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Topological Indices of Molecular Graphs Under Specific Chemical Reactions

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Abstract - Molecular graph serves as a convenient model for any real or abstract chemical compound. A topological index is the graph invariant number calculated from the graph representing the molecule. The advantage of topological indices is that it may be used directly as simple numerical descriptors in QSPR/QSAR models. Most of the topological descriptors are based either on atom-atom connectivity or on topological distances. A chemical reaction can be represented as the transformation of the chemical (Molecular) graph representing the reaction's substrate into another chemical graph representing the product. The type of chemical reaction where two substrates combine to form a single product (combination reaction) motivated us to study the effect of topological indices when a bridge is introduced between the respective vertices (of degree i, i=1, 2, 3) of two copies of the same graph. The graph obtained in this manner may or may not exist in reality, but it is the interest of the chemist to check the stability of the so obtained structure of the product. In this paper we present an algorithm to calculate the distance matrix of the resultant graph obtained after each iteration and thereby tabulate various topological indices. We also give the explicit formula for calculating Wiener index of the graph representing the resulting product.

Keywords: Graph, Molecules, Distance matrix, Topological indices, Wiener Index, Platt number.

I. INTRODUCTION

A topological index is a numerical descriptor of a molecule, based on a certain topological feature of the corresponding molecular graph. A representation of an object giving information only about the number of elements composing it and their connectivity is named as topological representation of an object. A topological representation of a molecule is called molecular graph. A molecular graph is a collection of points representing the atoms in the molecule and set of lines representing the covalent bonds. These points are named vertices and the lines are named edges in graph theory language. The advantage of topological indices is in that they may be used directly as simple numerical descriptors in a comparison with physical, chemical or biological parameters of molecules in Quantitative Structure Property Relationships (QSPR) and in Quantitative Structure Activity Relationships (QSAR). One of the most widely known topological descriptor is the Wiener index named after chemist Harold Wiener.

The Wiener index [5] of a graph is defined as the sum of distances between all vertices pairs in a connected graph. Wiener index correlates well with many physico-chemical properties of organic compounds and as such has been well studied over the last quarter of a century. The classical Zagreb group indices which are dependent on the degrees of adjacent vertices appeared in the topological formula for the π-electron energy of conjugated systems. Recently introduced Zagreb Coindices [1] are dependent on the degrees of non-adjacent vertices and thereby quantifying a possible influence of remote pairs of vertices to the molecule's properties. For many physico chemical properties the predictive power of GA index [9] is better than other connectivity indices. Platt number [5] was used to predict the physical parameters of alkanes. Reverse Wiener & Reciprocal reverse Wiener indices [10] are used to produce QSPR models for the alkane molar heat capacity. It has been demonstrated that Degree Distance [6] $DD(G)$ and $W(G)$ are closely mutually related for certain classes of molecular graphs. The Randic index [2] has been closely correlated with many chemical properties. The reciprocal complementary Wiener (RCW) number is one of the newest additions in the family of such descriptors. It was put forward by Ivanciuc and its (chemical) applications were discussed in [8].

II. MOTIVATION AND DEFINITIONS

The main paradigm of medicinal Chemistry is that biological activity, as well as physical, physicochemical and chemical properties of chemical compound depends on their molecular structure. Based on this paradigm Crum Brown and Fraser published the first quantitative structure activity relationship in 1868. This paradigm is guiding the discovery of new lead compounds. A lead compound is any chemical compound that shows the biological activity we are interested in. Combination reaction [7] is a general category of a chemical reaction. It may be defined as a chemical reaction in which two or more substances combine to form a single substance under suitable conditions. Combination reactions involve the formation of new bonds. Chemical reactions of the above type motivated us to study the effect of Topological indices when two copies of the graph representing the substrates combine to form a product graph in which an edge is introduced between respective vertices (of degree i, i=1,2,3) as given in Fig. 1. We give the following definitions used in our study.

Definition 2.1: The Weiner index [5] $\mathrm{W}(G)$ of a graph G is defined as the sum of half of the distances between every pair of vertices of G.

$\mathrm{W}(G)=\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} d(v_i,v_j)$, where $d(v_i,v_j)$ is the number of edges in a shortest path connecting the vertices v_i, v_j. We have an equivalent definition of Wiener index $\mathrm{W}(G)=\sum_{i<j} d(v_i,v_j)$.

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Wiener index of the cycle graph C_N, $W(C_N)=\begin{cases}\frac{N(N^2-1)}{8}, & N \text{ is odd}\\ \frac{N^3}{8}, & N \text{ is even}\end{cases}$

Wiener index of the path graph P_N, $W(P_N)=\frac{N^3-N}{6}$

Definition 2.2: The Platt number [5] $F(G)$ of a graph G is defined as the total sum of degrees of edges in a graph, $F(G)=\sum_{i=1}^{M} D(e_i)$ where $D(e_i)$ denotes degree of the edge e_i, i.e., number of edges adjacent to e_i and M denotes the number of edges.

Definition 2.3: The Zagreb group indexes [5] of a graph G denoted by $M_1(G)$ (first Zagreb index) and $M_2(G)$ (second Zagreb index) are defined as

$M_1(G)=\sum_{i=1}^{N} D_i^2$, $M_2(G)=\sum_{(i,j)} D_i D_j$ where D_i stands for the degree of a vertex i. The sum in $M_1(G)$ is over all vertices of G, while the sum in $M_2(G)$ is over all edges of G.

Definition 2.4: The Zagreb group coindices [1] of a graph G denoted by $\overline{M_1}(G)$ (first Zagreb co index) and $\overline{M_2}(G)$ (second Zagreb coindex) are defined as

$$\overline{M_1}(G)=\sum_{\substack{\text{over all edges } (v_i,v_j) \text{ of}\\ \text{the complement of } G}} (D_i+D_j),\quad \overline{M_2}(G)=\sum_{\substack{\text{over all edges } (v_i,v_j) \text{ of}\\ \text{the complement of } G}} (D_iD_j)$$

where D_i stands for the degree of the vertex v_i.

Definition 2.5: The geometric-arithmetic index [9] $GA(G)$ of a graph G is defined as

$GA(G)=\sum_{uv\in E(G)} \frac{\sqrt{D_u D_v}}{\left(\frac{D_u+D_v}{2}\right)}$ where $E(G)$ is the set of edges of the graph G and D_u denotes the degree of the vertex u.

Definition 2.6: The reverse Wiener and reciprocal reverse Wiener indices [10] of a graph G denoted by $\Lambda(G)$ and $R\Lambda(G)$ are defined as

$$\Lambda(G)=\sum_{i<j} r_{ij} \qquad (1)$$

$$R\Lambda(G)=\sum_{i<j} rr_{ij} \qquad (2)$$

where r_{ij} in (1) is defined as $r_{ij}=\begin{cases} d-d_{ij} & \text{if } i\neq j\\ 0 & \text{otherwise}\end{cases}$ d is the diameter of the graph G and d_{ij} is the distance (i.e., the number of edges of a shortest path) between the vertices v_i and v_j and rr_{ij} in (2) is defined as $rr_{ij}=\frac{1}{r_{ij}}=\begin{cases}\frac{1}{d-d_{ij}} & \text{if } i\neq j \ \&\ d_{ij}<d\\ 0 & \text{otherwise}\end{cases}$. The relation between Wiener index $W(G)$ and reverse Wiener index $\Lambda(G)$ is $\Lambda(G)=\sum_{i<j} r_{ij}=\frac{1}{2}N(N-1)d-W(G)$ where N denotes the number of vertices of the graph G.

Definition 2.7: The Reciprocal Complementary Wiener number [8] of the graph G is defined as $RCW(G)=\sum_{\{u,v\}\subseteq V(G)} \frac{1}{d+1-d(u,v)}$ where the summation is over all unordered pairs of distinct vertices of G. d is the diameter of the graph G and $d(u,v)$ is the number of edges in a shortest path connecting the vertices u,v.

Definition 2.8: The Randic′ index [2] of the graph G is defined as the sum of $(D_uD_v)^{-\frac{1}{2}}$ over all pairs of adjacent vertices u,v of G, where D_u is the degree of the vertex u in G.

Definition 2.9: The degree distance [6] of the graph G is defined as $DD(G)=\sum_{\{u,v\}\subseteq V(G)} (D_u+D_v)d(u,v)$ where the summation is over all unordered pairs of distinct vertices of G. D_u is the degree of the vertex u in G and $d(u,v)$ is the number of edges in a shortest path connecting the vertices u,v.

III. MAIN RESULTS

First we present an algorithm to calculate the distance matrix of the graph representing the product after each iteration and compute various topological indices. Topological indices for different graph structures (Examples 1 – 4) are obtained with the help of C program using the above algorithm and the results are tabulated (Tables 1 – 4). We also establish the explicit formula to calculate Wiener index up to second iteration for graph structures P_n, and that up to third iteration for graph structures $K_{1,5}$ and $K_{1,4}$.

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Algorithm 3.1:

Input: Enter N, the number of vertices and $A\left(G^{(0)}\right)$, the Adjacency Matrix of the given graph $G^{(0)}$.

Output: Topological Indices of the graph $G^{(i)}, i \le 3$.

Step 1. Choose $p = 0.$

Step 2. Calculate the degree of each of the vertex $v_j, j = 1, 2, ..., N$ and M, the number of edges of the graph $G^{(p)}$.

Step 3. Compute the degree of every edge $\left(v_j, v_k\right)$ of the graph $G^{(p)}$. $\left(\deg\left(v_j\right) + \deg\left(v_k\right) - 2\right)$

Step 4. For the vertex v_j, identify those vertices which are in the

k^{th} $\left(k = 1, 2, ..., N-1\right)$ neighborhood of v_j. Repeat Step 4 for each vertex $v_j, j = 1, 2, ..., N.$

Step 5. Form the Distance Matrix $D\left(G^{(p)}\right)$ of the graph $G^{(p)}$.

Step 6. Find the largest of the distances (diameter, d) between every pair of vertices of the graph $G^{(p)}$.

Step 7. From the values computed from Step 2 to Step 6 calculate various Topological Indices (Distance & Connectivity Indices).

Step 8. Find the number l of vertices of the graph $G^{(p)}$ whose degrees are less than 4. If $l = 0$

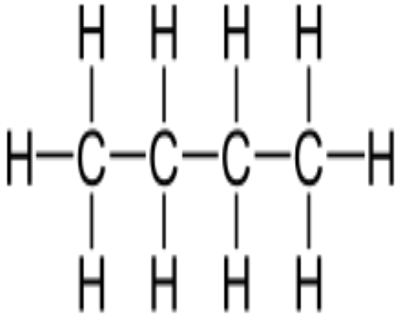
i.e. $G^{(p)}$ is 4-regular then go to End. Otherwise go to Step 9.

Step 9. Construct the graph $G^{(p+1)} = G^{(p)} \hat{e} G^{(p)}$ by taking two copies of $G^{(p)}$ and introducing edges between the respective vertices if the degree of the vertex is less than four. The resultant graph has $2N$ vertices and $\left(2M + l\right)$ edges.

Step 10. Find the Adjacency Matrix of the graph $A\left(G^{(p+1)}\right)$.

Step 11. Set $p = p + 1.$ Go to Step 2. End.

Example 1.



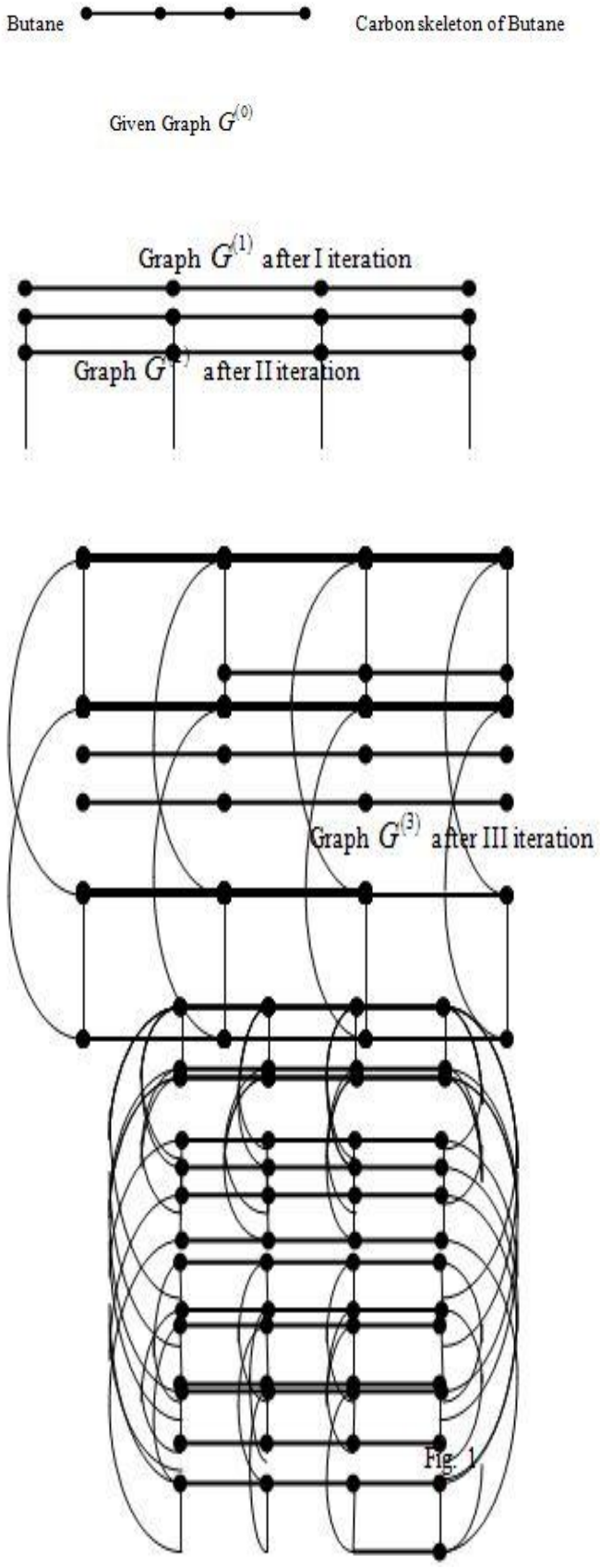


Fig. 1

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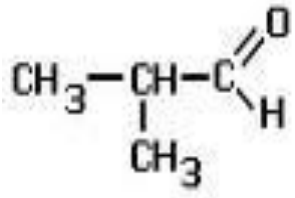
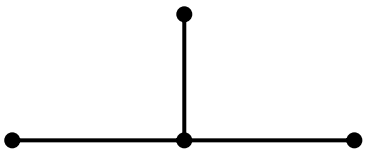
Table 1. Topological Indices of the product graph after each iteration

	Given Graph $G^{(0)}$	Product graph after I iteration $G^{(1)}$	Product graph after II iteration $G^{(2)}$	Product graph after III iteration $G^{(3)}$
Number of vertices	4	8	16	32
Number of edges	3	10	28	64
Topological Indices ↓				
Wiener (W)	10	56	288	1536
Reverse Wiener (RW)	8	56	312	1440
Reciprocal Complementary Wiener (RCW)	1	2	4	16
Reciprocal Reverse Wiener (RRW)	2	6	16	64
Platt Number (F)	4	32	144	384
First Zagreb index (M_1)	10	52	200	512
Second Zagreb index (M_2)	8	68	360	1024
First Zagreb coindex $(\overline{M_1})$	8	88	640	3456
Second Zagreb coindex $(\overline{M_2})$	5	106	1108	6912
Randic's Connectivity index (R)	1.91	3.97	7.98	16
Geometric Arithmetic index (GA)	3.83	10.90	29.24	64
Degree Distance (DD)	28	272	1984	12288

Example 2.



2-methylpropanal



Carbon skeleton of 2-methylpropanal

Table 2. Topological Indices of the product graph after each iteration

	Given Graph $G^{(0)}$	Product graph after I iteration $G^{(1)}$	Product graph after II iteration $G^{(2)}$	Product graph after III iteration $G^{(3)}$
Number of vertices	4	8	16	32
Number of edges	3	10	26	64
Topological Indices ↓				
Wiener (W)	9	52	280	1392
Reverse Wiener (RW)	3	32	200	1088
Reciprocal Complementary Wiener (RCW)	3	6	14	28
Reciprocal Reverse Wiener (RRW)	3	12	38	108
Platt Number (F)	6	36	120	384
First Zagreb index (M_1)	12	56	172	512
Second Zagreb index (M_2)	9	76	284	1024
First Zagreb coindex $(\overline{M_1})$	6	84	608	3456
Second Zagreb coindex $(\overline{M_2})$	3	96	982	6912
Randic's Connectivity index (R)	1.73	3.87	7.96	16.00
Geometric Arithmetic index (GA)	2.60	9.66	27.86	64.00
Degree Distance (DD)	24	248	1808	11136

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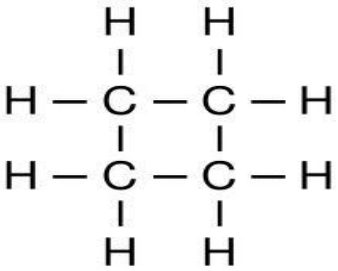
Example 3.



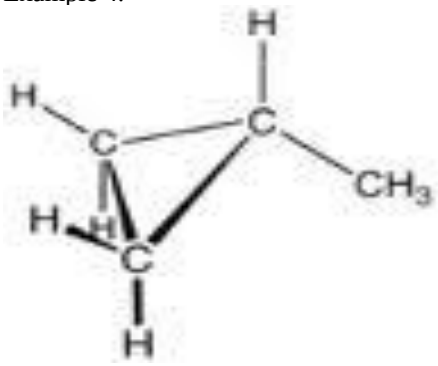
Cyclobutane

Carbon skeleton of Cyclobutane

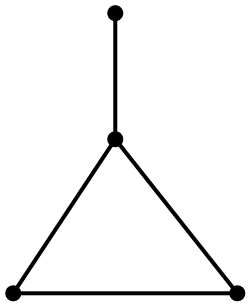
Table 3. Topological Indices of the product graph after each iteration

	Given Graph $G^{(0)}$	Product graph after I iteration $G^{(1)}$	Product graph after II iteration $G^{(2)}$
Number of vertices	4	8	16
Number of edges	4	12	32
Topological Indices ↓			
Wiener (W)	8	48	256
Reverse Wiener (RW)	4	36	224
Reciprocal Complementary Wiener (RCW)	2	4	8
Reciprocal Reverse Wiener (RRW)	4	12	32
Platt Number (F)	8	48	192
First Zagreb index $\left(\mathrm{M}_1\right)$	16	72	256
Second Zagreb index $\left(\mathrm{M}_2\right)$	16	108	512
First Zagreb coindex $\left(\overline{\mathrm{M}_1}\right)$	8	96	704
Second Zagreb coindex $\left(\overline{\mathrm{M}_2}\right)$	8	144	1408
Randic's Connectivity index (R)	2	4	8
Geometric Arithmetic index (GA)	4	12	32
Degree Distance (DD)	32	288	2048

Example 4.



Methylcyclopropane



Carbon skeleton of Methylcyclopropane

Theorem 3.2: The Wiener index of graphs $P_n^{(1)}$ and $P_n^{(2)}$ are respectively $W\left(P_n^{(1)}\right)=4W\left(P_n\right)+n^2$ and $W\left(P_n^{(2)}\right)=16W\left(P_n^{(1)}\right)+8n^2$.

Proof: (i) $W\left(P_n^{(1)}\right)=4W\left(P_n\right)+n^2$

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Table 4. Topological Indices of the product graph after each iteration

	Given Graph $G^{(0)}$	Product graph after I iteration $G^{(1)}$	Product graph after II iteration $G^{(2)}$	Product graph after III iteration $G^{(3)}$
Number of vertices	4	8	16	32
Number of edges	4	12	30	64
Topological Indices ↓				
Wiener (W)	8	48	264	1680
Reverse Wiener (RW)	4	36	216	1792
Reciprocal Complementary Wiener (RCW)	2	4	10	16
Reciprocal Reverse Wiener (RRW)	4	12	34	48
Platt Number (F)	10	52	168	384
First Zagreb index $\left(M_1\right)$	18	76	228	512
Second Zagreb index $\left(M_2\right)$	19	120	436	1024
First Zagreb coindex $\left(\overline{M_1}\right)$	6	92	672	3456
Second Zagreb coindex $\left(\overline{M_2}\right)$	4	130	1250	6912
Randic's Connectivity index (R)	1.89	3.95	7.99	16
Geometric Arithmetic index (GA)	4.32	12.5	30.62	64
Degree Distance (DD)	30	280	1968	13440

Let P_n be the path graph with vertices $(v_1, v_2, ...v_n)$. The graph $P_n^{(1)}$ is obtained by taking two copies of P_n and introducing edges between respective vertices $\left(v_1v_1^1, v_2v_2^1, ...v_nv_n^1\right)$. $\left(v_1^1, v_2^1, ...v_n^1\right)$ denote the vertices of the second copy of P_n .

By definition,

$$W\left(P_n^{(1)}\right)=\frac{1}{2}\left\{\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j^1\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^1,v_j\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^1,v_j^1\right)\right\}$$

$$W\left(P_n^{(1)}\right)=\frac{1}{2}\left\{\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+\left(\underbrace{1+1+...+1}_{n\ times}\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+n\left(n-1\right)\right.$$

$$\left.+\left(\underbrace{1+1+...+1}_{n\ times}\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+n\left(n-1\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)\right\}$$

$$W\left(P_n^{(1)}\right)=\frac{1}{2}\left\{2\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+2\left[\left(\underbrace{1+1+...+1}_{n\ times}\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+n\left(n-1\right)\right]\right\}$$

$$W\left(P_n^{(1)}\right)=\frac{1}{2}\left\{4\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+2n\left(n-1\right)+2n\right\}$$

$$W\left(P_n^{(1)}\right)=4W\left(P_n\right)+n^2$$

(ii) $W\left(P_n^{(2)}\right)=16W\left(P_n^{(1)}\right)+8n^2$

The graph $P_n^{(2)}$ is obtained by taking two copies of $P_n^{(1)}$ and introducing edges between respective vertices $\left(v_1v_1^2, v_1^1v_1^3, v_2v_2^2, v_2^1v_2^3 ..., v_nv_n^2, v_n^1v_n^3\right)$. First copy of $P_n^{(1)}$ has vertices $\left(v_1, v_2, ...v_n, v_1^1, v_2^1, ...v_n^1\right)$ and that the second copy $\left(v_1^2, v_2^2, ...v_n^2, v_1^3, v_2^3, ...v_n^3\right)$.

$$W\left(P_n^{(2)}\right)=\frac{1}{2}\left\{\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j^1\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j^2\right)\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j^3\right)\right.$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^1,v_j\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^1,v_j^1\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^1,v_j^2\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^1,v_j^3\right)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^2,v_j\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^2,v_j^1\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^2,v_j^2\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^2,v_j^3\right)$$

$$\left.+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^3,v_j\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^3,v_j^1\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^3,v_j^2\right)+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i^3,v_j^3\right)\right\}$$

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$$W\left(P_n^{(2)}\right)=\frac{1}{2}\left\{\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+2\left[\underbrace{\left(1+1+...+1\right)}_{n\,times}+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+n\left(n-1\right)\right]\right.$$
$$\left.+\left[\underbrace{\left(1+1+...+1\right)}_{n\,times}+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+n\left(n-1\right)+n^2\right]\right.$$

$$+2\left\{2\left[\underbrace{\left(1+1+...+1\right)}_{n\,times}+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+n\left(n-1\right)\right]+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)\right.$$
$$\left.\left.+\left[\underbrace{\left(1+1+...+1\right)}_{n\,times}+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+n\left(n-1\right)+n^2\right]\right\}\right.$$

$$W\left(P_n^{(2)}\right)=\frac{1}{2}\left\{\left\{4\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+8\left[\underbrace{\left(1+1+...+1\right)}_{n\,times}+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+n\left(n-1\right)\right]\right.\right.$$
$$\left.\left.+4\left[\underbrace{\left(1+1+...+1\right)}_{n\,times}+\sum_{i=1}^{n}\sum_{j=1}^{n}d\left(v_i,v_j\right)+n\left(n-1\right)+n^2\right]\right\}\right.$$

$$W\left(P_n^{(2)}\right)=16W\left(P_n\right)+8n^2$$

Theorem 3.3: The Wiener Index for the graph $K_{1,5}$ after each iteration is

(i) $W\left(K_{1,5}^{(1)}\right)=4W(K_{1,5})+27$

(ii) $W\left(K_{1,5}^{(2)}\right)=16W(K_{1,5})+212$

(iii) $W\left(K_{1,5}^{(3)}\right)=32W(K_{1,5})+488$

Proof: Using the same procedure as followed in Theorem 3.2 we get the above result.

Theorem 3.4: The Wiener Index for the graph $K_{1,4}$ after each iteration is

(i) $W\left(K_{1,4}^{(1)}\right)=4W(K_{1,4})+16$

(ii) $W\left(K_{1,4}^{(2)}\right)=16W(K_{1,4})+68$

(iii) $W\left(K_{1,4}^{(3)}\right)=64W(K_{1,4})+816$

Proof: Using the same procedure as followed in Theorem 3.2 we get the result.

IV. CONCLUSION

An effort is made to calculate topological indices for graphs obtained under specific chemical reactions (combination reactions). The graphs obtained in this manner may or may not represent a stable chemical compound in reality, but it is the interest of the chemist to check the so obtained structure of the resulting graph.

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