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CERTAIN TOPOLOGICAL INDICES AND RELATED POLYNOMIALS FOR POLYSACCHARIDES

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Abstract. A polysaccharide is a large molecule made of many smaller monosaccharides. Monosaccharides are simple sugars, like glucose. Special enzymes bind these small monomers together creating large sugar polymers or polysaccharides. A polysaccharide is also called a glycan. Starch, glycogen, and cellulose are examples of polysaccharides. Depending on their structure, polysaccharides can have a wide variety of functions in nature. Some polysaccharides are used for storing energy, some for sending cellular messages, and others for providing support to cells and tissues. In the present work, we focus on the polysaccharides, namely, amylose and blue starch-iodine complex. Several topological indices and polynomials are determined in view of edge dividing methods. Also, depict their graphic behavior.

Keywords: Amylose, blue starch-iodine complex, topological indices and polynomials.

2020 AMS Subject Classification: 05Cxx, 05C09, 05C31.

1. Introduction

Polysaccharides, particularly of plant origin, are prominent components in the diets are herbivores and omnivores. Amylose is a polysaccharide used in various industries as a functional biomaterial. It is mainly a linear component consisting of about $100 - 10,000$ glucose monomers linked by $\alpha(1 \to 4)$ bindings.

Amylose are used in permanent textile finishes, plastics, film making and paper pulp fibre bonding. High amylose starches have been used together with an instant starch or food gum as a binder to provide a crisp coating for french fries which also reduces oil absorption. Used as starches in the usage of sausage casings and food wrappers, incorporation into bread crusts and pasta for more uniform heating in the microwave.

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They are also used in foods legumes and beans, whole grains, vegetables and starchy fruits, rice and potatoes.

In 1814, Colin and Claubry discovered the starch-iodine reaction, which is well renowned to any chemist from basic courses in qualitative and quantitative analysis.

A topological index, which is a graph invariant it does not depend on the labeling or pictorial representation of the graph, is a numerical constant mathematically obtain from the graph structure. In Chemistry, topological indices have been found to be useful in discrimination, chemical documentation, structure property relationships, structure activity relationships and pharmaceutical drug design [4]. There are few main classes of topological indices, namely Wiener index, first and second Zagreb indices, forgotten index, Symmetric division degree index etc., that have been very often studied and investigated by the researchers [15, 16, 17, 18].

The first and second zagreb indices were introduced by Gutman and Trinajstic [9] which are defined as,

$$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)].$$

$$M_2(G) = \sum_{uv \in E(G)} [d(u)d(v)].$$

In 2015, Ediz, S. [6] defined reverse vertex degree and reverse Zagreb indices of a simple connected graphs. The reverse vertex degree of a vertex v of a simple connected graph G defined as;

$$c_v = \Delta - d_v + 1.$$

where Δ denotes the largest of all degrees of vertices of G and d_v denotes the number of edges incident to v.
The first reverse Zagreb beta index [7] of a graph G defined as;

$$CM_1^{\beta}(G) = \sum_{uv \in E(G)} c_u + c_v.$$

And the second reverse Zagreb index of a simple connected graph G defined as;

$$CM_2(G) = \sum_{uv \in E(G)} c_u c_v.$$

The concept of Sombor index was recently introduced by Gutman [8] in the chemical graph theory. It is a vertex-degree-based topological index and defined as;

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}.$$

Inspired by work on Sombor indices, V. R. Kulli, introduced the Nirmala index [11] of a graph G as follows;

$$N(G) = \sum_{uv \in E(G)} \sqrt{d_u + d_v}.$$

The irregularity index was introduced by Albertson [2] in and defined as;

$$M_i(G) = \sum_{uv \in E(G)} |d_u - d_v|.$$

Recently, minus F-index [12] of a graph G is introduced by V. R. Kulli, and defined as;

$$MF(G) = \sum_{uv \in E(G)} |d_u^2 - d_v^2|.$$

Square F-index is defined as;

$$QF(G) = \sum_{uv \in E(G)} (d_u^2 - d_v^2)^2.$$

V. R. Kulli defined the first Gourava index [13] of a graph G is defined as;

$$GO(G) = \sum_{uv \in E(G)} (d_u + d_v + d_u d_v).$$

Inspired by the works of Zagreb indices, Deepika T. introduced the VL index [5] of a graph G is defined as;

$$VL(G) = \frac{1}{2} \sum_{uv \in E(G)} [d_e + d_f + 4].$$

where $d_e = d_u + d_v - 2$ and $d_f = (d_u \times d_v) - 2$, such that d_u and d_v are the degree vertices of u and v in G respectively.

Alameri et.al., in 2020, introduced Y-index [1] defined as;

$$Y(G) = \sum_{u \in E(G)} (d^3(u) + d^3(v))$$

Numerous graph polynomials have been developed for measuring structural information of molecular graphs. Graphs polynomial of found applications in Chemistry in connection with the molecular orbital theory of unsaturated compounds and also an important source of structural descriptors used in developing structure property models. Degree based graph polynomials are useful because they contain a wealth of information about topological indices.

For a simply connected graph G, the first Zagreb beta polynomial [14] is defined as;

$$CM_1^{\beta}(G, x) = \sum_{uv \in E(G)} x^{c_u + c_v}.$$

The Second reverse Zagreb polynomial of a simple connected graph G defined as;

$$CM_2(G, x) = \sum_{uv \in E(G)} x^{c_u c_v}.$$

This paper is organized as follows. Section 1 consists of a brief introduction and literature review which is essential for the development of main results. Forthcoming two sections, we shall give the topological indices, polynomials of the amylose and blue starch-iodine complex. Also, depict their graphic behavior. Section 4 consists conclusion of this work.

2. Amylose

In this sector calculated the many standard topological indices and related polynomials for amylose by using the edge partition technique. Here, also obtained graphic comparison of topological indices of amylose.

Amylose was discovered in 1940, by Meyer and his co-workers found that properties were different from those of native maize starch. It is found in algae and other lower forms of plants. It is a spread polymer of around 6000 glucose deposits with branches on 1 in each 24 glucose ring. It plays an important role in the storage of plant energy and as plants do not require glucose to explode, its dense structure and slow breakdown features are under plant's growth [10].
The reader can find the molecular structure and molecular graphs of amylose in [3].

Theorem 2.1. *For all $n \geq 2$, let $\mathbb{A}$ be the structure of amylose, then*

1. $SO(\mathbb{A}) = 43.55n - 0.8865$.
2. $N(\mathbb{A}) = 26.71n - 8.472$.
3. $VL(\mathbb{A}) = 67n - 4$.
4. $M_i(\mathbb{A}) = 10n + 2$.
5. $MF(\mathbb{A}) = 44n + 6$.
6. $GO(\mathbb{A}) = 134n - 8$.
7. $CM_2(\mathbb{A}) = 26n + 2$.
8. $CM_1^{\beta}(\mathbb{A}) = 36n + 2$.
9. $QF(\mathbb{A}) = 262n + 3$.
10. $Y(\mathbb{A}) = 456n - 18$.

Proof. Here we noticed that in the graph of amylose vertices have degrees 1, 2 or 3. The number of the edges of types are given bellow.

$$E_1 = \{uv \in E(\mathbb{A}) : d_{\mathbb{A}}(u) = 1, d_{\mathbb{A}}(v) = 2\}.$$
$$E_2 = \{uv \in E(\mathbb{A}) : d_{\mathbb{A}}(u) = 1, d_{\mathbb{A}}(v) = 3\}.$$
$$E_3 = \{uv \in E(\mathbb{A}) : d_{\mathbb{A}}(u) = 2, d_{\mathbb{A}}(v) = 3\}.$$
$$E_4 = \{uv \in E(\mathbb{A}) : d_{\mathbb{A}}(u) = 3, d_{\mathbb{A}}(v) = 3\}.$$

One can calculate easily that $|E_1(\mathbb{A})| = n$, $|E_2(\mathbb{A})| = 2n + 2$, $|E_3(\mathbb{A})| = 5n - 2$, $|E_4(\mathbb{A})| = 4n$.

$$\begin{aligned}
\text{Let,}\quad SO(G) &= \sum_{u,v \in E(G)} \sqrt{d(u)^2 + d(v)^2} \\
SO(\mathbb{A}) &= \mid E_{(1,2)} \mid \sum_{u,v \in E_{(1,2)}(\mathbb{A})} \sqrt{d(u)^2 + d(v)^2} + \mid E_{(1,3)} \mid \sum_{u,v \in E_{(1,3)}(\mathbb{A})} \sqrt{d(u)^2 + d(v)^2} \\
&+ \mid E_{(2,3)} \mid \sum_{u,v \in E_{(2,3)}(\mathbb{A})} \sqrt{d(u)^2 + d(v)^2} + \mid E_{(3,3)} \mid \sum_{u,v \in E_{(3,3)}(\mathbb{A})} \sqrt{d(u)^2 + d(v)^2} \\
SO(\mathbb{A}) &= 43.55n - 0.8865.
\end{aligned}$$

Similarly, using the definitions of topological indices we obtain the results. □

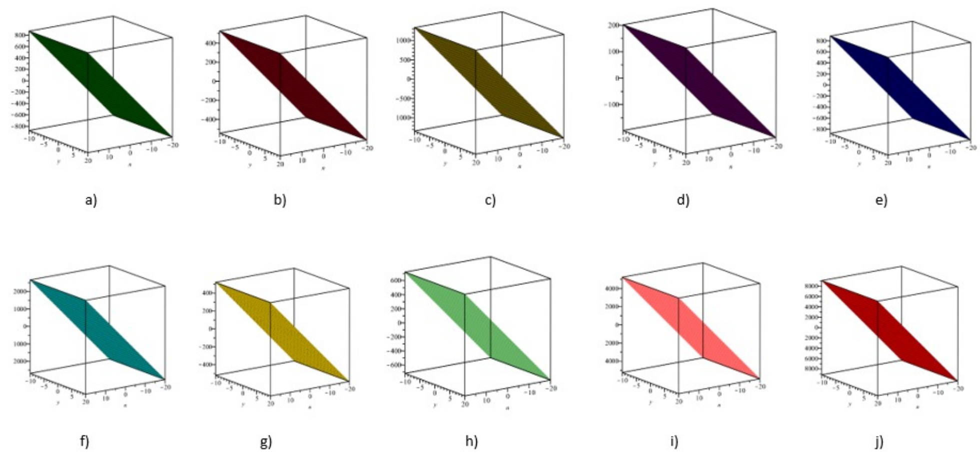

FIGURE 1. 3D plot of topological indices of amylose a) Sombor index b) Nirmala index c) VL index d) irregularity index e) minus F-index f) Gourava index g) Second zagreb index h) first zagreb beta index i) square F index j) Y index .

Theorem 2.2. *let $\mathbb{A}$ be the structure of amylose, then*

1. $SO(\mathbb{A},x) = nx^{\sqrt{5}} + (2n+2)x^{\sqrt{10}} + (5n-2)x^{\sqrt{13}} + 4nx^{\sqrt{18}}$.
2. $N(\mathbb{A},x) = nx^{\sqrt{13}} + (2n+2)x^{\sqrt{4}} + (5n-2)x^{\sqrt{5}} + 4nx^{\sqrt{6}}$.
3. $VL(\mathbb{A},x) = \frac{n}{2}x^5 + (n+1)x^7 + \frac{(5n-2)}{2}x^{11} + 2nx^{15}$.
4. $M_i(\mathbb{A},x) = (6n-2)x + (2n+2)x^2 + 4n$.
5. $MF(\mathbb{A},x) = \frac{n}{x^3} + \frac{2n+2}{x^8} + \frac{5n-2}{x^5} + 4n$.
6. $GO(\mathbb{A},x) = (6n-2) + (2n+2)x^7 + (5n-2)x^{11} + 4nx^{15}$.
7. $CM_2(\mathbb{A},x) = nx^6 + (2n+2)x^3 + (5n-2)x^2 + 4nx^1$.
8. $CM_1^{\beta}(\mathbb{A},x) = nx^5 + (2n+2)x^4 + (5n-2)x^3 + 4nx^2$.
9. $QF(\mathbb{A},x) = nx^9 + (2n+2)x^{64} + (5n-2)x^{25} + 4n$.
10. $Y(\mathbb{A},x) = nx^9 + (2n+2)x^{16} + (5n-2)x^{25} + 4nx^{36}$.

Proof. Using the information given in Theorem 1 and definition of Sombor polynomial, we have

$$
\begin{aligned}
\text{Let,}\quad SO(G,x) &= \sum_{u,v\in E(G)} x^{\sqrt{d(u)^2+d(v)^2}} \\
SO(\mathbb{A},x) &= \mid E_{(1,2)} \mid \sum_{u,v\in E_{(1,2)}(\mathbb{A})} x^{\sqrt{d(u)^2+d(v)^2}} + \mid E_{(1,3)} \mid \sum_{u,v\in E_{(1,3)}(\mathbb{A})} x^{\sqrt{d(u)^2+d(v)^2}} \\
&+ \mid E_{(2,3)} \mid \sum_{u,v\in E_{(2,3)}(\mathbb{A})} x^{\sqrt{d(u)^2+d(v)^2}} + \mid E_{(3,3)} \mid \sum_{u,v\in E_{(3,3)}(\mathbb{A})} x^{\sqrt{d(u)^2+d(v)^2}} \\
SO(\mathbb{A},x) &= nx^{\sqrt{5}} + (2n+2)x^{\sqrt{10}} + (5n-2)x^{\sqrt{13}} + 4nx^{\sqrt{18}}.
\end{aligned}
$$

In the similar method we also obtain results for other polynomials. Hence the Proof. □

3. Blue starch - iodine complex

In this sector calculated the many standard topological indices and related polynomials for blue starch - Iodine Complex by using the edge partition technique. Here, also obtained graphic comparison of topological indices of blue starch - iodine complex.

The main structure of amylose are cyclic degradants known as cyclodextrins. They are obtained enzymatically and may be considered as single turns of the helix of amylose imploding into a circular path. In all of these complexes, cyclodextrin molecules are positioned in front to form dimers and they are piled together to generate large cylinders that resemble the amylose helix in its global structure.

The reader can find the molecular structure and molecular graphs of blue starch - iodine complex in [3].

Theorem 3.1. *For all $n \geq 3$, let $\mathbb{B}$ be the structure of Blue starch - Iodine Complex, then*

1. $SO(\mathbb{B}) = 12.397n^2 + 10.986n + 1.773.$
2. $N(\mathbb{B}) = 7.708n^2 + 7.0817n + 0.944.$
3. $VL(\mathbb{B}) = 18.25n^2 + 71.75n + 8.$
4. $M_i(\mathbb{B}) = 4n^2 - 4.$
5. $MF(\mathbb{B}) = 19n^2 - 7n - 12.$
6. $GO(\mathbb{B}) = 36.5n^2 + 24.5n + 40.$
7. $CM_2(\mathbb{B}) = 7.5n^2 + 14.5n - 4.$
8. $CM_1^{\beta}(\mathbb{B}) = 11n^2 + 13n - 4.$
9. $QF(\mathbb{B}) = 107n^2 + 114n - 156.$
10. $Y(\mathbb{B}) = 119n^2 + 117n + 28.$

Proof. Let $\mathbb{B}$ be a blue starch - iodine complex graph. We have five partitions of the edge set $E(\mathbb{B})$ as follows:

$$E_1 = \{uv \in E(\mathbb{B}) : d_{\mathbb{B}}(u) = 1, d_{\mathbb{B}}(v) = 2\}.$$
$$E_2 = \{uv \in E(\mathbb{B}) : d_{\mathbb{B}}(u) = 1, d_{\mathbb{B}}(v) = 3\}.$$
$$E_3 = \{uv \in E(\mathbb{B}) : d_{\mathbb{B}}(u) = 2, d_{\mathbb{B}}(v) = 2\}.$$
$$E_4 = \{uv \in E(\mathbb{B}) : d_{\mathbb{B}}(u) = 2, d_{\mathbb{B}}(v) = 3\}.$$
$$E_5 = \{uv \in E(\mathbb{B}) : d_{\mathbb{B}}(u) = 3, d_{\mathbb{B}}(v) = 3\}.$$

One can calculate easily that $|E_1(\mathbb{B})| = 2n$, $|E_2(\mathbb{B})| = \sum_{i=1}^{n-1}(n+2) - 2$, $|E_3(\mathbb{B})| = n$, $|E_4(\mathbb{B})| = 4n.$, $|E_4(\mathbb{B})| = \sum_{i=1}^{n-1}(6n-2) + 2$, $|E_5(\mathbb{B})| = 4n$. The proof technique is similar as theorem 1. □

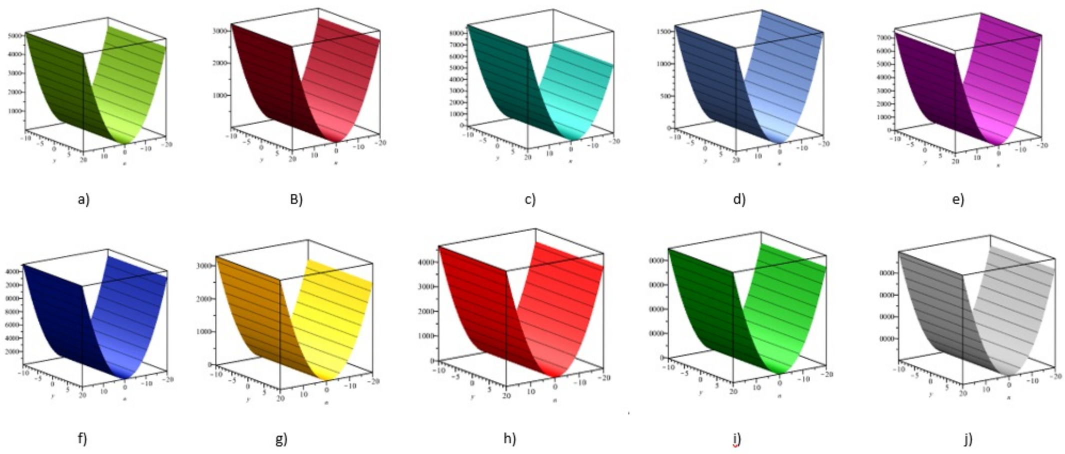

FIGURE 2. 3D plot of topological indices of blue starch - iodine complex graph a) Sombor index b) Nirmala index c) VL index d) irregularity index e) minus F-index f) Gourava index g) Second zagreb index h) first zagreb beta index i) square F index j) Y index.

Theorem 3.2. *let $\mathbb{B}$ be a blue starch - iodine complex graph, then*

1. $SO(\mathbb{B}, x) = 2nx^{\sqrt{5}} + \frac{(n^2+3n-8)}{2}x^{\sqrt{10}} + nx^{\sqrt{8}} + (3n^2-5n+4)x^{\sqrt{10}} + 4nx^{\sqrt{18}}$.
2. $N(\mathbb{B}, x) = 2nx^{\sqrt{13}} + \frac{n^2+5n-8}{2}x^2 + (3n^2-5n+4)x^{\sqrt{5}} + 4nx^{\sqrt{6}}$.
3. $VL(\mathbb{B}, x) = nx^5 + \frac{n^2+3n-8}{4}x^7 + \frac{3n^2-5n+4}{2}x^{11} + 2nx^{15} + nx^8$.
4. $M_i(\mathbb{B}, x) = 5n + (3n^2-3n+4)x + \frac{n^2+3n-8}{2}x^2$.
5. $MF(\mathbb{B}, x) = 5n + 2nx^{-3} + \frac{n^2+3n-8}{2}x^{-8} + (3n^2-5n+4)x^{-5}$.
6. $GO(\mathbb{B}, x) = 2nx^5 + \frac{n^2+3n-8}{2}x^7 + nx^8 + (3n^2-5n+4)x^{11} + 4nx^{15}$.
7. $CM_2(\mathbb{B}, x) = 2nx^6 + (\frac{n^2+3n-8}{2}x^3 + nx^4 + (3n^2-5n+4)x^3 + 4nx$.
8. $CM_1^{\beta}(\mathbb{B}, x) = 2nx^5 + (\frac{n^2+5n-8}{2}x^4 + (3n^2-5n+4)x^3 + 4nx^2$.
9. $QF(\mathbb{B}, x) = 5n + 2nx^9 + \frac{n^2+3n-8}{2}x^{64} + (3n^2-5n+4)x^{25}$.
10. $Y(\mathbb{B}, x) = 2nx^9 + \frac{n^2+3n-8}{2}x^{28} + nx^{16} + (3n^2-5n+4)x^{25} + 4nx^{54}$.

The proof technique is similar as theorem 2.

4. CONCLUSION:

It is important to calculate topological indices of amylose and blue starch-iodine complex because it is a proved fact that topological indices help to predict many properties without going to the wet lab. In the present work we evaluate some topological indices of the amylose and blue starch-iodine complex. First, we obtain degree based indices then recover some polynomial of the structures. Also, the findings are interpreted graphically.

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V. Lokesha for the photography and short autobiography, see TWMS J. App. and Eng. Math. V.6, N.2.

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S. Jain for the photography and short autobiography, see TWMS J. App. and Eng. Math. V.10, N.3.

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