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Degree-based topological indices and polynomials of cellulose

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Abstract

This work attempts to compute cellulose's chemical structure using topological indices based on the degree and its neighbourhood. The study of graphs using chemistry attracts a lot of researchers globally because of its enormous applications. One such application is discussed in this work, where the structure of cellulose is considered for which the computation of topological indices and analysis of the same are carried out. A polymer is a repeated chain of the same molecule stuck together. Glucose is a natural polymer also called, Polysaccharide. The diet of the humans include fibre which contains cellulose but direct consumption of the same may not be digestible by them.

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1. Introduction

Cellulose [1] is a tasteless, odourless, and biodegradable structural polysaccharides available in crystalline and non-crystalline form. The crystalline form is used in the manufacture of cotton. Cellulose can be digested by animals and hence they get the energy and nutrients required from grass. Cellulose has varied number of applications including its composition in cotton and paper making. It is chemically modified to produce substances like plastics, rayon, adhesives, explosives, and thickening agents. Also, it is used in moisture-proof coats. Cellulose is abundantly utilized in biomedicine and pharmaceuticals. Cellulose derivatives are also

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used in HIV drugs, five flavonoids, one pain reliever and two antibiotics among others. The most abundant biopolymer is cellulose, derived from biomass. It is the form of lignocellulose found in plants. For example, the cellulose content in cotton fibre and wood are (90–95)% and (40–50)% respectively. The structure and shape of plant cells is obtained by the physical and chemical bond with lignin and hemicelluloses. Besides extracting from plants, cellulose can also be obtained through the fermentation of bacterial species such as Acetobacter Xylinam.

In 1839, Anselme Payen first isolated cellulose from plant, it was noticed that the molecular formula was same for cellulose and starch but there were remarkable differences in the solubility and texture of both the compounds. This was the reason that a lot of research started and still is happening in the structure and composition of cellulose to understand the chemical and physical properties of the same. The purified and partially depolymerized cellulose has numerous applications especially as a thickening agent, filtration agent for drilling and waste water treatments. The presence of hydrogen bonds between hydroxyl groups and the oxygen atoms, it exhibits a crystalline fibre structure. The hydrogen bonds cause a limited solubility of cellulose in most solvents and aggregation. The origin of microbial and regenerated cellulose leads to different stability because of the location of hydrogen bonds within the strands.

In the world, cellulose is a chemical compound produced by plants that is available in large quantities. The most structural part of herbal cells and tissues is cellulose.

It is a natural polymer which plays a key role indirectly in the food chain of human beings. This polymer has adaptable uses in many products like veterinary foods, paper, fibres, clothing, cosmetic and pharmaceutical industries. Its derivatives are extensively used in pharmaceutical and cosmetic industries. The two main groups of cellulose family with different properties are cellulose ethers and cellulose esters.

Graph theory has varied tools that possess numerous applications [2, 3, 4]. One such tool is topological index. A topological index guides us about the structural properties of a chemical compound[5, 6, 7, 8, 9, 10, 11]. It acts as a backend data to the drug design where the chemists can fetch necessary information about the compound from its respective topological index. These indices are of highest importance in the study of quantitative structure activity relationship and quantitative structure toxicity relationship(QSAR and QSTR) [12, 13, 14, 15]. There is a growing interest in the study of topological indices through the length and breadth of the globe because of its varied applications[16, 17, 18, 19, 20, 21, 22]. An attempt is made to study the chemical structure known as cellulose as a molecular graph, where bonds and end points of bonds are regarded as edges and the vertices of the graph respectively.

Gutman and Trinajstic [23, 24] introduced the Zagreb indices in the year 1972 to study the pi-electron energy total on the structure of the molecule

$$M_1(G) = \sum_{\nu\omega \in E(G)} (d_\nu + d_\omega).$$

$$M_2(G) = \sum_{\nu\omega \in E(G)} (d_\nu \times d_\omega).$$

Randic proposed a new topological index in 1975 called, Randic index [25] to measure the extent of carbon atom skeleton branching of hydrocarbons.

$$R(G) = \sum_{\nu\omega \in E(G)} \frac{1}{\sqrt{(d_\nu \times d_\omega)}}.$$

Gutman et al. [26] introduced the reciprocal Randic index and it is defined as

$$RR(G) = \sum_{\nu\omega \in E(G)} \sqrt{(d_\nu \times d_\omega)}.$$

[27] introduced the sum-connectivity index that well correlates with the pi-electronic energy of hydrocarbons such as benzenoid structures

$$SCI(G) = \sum_{\nu\omega \in E(G)} \frac{1}{\sqrt{(d_\nu + d_\omega)}}.$$

Harmonic index [28] is a form of Randic index and is defined by

$$H(G) = \sum_{\nu\omega \in E(G)} \frac{2}{(d_\nu + d_\omega)}.$$

The hyper-Zagreb index [29] was introduced by Shirdel et al., in the year 2013 and it is defined as follows

$$HM(G) = \sum_{\nu\omega \in E(G)} (d_\nu + d_\omega)^2.$$

1^{st}, 2^{nd} and 3^{rd} redefined Zagreb indices were introduced by Ranjini et al., in 2016 [30] as

$$ReZG_1(G) = \sum_{\nu\omega \in E(G)} \frac{d_\nu + d_\omega}{d_\nu d_\omega}$$
$$ReZG_2(G) = \sum_{\nu\omega \in E(G)} \frac{d_\nu d_\omega}{d_\nu + d_\omega}$$
$$ReZG_3(G) = \sum_{\nu\omega \in E(G)} (d_\nu d_\omega)(d_\nu + d_\omega).$$

An attempt is made to define and introduce the general redefined Zagreb index, which is denoted by $ReZ_{(\alpha,\beta)}(G)$. It is defined as

$$ReZ_{(\alpha,\beta)}(G) = \sum_{\nu\omega \in E(G)} [d_\nu \times d_\omega]^\alpha [d_\nu + d_\omega]^\beta.$$

where α and β are real numbers. Opting $\alpha = 0$ and $\beta = \alpha$, $\beta \neq 0$, gives rise to the general sum-connectivity index, and defined as

$$\chi_\alpha(G) = \sum_{\nu\omega \in E(G)} [d_\nu + d_\omega]^\alpha,$$

whereas for $\alpha \neq 0$ and $\beta = 0$, the general Randic index R_α is obtained as

$$R_\alpha(G) = \sum_{\nu\omega \in E(G)} [d_\nu \times d_\omega]^\alpha.$$

Few degree-based indices of a graph G can be procured using the general ReZ index by permitting specific values for the parameters α and β are listed in Table 1.

The general polynomials [31, 32] for the graph G which give rise to the topological indices are listed below.

The general Randić polynomial is

$$R_\alpha(G, x) = \sum_{\nu\omega \in E(G)} x^{[d_\nu \times d_\omega]^\alpha}.$$

Table 1: The indices that are based on degree of vertices of a graph G are procured using the general ReZ index by permitting specific values for the parameters α & β

$Topological\ index$	$Corresponding\ ReZ_{(\alpha,\beta)}(G)$
$M_1(G) = 1^{st}\ Zagreb\ index$	$ReZ_{(0,1)}(G)$
$M_2(G) = 2^{nd}\ Zagreb\ index$	$ReZ_{(1,0)}(G)$
$R(G) = Randic\ index$	$ReZ_{(\frac{-1}{2},0)}(G)$
$RR(G) = Reciprocal\ Randic\ index$	$ReZ_{(\frac{1}{2},0)}(G)$
$SCI(G) = Sum-connectivity\ index$	$ReZ_{(0,\frac{1}{2})}(G)$
$H(G) = Harmonic\ index$	$2ReZ_{(0,-1)}(G)$
$HM(G) = Hyper\ Zagreb\ index$	$ReZ_{(0,2)}(G)$
$ReZG_1(G) = Redefined\ 1^{st}\ Zagreb\ index$	$ReZ_{(-1,1)}(G)$
$ReZG_2(G) = Redefined\ 2^{nd}\ Zagreb\ index$	$ReZ_{(1,-1)}(G)$
$ReZG_3(G) = Redefined\ 3^{rd}\ Zagreb\ index$	$ReZ_{(1,1)}(G)$
$\chi_\alpha(G) = General\ sum-connectivity\ index$	$ReZ_{(0,\alpha)}(G)$
$R_\alpha(G) = General\ Randic-connectivity\ index$	$ReZ_{(\alpha,0)}(G)$

The general sum-connectivity polynomial is

$$\chi_\alpha(G,x) = \sum_{\nu\omega\in E(G)} x^{[d_\nu+d_\omega]^\alpha}.$$

The generalized Zagreb polynomial is

$$M_{(\alpha,\beta)}(G,x) = \sum_{\nu\omega\in E(G)} x^{[(d_\nu)^\alpha\times(d_\omega)^\beta+(d_\omega)^\alpha\times(d_\nu)^\beta]}.$$

The redefined 3^{rd} Zagreb polynomial is defined as

$$ReZG_3(G,x) = \sum_{\nu\omega\in E(G)} x^{(d_\nu\times d_\omega)(d_\nu+d_\omega)}.$$

Inspired by these definitions, we introduce the general ReZ index polynomial of a graph G as

$$ReZ_{(\alpha,\beta)}(G,x) = \sum_{\nu\omega\in E(G)} x^{[d_\nu\times d_\omega]^\alpha[d_\nu+d_\omega]^\beta}.$$

where α and β are specific real numbers.

Table 2: Association of general ReZ index polynomial with other polynomials leading to topological indices

$Topological\ index$	$ReZ_{(\alpha,\beta)}(G,x)$
$M_1(G,x) = 1^{st}\ Zagreb\ polynomial$	$ReZ_{(0,1)}(G,x)$
$M_2(G,x) = 2^{nd}\ Zagreb\ polynomial$	$ReZ_{(1,0)}(G,x)$
$HM(G,x) = Hyper\ Zagreb\ polynomial$	$ReZ_{(0,2)}(G,x)$
$ReZG_3(G,x) = Redefined\ 3^{rd}\ Zagreb\ polynomial$	$ReZ_{(1,1)}(G,x)$
$\chi_\alpha(G,x) = General\ sum-connectivity\ polynomial$	$ReZ_{(0,\alpha)}(G,x)$
$R_\alpha(G,x) = General\ Randic-connectivity\ polynomial$	$ReZ_{(\alpha,0)}(G,x)$

Sourav Mondal et al., [33] proposed the neighbourhood version of the various indices and are defined as follows

$$NM_1(G) = \sum_{\nu\omega\in E(G)} (S_\nu + S_\omega).$$

$$NM_2(G) = \sum_{\nu\omega\in E(G)} (S_\nu \times S_\omega).$$

$$ND_4(G) = \sum_{\nu\omega\in E(G)} \frac{1}{\sqrt{(S_\nu \times S_\omega)}}.$$

$$ND_1(G) = \sum_{\nu\omega\in E(G)} \sqrt{(S_\nu \times S_\omega)}.$$

$$ND_2(G) = \sum_{\nu\omega\in E(G)} \frac{1}{\sqrt{(S_\nu + S_\omega)}}.$$

$$NH(G) = \sum_{\nu\omega\in E(G)} \frac{2}{(S_\nu + S_\omega)}.$$

$$HM_N(G) = \sum_{\nu\omega\in E(G)} (S_\nu + S_\omega)^2.$$

$$ND_6(G) = \sum_{\nu\omega\in E(G)} (S_\nu S_\omega)(S_\nu + S_\omega).$$

Neighborhood redefined 1^{st}, 2^{nd} Zagreb indices were proposed by Shanmukha et al., in 2020 [34] as

$$NReZ_1(G) = \sum_{\nu\omega\in E(G)} \frac{S_\nu + S_\omega}{S_\nu S_\omega}.$$

$$NReZ_2(G) = \sum_{\nu\omega\in E(G)} \frac{S_\nu S_\omega}{S_\nu + S_\omega}.$$

Recently, Shanmukha et al., [35] proposed the general neighborhood redefined Zagreb index, denoted by $NReZ_{(\alpha,\beta)}(G)$, and defined as

$$NReZ_{(\alpha,\beta)}(G) = \sum_{\nu\omega\in E(G)} [S_\nu \times S_\omega]^\alpha [S_\nu + S_\omega]^\beta.$$

where α and β are real numbers. By choosing $\alpha = 0$ and $\beta = \alpha, \beta \neq 0$, gives raise to the general neighborhood sum-connectivity index, and defined as

Table 3: The indices that are based on degree of vertices of a graph G are procured using the general $NReZ$ index by permitting specific values for the parameters α & β

$Topological\ index$	$NReZ_{(\alpha,\beta)}(G)$
$NM_1(G) = Neighborhood\ 1^{st}\ Zagreb\ index$	$NReZ_{(0,1)}(G)$
$NM_2(G) = Neighborhood\ 2^{nd}\ Zagreb\ index$	$NReZ_{(1,0)}(G)$
$ND_4(G) = Neighborhood\ Randic\ index$	$NReZ_{(\frac{-1}{2},0)}(G)$
$ND_1(G) = Neighborhood\ reciprocal\ Randic\ index$	$NReZ_{(\frac{1}{2},0)}(G)$
$ND_2(G) = Neighborhood\ sum-connectivity\ index$	$NReZ_{(0,\frac{1}{2})}(G)$
$NH(G) = Neighborhood\ harmonic\ index$	$2NReZ_{(0,-1)}(G)$
$HM_N(G) = Neighborhood\ hyper\ Zagreb\ index$	$NReZ_{(0,2)}(G)$
$NReZ_1(G) = Neighborhood\ redefined\ 1^{st}\ Zagreb\ index$	$NReZ_{(-1,1)}(G)$
$NReZ_2(G) = Neighborhood\ redefined\ 2^{nd}\ Zagreb\ index$	$NReZ_{(1,-1)}(G)$
$ND_6(G) = Neighborhood\ redefined\ 3^{rd}\ Zagreb\ index$	$NReZ_{(1,1)}(G)$
$N\chi_\alpha(G) = Neighborhood\ general\ sum-connectivity\ index$	$NReZ_{(0,\alpha)}(G)$
$NR_\alpha(G) = Neighborhood\ general\ Randic-connectivity\ index$	$NReZ_{(\alpha,0)}(G)$

$$N\chi_\alpha(G) = \sum_{\nu\omega\in E(G)} [S_\nu + S_\omega]^\alpha.$$

whereas for $\alpha \neq 0$ and $\beta = 0$, the general neighborhood Randic index R_α is obtained as

$$NR_\alpha(G) = \sum_{\nu\omega\in E(G)} [S_\nu \times S_\omega]^\alpha.$$

We define few general neighborhood graph polynomials leading to topological indices. They are given below

The general neighborhood Randic polynomial of a graph G is

$$NR_\alpha(G,x) = \sum_{\nu\omega\in E(G)} x^{[S_\nu \times S_\omega]^\alpha}.$$

The general neighborhood sum-connectivity polynomial is

$$N\chi_\alpha(G,x) = \sum_{\nu\omega\in E(G)} x^{[S_\nu + S_\omega]^\alpha}.$$

The general neighborhood Zagreb polynomial is

$$NM_{(\alpha,\beta)}(G,x) = \sum_{\nu\omega\in E(G)} x^{[(S_\nu)^\alpha \times (S_\omega)^\beta + (S_\omega)^\alpha \times (S_\nu)^\beta]}.$$

The neighborhood redefined 3^{rd} Zagreb polynomial is defined as

$$ND_6(G,x) = \sum_{\nu\omega\in E(G)} x^{(S_\nu \times S_\omega)(S_\nu + S_\omega)}.$$

Inspired by these definitions, we introduce the general neighborhood redefined Zagreb polynomial of a graph G as

$$NReZ_{(\alpha,\beta)}(G,x) = \sum_{\nu\omega\in E(G)} x^{[S_\nu \times S_\omega]^\alpha [S_\nu + S_\omega]^\beta}.$$

where α and β are specific real numbers.

Table 4: Association of general neighborhood polynomial and other polynomials leading to topological indices

Topological index	$NReZ_{(\alpha,\beta)}(G,x)$
$NM_1(G,x) =$ *Neighborhood* 1^{st} *Zagreb polynomial*	$NReZ_{(0,1)}(G,x)$
$NM_2(G,x) =$ *Neighborhood* 2^{nd} *Zagreb polynomial*	$NReZ_{(1,0)}(G,x)$
$HM_N(G,x) =$ *Neighborhood hyper Zagreb polynomial*	$NReZ_{(0,2)}(G,x)$
$ND_6(G,x) =$ *Neighborhood redefined* 3^{rd} *Zagreb polynomial*	$NReZ_{(1,1)}(G,x)$
$N\chi_\alpha(G,x) =$ *Neighborhood general sum connectivity polynomial*	$NReZ_{(0,\alpha)}(G,x)$
$NR_\alpha(G,x) =$ *Neighborhood general Randic connectivity index*	$NReZ_{(\alpha,0)}(G,x)$

2. Methodology

Initially, the topological indices are defined and subsequently the general formulae for graph polynomials of the indices are formulated. Following the general formulae, the topological indices are computed. In this process, the methods used are the computational tools like vertex partition method, vertex neighborhood method and edge partition method.

3. Cellulose graph

Cellulose is the most common abundant organic polymer. The cellulose contains cotton fibre, wood and hemp that is dried as its composition. Cellulose is more crystalline in comparison to starch. When heated in water, starch transforms from crystalline to amorphous, while cellulose needs more temperature and pressure to become non-crystalline in water. The structure of cellulose $(C_6H_{10}O_5)_n$ is depicted in Figure 1. The details of cardinality of vertices and edges are given below. The molecular graph of cellulose G_n is as shown in Figure 1. It can be observed that in general $|V(G_n)| = 22n + 1$ and $|E(G_n)| = 24n$.

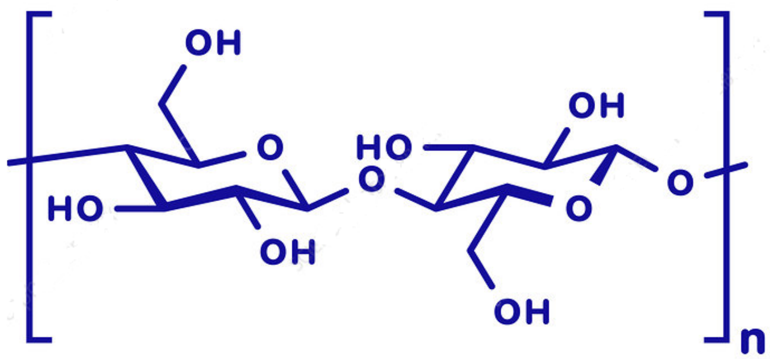

Figure 1: The molecular structure of cellulose.

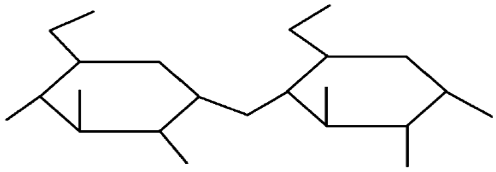

Figure 2: Corresponding molecular graph of cellulose G_1: n=1.

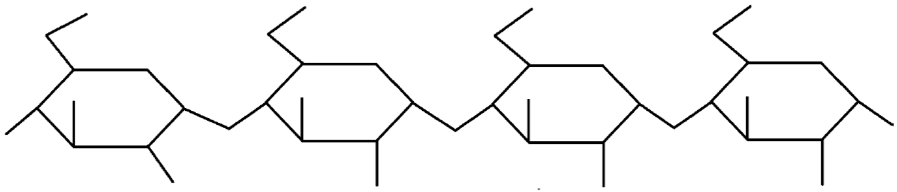

Figure 3: Corresponding molecular graph of cellulose G_2: n=2.

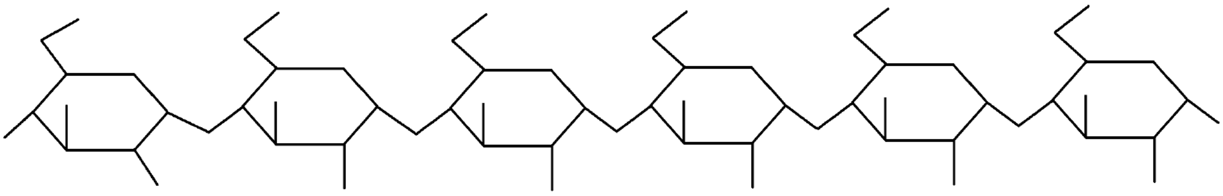

Figure 4: Corresponding molecular graph of cellulose G_3: n=3.

3.1. Results for molecular structure of cellulose graph using degrees of the end vertices

From Figure 1, the degree of incident vertices can be calculated for cellulose graph. The cardinality of the set of vertices is $|V(G_n)| = 22n + 1$. There are four types of vertices with degree 1, degree 2 and degree 3, tabulated in Table 5. The types of edges are tabulated in Table 6:

Table 5: The vertex partition of molecular structure of cellulose graph

$d_\nu \backslash \nu \in V(G)$	$No.\ of\ vertices$
1	$6n + 2$
2	$6n - 1$
3	$10n.$

Table 6: The edge partition of molecular structure of cellulose graph based on degrees of the end vertices of each edge

$(d_\nu, d_\omega)\ where\ \nu\omega \in E(G)$	$No.\ of\ edges$
$E_1 = (1, 2)$	$2n$
$E_2 = (1, 3)$	$4n + 2$
$E_3 = (2, 3)$	$10n - 2$
$E_4 = (3, 3)$	$8n$

Theorem 3.1. *The general redefined Zagreb index $ReZ_{(\alpha,\beta)}$ of cellulose graph is given by*

$$ReZ_{(\alpha,\beta)}(G_n) = 2n[2]^\alpha[3]^\beta + (4n + 2)[3]^\alpha[4]^\beta + (10n - 2)[6]^\alpha[5]^\beta + 8n[9]^\alpha[6]^\beta.$$

Proof. Applying the definition of general $ReZ_{(\alpha,\beta)}$-index on cellulose molecular graph G_n, we get

$$\begin{aligned} ReZ_{(\alpha,\beta)}(G_n) &= \sum_{\nu\omega\in E(G)} [d_\nu \times d_\omega]^\alpha [d_\nu + d_\omega]^\beta \\ &= 2n[2]^\alpha[3]^\beta + (4n+2)[3]^\alpha[4]^\beta + (10n-2)[6]^\alpha[5]^\beta + 8n[9]^\alpha[6]^\beta. \end{aligned}$$

□

Substituting the values of α and β according to Table 1 in the above general equation results in the following topological indices.

Corollary 3.2. *Let G_n be the cellulose graph then,*

i. $M_1(G_n) = 120n - 2$,
ii. $M_2(G_n) = 148n - 6$,
iii. $R(G_n) = \frac{1309}{125}n - \frac{443}{500}$,
iv. $RR(G_n) = \frac{14563}{250}n - \frac{287}{200}$,
v. $SCI(G_n) = \frac{2071}{50}n - \frac{59}{125}$,
vi. $H(G_n) = 10n + \frac{2}{10}$,
vii. $HM(G_n) = 620n - 18$,
viii. $ReZG_1(G_n) = \frac{16167}{500}n + \frac{267}{1000}$,
ix. $ReZG_2(G_n) = 18n - \frac{833}{5000}$,
x. $ReZ_3(G_n) = 792n - 36$,
xi. $\chi_\alpha(G_n) = 2n[3]^\alpha + (4n+2)[4]^\alpha + (10n-2)[5]^\alpha + 8n[6]^\alpha$,
xii. $R_\alpha(G_n) = 2n[2]^\alpha + (4n+2)[3]^\alpha + (10n-2)[6]^\alpha + 8n[9]^\alpha$.

Similarly, the following theorem for general redefined Zagreb polynomial of cellulose graph is obtained.

Theorem 3.3. *The general redefined Zagreb polynomial $ReZ_{(\alpha,\beta)}(G_n, x)$ of cellulose graph is given by*

$$ReZ_{(\alpha,\beta)}(G_n, x) = (2n)x^{[2]^\alpha[3]^\beta} + (4n+2)x^{[3]^\alpha[4]^\beta} + (10n-2)x^{[6]^\alpha[5]^\beta} + (8n)x^{[9]^\alpha[6]^\beta}.$$

Proof.

$$\begin{aligned} ReZ_{(\alpha,\beta)}(G_n, x) &= \sum_{\nu\omega\in E(G)} x^{[d_\nu \times d_\omega]^\alpha [d_\nu + d_\omega]^\beta} \\ &= (2n)x^{[2]^\alpha[3]^\beta} + (4n+2)x^{[3]^\alpha[4]^\beta} + (10n-2)x^{[6]^\alpha[5]^\beta} + (8n)x^{[9]^\alpha[6]^\beta}. \end{aligned}$$

□

Substituting the values of α and β according to Table 2, in the above general polynomial equation results in the following polynomials of topological indices.

Corollary 3.4. *Let G_n be the cellulose graph then,*

i. $M_1(G_n, x) = n(2x^3 + 4x^4 + 10x^5 + 8x^6) + 2x^4 - 2x^5$,
ii. $M_2(G_n, x) = n(2x^2 + 4x^3 + 10x^6 + 8x^9) + 2x^3 - 2x^6$,
iii. $HM(G_n, x) = n(2x^9 + 4x^{16} + 10x^{25} + 8x^{36}) + 2x^{16} - 2x^{25}$,
iv. $ReZ_3(G_n, x) = n(2x^6 + 4x^{12} + 10x^{30} + 8x^{54}) + 2x^{12} - 2x^{30}$,
xi. $\chi_\alpha(G_n, x) = n(2x^{3^\alpha} + 4x^{4^\alpha} + 10x^{5^\alpha} + 8x^{6^\alpha}) + 2x^{4^\alpha} - 2x^{5^\alpha}$,
xii. $R_\alpha(G_n, x) = n(2x^{2^\alpha} + 4x^{3^\alpha} + 10x^{6^\alpha} + 8x^{9^\alpha}) + 2x^{3^\alpha} - 2x^{6^\alpha}$.

The results are demonstrated using an Example 3.5.

Example 3.5. Consider the molecular graph G_2 of cellulose graph shown in Figure 3. For G_2 we have 45 vertices and 48 edges and the edge set have four partitions, $|E_1(G_2)| = 4$, $|E_2(G_2)| = 10$, $|E_3(G_2)| = 18$, $|E_4(G_2)| = 16$.

Using Theorem 3.1, we have

$$ReZ_{(\alpha,\beta)}(G_n) = 2n[2]^\alpha[3]^\beta + (4n+2)[3]^\alpha[4]^\beta + (10n-2)[6]^\alpha[5]^\beta + 8n[9]^\alpha[6]^\beta.$$

Further using particular values of α and β as discussed in Corollary 3.2, we have

i. $M_1(G_2) = 238$,
ii. $M_2(G_2) = 290$,
iii. $R(G_2) = 20.058$,
iv. $RR(G_2) = 115.069$,
v. $SCI(G_2) = 82.368$,
vi. $H(G_2) = 20.2$,
vii. $HM(G_2) = 1222$,
viii. $ReZG_1(G_2) = 64.9326$,
ix. $ReZG_2(G_2) = 35.8334$,
x. $ReZ_3(G_2) = 1548$,
xi. $\chi_1(G_2) = 238$,
xii. $R_1(G_2) = 290$.

As already discussed, the polynomials of degree-based indices provide interesting and relevant information of the graph. For illustration, the first Zagreb index $M_1(G_2)$ and second Zagreb index $M_2(G_2)$ as computed above can be obtained by taking the first derivative of $M_1(G_2, x)$ and $M_2(G_2, x)$ at $x = 1$, respectively. By Corollary 3.4, we have

$$M_1'(G_2, x) = 2(6x^2 + 16x^3 + 50x^4 + 48x^5) + 8x^3 - 10x^4$$

which gives

$$M_1'(G_2, 1) = 238.$$

Similarly

$$M_2'(G_2, x) = 2(4x^1 + 12x^2 + 60x^5 + 72x^8) + 6x^2 - 12x^5$$

which gives

$$M_2'(G_2, 1) = 290.$$

3.2. Results for molecular structure of cellulose graph through neighbourhood degrees of the end vertices

From Figure 1, the degrees of neighbouring vertices are calculated for molecular structure of cellulose graph. The cardinality of the vertex set is $|V(G_n)| = 22n + 1$. There are six types of vertices of degrees 2, 3, 4, 6, 7 and 8 as tabulated in Table 7. The different forms of edges in neighbour degree of vertices are tabulated in Table 8.

Theorem 3.6. *The general neighborhood redefined Zagreb index $NReZ_(\alpha, \beta)$ of cellulose graph is given by*

$$\begin{aligned} NReZ_{(\alpha,\beta)}(G_n) =& 2n[8]^\alpha[6]^\beta + 2[18]^\alpha[9]^\beta + 4n[21]^\alpha[10]^\beta + 2n[28]^\alpha[11]^\beta + (2n+1)[36]^\alpha[12]^\beta \\ &+ (6n-1)[42]^\alpha[13]^\beta + (2n-1)[48]^\alpha[14]^\beta + (2n+1)[49]^\alpha[14]^\beta + (4n-2)[56]^\alpha[15]^\beta. \end{aligned}$$

Table 7: The vertex partition of cellulose graph based on sum of neighbour degrees of the end vertices of each edge

$S_\nu \backslash \nu \in V(G)$	$No.\ of\ Vertices$
2	$2n$
3	$4n+2$
4	$2n$
6	$4n$
7	$8n$
8	$2n-1$

Table 8: The edge partition of cellulose graph based on sum of neighbor degrees of the end vertices of each edge

$(S_\nu, S_\omega)\ Where\ \nu\omega \in E(G)$	$No.\ of\ Edges$
$E_1 = (2,4)$	$2n$
$E_2 = (3,6)$	2
$E_3 = (3,7)$	$4n$
$E_4 = (4,7)$	$2n$
$E_5 = (6,6)$	$2n+1$
$E_6 = (6,7)$	$6n-1$
$E_7 = (6,8)$	$2n-1$
$E_8 = (7,7)$	$2n+1$
$E_9 = (7,8)$	$4n-2$

Proof.

$$\begin{aligned} NReZ_{(\alpha,\beta)}(G_n) = &\sum_{\nu\omega\in E(G)} [S_\nu \times S_\omega]^\alpha [S_\nu + S_\omega]^\beta \\ =&2n[8]^\alpha[6]^\beta + 2[18]^\alpha[9]^\beta + 4n[21]^\alpha[10]^\beta + 2n[28]^\alpha[11]^\beta + (2n+1)[36]^\alpha[12]^\beta \\ &+ (6n-1)[42]^\alpha[13]^\beta + (2n-1)[48]^\alpha[14]^\beta + (2n+1)[49]^\alpha[14]^\beta + (4n-2)[56]^\alpha[15]^\beta. \end{aligned}$$

□

Substituting the values of α and β according to Table 3 in the above general equation results in the following neighborhood topological indices.

Corollary 3.7. *Let G_n be the cellulose graph then,*

i. $NM_1(G_n) = 292n - 13$,
ii. $NM_2(G_n) = 898n - 81$,
iii. $ND_4(G_n) = \frac{1317}{250}n + \frac{43}{200}$,
iv. $ND_1(G_n) = \frac{35811}{250}n - \frac{689}{100}$,
v. $ND_2(G_n) = \frac{17473}{125}n - \frac{1191}{100}$,
vi. $NH(G_n) = \frac{524}{125}n + \frac{953}{5000}$,
vii. $HM_N(G_n) = 3700n - 313$,
viii. $NReZ_1(G_n) = \frac{447}{50}n + \frac{241}{500}$,
ix. $NReZ_2(G_n) = \frac{17583}{250}n - \frac{1813}{500}$,
x. $ND_6(G_n) = 11768n - 1456$,
xi. $N\chi_\alpha(G_n) = 2n[6]^\alpha + 2[9]^\alpha + 4n[10]^\alpha + 2n[11]^\alpha + (2n+1)[12]^\alpha + (6n-1)[13]^\alpha + (2n-1)[14]^\alpha + (2n+1)[14]^\alpha + (4n-2)[15]^\alpha$,
xii. $NR_\alpha(G_n) = 2n[8]^\alpha + 2[18]^\alpha + 4n[21]^\alpha + 2n[28]^\alpha + (2n+1)[36]^\alpha + (6n-1)[42]^\alpha + (2n-1)[48]^\alpha + (2n+1)[49]^\alpha + (4n-2)[56]^\alpha$.

In the same lines, we get the following theorem for general neighborhood redefined Zagreb polynomial of cellulose graph.

Theorem 3.8. *The general neighborhood redefined Zagreb polynomial $NReZ_{(\alpha,\beta)}(G_n, x)$ of cellulose graph is given by*

$$\begin{aligned}NReZ_{(\alpha,\beta)}(G_n, x) =&(2n)x^{[8]^\alpha[6]^\beta} + (2)x^{[18]^\alpha[9]^\beta} + (4n)x^{[21]^\alpha[10]^\beta} + (2n)x^{[28]^\alpha[11]^\beta}\\&+ (2n+1)x^{[36]^\alpha[12]^\beta} + (6n-1)x^{[42]^\alpha[13]^\beta} + (2n-1)x^{[48]^\alpha[14]^\beta} + (2n+1)x^{[49]^\alpha[14]^\beta}\\&+ (4n-2)x^{[56]^\alpha[15]^\beta}.\end{aligned}$$

Proof.

$$\begin{aligned}NReZ_{(\alpha,\beta)}(G_n, x) =& \sum_{\nu\omega\in E(G)} x^{[S_\nu\times S_\omega]^\alpha[S_\nu+S_\omega]^\beta}\\=&(2n)x^{[8]^\alpha[6]^\beta} + (2)x^{[18]^\alpha[9]^\beta} + (4n)x^{[21]^\alpha[10]^\beta} + (2n)x^{[28]^\alpha[11]^\beta}\\&+ (2n+1)x^{[36]^\alpha[12]^\beta} + (6n-1)x^{[42]^\alpha[13]^\beta} + (2n-1)x^{[48]^\alpha[14]^\beta} + (2n+1)x^{[49]^\alpha[14]^\beta}\\&+ (4n-2)x^{[56]^\alpha[15]^\beta}.\end{aligned}$$

□

Substituting the values of α and β according to Table 4, in the above general polynomial equation results in the following polynomials of neighborhood topological indices.

Corollary 3.9. *Let G_n be the cellulose graph then,*

i. $NM_1(G_n, x) = n(2x^6 + 4x^{10} + 2x^{11} + 2x^{12} + 6x^{13} + 4x^{14} + 4x^{15}) + 2x^9 + x^{12} - x^{13} - 2x^{15}$,
ii. $NM_2(G_n, x) = n(2x^8+4x^{21}+2x^{28}+2x^{36}+6x^{42}+2x^{48}+2x^{49}+4x^{56})+2x^{18}+x^{36}-x^{42}-x^{48}+x^{49}-2x^{56}$,
iii. $HM_N(G_n, x) = n(2x^{36} + 4x^{100} + 2x^{121} + 2x^{144} + 6x^{169} + 4x^{196} + 4x^{225}) + 2x^{81} + x^{144} - x^{169} - 2x^{225}$,
iv. $ND_6(G_n, x) = n(2x^{48} + 4x^{210} + 2x^{308} + 2x^{432} + 6x^{546} + 2x^{672} + 2x^{686} + 2x^{840}) + 2x^{162} + x^{432} - x^{546} - x^{672} + x^{686} - 2x^{840}$,
xi. $N\chi_\alpha(G_n, x) = n(2x^{6^\alpha} + 4x^{10^\alpha} + 2x^{11^\alpha} + 2x^{12^\alpha} + 6x^{13^\alpha} + 4x^{14^\alpha} + 4x^{15^\alpha}) + 2x^{9^\alpha} + x^{12^\alpha} - x^{13^\alpha} - 2x^{15^\alpha}$,
xii. $NR_\alpha(G_n, x) = n(2x^{8^\alpha} + 4x^{21^\alpha} + 2x^{28^\alpha} + 2x^{36^\alpha} + 6x^{42^\alpha} + 2x^{48^\alpha} + 2x^{49^\alpha} + 4x^{56^\alpha}) + 2x^{18^\alpha} + x^{36^\alpha} - x^{42^\alpha} - x^{48^\alpha} + x^{49^\alpha} - 2x^{56^\alpha}$.

The results are demonstrated using an Example 3.10.

Example 3.10. Consider the molecular graph G_2 of cellulose graph shown in Figure 3. For G_2 we have 45 vertices and 48 edges and the edge set have nine partitions, $|E_1(G_2)| = 4$, $|E_2(G_2)| = 2$, $|E_3(G_2)| = 8$, $|E_4(G_2)| = 4$, $|E_5(G_2)| = 5$, $|E_6(G_2)| = 11$, $|E_7(G_2)| = 3$, $|E_8(G_2)| = 5$, $|E_9(G_2)| = 6$.

Using Theorem , we have

$$\begin{aligned}NReZ_{(\alpha,\beta)}(G_n) =&2n[8]^\alpha[6]^\beta + 2[18]^\alpha[9]^\beta + 4n[21]^\alpha[10]^\beta + 2n[28]^\alpha[11]^\beta + (2n+1)[36]^\alpha[12]^\beta\\&+ (6n-1)[42]^\alpha[13]^\beta + (2n-1)[48]^\alpha[14]^\beta + (2n+1)[49]^\alpha[14]^\beta + (4n-2)[56]^\alpha[15]^\beta.\end{aligned}$$

Further using particular values of α and β as discussed in Corollary 3.7, we have

i. $NM_1(G_2) = 571$,
ii. $NM_2(G_2) = 1715$,
iii. $ND_4(G_2) = 10.751$,
iv. $ND_1(G_2) = 279.598$,

v. $ND_2(G_2) = 267.658$,
vi. $NH(G_2) = 8.5746$,
vii. $HM_N(G_2) = 7087$,
viii. $NReZ_1(G_2) = 18.362$,
ix. $NReZ_2(G_2) = 137.038$,
x. $ND_6(G_2) = 22080$,
xi. $N\chi_1(G_2) = 571$,
xii. $NR_1(G_2) = 1715$.

As already discussed the degree-based topological polynomials provide riveting and important data about the graph. For instance, the neighborhood first Zagreb index $NM_1(G_2)$ and neighborhood second Zagreb index $NM_2(G_2)$ as computed above can be obtained by taking the first derivative of $NM_1(G_2, x)$ and $NM_2(G_2, x)$ at $x = 1$, respectively. By Corollary 3.9, we have

$M_1'(G_2, x) = 2(12x^5 + 40x^9 + 22x^{10} + 24x^{11} + 78x^{12} + 56x^{13} + 60x^{14}) + 18x^8 + 12x^{11} - 13x^{12} - 30x^{14}$ which gives $NM_1'(G_2, 1) = 571$.

Similarly $NM_2'(G_2, x) = 2(16x^7 + 84x^{20} + 56x^{27} + 72x^{35} + 252x^{41} + 96x^{47} + 98x^{48} + 224x^{55}) + 36x^{17} + 36x^{35} - 42x^{41} - 48x^{47} + 49x^{48} - 112x^{55}$ which gives $NM_2'(G_2, 1) = 1715$.

4. Conclusion

The chemical compound considered under the study is a natural polymer known as cellulose. Cellulose is a polysaccharide comprising of several thousands of glucose units which are connected linearly. It is found on the cell walls of green plants especially in the forms of algae and oomycetes. Cellulose is widely used in pharmaceutical industries because of its exceptional compressibility properties used in solid forms of dosage like tablets. Because of the presence of cellulose, even when tablets are made stiff and hard they dissolve easily. Cellulose derivatives are also used in HIV drugs, five flavonoids, pain reliever and antibiotics among others. This work may be further studied by researchers to widen the applications of cellulose.

References

[1] Gupta, P. K., Raghunath, S. S., Prasanna, D. V., Venkat, P., Shree, V., Chithananthan, C., ... & Geetha, K. (2019). An update on overview of cellulose, its structure and applications. *Cellulose,* 846-1297. 1

[2] Biggs, N., Lloyd, E. K., & Wilson, R. J. (1986). *Graph Theory,* 1736-1936. Oxford University Press. 1

[3] Van Steen, M. (2010). *Graph Theory and Complex Networks.* An introduction, 144. 1

[4] Trinajstic, N. (1992). *Chemical Graph Theory,* 2nd revised CRC Press. Boca Raton, FL. 1

[5] Bonchev, D. (1983). *Information theoretic indices for characterization of chemical structures* (No. 5). Research Studies Press. 1

[6] Estrada, E., Torres, L., Rodriguez, L., & Gutman, I. (1998). An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes. *Indian Journal of Chemistry, 37*(1998), 849-855. 1

[7] Furtula, B., Graovac, A., & Vukicevic, D. (2010). Augmented zagreb index. *Journal of Mathematical Chemistry, 48*(2), 370-380. 1

[8] Ghorbani, M., & Hosseinzadeh, M. A. (2010). Computing ABC_4 index of nanostar dendrimers. *Optoelectronics and Advanced Materials-Rapid Communications*, (4 September 2010), 1419-1422. 1

[9] Gutman, I., & Polansky, O. E. (2012). *Mathematical Concepts in Organic Chemistry.* Springer Science & Business Media. 1

[10] Gutman, I. (1993). Some properties of the Wiener polynomial. *Graph Theory Notes New York, 125*, 13-18. 1

[11] Graovac, A., Ghorbani, M., & Hosseinzadeh, M. A. (2011). Computing fifth geometric-arithmetic index for nanostar dendrimers. *Journal of Mathematical Nanoscience, 1*(1-2), 33-42. 1

[12] Randic, M. (1996). Quantitative structure-property relationship. Boiling points of planar benzenoids. *New Journal of Chemistry, 20*(10), 1001-1009. 1

[13] Hayat, S., Imran, M., & Liu, J. B. (2019). Correlation between the Estrada index and p-electronic energies for benzenoid hydrocarbons with applications to boron nanotubes. *International Journal of Quantum Chemistry, 119*(23), e26016. 1

[14] Shanmukha, M. C., Basavarajappa, N. S., & Shilpa, K. C. (2020). Degree-Based Topological Indices on Asthma Drugs with QSPR Analysis during Covid-19. *European Journal of Molecular & Clinical Medicine, 7*(10), 53-66. 1

[15] Ulanowicz, R. E. (2004). Quantitative methods for ecological network analysis. *Computational Biology and Chemistry, 28*(5-6), 321-339. 1

[16] Hosoya, H. (1988). On some counting polynomials in chemistry. *Discrete Applied Mathematics, 19*(1-3), 239-257. 1

[17] Ranjini, P. S., Lokesha, V., & Usha, A. (2013). Relation between phenylene and hexagonal squeeze using harmonic index. *International Journal of Graph Theory, 1*(4), 116-121. 1

[18] Todeschini, R., & Consonni, V. (2008). *Handbook of Molecular Descriptors* (Vol. 11). John Wiley & Sons. 1

[19] Todeschini, R., & Consonni, V. (2009). *Molecular Descriptors for Chemoinformatics: Volume I: Alphabetical Listing/Volume II: Appendices, References* (Vol. 41). John Wiley & Sons. 1

[20] Vukicevic, D., & Furtula, B. (2009). Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. *Journal of Mathematical Chemistry, 46*(4), 1369-1376. 1

[21] Gao, W., Siddiqui, M. K., Naeem, M., & Imran, M. (2018). Computing multiple ABC index and multiple GA index of some grid graphs. *Open Physics, 16*(1), 588-598. 1

[22] Gao, W., Farahani, M. R., Jamil, M. K., & Siddiqui, M. K. (2016). The redefined first, second and third Zagreb indices of Titania nanotubes $TiO_2[m;n]$. *The Open Biotechnology Journal, 10*, 272-277. 1

[23] Gutman, I., & Trinajstic, N. (1972). Graph theory and molecular orbitals. Total $\phi-$electron energy of alternant hydrocarbons. *Chemical Physics Letters, 17*(4), 535-538. 1

[24] Gutman, I., & Das, K. C. (2004). The first Zagreb index 30 years after. *MATCH Communications in Mathematical and in Computer Chemistry, 50*, 83-92. 1

[25] Randić, M. (1975). Characterization of molecular branching. *Journal of the American Chemical Society, 97*(23), 6609-6615. 1

[26] Gutman, I., Furtula, B., & Elphick, C. (2014). Three new/old vertex-degree-based topological indices. *MATCH Communications in Mathematical and in Computer Chemistry, 72*(3), 617-632. 1

[27] Du, Z., Zhou, B., & Trinajstic, N. (2011). On the general sum-connectivity index of trees. *Applied Mathematics Letters, 24*(3), 402-405. 1

[28] Li, J., & Shiu, W. C. (2014). The harmonic index of a graph. *The Rocky Mountain Journal of Mathematics, 44*(5), 1607-1620. 1

[29] Shirdel, G. H., Rezapour, H., & Sayadi, A. M. (2013). The hyper-Zagreb index of graph operations. *Iranian Journal of Mathematical Chemistry, 4*(2), 213-220. 1

[30] Lokesha, V., Usha, A., Ranjini, P. S., & Deepika, T. (2016). Harmonic index, redefined Zagreb indices of Dragon graph with complete graph. *Asian Journal of Mathematics and Computer Research, 9*, 161-166. 1

[31] Ali, P., Kirmani, S. A. K., Rugaie, O. A., & Azam, F. (2020). Degree-based indices and polynomials of hyaluronic acid-curcumin conjugates. *Saudi Pharmaceutical Journal, 28*, 1093-1100. 1

[32] Vetrik, V. (2019). Polynomials of degree-based indices for hexagonal nanotubes. *UPB Scientific Bulletin, Series B: Chemistry and Materials Science, 81*, 109-120. 1

[33] Mondal, S., De, N., & Pal, A. (2019). Topological properties of graphene using some novel neighborhood degree-based topological indices. *International Journal of Mathematics for Industry, 11*, 1950006-1950014. 1

[34] Shanmukha, M. C., Basavaraappa, N. S., Usha, A., & Shilpa, K. C. (2020). Novel neighbourhood redefined first and second Zagreb indices on Carborundum structures. *Journal of Applied Mathematics and Computing, 2020*, 1-14. 1

[35] Shanmukha, M. C., Usha, A., Basavarajappa, N. S., Savitha, K. C., & Shilpa, K. C. (2021). A general neighborhood redefined Zagreb index on Boron nanotubes. *Malya Journal of Matematik, 9*, 836-843. 1