



HAL
open science

Degree-Based Topological Indices of Polysaccharides: Amylose and Blue Starch-Iodine Complex

Anam Rani, Usman Ali

► **To cite this version:**

Anam Rani, Usman Ali. Degree-Based Topological Indices of Polysaccharides: Amylose and Blue Starch-Iodine Complex. *Journal of Chemistry*, 2021, 2021, pp.1-10. 10.1155/2021/6652014. hal-03228318

HAL Id: hal-03228318

<https://hal.sorbonne-universite.fr/hal-03228318>

Submitted on 18 May 2021

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Degree-based Topological Indices of Polysaccharides: Amylose and Blue Starch Iodine Complex

Anam Rani¹, Usman Ali^{2,3,*}

¹ Department of Basics Sciences, Deanship of Preparatory Year King Faisal University Al Ahsa, Saudi Arabia

² Institute de Mathematiques de Jussieu-Paris Rive Gauche -Paris, France (Universite de Paris/Sorbonne Universite)

³ CASPAM, Bahauddin Zakariya University, Multan 66000, Pakistan

arani@kfu.edu.sa, uali@bzu.edu.pk

Abstract

Starch is a polymer of glucose where alpha-linkages associated with glucopyranose units. It comprises a mixture of Amylose and Amylopectin. Furthermore, Amylose is a linear chain of hundreds of glucose molecules. Starches are not allowed to be dissolved in water. They can be digested by breaking down alpha bonds (glycosidic bonds). Its cyclic degradation products, called cyclodextrins, are the best role models for Amylose. They can be considered simple turns of the Amylose propeller that has imploded into a circular path. Both humans and animals have Amylases, which allow them to digest starches. The important sources of starch include potatoes, rice, wheat and maize for human consumption. The production of starches is how plants store glucose. The blue colour of starch produced by an iodine solution or iodine reaction is used for its identification. Polysaccharides with a reduced degree of polymerization, known as dextrins, are produced in the starch's partial acid hydrolysis. Complete hydrolysis leads to glucose. In this article, we compute the topological properties: *Zagreb index* $M_1(\Gamma)$ and $M_2(\Gamma)$, *Randić index* $R_\alpha(\Gamma)$ for $\alpha = -\frac{1}{2}, -1, \frac{1}{2}, 1$, *Atom-bond connectivity index* $ABC(\Gamma)$, *Geometric arithmetic index* $GA(\Gamma)$, *fourth Atom-bond connectivity index* $ABC_4(\Gamma)$ and *fifth Geometric arithmetic index* $GA_5(\Gamma)$, degree-based topological indices a graph Γ representing Polysaccharides, namely, Amylose and Blue Starch Iodine Complex. In the end, we compare these indices and depict their graphic behavior.

Keywords: Polysaccharides, Amylose, Blue Starch Iodine Complex, Zagreb index, Randić index, Atom-bond connectivity index, Geometric arithmetic index

1 Introduction

Amylose has the most basic structure of all nutritional polysaccharides, composed purely of glucose polymers connected only by $\alpha(1-4)$ bonds. Notice that *starch* is, in fact, a combination of Amylose and Amylopectin. Amylose is not allowed to be dissolved in water and is more difficult to digest compared to Amylopectin. The complexing of Amylopectin with Amylose facilitates its water- another view of Amylose solubility and digestibility. Amylose 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. Another function of polysaccharides within cells refers to structural support. Besides, hemicelluloses is another group of polysaccharides located in plant cell walls.

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.

*Corresponding author

The first topological index was derived in 1947 when Wiener worked on the boiling point of paraffin, alkanes. It was known as the Wiener number. Later on, it is called a path number. The work [2] described the M-polynomial and degree-based topological indices of graphs. The articles [7, 9] discussed the symmetric divisor deg index of graphs, first Zegreb after 30 years in changed form and topological indices of molecular structure. The authors in [10] also discussed the π electron energy of hydrocarbons. In the recent years, Hasni et al. computed the degree based topological indices of line graph of benzene ring embedded in P-type-surface in 2D network [1]. In [11] the authors calculated the index numbers for the edge version of geometric-arithmetic index of nanocones. Much research has been done to explain the nature of chromophore absorption at 620 nm that yields starch-iodine complex, the distinctive dark blue colour. Still, there seem to have been many disputes that might be addressed to some extent in recent decades.

Let Γ be connected simple graph with $V(\Gamma)$ a set of vertices and $E(\Gamma)$ a set of edges. Let $u \in V(\Gamma)$ and its degree is represented by \mathfrak{R}_u . The idea of degree-based topological indices began from Wiener index, in 1945, Wiener defined them while studying alkane's boiling point cf. [15]. The first degree-based topological index is *Randić index* given by Milan Randić in [12] and is described as:

$$R_{-\frac{1}{2}} = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}}$$

Generalized Randić index (denoted as $R_\alpha(\Gamma)$) is described as:

$$R_\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} (\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v)^\alpha \quad \alpha = 1, \frac{1}{2}, -\frac{1}{2}, -1 \quad (1)$$

Inverse generalized Randić index (denoted as $RR_\alpha(\Gamma)$) is described as:

$$RR_\alpha(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{(\sqrt{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v})^\alpha}$$

In [8, 10] and [13], Gutman and Trinajstić introduced and defined the *first Zagreb index* (denoted as $M_1(\Gamma)$) and *second Zagreb index* (denoted as $M_2(\Gamma)$) as:

$$\begin{aligned} M_1(\Gamma) &= \sum_{uv \in E(\Gamma)} (\widetilde{\mathfrak{R}}_u + \widetilde{\mathfrak{R}}_v) \\ M_2(\Gamma) &= \sum_{uv \in E(\Gamma)} (\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v) \end{aligned} \quad (2)$$

In [3], Estrada introduced and studied about the *Atom-bond connectivity index* (denoted as $ABC(\Gamma)$). It is defined as:

$$ABC(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\frac{\widetilde{\mathfrak{R}}_u + \widetilde{\mathfrak{R}}_v - 2}{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}} \quad (3)$$

Geometric-arithmetic index (denoted as $GA(\Gamma)$) was given by Vukičević cf. [14] and is defined as:

$$GA(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{2\sqrt{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}}{\widetilde{\mathfrak{R}}_u + \widetilde{\mathfrak{R}}_v} \quad (4)$$

The *fourth version of the ABC index* (denoted as $ABC_4(\Gamma)$) was introduced by Ghorbani in [4] and is defined as:

$$ABC_4(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \quad (5)$$

where $S_u = \sum_{v=N_\Gamma(u)} \widetilde{\mathfrak{R}}_v$ and $N_\Gamma(u) = \{v \in V(\Gamma) | uv \in E(\Gamma)\}$

The fifth version of the GA index (denoted as $GA_5(\Gamma)$) was given by Graovac cf. [5] and is defined as:

$$GA_5(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{2\sqrt{S_u S_v}}{S_u + S_v} \quad (6)$$

2 Result for Amylose

Starch is a polymer of glucose whose glucopyranose alpha bonds bind cells. It is a mixture of Amylose and Amylopectin. Amylose is a linear chain of hundreds of glucose molecules. Starches cannot be dissolved in water. They can be digested by breaking the alpha-bonds (glycosidic bonds). Amylose is a polysaccharide composed of α -D-glucose units, linked by $\alpha(1-4)$ glycosidic bonds. It is one of the two starch components that make up about 20 to 30 percent. Due to its tight spiral structure, Amylose seems to be more resilient to digestion than other starch molecules and is, thus, a significant form of resistant starch [6] (see Figure1 for a molecular structure of Amylose and Figure2 for its unit graph and the graph model corresponding to Amylose for $n=4$, where n is the number of units). In Amylose, there are three types of vertices having degrees 1, 2, and 3. For $n \geq 2$, Amylose has four types of edge partitions as:

$$E_{1,2}(\Gamma) = \{\widetilde{\mathfrak{R}}_u = 1, \widetilde{\mathfrak{R}}_v = 2 \text{ and } u, v \in V(\Gamma)\}$$

$$E_{1,3}(\Gamma) = \{\widetilde{\mathfrak{R}}_u = 1, \widetilde{\mathfrak{R}}_v = 3 \text{ and } u, v \in V(\Gamma)\}$$

$$E_{2,3}(\Gamma) = \{\widetilde{\mathfrak{R}}_u = 2, \widetilde{\mathfrak{R}}_v = 3 \text{ and } u, v \in V(\Gamma)\}$$

$$E_{3,3}(\Gamma) = \{\widetilde{\mathfrak{R}}_u = 3, \widetilde{\mathfrak{R}}_v = 3 \text{ and } u, v \in V(\Gamma)\}$$

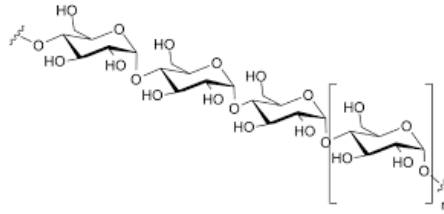


Figure 1: Molecular structure of Amylose

Types of edges	$E_{\{1,2\}}$	$E_{\{1,3\}}$	$E_{\{2,3\}}$	$E_{\{3,3\}}$
Edges	(1,2)	(1,3)	(2,3)	(3,3)
Frequency	n	$2n + 2$	$5n - 2$	$4n$

Table 1: Edge partition of edges based on degree of vertices

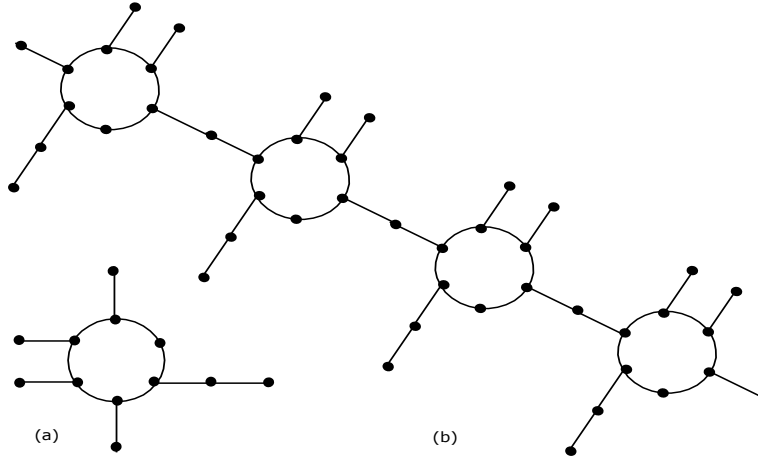


Figure 2: (a) Graph of Amylose for $n=1$ (b) Graph of Amylose for $n=4$

Theorem 1. For all $n \geq 2$, the graph Γ of Amylose, we have the following:

$$\begin{aligned}
 R_1(\Gamma) &= 74n - 6 \\
 R_{\frac{1}{2}}(\Gamma) &= 29.1258n - 1.4349 \\
 R_{-\frac{1}{2}}(\Gamma) &= 5.2363n + 0.3382 \\
 R_{-1}(\Gamma) &= 2.4444n + 0.3334
 \end{aligned}$$

Proof. The general Randić connectivity index $R_\alpha(\Gamma)$ for $\alpha = 1$ is

$$R_1(\Gamma) = \sum_{uv \in E(\Gamma)} \widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v$$

From Table 1 and Equation 1, we get

$$\begin{aligned}
 R_1(\Gamma) &= n(1 \times 2) + (2n + 2)(1 \times 3) + (5n - 2)(2 \times 3) + 4n(3 \times 3) \\
 &= 74n - 6
 \end{aligned}$$

Now, for $\alpha = \frac{1}{2}$, the general Randić connectivity index $R_\alpha(\Gamma)$ is

$$R_{\frac{1}{2}}(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}$$

Again, from Table 1 and Equation 1, we have

$$\begin{aligned}
 R_{\frac{1}{2}}(\Gamma) &= n\sqrt{(1 \times 2)} + (2n + 2)\sqrt{(1 \times 3)} + (5n - 2)\sqrt{(2 \times 3)} + 4n\sqrt{(3 \times 3)} \\
 &= 29.1258n - 1.4349
 \end{aligned}$$

If $\alpha = -\frac{1}{2}$, then

$$R_{-\frac{1}{2}}(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}}$$

From Table 1 and Equation 1, it follows that

$$\begin{aligned} R_{-\frac{1}{2}}(\Gamma) &= \frac{n}{\sqrt{(1 \times 2)}} + \frac{(2n+2)}{\sqrt{(1 \times 3)}} + \frac{(5n-2)}{\sqrt{(2 \times 3)}} + \frac{4n}{\sqrt{(3 \times 3)}} \\ &= 5.2363n + 0.3382 \end{aligned}$$

Now, for $\alpha = -1$, we have

$$R_{-1}(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}$$

From Table 1 and Equation 1, we get

$$\begin{aligned} R_{-1}(\Gamma) &= \frac{n}{(1 \times 2)} + \frac{(2n+2)}{(1 \times 3)} + \frac{(5n-2)}{(2 \times 3)} + \frac{4n}{(3 \times 3)} \\ &= 2.4444n + 0.3334 \end{aligned}$$

□

Theorem 2. For all $n \geq 2$, Γ be the graph of Amylose. Then we have the following:

$$\begin{aligned} M_1(\Gamma) &= 60n - 2 \\ M_2(\Gamma) &= 74n - 6 \\ ABC(\Gamma) &= 8.5423n + 0.2188 \\ GA(\Gamma) &= 11.5738n - 0.2276 \end{aligned}$$

Proof. By using Table 1 and Equation 2, we get

$$\begin{aligned} M_1(\Gamma) &= \sum_{uv \in E(\Gamma)} (\widetilde{\mathfrak{R}}_u + \widetilde{\mathfrak{R}}_v) \\ &= n(1+2) + (2n+2)(1+3) + (5n-2)(2+3) + 4n(3+3) \\ &= 60n - 2 \end{aligned}$$

$$\begin{aligned} M_2(\Gamma) &= \sum_{uv \in E(\Gamma)} \widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v \\ &= n(1 \times 2) + (2n+2)(1 \times 3) + (5n-2)(2 \times 3) + 4n(3 \times 3) \\ &= 74n - 6 \end{aligned}$$

By using Table 1 and Equation 3, we get

$$\begin{aligned} ABC(\Gamma) &= \sum_{uv \in E(\Gamma)} \sqrt{\frac{\widetilde{\mathfrak{R}}_u + \widetilde{\mathfrak{R}}_v - 2}{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}} \\ &= n\sqrt{\frac{1+2-2}{1 \times 2}} + (2n+2)\sqrt{\frac{1+3-2}{1 \times 3}} + (5n-2)\sqrt{\frac{2+3-2}{2 \times 3}} + 4n\sqrt{\frac{3+3-2}{3 \times 3}} \\ &= 8.5423n + 0.2188 \end{aligned}$$

By using Table 1 and Equation 4, we get

$$\begin{aligned}
GA(\Gamma) &= \sum_{uv \in E(\Gamma)} \frac{2\sqrt{\mathfrak{R}_u \mathfrak{R}_v}}{\mathfrak{R}_u + \mathfrak{R}_v} \\
&= 2 \left(n \frac{\sqrt{1 \times 2}}{(1+2)} + (2n+2) \frac{\sqrt{1 \times 3}}{(1+3)} + (5n-2) \frac{\sqrt{2 \times 3}}{(2+3)} + 4n \frac{\sqrt{3 \times 3}}{(3+3)} \right) \\
&= 11.5738n - 0.2276
\end{aligned}$$

□

In the following table, we give the edge partition centered on degree sum of end vertices for each edge.

Types of edges	$E_{\{2,4\}}$	$E_{\{3,6\}}$	$E_{\{3,7\}}$	$E_{\{4,7\}}$	$E_{\{6,6\}}$	$E_{\{6,7\}}$	$E_{\{6,8\}}$	$E_{\{7,7\}}$	$E_{\{7,8\}}$
Number of edges	(2,4)	(3,6)	(3,7)	(4,7)	(6,6)	(6,7)	(6,8)	(7,7)	(7,8)
Frequency	n	1	$2n+1$	n	1	$3n-1$	$n-1$	$2n+1$	$2n-2$

Table 2: Edge partition based on degree sum of end vertices of each edge

Theorem 3. For all $n \geq 2$, the graph Γ of Amylose, we have

$$ABC_4(\Gamma) = 6.4972n + 0.2874$$

$$GA_5(\Gamma) = 11.7142n - 0.123$$

Proof. By using Table 2 and Equation 5, we get

$$\begin{aligned}
ABC_4(\Gamma) &= \sum_{uv \in E(\Gamma)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \\
&= n \sqrt{\frac{2+4-2}{2 \times 4}} + \sqrt{\frac{3+6-2}{3 \times 6}} + (2n+1) \sqrt{\frac{3+7-2}{3 \times 7}} + n \sqrt{\frac{4+7-2}{4 \times 7}} + \sqrt{\frac{6+6-2}{6 \times 6}} \\
&\quad + (3n-1) \sqrt{\frac{6+7-2}{6 \times 7}} + (n-1) \sqrt{\frac{6+8-2}{6 \times 8}} + (2n+1) \sqrt{\frac{7+7-2}{7 \times 7}} + (2n-2) \sqrt{\frac{7+8-2}{7 \times 8}} \\
&= 6.4972n + 0.2874
\end{aligned}$$

By using Table 2 and Equation 6, we get

$$\begin{aligned}
GA_5(\Gamma) &= \sum_{uv \in E(\Gamma)} \frac{2\sqrt{S_u S_v}}{S_u + S_v} \\
&= 2 \left(n \frac{\sqrt{2 \times 4}}{(2+4)} + \frac{\sqrt{3 \times 6}}{(3+6)} + (2n+1) \frac{\sqrt{3 \times 7}}{(3+7)} + n \frac{\sqrt{4 \times 7}}{(4+7)} + \frac{\sqrt{6 \times 6}}{(6+6)} + (3n-1) \frac{\sqrt{6 \times 7}}{(6+7)} \right. \\
&\quad \left. + (n-1) \frac{\sqrt{6 \times 8}}{(6+8)} + (2n+1) \frac{\sqrt{7 \times 7}}{(7+7)} + (2n-2) \frac{\sqrt{7 \times 8}}{(7+8)} \right) \\
&= 11.7142n - 0.123
\end{aligned}$$

□

Table 3: Numerical Comparison of $M_1(G)$, $M_2(\Gamma)$, $ABC(\Gamma)$, $GA(\Gamma)$, $R_1(\Gamma)$, $R_{-1}(\Gamma)$, $R_{\frac{1}{2}}(\Gamma)$, and $R_{-\frac{1}{2}}(\Gamma)$

n	$M_1(\Gamma)$	$M_2(\Gamma)$	$ABC(\Gamma)$	$GA(\Gamma)$	$R_1(\Gamma)$	$R_{-1}(\Gamma)$	$R_{\frac{1}{2}}(\Gamma)$	$R_{-\frac{1}{2}}(\Gamma)$
1	58	68	8.7611	11.3462	68	2.7778	27.6909	5.5746
2	118	142	17.3034	22.92	142	5.2222	56.8166	10.8109
3	178	216	25.8457	34.4938	216	7.6667	85.9424	16.0474
4	238	290	34.388	46.0676	290	10.1111	115.0682	21.2837
5	298	364	42.9303	57.6414	364	12.5556	144.1939	26.5201
6	358	438	51.4726	69.2152	438	15	173.3197	31.7565
7	418	512	60.0149	80.789	512	17.4444	202.4455	36.9929
8	478	586	68.5572	92.3628	586	19.8889	231.5712	42.2293
9	538	660	77.0995	103.9366	660	22.3333	260.6969	47.4656
10	598	734	85.6418	115.5104	734	24.7778	289.8228	52.7020

Table 4: Numerical Comparison of $ABC_4(\Gamma)$ and $GA_5(\Gamma)$

n	1	2	3	4	5	6	7	8	9	10
$ABC_4(\Gamma)$	6.785	13.282	19.779	26.276	32.773	39.271	45.768	52.265	58.762	65.259
$GA_5(\Gamma)$	11.591	23.305	35.019	46.734	58.448	70.162	81.876	93.5906	105.305	117.019

3 Numerical and Graphical Representation

The numeric representation of the results calculated above is illustrated in Tables 3 and 4, while the graphic representation is devoted to Figures 3 and 4.

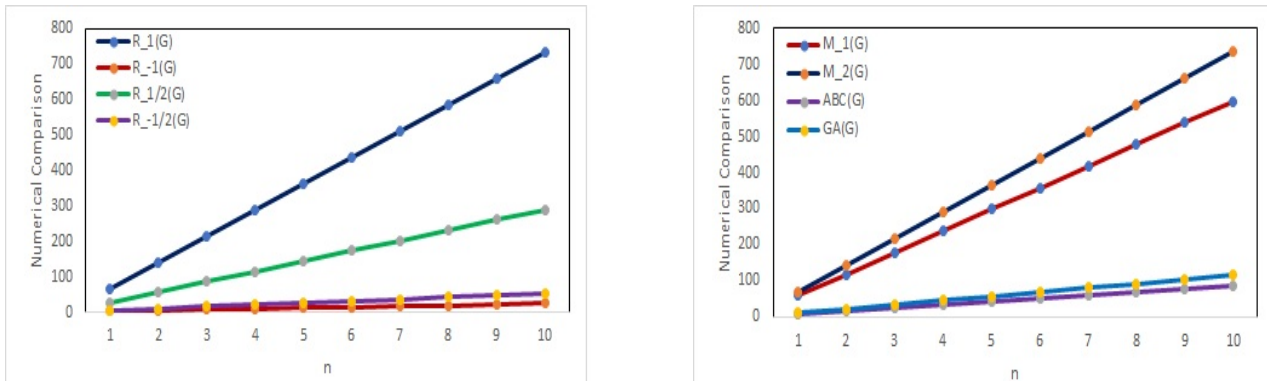


Figure 3: (a) Comparison of R_α for $\alpha = 1, -1, \frac{1}{2}, -\frac{1}{2}$, (b) Comparison of $M_1(\Gamma)$, $M_2(\Gamma)$, $ABC(\Gamma)$ and $GA(\Gamma)$

4 Results for Blue Starch-Iodine Complex

The main structure for 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

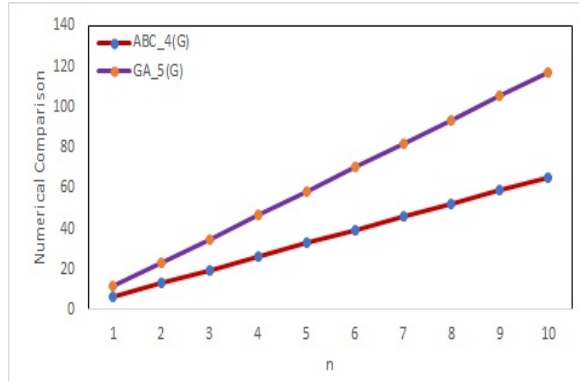


Figure 4: Comparison of $ABC_4(\Gamma)$, $GA_5(\Gamma)$

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 most interesting one is (trimesic acid H_2O)₁₀ HI_5 with linear polyiodide chain. Even though this structural model was accepted. But, unfortunately, cannot shed light on the actual configuration of the polyiodide chain (see Figure5 for Molecular structure of Blue Starch-Iodine and Figure6 for its unit graph and the graph model corresponding to Blue Starch-Iodin for $n=6$, where n is the number of units)). In starch iodine there are three types of vertices having degrees 1, 2, and 3. For $n \geq 3$, Blue Starch-Iodine Complex has five types of edge partitions as:

$$E_{1,2}(\Gamma) = \{\tilde{\mathfrak{R}}_u = 1, \tilde{\mathfrak{R}}_v = 2 \text{ and } u, v \in V(\Gamma)\}$$

$$E_{1,3}(\Gamma) = \{\tilde{\mathfrak{R}}_u = 1, \tilde{\mathfrak{R}}_v = 3 \text{ and } u, v \in V(\Gamma)\}$$

$$E_{2,2}(\Gamma) = \{\tilde{\mathfrak{R}}_u = 2, \tilde{\mathfrak{R}}_v = 2 \text{ and } u, v \in V(\Gamma)\}$$

$$E_{2,3}(\Gamma) = \{\tilde{\mathfrak{R}}_u = 2, \tilde{\mathfrak{R}}_v = 3 \text{ and } u, v \in V(\Gamma)\}$$

$$E_{3,3}(\Gamma) = \{\tilde{\mathfrak{R}}_u = 3, \tilde{\mathfrak{R}}_v = 3 \text{ and } u, v \in V(\Gamma)\}$$

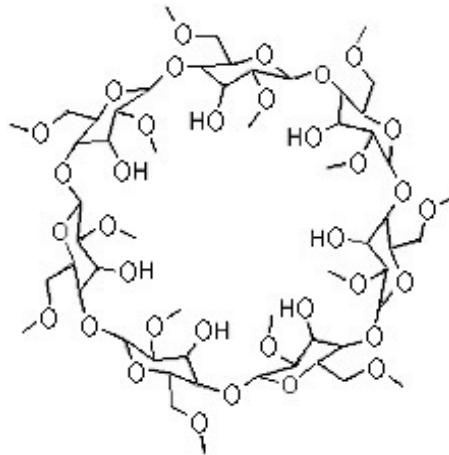


Figure 5: (Molecular structure of Blue Starch-Iodine)

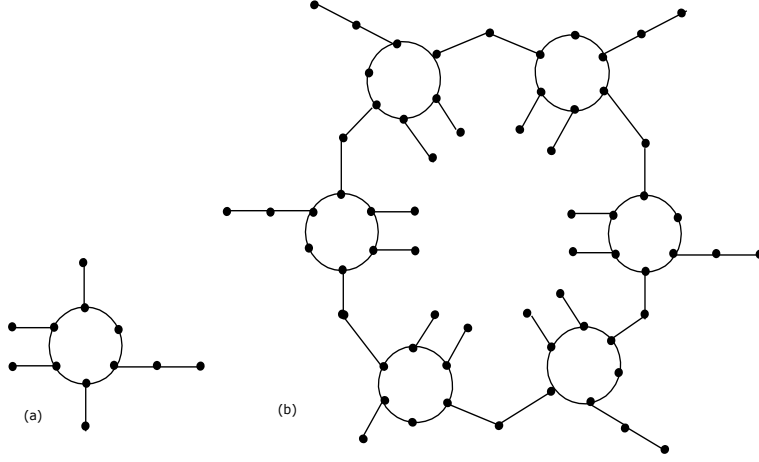


Figure 6: (a) Graph of Blue Starch-Iodine for n=1 (b) Graph of Blue Starch-Iodine for n=6)

Types of edges	$E_{\{1,2\}}$	$E_{\{1,3\}}$	$E_{\{2,2\}}$	$E_{\{2,3\}}$	$E_{\{3,3\}}$
Number of edges	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Frequency	$2n$	$\sum_{i=1}^{n-1} (n+2) - 2$	n	$\sum_{i=1}^{n-1} (6n-2) + 2$	$4n$

Table 5: Edge partition based on degree of vertices

Theorem 4. For all $n \geq 3$, the graph Γ of blue starch-iodine complex, we have the following $R_\alpha(\Gamma)$, $\alpha \in R$:

$$R_1(\Gamma) = 39n^2 - n + 12$$

$$R_{\frac{1}{2}}(\Gamma) = 16.429n^2 - 1.0354 + 2.8695$$

$$R_{-\frac{1}{2}}(\Gamma) = 3.0272n^2 + .5585n - 0.6764$$

$$R_{-1}(\Gamma) = 0.75n^2 + 0.6944n - 0.6667$$

Proof. For $\alpha=1$, the general Randić connectivity index is

$$R_1(\Gamma) = \sum_{uv \in E(\Gamma)} \widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v$$

From Table 5 (for edge partition) and Equation 1, we get

$$\begin{aligned} R_1(\Gamma) &= 2n(1 \times 2) + \left[\sum_{i=1}^{n-1} (n+2) - 2 \right] (1 \times 3) + n(2 \times 2) + \left[\sum_{i=1}^{n-1} (6n-2) + 2 \right] (2 \times 3) + 4n(3 \times 3) \\ &= 39n^2 - n + 12 \end{aligned}$$

Now, for $\alpha = \frac{1}{2}$, we have

$$R_{\frac{1}{2}}(\Gamma) = \sum_{uv \in E(\Gamma)} \sqrt{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}$$

By using Table 5 and Equation 1, after simplification, we have

$$\begin{aligned} R_{\frac{1}{2}}(\Gamma) &= 2n\sqrt{(1 \times 2)} + \left[\sum_{i=1}^{n-1} (n+2) - 2 \right] \sqrt{(1 \times 3)} + n\sqrt{(2 \times 2)} + \left[\sum_{i=1}^{n-1} (6n-2) + 2 \right] \sqrt{(2 \times 3)} + 4n\sqrt{(3 \times 3)} \\ &= 16.429n^2 - 1.0354 + 2.8695 \end{aligned}$$

For $\alpha = -\frac{1}{2}$, we have

$$R_{-\frac{1}{2}}(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\sqrt{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}}$$

From Table 5 and Equation 1, it follows that

$$\begin{aligned} R_{-\frac{1}{2}}(\Gamma) &= \frac{2n}{\sqrt{(1 \times 2)}} + \frac{[\sum_{i=1}^{n-1} (n+2) - 2]}{\sqrt{(1 \times 3)}} + \frac{n}{\sqrt{(2 \times 2)}} + \frac{[\sum_{i=1}^{n-1} (6n-2) + 2]}{\sqrt{(2 \times 3)}} + \frac{4n}{\sqrt{(3 \times 3)}} \\ &= 3.0272n^2 + .5585n - 0.6764 \end{aligned}$$

For $\alpha = -1$, we have

$$R_{-1}(\Gamma) = \sum_{uv \in E(\Gamma)} \frac{1}{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}$$

Again by using Table 5 and Equation 1, we get

$$\begin{aligned} R_{-1}(\Gamma) &= \frac{2n}{(1 \times 2)} + \frac{[\sum_{i=1}^{n-1} (n+2) - 2]}{(1 \times 3)} + \frac{n}{(2 \times 2)} + \frac{[\sum_{i=1}^{n-1} (6n-2) + 2]}{(2 \times 3)} + \frac{4n}{(3 \times 3)} \\ &= 0.75n^2 + 0.6944n - 0.6667 \end{aligned}$$

□

Theorem 5. For all $n \geq 3$, Γ be the graph of blue starch-iodine complex. Then we have the following:

$$\begin{aligned} M_1(\Gamma) &= 34n^2 - 2n + 4 \\ M_2(\Gamma) &= 39n^2 - n + 12 \\ ABC(\Gamma) &= 5.0591n^2 - 0.0523n - 0.4376 \\ GA(\Gamma) &= 6.7448n^2 - 3.0868n + 0.4552 \end{aligned}$$

Proof. By using Table 5 and Equation 2, we get

$$\begin{aligned} M_1(\Gamma) &= \sum_{uv \in E(\Gamma)} (\widetilde{\mathfrak{R}}_u + \widetilde{\mathfrak{R}}_v) \\ &= 2n(1+2) + [\sum_{i=1}^{n-1} (n+2) - 2](1+3) + n(2+2) + [\sum_{i=1}^{n-1} (6n-2) + 2](2+3) + 4n(3+3) \\ &= 34n^2 - 2n + 4 \end{aligned}$$

$$\begin{aligned} M_2(\Gamma) &= \sum_{uv \in E(\Gamma)} \widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v \\ &= 2n(1 \times 2) + [\sum_{i=1}^{n-1} (n+2) - 2](1 \times 3) + n(2 \times 2) + [\sum_{i=1}^{n-1} (6n-2) + 2](2 \times 3) + 4n(3 \times 3) \\ &= 39n^2 - n + 12 \end{aligned}$$

By using Table 5 and Equation 3, we get

$$\begin{aligned}
ABC(\Gamma) &= \sum_{uv \in E(\Gamma)} \sqrt{\frac{\widetilde{\mathfrak{R}}_u + \widetilde{\mathfrak{R}}_v - 2}{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}} \\
&= 2n\sqrt{\frac{1+2-2}{1 \times 2}} + \left[\sum_{i=1}^{n-1} (n+2) - 2 \right] \sqrt{\frac{1+3-2}{1 \times 3}} + n\sqrt{\frac{2+2-2}{2 \times 2}} + \left[\sum_{i=1}^{n-1} (6n-2) + 2 \right] \sqrt{\frac{2+3-2}{2 \times 3}} \\
&\quad + 4n\sqrt{\frac{3+3-2}{3 \times 3}} \\
&= 5.0591n^2 - 0.0523n - 0.4376
\end{aligned}$$

By using Table 5 and Equation 4, we get

$$\begin{aligned}
GA(\Gamma) &= \sum_{uv \in E(\Gamma)} \frac{2\sqrt{\widetilde{\mathfrak{R}}_u \widetilde{\mathfrak{R}}_v}}{(\widetilde{\mathfrak{R}}_u + \widetilde{\mathfrak{R}}_v)} \\
&= 2 \left(2n \frac{\sqrt{1 \times 2}}{(1+2)} + \left[\sum_{i=1}^{n-1} (n+2) - 2 \right] \frac{\sqrt{1 \times 3}}{(1+3)} + n \frac{\sqrt{2 \times 2}}{(2+2)} + \left[\sum_{i=1}^{n-1} (6n-2) + 2 \right] \frac{\sqrt{2 \times 3}}{(2+3)} + 4n \frac{\sqrt{3 \times 3}}{(3+3)} \right) \\
&= 6.7448n^2 - 3.0868n + 0.4552
\end{aligned}$$

□

Types of edges	$E_{\{2,3\}}$	$E_{\{2,4\}}$	$E_{\{3,5\}}$	$E_{\{3,6\}}$	$E_{\{3,7\}}$	$E_{\{4,8\}}$
No. of edges	(2,3)	(2,4)	(3,5)	(3,6)	(3,7)	(4,8)
Frequency	n	n	n	$\sum_{i=1}^{n-1} (1) - 1$	$\sum_{i=1}^{n-1} (n) - 1$	n
Types of edges	$E_{\{5,7\}}$	$E_{\{6,6\}}$	$E_{\{6,7\}}$	$E_{\{6,8\}}$	$E_{\{7,7\}}$	$E_{\{7,8\}}$
No. of edges	(5,7)	(6,6)	(6,7)	(6,8)	(7,7)	(7,8)
Frequency	n	$\sum_{i=1}^{n-1} (1) - 1$	$\sum_{i=1}^{n-1} (3n-2) + 2$	n	$\sum_{i=1}^{n-1} (2) - 2$	$\sum_{i=1}^{n-1} (4n-3) + 3$

Table 6: Edge partition based on degree sum of end vertices of each edge

Theorem 6. For all $n \geq 3$, the graph Γ of blue starch-iodine complex, we have

$$ABC_4(\Gamma) = 4.0798n^2 - 0.7682n + 0.04$$

$$GA_5(\Gamma) = 7.8987n^2 - 3.1339n + 1.1727$$

Proof. By using Table 6 and Equation 5, we get

$$\begin{aligned}
ABC_4(\Gamma) &= \sum_{uv \in E(\Gamma)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \\
&= n\sqrt{\frac{2+3-2}{2 \times 3}} + n\sqrt{\frac{2+4-2}{2 \times 4}} + n\sqrt{\frac{3+5-2}{3 \times 5}} + (n-2)\sqrt{\frac{3+6-2}{3 \times 6}} + (n^2 - n - 1)\sqrt{\frac{3+7-2}{3 \times 7}} \\
&\quad + n\sqrt{\frac{4+8-2}{4 \times 8}} + n\sqrt{\frac{5+7-2}{5 \times 7}} + (n-2)\sqrt{\frac{6+6-2}{6 \times 6}} + (3n^2 - 5n + 4)\sqrt{\frac{6+7-2}{6 \times 7}} \\
&\quad + n\sqrt{\frac{6+8-2}{6 \times 8}} + (2n-4)\sqrt{\frac{7+7-2}{7 \times 7}} + (4n^2 - 7n + 6)\sqrt{\frac{7+8-2}{7 \times 8}} \\
&= 4.0798n^2 - 0.7682n + 0.04
\end{aligned}$$

By using Table 6 and Equation 6, we get

$$\begin{aligned}
 GA_5(\Gamma) &= \sum_{uv \in E(\Gamma)} \frac{2\sqrt{S_u S_v}}{(S_u + S_v)} \\
 &= 2 \left(n \frac{\sqrt{2 \times 3}}{(2+3)} + n \frac{\sqrt{2 \times 4}}{(2+4)} + n \frac{\sqrt{3 \times 5}}{(3+5)} + (n-2) \frac{\sqrt{3 \times 6}}{(3+6)} + (n^2 - n - 1) \frac{\sqrt{3 \times 7}}{(3+7)} + n \frac{\sqrt{4 \times 8}}{(4+8)} + n \frac{\sqrt{5 \times 7}}{(5+7)} \right) \\
 &\quad + (n-2) \frac{\sqrt{6 \times 6}}{(6+6)} + (3n^2 - 5n + 4) \frac{\sqrt{6 \times 7}}{(6+7)} + n \frac{\sqrt{6 \times 8}}{(6+8)} + (2n-4) \frac{\sqrt{7 \times 7}}{(7+7)} + (4n^2 - 7n + 6) \frac{\sqrt{7 \times 8}}{(7+8)} \\
 &= 7.8987n^2 - 3.1339n + 1.1727
 \end{aligned}$$

□

5 Numerical and Graphical Representation

Here, we give numeric and graphic representation for the results calculated in the above section (see Table 7 and 8).

Table 7: Numerical Comparison of $M_1(\Gamma)$, $M_2(\Gamma)$, $ABC(\Gamma)$, $GA(\Gamma)$, $R_1(\Gamma)$, $R_{-1}(\Gamma)$, $R_{\frac{1}{2}}(\Gamma)$, and $R_{-\frac{1}{2}}(\Gamma)$

n	$M_1(\Gamma)$	$M_2(\Gamma)$	$ABC(\Gamma)$	$GA(\Gamma)$	$R_1(\Gamma)$	$R_{-1}(\Gamma)$	$R_{\frac{1}{2}}(\Gamma)$	$R_{-\frac{1}{2}}(\Gamma)$
1	36	50	4.5692	4.1132	50	1.361	18.2633	2.9093
2	136	166	19.6942	21.2608	166	6.0553	66.5148	12.5488
3	304	360	44.9374	51.898	360	13.4162	147.6243	28.2419
4	540	632	80.2988	96.0248	632	23.4437	261.5918	49.9887
5	844	982	125.7784	153.6412	982	36.1378	408.4173	77.7891
6	1216	1410	181.3762	224.7472	1410	51.4985	588.1007	111.6433
7	1656	1916	247.0922	309.3428	1916	69.5258	800.6421	151.5512
8	2164	2500	322.9264	407.428	2500	90.2197	1046.0415	197.5126
9	2740	3162	408.8788	519.0028	3162	113.5802	1324.2989	249.5278
10	3384	3902	504.9494	644.0672	3902	139.6073	1635.4143	307.5967

Table 8: Numerical Comparison of $ABC_4(\Gamma)$ and $GA_5(\Gamma)$

n	1	2	3	4	5	6	7	8	9	10
$ABC_4(\Gamma)$	3.35	14.82	34.45	62.24	98.19	142.30	194.57	255	323.59	400.34
$GA_5(\Gamma)$	5.94	26.49	62.86	115.02	182.97	266.72	366.27	481.62	612.76	759.70

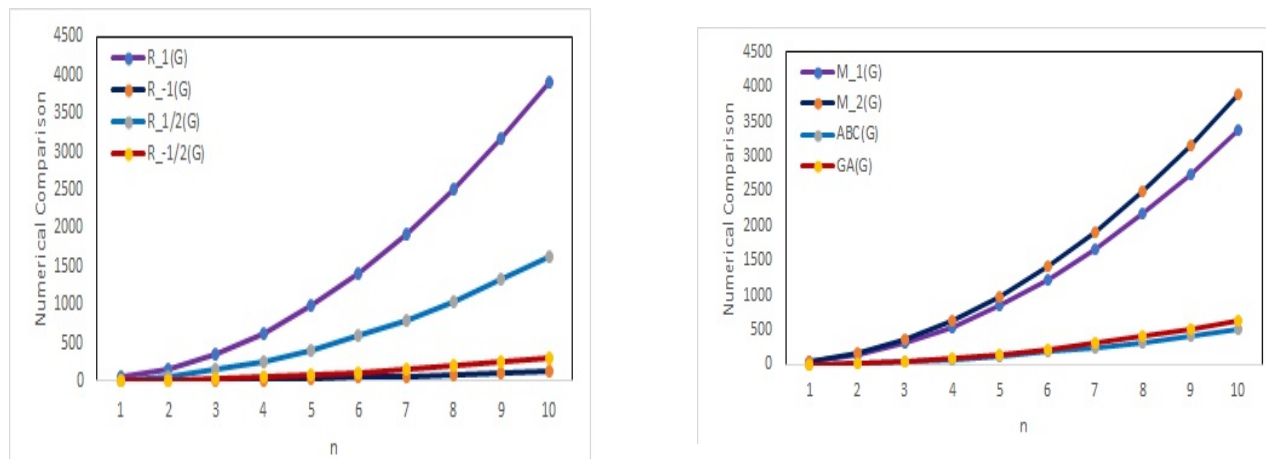


Figure 7: (a) Comparison of $R_\alpha(\Gamma)$ for $1, -1, \frac{1}{2}, -\frac{1}{2}$, (b) Comparison of $M_1(\Gamma), M_2(\Gamma), ABC(\Gamma)$ and $GA(\Gamma)$

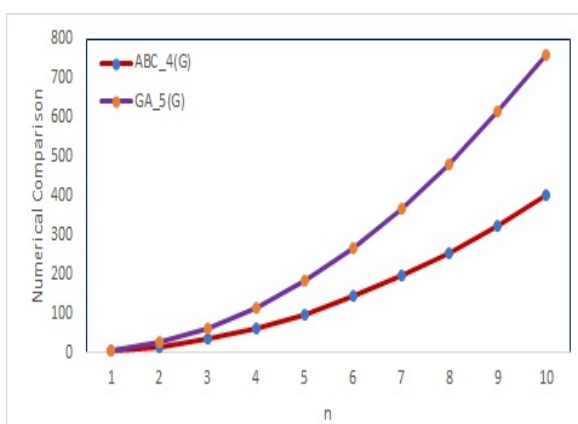


Figure 8: Comparison of $ABC_4(G), GA_5(G)$

6 Conclusion

Amylose has a significant function in the storage of plant energy. It is not easy to digest Amylopectin; however, it occupies less space than Amylopectin due to its spiral structure. Consequently, for storage in plants, it is the preferred starch. A mixture of iodine and potassium iodide in water is light orange-brown. When added to a sample containing starch, such as the bread pictured above, the color will change to a deep blue (see the comparison of different indices in Figures 7 and 8). In this study, we have calculated degree-dependent topological-indices of Amylose and Blue Starch-Iodine. We observed that $R_{-\frac{1}{2}}$ is closely related to geometric arithmetic, R_{-1} is closely related to atom bond connectivity bond and modified atom bond connectivity, the second zegrab is the first Randic index, while $R_{\frac{1}{2}}$ is approximately equal to the modified geometric arithmetic of Amylose. Similarly, Other observations can take place from the graphical representations given in this paper.

7 Funding

This project is sponsored by the Deanship of Scientific Research under Nasher Proposal No. 206152, King Faisal University.

References

- [1] A. Ahmad, K. Elahi, R. Hasni and M. F. Nadeem, Computing the degree based topological indices of line graph of benzene ring embedded in P-type-surface in 2D network, *J. Inf. Optim. Sci.*, 40(7)(2019), 1511-1528.
- [2] E. Deutsch and S. Klavžar, M-polynomial and degree-based topological indices, *Iran. J. Math. Chem.*, 6(2)(2015), 93-102.
- [3] E. Estrada and L. Torres, L. Rodríguez and I. Gutman, An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes, *Indian J. Chem.*, 37A(1998), 849-855.
- [4] M. Ghorbani and M. Hosseinzadeh, Computing ABC_4 index of nanostar dendrimers, *Optoelectron. Adv. Mater. Rapid Commun.*, 4(2010), 1419-1422.
- [5] A. Graovac, M. Ghorbani and M. Hosseinzadeh, Computing fifth geometric-arithmetic index for nanostar dendrimers, *J. Math. Nanosci.*, 1(2011), 33-42.
- [6] M. Green, G. Blankenhorn and H. Hart, Which starch fraction is water-soluble, Amylose or Amylopectin? *J. Chem. Educ.*, 52(11)(1975), 729.
- [7] C. Gupta, V. Lokesh, S. Shwetha and P. Ranjini, On the symmetric division deg index of graph, *Southeast Asian Bull. Math.*, 40(1)(2016), 41-51.
- [8] I. Gutman and K. Das, The first zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem*, 50(1)(2004), 83-92.
- [9] I. Gutman and O. Polansky, Topological indices, *Mathematical Concepts in Organic Chemistry*, Springer, 1986.
- [10] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. total ϕ -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, 17(4)(1972), 535-538.
- [11] M. F. Nadeem, S. Zafar and Z. Zahid, On the edge version of geometric-arithmetic index of nanocones, *Stud. Univ. Babeş-Bolyai Chemia.*, 61(1)(2016), 273-282.
- [12] M. Randić, Characterization of molecular branching, *J. Amer. Chem. Soc.*, 97(23)(1975), 6609-6615.
- [13] N. Trinajstić, S. Nikolić, A. Miličević and I. Gutman, About the zagreb indices, *Kemija u industriji: Časopis kemičara i kemijskih inženjera Hrvatske*, 59(12)(2010), 577-589.
- [14] D. Vukičević and B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degree of edges, *J. Math. Chem.*, 46(2009), 1369-1376.
- [15] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.*, 69(1)(1947), 17-20.