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Topological Indices: Study of a Chemical Molecular Structure

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Abstract**:** There is an inherent connection between the chemical properties of chemical compounds and drugs (eg: boiling point and melting point) and their molecular structure. The physical features, chemical reactivity and biological activity of the chemical molecular structures can be understood by topological indices. The lack of chemical experiments can make up the study of topological indices on chemical structure of chemical materials and drugs and it can provide a theoretical basis for manufacturing drugs and chemical materials. In this paper some chemical characteristics of chemical compounds are revealed using topological indices, which may help in pharmaceutical engineering.

Keywords :Sum Connectivity Index, General Randić Index, General Harmonic Index, The first and second Zagreb Indices, The third Zagreb Index, Multiplicative version of first and second Zagreb Indices ,Redefined version of Zagreb Indices.

1.INTRODUCTION

Chemical and pharmaceutical techniques are rapidly increasing in these years. To determine the chemical and physical properties of a chemical compound, we need too many chemically based experiments. But the topological indices reduce the work of chemical experiments. Using topological indices, we can find out physical or chemical and biological features of a molecular structure.

The topological index of a molecular structure is a numerical quantity which gives values to the molecular structure and its branching pattern. There are various indices applied in chemical engineering which helps to find out the relationship between molecular structure and their chemical– physical characteristics. It includes Zagreb Index [1], Randić Index [2], Harmonic Index, General Sum Connectivity Index [3,4].

In mathematical chemistry, chemical compounds are expressed as graphs in which each vertex represents an atom of a molecule structure and each edge implies covalent bonds between two atoms.

Let G = (V, E) be a simple graph with vertex set V(G) = $v_1, v_2, v_3, \dots v_n$ and edge set E(G) = $e_1, e_2, e_3, \dots e_n$ and $|V(G)|$ and $|E(G)|$ are cardinalities of V(G) and E(G). d(u) denote the

ISSN:0971-1260
Vol-22- Issue-14-December-2019

degree of the vertex u and d (u, v) denote the length of the shortest path between any two vertices u and v connected with each other.

Definition-1 [2] The oldest degree based topological index, the Randić Index, denoted by $R_{-\frac{1}{2}}$(G) is defined as, $R_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$

Definition-2 [5] For any real number k∈ R, the General Randić Index, denoted by R_k(G) is defined as,

$$R_k(G) = \sum_{uv \in E(G)} (d(u)d(v))^k$$

Definition-3 [1] The first and second Zagreb index are defined as

$$M_1(G) = \sum_{uv \in E(G)} (d(u))^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} (d(u)d(v))$$

Some authors call M_1(G) as Gutman Index.

Definition-4 [6] The third Zagreb index were defined as $M_3(G) = \sum_{uv \in E(G)} |d(u) - d(v)|$

Definition-5 [6] The modified Second Zagreb index M_2^*(G) is defined as

$$M_2^*(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}$$

The modified Second Zagreb Index can be obtained by setting k = -1 on General Randić Index.

Definition-6 [6] The Sum Connectivity Index χ(G) of a molecular graph G was defined by

$$\chi(G) = \sum_{uv \in E(G)} (d(u) + d(v))^{\frac{-1}{2}}$$

Definition-7 [6] Zhou and Trinajstic extended the concept of Sum Connectivity Index and introduced the General Sum Connectivity Index and introduced the General Sum Connectivity Index as follows.

$$\chi_k(G) = \sum_{uv \in E(G)} (d(u) + d(v))^k$$

Definition-8 [7] The Hyper Zagreb Index can be defined as $HM(G) = \sum_{uv \in E(G)} (d(u) + d(v))^2$

Hyper Zagreb Index can be obtained from General Sum Connectivity Index by setting k = 2

Definition-9[8] The harmonic index for a molecular graph G is defined as,

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}$$

Zhong obtained the minimum and maximum values of the harmonic index for connected molecular graphs and trees [10].

ISSN:0971-1260
Vol-22- Issue-14-December-2019

Definition-10 [9] The general version of Harmonic Index is defined as,

$$H_k(G) = \sum_{uv \in E(G)} \left(\frac{2}{d(u)+d(v)}\right)^k$$

Definition-11 [10] The Geometric Arithmetic Index is defined as, $GA_1(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$

Definition-12 [11] Eliasi and Iranmanesh proposed Ordinary Generalised Arithmetic Index which is defined as

$$OGA_k(G) = \sum_{uv \in E(G)} \left(\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}\right)^k$$

Definition-13 [14] The Generalised version of Zagreb Index was introduced by Azari and Iranmanesh and is defined as

$M_{t_1,t_2}(G) = \sum_{e=uv}(d(u)^{t_1}d(v)^{t_2} + d(u)^{t_2}d(v)^{t_1})$, where the parameters t_1 and t_2 are arbitrary nonnegative integers.

Definition-14 [15,16] Gutman and Ghorbani and Azimi introduced the multiplicative version of first and second Zagreb indices of a molecular graph G. The first multiplicative Zagreb index is denoted as $PM_1(G)$ and the second multiplicative Zagreb index is denoted as $PM_2(G)$.

$$PM_1(G) = \prod_{uv \in E(G)}(d(u) + d(v)), PM_2(G) = \prod_{uv \in E(G)}(d(u)\, d(v))$$

Definition-15 [17] Ranjini et.al introduced the redefined version of Zagreb Indices of a molecular graph G.

$$ReZG_1(G) = \sum_{uv \in E(G)} \frac{d(u)+d(v)}{d(u)d(v)}$$

$$ReZG_2(G) = \sum_{uv \in E(G)} \frac{d(u)d(v)}{d(u)+d(v)}$$

$$ReZG_3(G) = \sum_{uv \in E(G)}(d(u)d(v))\,(d(u) + d(v))$$

Here, $ZG_1(G)$, $ZG_2(G)$ and $ZG_3(G)$ are the first, second and third redefined Zagreb Indices.

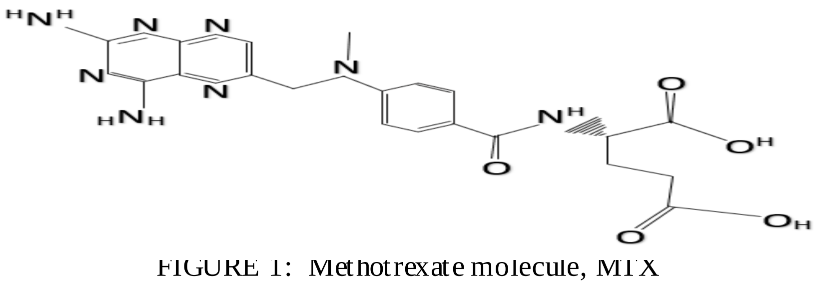

FIGURE 1: Methotrexate molecule, MTX

ISSN:0971-1260
Vol-22- Issue-14-December-2019

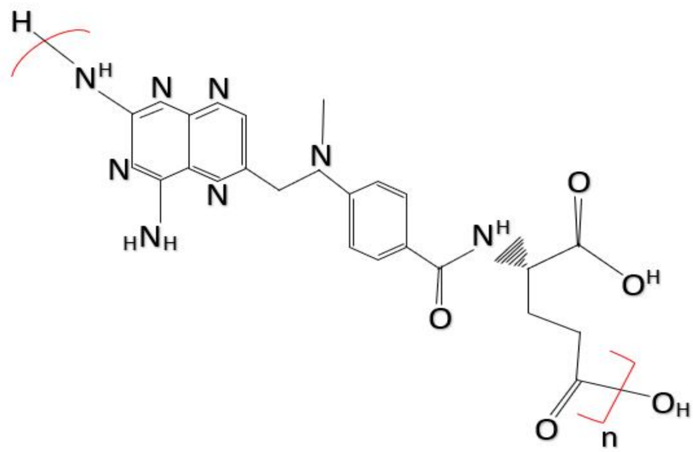

FIGURE 2: Methotrexate block chain, MTX[n]

In the following sections, we first introduce the methotrexate block polymer and the importance of this molecular structure. In section 3, we will present our important results and detailed proof.

2.MOTIVATION

Methotrexate (MTX) molecules are used as a chemotherapy agent and immune system suppressant. Methotrexate is a powerful molecule which is used to treat cancer. It was originally developed to treat against leukemia in the 1940's. But now it is used to treat cancer, autoimmune diseases, ectopic pregnancy and for medical abortions.

Types of cancers it is used for include breast cancer, leukemia, lung cancer, lymphoma and osteosarcoma.Types of autoimmune diseases it is used for include psoriasis, rheumatoid arthritis and Crohn's disease.

Methotrexate belongs to a class of drugs known as antimetabolites. It works by slowing or stopping the growth of cancer cells and suppressing the immune system. It may also be used to control juvenile rheumatoid arthritis. Since 1958, Methotrexate is used in patients with moderate or severe psoriasis [12]. Thus, it is a powerful tool in many severe diseases, especially in anticancer activity. It is widely considered in the pharmacy field [13].Also, we are motivated by the work of Wei Gao, Weifan Wang and Mohammad Reza Farahani on *Topological Indices Study of Molecular Structure in Anticancer Drugs*[6].

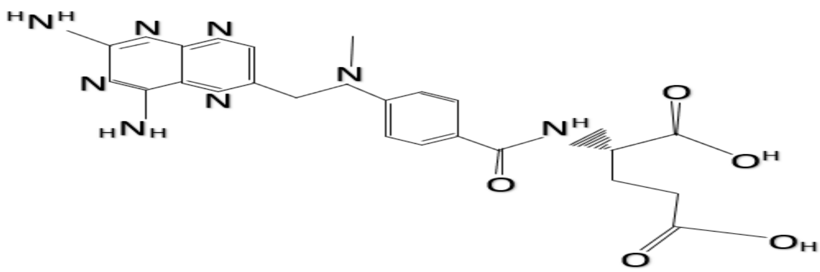

FIGURE 3: The molecular structure of MTX [1]

ISSN:0971-1260
Vol-22- Issue-14-December-2019

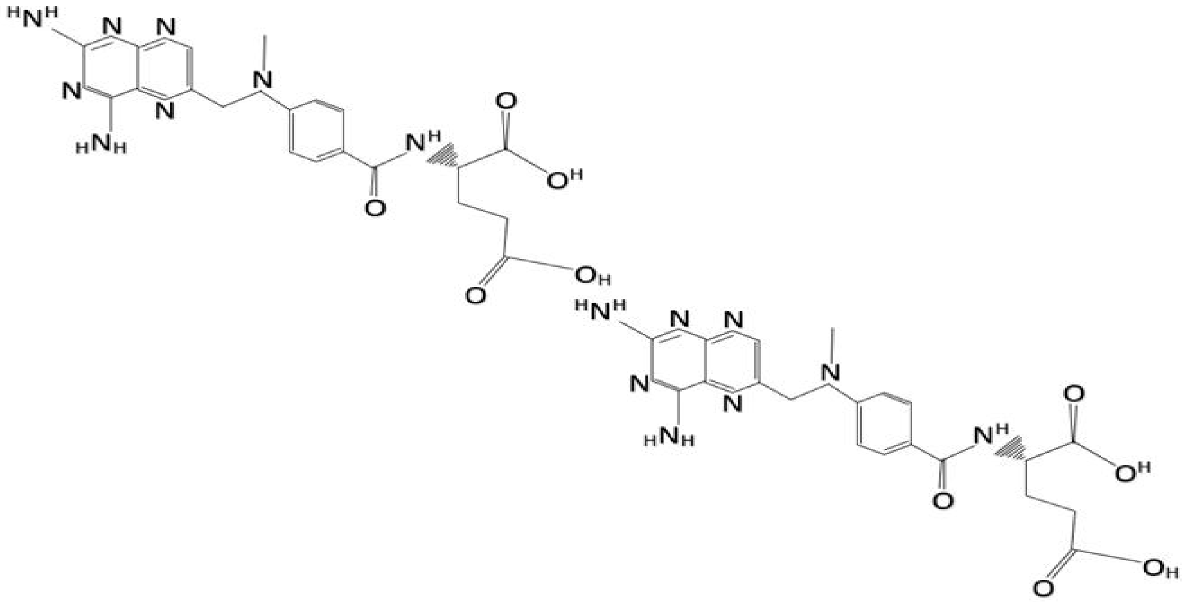

FIGURE 4: The molecular structure of MTX [2]

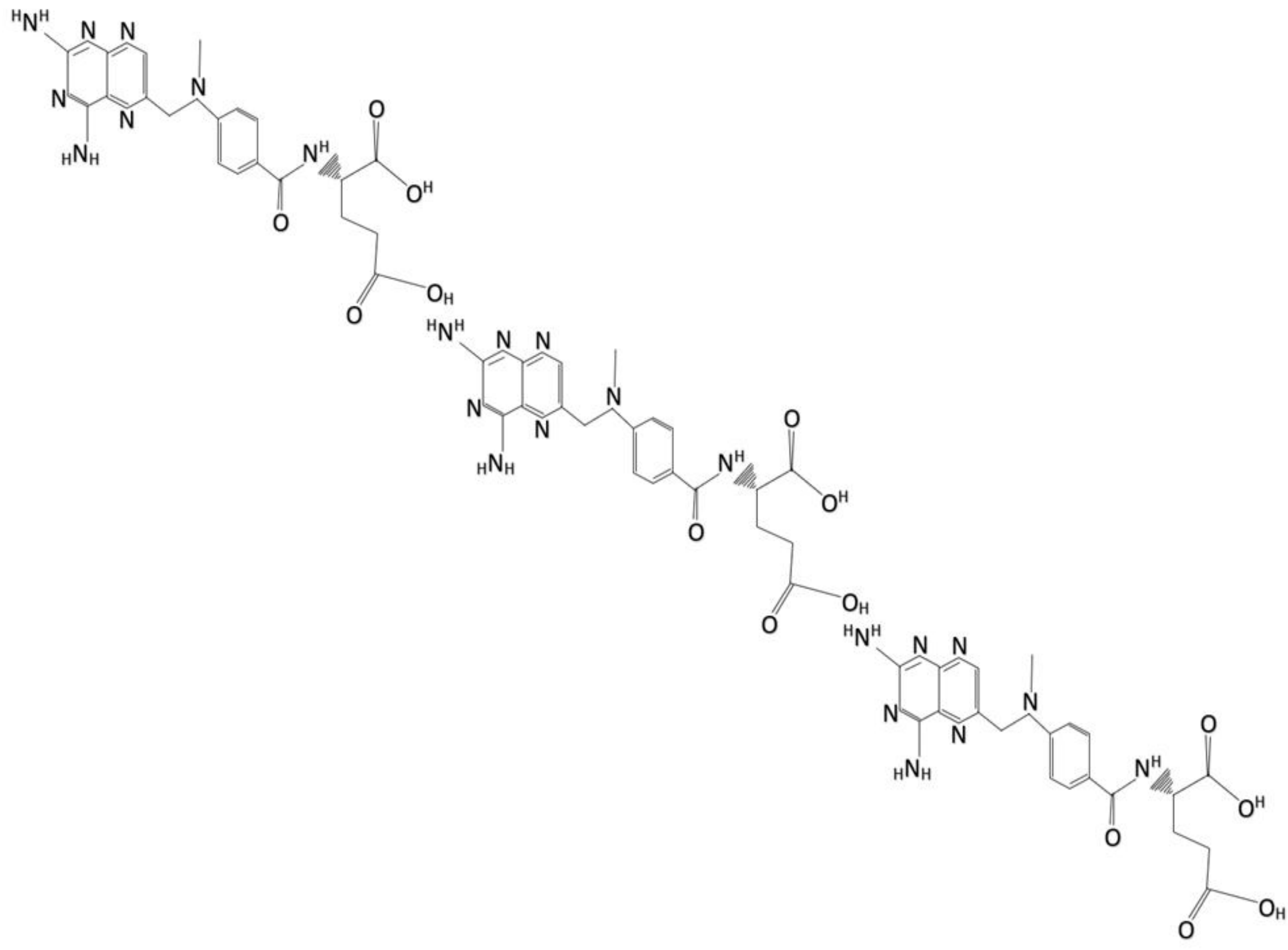

FIGURE 5: The molecular structure of MTX [3]

ISSN:0971-1260
Vol-22- Issue-14-December-2019

In MTX [n], when n = 1,2 and 3 (see figures 3,4 and 5 respectively) we can find the methotrexate molecules in blocks. When n = 2, two methotrexate molecules combines and a water molecule forms. The study of topological indices on MTX [n] molecules are limited. This kind of polymer structure is widely used in pharmaceutical field and medical science. It plays a key role in the development of anticancer drugs. The industrial interest and academic interest of this molecular structure can be researched from a mathematical point of view by using various topological indices.

3. MAIN RESULTS AND PROOFS

Here we are discussing the main results of this paper. We use the techniques of edge dividing.

Theorem 1 Let MTX [n] be the methotrexate block polymer. Then one has,

χ_k(MTX [n]) = (10n + 2) 4^k+ (20n - 2) 5^k+ 5n (6^k)

R_k(MTX [n]) = (6n + 2) 3^k + (4n) 4^k+ (20n - 2) 6^k+ 5n (9^k)

Proof

Let δ and Δ be the minimum degree and maximum degree of MTX [n], respectively. Divide the edge set of E(MTX [n]) into several partitions.

(i) For any i, $2\delta(G) \leq i \leq 2\Delta(G)$, let $E_i = \{e = uv \in E(G) \,/ d(u) + d(v) = i\}$

(ii) For any j, $\delta^2(G) \leq i \leq \Delta^2(G)$, let $E_j^* = \{e = uv \in E(G) \,/ d(u)d(v) = j\}$

By observation and calculation, the edge set of MTX[n] can be divided into following edge subsets.

E_4 or E_3^* : d(u) = 1 and d(v) = 3

E_9^* : d(u) = 3 and d(v) = 3

$E_4 \cap E_4^*$: d(u) = 2 and d(v) = 2

E_6^* : d(u) = 2 and d(v) = 3

Also, we can calculate that $|V(MTX[n]|$ = 32n + 1 and $|E(MTX[n]|$ = 35n

We can deduce the edge subset as,

$|E_4| = |E_3^*|$ = 6n + 2

$|E_5| = |E_6^*|$ = 20n - 2

$|E_4 \cap E_4^*|$ = 4n

$|E_6| = |E_9^*|$ = 5n

By the definition of General Sum Connectivity Index (definition -7),

$$\chi_k(\text{MTX }[n]) = \sum_{uv \in E(G)} (d(u) + d(v))^k$$

$$= \sum_{uv \in E_3^*} (d(u) + d(v))^k + \sum_{uv \in E_4 \cap E_4^*} (d(u) + d(v))^k$$

$$+ \sum_{uv \in E_6^*} (d(u) + d(v))^k + \sum_{uv \in E_9^*} (d(u) + d(v))^k$$

= (6n + 2) 4^k + (4n) 4^k+ (20n - 2) 5^k+ 5n (6^k)

ISSN:0971-1260
Vol-22- Issue-14-December-2019

$= (10n + 2)\ 4^k + (20n - 2)\ 5^k + 5n\ (6^k)$

By the definition of General Randić Index (definition -2),

R_k(MTX [n]) = $\sum_{uv \in E(G)}(d(u)d(v))^k$

$= \sum_{uv \in E_3^*}(d(u)\ d(v))^k + \sum_{uv \in E_4 \cap E_4^*}(d(u)\ d(v))^k + \sum_{uv \in E_6^*}(d(u)\ d(v))^k$

$+ \sum_{uv \in E_9^*}(d(u)\ d(v))^k$

$= (6n + 2)\ 3^k + (4n)\ 4^k + (20n - 2)\ 6^k + 5n\ (9^k)$

Hence, we get the desired proof.

Corollary -1 When we put k = $\frac{-1}{2}$ on χ_k(MTX [n]) = $\sum_{uv \in E(G)}(d(u) + d(v))^k$, we get the Sum Connectivity Index.

$\chi_{\frac{-1}{2}}$(MTX [n]) = $\sum_{uv \in E(G)}(d(u) + d(v))^{\frac{-1}{2}}$

$= (10n + 2)\ 4^{\frac{-1}{2}} + (20n - 2)\ 5^{\frac{-1}{2}} + (5n)\ 6^{\frac{-1}{2}}$

$= \frac{10n+2}{2} + \frac{20n-2}{\sqrt{5}} + \frac{5n}{\sqrt{6}}$

Corollary -2 When we put k = 2 on χ_k(MTX [n]) = $\sum_{uv \in E(G)}(d(u) + d(v))^k$, we get the Hyper Zagreb Index.

HM (MTX [n]) = $\sum_{uv \in E(G)}(d(u) + d(v))^2$

$= (10n + 2)\ 4^2 + (20n - 2)\ 5^2 + (5n)\ 6^2$

$= (10n + 2)\ 16 + (20n - 2)25 + (5n)\ 36$

$= 840n - 18$

Corollary -3 When we put k = $\frac{-1}{2}$ on R_k (MTX [n]) = $\sum_{uv \in E(G)}(d(u)\ d(v))^k$, we get the Randić Index.

$R_{\frac{-1}{2}}$(MTX [n]) = $\sum_{uv \in E(G)}(d(u)\ d(v))^{\frac{-1}{2}}$

$= (6n + 2)\ 3^{\frac{-1}{2}} + (4n)\ 4^{\frac{-1}{2}} + (20n-2)\ 6^{\frac{-1}{2}} + (5n)\ 9^{\frac{-1}{2}}$

$= \frac{6n+2}{\sqrt{3}} + \frac{20n-2}{\sqrt{6}} + \frac{5n}{3} + 2n$

Corollary -4 When we put k = 1 on R_k (MTX [n]) = $\sum_{uv \in E(G)}(d(u)\ d(v))^k$, we get the Second Zagreb Index.

ISSN:0971-1260
Vol-22- Issue-14-December-2019

R_1(MTX [n]) = $\sum_{uv \in E(G)} (d(u)\ d(v))^{-1}$

= (6n + 2) 3^{-1}+ (4n) 4^{-1}+(20n-2) 6^{-1} +(5n) 9^{-1}

= 199n – 6

Corollary -5 When we put k = -1 on R_k (MTX [n]) = $\sum_{uv \in E(G)} (d(u)\ d(v))^{k}$, we get the Modified Second Zagreb Index.

R_{-1}(MTX [n]) = $\sum_{uv \in E(G)} (d(u)\ d(v))^{-1}$

= (6n + 2) 3^{-1}+ (4n) 4^{-1}+(20n-2) 6^{-1} +(5n) 9^{-1}

= $\frac{6n+2}{3} + \frac{4n}{4} + \frac{20n-2}{6} + \frac{5n}{9}$

= $\frac{62n+3}{9}$

Theorem-2 The General Harmonic Index of MTX[n] is

$$H_k(MTX[n]) = (10n + 2)\left(\frac{1}{2}\right)^k + (20n - 2)\left(\frac{2}{5}\right)^k + (5n)\left(\frac{1}{3}\right)^k$$

Proof

We will prove the theorem by edge dividing method as mentioned in theorem-1

H_k(MTX[n]) = $\sum_{uv \in E(G)} \left(\frac{2}{d(u)+d(v)}\right)^k$, by definition 10

$$= \sum_{uv \in E_3^*} \left(\frac{2}{d(u)+d(v)}\right)^k + \sum_{uv \in E_4 \cap E_4^*} \left(\frac{2}{d(u)+d(v)}\right)^k + \sum_{uv \in E_6^*} \left(\frac{2}{d(u)+d(v)}\right)^k + \sum_{uv \in E_9^*} \left(\frac{2}{d(u)+d(v)}\right)^k$$

$$= (6n + 2)\left(\frac{2}{4}\right)^k + (4n)\left(\frac{2}{4}\right)^k + (20n-2)\left(\frac{2}{5}\right)^k + (5n)\left(\frac{2}{6}\right)^k$$

$$= (6n + 2)\left(\frac{1}{2}\right)^k + (4n)\left(\frac{1}{2}\right)^k + (20n-2)\left(\frac{2}{5}\right)^k + (5n)\left(\frac{1}{3}\right)^k$$

$$= (10n + 2)\left(\frac{1}{2}\right)^k + (20n - 2)\left(\frac{2}{5}\right)^k + (5n)\left(\frac{1}{3}\right)^k$$

Hence, we get the desired proof.

Corollary – 1 When we put k = 1 on $H_k(G) = \sum_{uv \in E(G)} \left(\frac{2}{d(u)+d(v)}\right)^k$ we get,

ISSN:0971-1260
Vol-22- Issue-14-December-2019

$$H_1(G) = \sum_{uv \in E(G)} \left(\frac{2}{d(u)+d(v)}\right)^1$$

$$= (10n + 2)\frac{1}{2} + (20n - 2)\frac{2}{5} + 5n\frac{1}{3}$$

$$= \frac{220n+3}{15}$$

By using the method of edge dividing, we get several expressions for several important indices.

Theorem-3 The Ordinary Geometric Arithmetic Index of MTX[n] is

$$OGA_k(MTX[n]) = (6n + 2)\left(\frac{\sqrt{3}}{2}\right)^k + (20n - 2)\left(\frac{2\sqrt{6}}{5}\right)^k + (9n)$$

Theorem-4 The generalised version of Zagreb Indices of MTX [n] is

$$M_{t_1,t_2}(MTX[n]) = (6n+2)(3^{t_2} + 3^{t_1}) + (20n-2)(3^{t_1}2^{t_2} + 3^{t_2}2^{t_1}) + 10n3^{t_1+t_2} + 4n2^{1+t_1+t_2}$$

Theorem-5 The First Zagreb Index of MTX [n] is

$$M_1(MTX [n]) = (6n + 2) + (28n - 2)\, 2^2 + (36n)\, 3^2$$

Theorem-6 The Third Zagreb Index of MTX [n] is $M_3(MTX [n]) = 32n + 2$

Theorem-7 The Multiplicative Zagreb Indices of MTX [n] are

$$PM_1(MTX [n]) = 4^{10n+2}5^{20n-2}6^{5n} \text{ and } PM_2(MTX [n]) = 3^{6n+2}4^{4n}6^{20n-2}9^{5n}$$

Theorem-8 The Redefined Zagreb Indices of MTX [n] are $REZG_1(MTX [n]) = 32n – 1$, $REZG_2(MTX [n]) = 40n - \frac{9}{10}$ and $REZG_3(MTX [n]) = 1006 n – 36$

4.CONCLUSION

In this paper we introduced theoretical expressions of various topological indices of Methotrexate (MTX) molecule. By edge dividing technique we obtained general expressions for various indices including Sum Connectivity Index, General Randić Index, General Harmonic Index, The first and second Zagreb Indices, The third Zagreb Index, Multiplicative version of first and second Zagreb Indices and Redefined version of Zagreb Indices. The results obtained in this paper will promote advanced study of the Methotrexate block polymer in chemical and pharmacy engineering.

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