Put $E^c = \{\{u,v\} \in V(G) \mid uv \notin E(G)\}$. Thus $|E^c| = \frac{1}{2} \binom{n}{k} \left[\binom{n}{k} - 1 \right]$.

If $n < 2k$, then any vertex is adjacent with other vertices. Therefore $WW(\Gamma^{\{k\}}) = |E(\Gamma^{\{k\}})|$ and in this case $|E(\Gamma^{\{k\}})| = \frac{1}{2} \binom{n}{k} \left[\binom{n}{k} - 1 \right]$.

Now if $n \geq 2k$, then the distance any two vertices of $\Gamma^{\{k\}}$ is 1 or 2, according to [1, proposition 1], so $WW(G) = \frac{1}{2} \sum_{uv \in E(G)} 2 + \frac{1}{2} \sum_{uv \notin E(G)} 6 = |E| + |E^c|$. But in this case $|E| = \frac{1}{2} \binom{n}{k} \left[\binom{n}{k} - \binom{n-k}{k} - 1 \right]$. Hence $WW(\Gamma^{\{k\}}) = \frac{1}{2} \binom{n}{k} \left[\binom{n}{k} + 2 \binom{n-k}{k} - 1 \right]$ if $n \geq 2k$. The result now follows. \square

The following lemma is basic.

LEMMA 3.2 [1]. *The automorphism group of $\Gamma^{\{k\}}$ on the set E of edge of $\Gamma^{\{k\}}$ has $k-1$ orbits if $n \geq 2k$ and has $n-k$ orbits if $n < 2k$. The size each orbit is $\frac{1}{2} \binom{n}{k} \binom{k}{i} \binom{n-k}{k-i}$, $1 \leq i \leq k-1$ or $\frac{1}{2} \binom{n}{k} \binom{k}{k-j} \binom{n-k}{j}$, $1 \leq j \leq n-k$ in the respective case $n \geq 2k$ or $n < 2k$.*

THEOREM 3.2. *The revised Szeged index of $\Gamma^{\{k\}}$ is as follows:*

$$Sz^*(\Gamma^{\{k\}}) = \frac{1}{2} \binom{n}{k} \times \begin{cases} \sum_{i=1}^{k-1} \binom{k}{i} \binom{n-k}{k-i} & n \geq 2k \\ \sum_{j=1}^{n-k} \binom{k}{k-j} \binom{n-k}{j} & n < 2k \end{cases}$$

Proof. It is clear that see $n_0(e|G) = |V(G)| - (n_u(e|G) + n_v(e|G))$. Since in Graph $\Gamma^{\{k\}}$, $n_u(e|G) = n_v(e|G)$. Thus $n_u(e|G) + \frac{1}{2} n_0(e|G) = n_v(e|G) + \frac{1}{2} n_0(e|G) = |V(G)|$. Therefore by Result 2.3 and Lemma 3.2, the theorem is proved. \square

Now we calculate the PI index of $\Gamma^{\{k\}}$ which is one of the main result in this paper.

THEOREM 3.3. *Let $n \geq 2k$. Then the PI index of $\Gamma^{\{k\}}$ is as follows:*

$$PI(\Gamma^{\{k\}}) = \binom{n}{k} \sum_{i=1}^{k-1} \binom{k}{i} \binom{n-k}{k-i} \left[\frac{\sum_{j=1}^{k-i} \binom{k-j}{j} \binom{n-2k+1}{k-j}}{2} \right] + \binom{n}{k} - \binom{n-k}{k} - 2$$

Proof. Let E_i , $1 \leq i \leq k-1$ be the orbits of $\text{Aut}(\Gamma^{\{k\}})$ on the set of edges of $\Gamma^{\{k\}}$, according to Lemma 3.2. By result 2.2, we have $PI(G) = \sum_{i=1}^{k-1} |E_i| [m_{u_i}(e_i|G) + m_{v_i}(e_i|G)]$.

Consider the edge $e = uv$ in the orbit E_i . It is clear that the edge $f = uw$ lying closer to u than to v whenever the vertex w be adjacent with both u and v . On the other hand, if $x, y \in N_u(e | G)$, then the edge $f = xy$ lying closer to u than to v . Therefore $m_u(e | G)$ is sum the number of edges of set $N_u(e | G)$ and the number of vertices of set $\Delta = \{w \in V(G) | uw, vw \in E(G)\}$. It is clear that the number of edges of set $N_u(e | G)$ is $\binom{|N_u(e | G)|}{2}$ and $|\Delta| = d(u) - |N_u(e | G)|$. Hence

$$m_u(e | G) = \binom{n_u(e | G)}{2} + d(u) - n_u(e | G).$$

Now with an easy calculation we obtain $m_u(e | G) = \binom{n_u(e | G) - 1}{2} + d(u) - 1$. If $n \geq 2k$, then $d(u) = \binom{n}{k} - \binom{n-k}{k} - 1$, and by [1, Proposition 2], $n_u(e | G) = 1 + \sum_{j=1}^{k-i} \binom{k-j}{j} \binom{n-2k+1}{k-j}$. Hence

$$m_u(e | G) = \left(\sum_{j=1}^{k-i} \binom{k-j}{j} \binom{n-2k+1}{k-j} \right) + \binom{n}{k} - \binom{n-k}{k} - 2.$$

In a similar manner we obtain $m_u(e | G) = m_v(e | G)$.

Now by Lemma 3.2, the proof is completed.

In the case that $n < 2k$, $n_u(e | \Gamma^{\{k\}}) = 1$, so $m_u(e | \Gamma^{\{k\}}) = d(u) - 1$. But in this case $d(u) = \binom{n}{k} - 1$. Hence $m_u(e | \Gamma^{\{k\}}) = \binom{n}{k} - 2$. Therefore by Lemma 3.2 and Result 2.2, we obtain

$$PI(\Gamma^{\{k\}}) = \binom{n}{k} \sum_{j=1}^{n-k} \binom{k}{k-j} \binom{n-k}{j} \left[\binom{n}{k} - \binom{n-k}{k} - 1 \right].$$

4. CONCENTRIC WHEELS GRAPH

Let n concentric cycles divided m parts. This graph is showed by $W_{m,n}$. We show the center this graph with v_0 and also i^{th} vertex in j^{th} cycle with $v_{\{i,j\}}$, for $1 \leq i \leq m$, $1 \leq j \leq n$. Thus $W_{m,n}$ has $mn + 1$ vertices and $2mn$ edges.

In this section we compute the mentioned indices of this graph with different method. We first obtain a formula for the Wiener index of this graph using recursion relation.

For a graph which repeats a certain shape several times the best method of calculating the Wiener index is by recursion process. In this case we assume the graph G consists of a certain shape n times and let u_n denote the Wiener index of G . If we can obtain a Fibonacci-like relation between u_n and the u_k , $k < n$, then we are concerned with solving a difference equation. Solving this difference equation will result in finding the Wiener index of G .

THEOREM 4.1. *The Wiener index of $W_{m,n}$ is equal to*

$$W(W_{m,n}) = m^2 \binom{n+1}{3} + m \binom{n+1}{2} + \begin{cases} \frac{1}{8} n^2 m^3 & 2 \mid n \\ \frac{1}{8} n^2 m(m^2 - 1) & 2 \nmid n \end{cases}.$$

Proof. Let u_n denotes the Wiener index of $W_{m,n}$. Then we have $u_n = u_{n-1} + f(n)$ where $f(n)$ is equal to the sum of distances of each of the vertices $v_{\{j,n\}}$, $1 \leq j \leq m$ from each other and from each of the vertices of $W_{m,n-1}$, so $f(n) = W(C_m) + \sum_{j=1}^m \sum_{x \in V(W_{m,n-1})} d(x, v_{\{j,n\}})$, where C_m is a cycle with m vertices.

Consider the vertex $v_{\{1,n\}}$ on n^{th} cycle of $W_{m,n}$. Let X be the sum of distance $v_{1,n}$ with vertices $v_{j,n}$, $2 \leq j \leq m$ of n^{th} cycle. Then the sum of distance vertex $v_{\{1,n\}}$ with vertices $v_{\{j,n-k\}}$, $1 \leq j \leq m$, $1 \leq k \leq n-1$, is $km + X$. Also we have $d(v_0, v_{\{1,n\}}) = n$. Hence

$$\sum_{x \in V(W_{m,n-1})} d(x, v_{1,n}) = n + \sum_{k=1}^{n-1} (km + X) = n + (n-1)X + m \binom{n}{2}.$$

Therefore $f(n) = W(C_m) + nm + (n-1)mX + m^2 \binom{n}{2}$. But $mX = 2W(C_m)$, so

$$f(n) = (2n-1)W(C_m) + nm + m^2 \binom{n}{2}.$$

Now using the above recursion relation we are able to find u_n as follows:

$$u_n - u_0 = \sum_{k=1}^n f(k) = W(C_m) \sum_{k=1}^n (2k-1) + m \sum_{k=1}^n k + m^2 \sum_{k=1}^n \binom{k}{2}.$$

We have $u_0 = 0$ and $W(C_m) = \begin{cases} \frac{1}{8}m^3 & 2 \mid m \\ \frac{1}{8}m(m^2-1) & 2 \nmid m \end{cases}$, the proof is completed.

Next, we will calculate the rest of the index. To do this we the set of edges of $W_{m,n}$ are divided into the set of edges on circles, the set of edges between circles and the set of edges between center and first circle, and are defined as follows:

$$A_j = \{v_{\{i,j\}}v_{\{i+1,j\}} \in E(G) \mid i = 1, 2, \dots, m-1\}, 1 \leq j \leq n,$$

$$B_i = \{v_{\{i,j\}}v_{\{i,j+1\}} \in E(G) \mid j = 1, 2, \dots, n-1\}, 1 \leq i \leq m, \text{ and } C_k = \{v_0v_{\{k,1\}} \in E(G)\}, 1 \leq k \leq m.$$

Thus $E(W_{m,n}) = A \cup B \cup C$, where $A = \bigcup_{j=1}^n A_j$, $B = \bigcup_{i=1}^m B_i$ and $C = \bigcup_{k=1}^m C_k$. Obviously, the sets A , B and C are partitions of the edges of $W_{m,n}$ $|A| = mn$, $|B| = (n-1)m$ and $|C| = m$.

THEOREM 4.2. *The Szeged index of $W_{m,n}$ is equal to*

$$Sz(W_{m,n}) = \frac{5}{12}n^3m^3 + \frac{3}{2}n^2m^2 + nm - 3n^2m - \frac{1}{6}nm^3 - \frac{1}{2}nm^2 + \begin{cases} 0 & 2 \mid m \\ 3n^3m(1-2m) & 2 \nmid m \end{cases}.$$

Proof. By definition,

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e|G)n_v(e|G) = \sum_{e=uv \in A} n_u(e|G)n_v(e|G) + \sum_{e=uv \in B} n_u(e|G)n_v(e|G) + \sum_{e=uv \in C} n_u(e|G)n_v(e|G).$$

Let $e = uv$ be an edge of $W_{m,n}$ in the set of A . Then $n_u(e|G) = n_v(e|G)$ is equal to $\frac{1}{2}nm$ if m is even and is equal to $\frac{1}{2}n(m-1)$ if m is odd. Hence

$$Sz(A) = \begin{cases} \frac{1}{4}n^3m^3 & 2 \mid m \\ \frac{1}{4}n^3m(m-1)^2 & 2 \nmid m \end{cases} \quad (1)$$

Now Suppose $e = uv$ be an edge of $W_{m,n}$ in the set of B . Let us choose $u = v_{\{i,j\}}$ and $v = v_{\{i,j+1\}}$ as vertices of the edge $e = uv$. We have $n_u(e \mid G) = jm + 1$ and $n_v(e \mid G) = (n - j)m$, so

$$Sz(B) = \sum_{i=1}^m \sum_{j=1}^{n-1} [nm + (nm - 1)mj - m^2j^2] = \frac{1}{6}(n^3m^3 + n^2m^2 - nm^3 - 3nm^2). \quad (2)$$

Finally if $e = uv$ is an edge of $W_{m,n}$ in the set of C . Suppose us choose $u = v_0$ and $u = v_{\{1,1\}}$. Thus $n_u(e \mid G) = (m - 3)n + 1$ and $n_v(e \mid G) = n$. Hence

$$Sz(C) = n^2m^2 + nm - 3n^2m. \quad (3)$$

Now, by sum of the equations (1), (2) and (3) the proof is completed.

THEOREM 4.3. *The revised Szeged index of $W_{m,n}$ is equal to*

$$Sz^*(W_{m,n}) = \frac{1}{12}(5n^3m^3 + 36n^2m^2 + 27nm - 48n^2m - 2nm^3 - 6nm^2).$$

Proof. By definition, $Sz^*(W_{m,n}) = Sz^*(A) + Sz^*(B) + Sz^*(C)$. But

$n_0(e \mid G) = |V(G)| - (n_u(e \mid G) + n_v(e \mid G))$, so according to pervious theorem we have:

(a) If the edge $e = uv \in A$, then $n_0(e \mid G)$ is equal to 1 or $n+1$ in respective case m is even or odd.

(b) If the edge $e = uv \in B$, then $n_0(e \mid G) = 0$.

(c) If the edge $e = uv \in C$, then $n_0(e \mid G) = 2n$.

Thus by Theorem 4.2, we have

$$Sz^*(W_{m,n}) = \sum_{e \in A} \left(\frac{nm+1}{2}\right)^2 + \sum_{e \in B} [m(n-j)(jm+1)] + \sum_{e \in C} 2n(nm - 2n + 1).$$

Now by some calculations the proof is completed.

Suppose G is a graph, $e = uv \in E(G)$ and $w \in V(G)$. Define $d(w, e) = \min\{d(u, w), d(v, w)\}$. We say that e is parallel to f if $d(u, f) = d(v, f)$. We define $M(e)$ be the number of all edges parallel to e , so $M(e) = |E(G)| - (m_u(e \mid G) + m_v(e \mid G))$. Therefore

$$PI(G) = |E(G)|^2 - \sum_{e \in E(G)} M(e). \quad (4)$$

Now, using this method we will calculate PI index of $W_{m,n}$.

THEOREM 4.4. *The PI index of $W_{m,n}$ is equal to*

$$PI(W_{m,n}) = 4n^2m^2 + nm^2 + m(2 - m) + \begin{cases} 2n^2m & 2 \mid m \\ n^2m & 2 \nmid m \end{cases}.$$

Proof. If $e \in A$, then $M(e)$ is equal to $2n$ or n in the respective cases m is even or odd. If $e \in B$, then $M(e) = m$ and if $e \in C$, then $M(e) = 2$. Therefore

$$\sum_{e \in E(G)} M(e) = \sum_{e \in A} M(e) + \sum_{e \in B} M(e) + \sum_{e \in C} M(e) = \begin{cases} 2n^2m + m^2(n-1) + 2m & 2 \mid m \\ n^2m + m^2(n-1) + 2m & 2 \nmid m \end{cases}.$$

Since $|E(W_{m,n})| = 2mn$, so by equation (4), the proof is completed.

4. CONCLUSION

In this paper some topological indices for various graphs using the group of automorphisms of G and using recursion method are determined. These formulas to be used in theoretical chemistry molecular structure descriptor. Computing topological indices for molecular graphs (such as dendrimers, nanotubes and nanotori) is left to future investigations.

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