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SOME BOND-ADDITIVE INDICES AND ITS POLYNOMIAL OF CELLULOSE

P. Kandan[1,2], S. Subramanian[2]

[1,*]Department of Mathematics, Annamalai University, Annamalai Nagar-608 002, India, kandan2k@gmail.com

[2]Department of Mathematics, Government Arts College, Chidambaram-608 102, India, sssubramanian87@gmail.com

Abstract. Cellulose is one of the natural bio-polymers which have been extensively used in various fields due to their valuable and remarkable chemical and physical properties. Due to a key ingredients of cellulose in various product, it's applications have widely been recognized in many industries like pharmaceutical, bio-fuel, textiles, etc. The study of graphs using chemistry attracts a lot of researchers globally because of its enormous application. One such application is studying topological indices of a chemical graph associated to a molecular structure. In this this work we have obtained the exact value of szeged, Padmakar-Ivan(PI), additively weighted PI index, multiplicatively weighted PI index, additively weighted szeged index, multiplicatively weighted szeged index and its polynomial for cellulose chemical structure. Moreover we derived the relation between these indices for the cellulose.

Key words and Phrases: Cellulose, Szeged index, Padamakar-Ivan index, Padmakar-Ivan polynomial, Szeged polynomial

1. INTRODUCTION

Most of the chemical compounds under consideration are carbon-based. Often one uses the term chemical graphs (molecular structure) of a compound is presented with a graph, where the edges indicate the links and the vertices represent the atoms. Both in the context of complex networks and in more traditional applications of chemical graph theory, it garnered a great deal of interest. It aids in the modeling of a wide range of systems, the structure and operation of which are influenced by the connection patterns of its constituent parts. Modern materials science needs have encouraged the creation of a wide range of bio-based materials, in which cellulose and its derivatives play a significant part, as a reaction to environmental concerns in[3, 8, 11, 18, 21, 29]. Because of cellulose's exceptional and one-of-a-kind chemical and physical properties, it has received wide recognition in a number of industries. The main cause of this is because cellulose is extremely rigid due to the tight link between its molecules. It is the most prevalent organic substance on the planet in terms of chemistry. The molecules of cellulose are strongly bonded by hydrogen bonds as a result of their intricate intra- and extra molecular interactions. As a result, they are insoluble in typical polar solvents like water,

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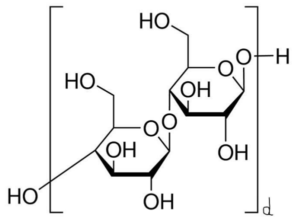

Figure 1. The molecular structure of Cellulose.

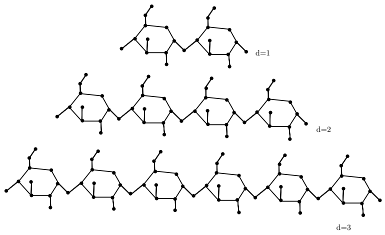

Figure 2. The chemical graph of Cellulose.

alcohols, and amines, which makes it challenging to process into the proper shape. The three-dimensional structure of the cellulose network $(C_6H_{10}O_5)_d$ is denoted by CL_d, where d is the countable of cellulose units, Figure 1. is the molecular structure, represented of cellulose network and Figure 2. represented the chemical graph of cellulose on $d = 1$, $d = 2$ and $d = 3$ units.

Over the last two decades, a lot of different of numerical values have been suggested and investigated, referred to variably as structural invariants, topological indices, or molecular descriptors. A molecule's topology is expressed numerically as a topological description. In Quantitative Structure-Property Relationship (QSPR) and Quantitative Structure-Activity Relationship (QSAR) investigations, these topological descriptors are utilized to estimate the physicochemical and/or biological characteristics of molecules[20, 41]. Several degree, spectrum, matching, and distance-based topological descriptors have been suggested and explored in the literature [37, 42, 5], some of the interesting indices are Sombor index, Steiner Gutman Index, Estrada index and Laplacian Estrada index of a graphs, see [43, 38, 39, 44]. One of the oldest topological indices and most investigated is the Wiener index, after the successful of this index, Gutman et al.[16] introduced the generalization of the Wiener index for a acyclic graph known as szeged(Sz) index. Consequentially, another szeged like index called Padmakar-Ivan index(PI) proposed by Kahadikar et al.[31].

Recently *Došlić* et al. [13], introduced a distance based topological index called Mostar index, which measure of the global peripherality of a molecular structure. PI, szeged, and Mostar indices are the interesting bond-additive type indices which quantities the degree of peripherality of particular edge and of the graph as a whole. Very recently Kandan et al., derived some bond-additive topological indices and their polynomial see [22, 23, 24, 25, 26, 27, 28]. For a connected $G = (V(G), E(G))$, the Padmakar-Ivan and szeged indices of G defined as

$$Sz(G) = \sum_{e=ab\epsilon E(G)} \aleph_a(ab|G)\aleph_b(ab|G)$$

and

$$PI(G) = \sum_{e=ab\epsilon E(G)} (\aleph_a(ab|G) + \aleph_b(ab|G))$$

respectively, where $\aleph_a(ab|G)$ denotes the number of vertices of G closer to a than to b and $\aleph_b(ab|G)$ denotes the number of vertices of G closer to b than to a. Note that in this definitions the equidistant vertices not counted for any edge of G. In the literature, many researchers found the applications and were extensively studied for various molecular structure to these indices see[17, 30, 32, 35] and for some recent investigation see[1, 12, 36, 40]. Inspired by this extension of szeged and the PI index, Ili$\acute{c}$ and Milosavljev$\acute{i}$c [19] proposed weighted version named as the additively weighted szeged and the additively weighted PI index, respectively which are defined as

$$Sz_A(G) = \sum_{e=ab\epsilon E(G)} (\wedge_a(ab|G) + \wedge_b(ab|G))\aleph_a(ab|G)\aleph_b(ab|G)$$

and

$$PI_A(G) = \sum_{e=ab\epsilon E(G)} (\wedge_a(ab|G) + \wedge_b(ab|G))\left(\aleph_a(ab|G) + \aleph_b(ab|G)\right).$$

Laterly, Arockiaraj et al.[6] introduced the multiplicatively weighted szeged and PI index respectively which are defined as

$$Sz_M(G) = \sum_{e=ab\epsilon E(G)} (\wedge_a(ab|G). \wedge_b (ab|G))\aleph_a(ab|G)\aleph_b(ab|G)$$

and

$$PI_M(G) = \sum_{e=ab\epsilon E(G)} (\wedge_a(ab|G). \wedge_b (ab|G))\left(\aleph_a(ab|G) + \aleph_b(ab|G)\right)$$

where $\wedge_a(ab|G), \wedge_b(ab|G)$ denotes the degree of vertex a, b respectively. For more works on these weighted indices, see[4, 6, 9].

Non-isomorphic graphs can be distinguished using a graph polynomial. Many graph polynomials have been created for quantifying the structural information of molecular graphs related for quantifying the structural information of molecular graphs. Graph polynomials were utilized in chemistry in conjunction with the molecular orbital theory of unsaturated compounds, and they were also a valuable source of structural descriptors used in constructing structure property models. [7, 14, 15, 33, 42]. Distance-based and degree-based graph polynomials are useful because they contain a wealth of information about topological indices. In [14] Szeged and PI polynomial of a graph G respectively defined as

$$Sz(G, x) = \sum_{e=ab\epsilon E(G)} x^{\aleph_a(ab|G)\aleph_b(ab|G)}$$

and

$$PI(G, x) = \sum_{e=ab\epsilon E(G)} x^{\aleph_a(ab|G)+\aleph_b(ab|G)}.$$

Since many graph parameter are derived from the graph polynomial, it is interesting to study new graph polynomial, which are used to model a the behavior of physical, chemical or biological system. Various topological indices can be derived from polynomials by taking their value at some point directly, or by taking integrals or derivatives. In light of the preceding condition and the newly proposed weighted version, very recently, Kandan et al.[28] introduced the weighted version polynomial of szeged and PI of a graph and derived it for some graphs. The Additively weighted szeged polynomial of a graph G is defined as

$$Sz_A(G, x) = \sum_{e=ab\epsilon E(G)} x^{(\wedge_a(ab|G)+\wedge_b(ab|G))\aleph_a(ab|G)\aleph_b(ab|G)}.$$

The Multiplicatively weighted szeged polynomial of G is defined as

$$Sz_M(G, x) = \sum_{e=ab\epsilon E(G)} x^{(\wedge_a(ab|G).\wedge_b(ab|G))\aleph_a(ab|G)\aleph_b(ab|G)}.$$

The Additively weighted Padmakar-Ivan polynomial of G is defined as

$$PI_A(G, x) = \sum_{e=ab\epsilon E(G)} x^{(\wedge_a(ab|G)+\wedge_b(ab|G))\aleph_a(ab|G)+\aleph_b(ab|G)}.$$

The Multiplicatively weighted padmakar-Ivan polynomial of G is defined as

$$PI_M(G,x) = \sum_{e=ab\epsilon E(G)} x^{(\wedge_a(ab|G).\wedge_b(ab|G))\aleph_a(ab|G)+\aleph_b(ab|G)}.$$

Recently, Kahalaf et al.[21] derived several graph polynomials of cellulose and for more results on polynomials see [2, 10, 34]. As the main result of this paper is to compute the exact form of szeged, PI, weighted szeged, weighted PI and their polynomial of cellulose. As a main result, in Section 3, we obtain the exact value of szeged index, additively weighted szeged index , Multiplicatively weighted szeged index and its polynomial. Moreover using these results we derived their relation and bounds for cellulose. In Section 4, similar results obtained for the Padmakar-Ivan index, additively weighted Padmakar-Ivan index, Multiplicatively weighted Padmakar-Ivan index and its polynomial. Further we obtained their relations and boundness of cellulose.

2. MAIN RESULT

By chemical graph structure analysis and observation on CL_d, we note that the edge set $E(CL_d)$ can be divided into five groups based on degree, which are summarized as follows see Figure 2.

$E_1(CL_d) = \{e = ab\epsilon E(CL_d) : \wedge_a(ab|CL_d) = 1, \wedge_b(ab|CL_d) = 2\}$, $|E_1| = 2d$
$E_2(CL_d) = \{e = ab\epsilon E(CL_d) : \wedge_a(ab|CL_d) = 1, \wedge_b(ab|CL_d) = 3\}$, $|E_2| = 4d + 2$
$E_3(CL_d) = \{e = ab\epsilon E(CL_d) : \wedge_a(ab|CL_d) = 2, \wedge_b(ab|CL_d) = 3\}$, $|E_3| = 10d - 2$
$E_4(CL_d) = \{e = ab\epsilon E(CL_d) : \wedge_a(ab|CL_d) = 3, \wedge_b(ab|CL_d) = 3\}$, $|E_4| = 8d$

It can be observed that in general, $|V(CL_d)| = 22d+1$, $|E(CL_d)| = 24d$. As a part of the main proof we use the above classification of edge partition of cellulose, now we summarize the value of $\aleph_a(ab|CL_d)$, $\aleph_b(ab|CL_d)$ in the Table 1.

3. SZEGED INDEX AND ITS POLYNOMIAL

Using the Table 1, we have the following results on szeged related indices of cellulose.

Theorem 3.1. *Let CL_d be the chemical graph of the cellulose,*

$$\begin{aligned} Sz(CL_d) &= 2d(22d) + (4d+2)22d + 4d(22d-1) + (d^2+d)\left(1452\frac{d-1}{3} + 1001\right) \\ &\quad + 935(d-d^2) - 1332d + 22d(d-1)\left(\frac{22d+25}{3}\right) + \left(d^2+d\right) \\ &\quad \left(1936\left(\frac{d-1}{3}\right) + 990\right) + 902(d-d^2) - 1166d. \end{aligned}$$

Proof. To obtain the Szeged index of cellulose, by the definition of szeged index and from the Table 1. we have

$$\begin{aligned} Sz(CL_d) &= \sum_{e=ab\in E(CL_d)} \aleph_a(ab|CL_d)\aleph_b(ab|CL_d) \\ &= \sum_{e=ab\in E_1(CL_d)} \aleph_a(ab|CL_d)\aleph_b(ab|CL_d) + \sum_{e=ab\in E_2(CL_d)} \aleph_a(ab|CL_d)\aleph_b(ab|CL_d) \\ &\quad + \sum_{e=ab\in E_3(CL_d)} \aleph_a(ab|CL_d)\aleph_b(ab|CL_d) + \sum_{e=ab\in E_4(CL_d)} \aleph_a(ab|CL_d)\aleph_b(ab|CL_d) \end{aligned}$$

TABLE 1. Edge partitions and $\aleph_a, \aleph_b$ value of cellulose

Cellulose $CL_{i=1,2,\ldots,d}$,					
E	$(\wedge_a, \wedge_b)$	$\lvert E\rvert$	$\aleph_a(ab\lvert CL_d)$	$\aleph_b(ab\lvert CL_d)$	$\sum_i \aleph_a(ab\lvert CL_d)\aleph_b(ab\lvert CL_d)$
E_1	(1,2)	2d	1	22d	2d(22d)
E_2	(1,3)	4d+2	1	22d	(4d+2)22d
E_3	(2,3)	2d	2	22d-1	(2d)44d-2
	(3,2)	d	22i-15	22d+16-22i	$(d^2+d)(242\frac{d-1}{3}+176)+165(d-d^2)-240d$
	(2,3)	d	22i-16	22d+17-22i	$(d^2+d)(242\frac{d-1}{3}+187)+176(d-d^2)-272d$
	(3,2)	d	22i-11	22d+12-22i	$(d^2+d)(242\frac{d-1}{3}+132)+121(d-d^2)-132d$
	(2,3)	d	22i-10	22d+11-22i	$(d^2+d)(242\frac{d-1}{3}+121)+110(d-d^2)-110d$
	(3,2)	d	22d+18-22i	22i-17	$(d^2+d)(242\frac{d-1}{3}+198)+187(d-d^2)-306d$
Cellulose $CL_{i=1,2,\ldots,d}$,					
E	$(\wedge_a, \wedge_b)$	$\lvert E\rvert$	$\aleph_a(ab\lvert CL_d)$	$\aleph_b(ab\lvert CL_d)$	$\sum_i \aleph_a(ab\lvert CL_d)\aleph_b(ab\lvert CL_d)$
	(2,3)	d	22d+17-22i	22i-16	$(d^2+d)(242\frac{d-1}{3}+187)+176(d-d^2)-272d$
	(2,3)	d-1	22(i-1)	22d+1-22(i-1)	$11d(d-1)(\frac{22d+25}{3})$
	(3,2)	d-1	22(i-1)+1	22d-22(i-1)	$11d(d-1)(\frac{22d+25}{3})$
E_4	(3,3)	3d	22d+17-22i	22i-16	$(d^2+d)(242\frac{d-1}{3}+187)+176(d-d^2)-272d$
	(3,3)	d	22i-15	22d+16-22i	$(d^2+d)(242\frac{d-1}{3}+176)+165(d-d^2)-240d$
	(3,3)	3d	22i-5	22d+6-22i	$(d^2+d)(242\frac{d-1}{3}+66)+55(d-d^2)-30d$
	(3,3)	d	22i-4	22d+5-22i	$(d^2+d)(242\frac{d-1}{3}+55)+44(d-d^2)-20d$

For convenient, we have calculated each summation separately to the corresponding edge partition as mentioned early.
For the edge partition E_1:

$$\sum_{e=ab\in E_1(CL_d)} \aleph_a(ab|CL_d)\aleph_b(ab|CL_d) = 2d(22d)$$

For the edge partition E_2:

$$\sum_{e=ab\in E_2(CL_d)} \aleph_a(ab|CL_d)\aleph_b(ab|CL_d) = (4d+2)22d$$

For the edge partition E_3:

$$\sum_{e=ab\in E_3(CL_d)} \aleph_a(ab|CL_d)\aleph_b(ab|CL_d) = 2d(44d-2)$$

$$
\begin{aligned}
&+\sum_{i=1}^{d}(22i-15)(22d+16-22i)+\sum_{i=1}^{d}(22i-16)(22d+17-22i)\\
&+\sum_{i=1}^{d}(22i-11)(22d+12-22i)+\sum_{i=1}^{d}(22i-10)(22d+11-22i)\\
&+\sum_{i=1}^{d}(22i+18-22i)(22i-17)+\sum_{i=1}^{d}(22i-16)(22d+17-22i)\\
&+\sum_{i=1}^{d-1}22(i-1)(22d+1-22(i-1))+\sum_{i=1}^{d-1}(22(i-1)+1)(22d-22(i-1))\\
&=2d(44d-2)+(d^2+d)\left(242\frac{d-1}{3}+176\right)+165(d-d^2)\\
&-240d+(d^2+d)\left(242\frac{d-1}{3}+187\right)+176(d-d^2)-272d+(d^2+d)\left(242\frac{d-1}{3}+132\right)\\
&+121(d-d^2)-132d+(d^2+d)\left(242\frac{d-1}{3}+121\right)+110(d-d^2)-110d\\
&+(d^2+d)\left(242\frac{d-1}{3}+198\right)+187(d-d^2)-306d+(d^2+d)\left(242\frac{d-1}{3}+187\right)\\
&+176(d-d^2)-272d+11d(d-1)\left(\frac{22d+25}{3}\right)+11d(d-1)\left(\frac{22d+25}{3}\right)\\
&=4d(22d-1)+(d^2+d)\left(1452\frac{d-1}{3}+1001\right)+935(d-d^2)-1332d+22d(d-1)\left(\frac{22d+25}{3}\right)
\end{aligned}
$$

For the edge partition E_4:

$$
\begin{aligned}
\sum_{e=ab\in E_4(CL_d)}\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)&=3\sum_{i=1}^{d}(22i-16)(22d+17-22i)+\sum_{i=1}^{d}(22i-15)(22d+16-22i)\\
&+3\sum_{i=1}^{d}(22i-5)(22i+6-22i)+\sum_{i=1}^{d}(22i-4)(22d+5-22i)\\
&=3\sum_{i=1}^{d}484(di-i^2)+374i+352(d-i)-272+\sum_{i=1}^{d}484(di-i^2)+352i+330(i-d)-240\\
&+3\sum_{i=1}^{d}484(di-i^2)+132i+110(i-d)-30+\sum_{i=1}^{d}484(di-i^2)+110i+88(i-d)-20\\
&=\sum_{i=1}^{d}(3(484(di-i^2)+374i+352(d-i)-272)+484(di-i^2)+352i+330(i-d)-240\\
&+3(484(di-i^2)+132i+110(i-d)-30)+484(di-i^2)+110i+88(i-d)-20)\\
&=3\left((d^2+d)\left(242\frac{d-1}{3}+187\right)+176(d-d^2)-272d\right)+(d^2+d)\left(242\frac{d-1}{3}+176\right)\\
&+165(d-d^2)-240d+3\left((d^2+d)\left(242\frac{d-1}{3}+66\right)+55(d-d^2)-30d\right)\\
&+(d^2+d)\left(242\frac{d-1}{3}+55\right)+44(d-d^2)-20d
\end{aligned}
$$

$$= (d^2 + d)\left(1936\left(\frac{d-1}{3}\right) + 990\right) + 902(d - d^2) - 1166d$$

Hence by summing up these values we have

$$\begin{aligned} Sz(CL_d) &= 2d(22d) + (4d + 2)22d + 4d(22d - 1) + (d^2 + d)\left(1452\frac{d-1}{3} + 1001\right) \\ &+ 935(d - d^2) - 1332d + 22d(d - 1)\left(\frac{22d + 25}{3}\right) + (d^2 + d)\left(1936\left(\frac{d-1}{3}\right) + 990\right) \\ &+ 902(d - d^2) - 1166d \end{aligned}$$

Hence the theorem. □

Next, we obtained obtained the weighted version of szeged index in the consecutive theorems.

Theorem 3.2. *Let CL_d be the chemical graph of cellulose,*

$$\begin{aligned} Sz_A(CL_d) &= 3(2d(22d)) + 4((4d + 2)22d) + 5\left(4d(22d - 1) + (d^2 + d)\left(1452\frac{d-1}{3} + 1001\right)\right. \\ &\left. +935(d - d^2) - 1332d + 22d(d - 1)\left(\frac{22d + 25}{3}\right)\right) + 6\left((d^2 + d)\left(1936\left(\frac{d-1}{3}\right) + 990\right)\right. \\ &\left. +902(d - d^2) - 1166d\right) \end{aligned}$$

Proof. To obtain the additively weighted szeged index of the CL_d, by the definition of Additively weighted szeged index and from the Table 1. we have

$$\begin{aligned} Sz_A(CL_d) &= \sum_{e=ab\epsilon E(CL_d)} (\wedge_a(ab|CL_d) + \wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d) \\ &= \sum_{\substack{i=1,2,3,4. \\ e=ab\epsilon E_i(CL_d)}} (\wedge_a(ab|CL_d) + \wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d) \end{aligned}$$

By using Theorem 3.1, we have

$$\begin{aligned} Sz_A(CL_d) &= (1 + 2)(Sz(E_1)) + (1 + 3)(Sz(E_2)) + (2 + 3)(Sz(E_3)) + (3 + 3)(Sz(E_4)) \\ &= 3(2d(22d)) + 4((4d + 2)22d) + 5(4d(22d - 1) + (d^2 + d)\left(1452\frac{d-1}{3} + 1001\right) \\ &+ 935(d - d^2) - 1332d + 22d(d - 1)\left(\frac{22d + 25}{3}\right) \\ &+ 6\left((d^2 + d)\left(1936\left(\frac{d-1}{3}\right) + 990\right) + 902(d - d^2) - 1166d\right) \end{aligned}$$

Hence the theorem. □

Theorem 3.3. *Let CL_d be the chemical graph of cellulose,*

$$\begin{aligned} Sz_M(CL_d) &= 2(2d(22d)) + 3((4d + 2)22d) + 6\left(4d(22d - 1) + (d^2 + d)\right. \\ &\left(1452\frac{d-1}{3} + 1001\right) + 935(d - d^2) - 1332d + 22d(d - 1) \\ &\left.\left(\frac{22d + 25}{3}\right)\right) + 9((d^2 + d)\left(1936\left(\frac{d-1}{3}\right) + 990\right) + 902(d - d^2) - 1166d) \end{aligned}$$

.

Proof. To obtained the Multiplicatively weighted szeged index of CL_d, by the definition of Multiplicatively weighted szeged index and from the Table 1. we have

$$Sz_M(CL_d) = \sum_{e=ab\in E(CL_d)} (\wedge_a(ab|CL_d). \wedge_b (ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)$$
$$= \sum_{\substack{i=1,2,3,4.\\ e=ab\in E_i(CL_d)}} (\wedge_a(ab|CL_d). \wedge_b (ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)$$

By using Theorem 3.1, we have

$$Sz_M(CL_d) = (1.2)(Sz(E_1)) + (1.3)(Sz(E_2)) + (2.3)(Sz(E_3)) + (3.3)(Sz(E_4))$$
$$= 2(2d(22d)) + 3((4d + 2)22d) + 6\left(4d(22d-1) + (d^2+d)\left(1452\frac{d-1}{3} + 1001\right)\right.$$
$$\left.+935(d-d^2) - 1332d + 22d(d-1)\left(\frac{22d+25}{3}\right)\right) + 9((d^2+d)\left(1936\left(\frac{d-1}{3}\right) + 990\right)$$
$$+ 902(d-d^2) - 1166d)$$

Hence the theorem. □

To the continuity of the above result, now we derive the exact expression of szeged and its related polynomial

Theorem 3.4. *Let CL_d be the chemical graph of cellulose,*

$$Sz(CL_d, x) = 2dx^{22d} + (4d+2)x^{22d} + 2dx^{(44d-2)} + \sum_{i=1}^{d}\left(2\left(x^{484(di-i^2)+352i+330(i-d)-240}\right)\right.$$
$$+ 5\left(x^{484(di-i^2)+374i+352(i-d)-272}\right) + x^{484(id-i^2)+264i+242(i-d)-132}$$
$$+ x^{484(id-i^2)+242i+220(i-d)-110} + x^{484(di-i^2)+374(i-d)+396i-306}$$
$$\left.+3\left(x^{484(di-i^2)+132i+110(i-d)-30}\right) + x^{484(di-i^2)+110i+88(i-d)-20}\right)$$
$$+\sum_{i=1}^{d-1} x^{22((22d+1)(i-1)-22(i-1)^2)} + \sum_{i=1}^{d-1} x^{22d((22(i-1)+1))-(22(i-1)+1)(i-1)}.$$

Proof. To obtained the szeged polynomial of CL_d, by the definition of szeged polynomial and applying the Table 1., we have

$$Sz(CL_d, x) = \sum_{e=ab\epsilon E(CL_d)} x^{\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)}$$
$$Sz(CL_d, x) = \sum_{e=ab\epsilon E_1(CL_d)} x^{\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} + \sum_{e=ab\epsilon E_2(CL_d)} x^{\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)}$$
$$+ \sum_{e=ab\epsilon E_3(CL_d)} x^{\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} + \sum_{e=ab\epsilon E_4(CL_d)} x^{\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)}$$

For convenient, we have calculated each summation separately to the corresponding edge partitions as mentioned early.
For the edge partition E_1:

$$\sum_{e=ab\epsilon E_1(CL_d)} x^{\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} = \sum_{e=ab\epsilon E_1(CL_d)} x^{22d} = 2dx^{22d}$$

For edge partition E_2:

$$\sum_{e=ab\epsilon E_2(CL_d)} x^{\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} = \sum_{e=ab\epsilon E_2(CL_d)} x^{22d} = (4d+2)x^{22d}$$

For edge partition E_3:

$$\begin{aligned}
\sum_{e=ab\epsilon E_3(CL_d)} x^{\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} &= 2dx^{(44d-2)} + \sum_{i=1}^{d} x^{(22i-15)(22d+16-22i)} \\
&+ \sum_{i=1}^{d} x^{(22i-16)(22d+17-22i)} + \sum_{i=1}^{d} x^{(22i-11)(22d+12-22i)} \\
&+ \sum_{i=1}^{d} x^{(22i-10)(22d+11-22i)} + \sum_{i=1}^{d} x^{(22i+18-22i)(22i-17)} \\
&+ \sum_{i=1}^{d} x^{(22i-16)(22d+17-22i)} + \sum_{i=1}^{d} x^{22(i-1)(22d+1-22(i-1))} \\
&+ \sum_{i=1}^{d} x^{(22(i-1)+1)(22d-22(i-1))} \\
&= 2dx^{(44d-2)} + \sum_{i=1}^{d} x^{484(di-i^2)+352i+330(i-d)-240} \\
&+ 2\sum_{i=1}^{d} x^{484(di-i^2)+374i+352(i-d)-272} + \sum_{i=1}^{d} x^{484(id-i^2)+264i+242(i-d)-132} \\
&+ \sum_{i=1}^{d} x^{484(id-i^2)+242i+220(i-d)-110)} + \sum_{i=1}^{d} x^{484(di-i^2)+374(i-d)+396i-306} \\
&+ \sum_{i=1}^{d-1} x^{22((22d+1)(i-1)-22(i-1)^2)} + \sum_{i=1}^{d-1} x^{22d(d(22(i-1)+1))-(22(i-1)+1)(i-1)} \\
&= 2dx^{(44d-2)} + \sum_{i=1}^{d} \Big(x^{484(di-i^2)+352i+330(i-d)-240} \\
&+ 2\left(x^{484(di-i^2)+374i+352(i-d)-272} \right) + x^{484(id-i^2)+264i+242(i-d)-132} \\
&+ x^{484(id-i^2)+242i+220(i-d)-110} + x^{484(di-i^2)} \\
&+ 374(i-d) + 396i - 306 + \sum_{i=1}^{d-1} x^{22((22d+1)(i-1)-22(i-1)^2)} \\
&+ \sum_{i=1}^{d-1} x^{22d(22(i-1)+1)-(22(i-1)+1)(i-1)} \Big)
\end{aligned}$$

For edge partition E_4:

$$\sum_{e=ab\epsilon E_4(CL_d)} x^{\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} = 3\sum_{i=1}^{d} x^{(22i-16)(22d+17-22i)}$$

$$+\sum_{i=1}^{d} x^{(22i-15)(22d+16-22i)} + 3\sum_{i=1}^{d} x^{(22i-5)(22i+6-22i)}$$
$$+\sum_{i=1}^{d} x^{(22i-4)(22d+5-22i)}$$
$$= 3\sum_{i=1}^{d} x^{484(di-i^2)+374i+352(d-i)-272} + \sum_{i=1}^{d} x^{484(di-i^2)+352i+330(i-d)-240}$$
$$+ 3\sum_{i=1}^{d} x^{484(di-i^2)+132i+110(i-d)-30} + \sum_{i=1}^{d} x^{484(di-i^2)+110i+88(i-d)-20}$$
$$= \sum_{i=1}^{d} \Big(3\left(x^{484(di-i^2)+374i+352(d-i)-272}\right) + x^{484(di-i^2)+352i+330(i-d)-240}$$
$$+3\left(x^{484(di-i^2)+132i+110(i-d)-30}\right) + x^{484(di-i^2)+110i+88(i-d)-20}\Big)$$

Hence by summarizing these values obtained here for the partitions E_1,E_2,E_3 and E_4, we have

$$Sz(CL_d,x) = 2dx^{22d} + (4d+2)x^{22d} + 2dx^{(44d-2)} + \sum_{i=1}^{d}\Big(2\left(x^{484(di-i^2)+352i+330(i-d)-240}\right)$$
$$+ 5\left(x^{484(di-i^2)+374i+352(i-d)-272}\right) + x^{484(id-i^2)+264i+242(i-d)-132}$$
$$+ x^{484(id-i^2)+242i+220(i-d)-110} + x^{484(di-i^2)+374(i-d)+396i-306}$$
$$+3\left(x^{484(di-i^2)+132i+110(i-d)-30}\right) + \sum_{i=1}^{d} x^{484(di-i^2)+110i+88(i-d)-20}\Big)$$
$$+\sum_{i=1}^{d-1} x^{22((22d+1)(i-1)-22(i-1)^2)} + \sum_{i=1}^{d-1} x^{22d((22(i-1)+1))-(22(i-1)+1)(i-1)}$$

Hence the theorem. □

Theorem 3.5. *Let CL_d be the chemical graph of cellulose,*

$$Sz_A(CL_d,x) = 2dx^{3(22d)} + (4d+2)x^{4(22d)} + 2dx^{5(44d-2)}$$
$$+\sum_{i=1}^{d}\Big(x^{5(484(di-i^2)+352i+330(i-d)-240)} + 2\left(x^{5(484(di-i^2)+374i+352(i-d)-272)}\right)$$
$$+ x^{5(484(id-i^2)+264i+242(i-d)-132)} + x^{5(484(id-i^2)+242i+220(i-d)-110)}$$
$$+ x^{5(484(di-i^2)+374(i-d)+396i-306)} + 3\left(x^{6(484(di-i^2)+374i+352(i-d)-272)}\right)$$
$$+ x^{6(484(di-i^2)+352i+330(i-d)-240)} + 3\left(x^{6(484(di-i^2)+132i+110(i-d)-30)}\right)$$
$$+x^{6(484(di-i^2)+110i+88(i-d)-20)}\Big) + \sum_{i=1}^{d-1} x^{5(22((22d+1)(i-1)-22(i-1)^2))}$$
$$+\sum_{i=1}^{d-1} x^{5(22d((22(i-1)+1))-(22(i-1)+1)(i-1))}.$$

Proof. To obtained the Additively weighted szeged polynomial of CL_d, by the definition of Additively weighted szeged polynomial and from the Table 1., we have

$$Sz_A(CL_d,x) = \sum_{e=ab\epsilon E(CL_d)} x^{(\wedge_a(ab|CL_d)+\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)}$$

$$\begin{aligned} Sz_A(CL_d,x) = & \sum_{e=ab\epsilon E_1(CL_d)} x^{(\wedge_a(ab|CL_d)+\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} \\ & + \sum_{e=ab\epsilon E_2(CL_d)} x^{(\wedge_a(ab|CL_d)+\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} \\ & + \sum_{e=ab\epsilon E_3(CL_d)} x^{(\wedge_a(ab|CL_d)+\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} \\ & + \sum_{e=ab\epsilon E_4(CL_d)} x^{(\wedge_a(ab|CL_d)+\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} \end{aligned}$$

For our convenient, now we calculate each summation separately to the corresponding edge partition as mentioned early.
For edge partition E_1:

$$\sum_{e=ab\epsilon E_1(CL_d)} x^{(\wedge_a(ab|CL_d)+\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} = 2dx^{(3)22d}$$

For edge partition E_2:

$$\begin{aligned} \sum_{e=ab\epsilon E_2(CL_d)} x^{(\wedge_a(ab|CL_d)+\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} &= \sum_{e=ab\epsilon E_2(CL_d)} x^{(1+3)22d} \\ &= (4d+2)x^{(4)22d} \end{aligned}$$

For edge partition E_3:

$$\begin{aligned} & \sum_{e=ab\epsilon E_3(CL_d)} x^{(\wedge_a(ab|CL_d)+\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} \\ &= 2dx^{(2+3)(44d-2)} + \sum_{i=1}^{d} x^{(3+2)(22i-15)(22d+16-22i)} + \sum_{i=1}^{d} x^{(2+3)(22i-16)(22d+17-22i)} \\ &+ \sum_{i=1}^{d} x^{(3+2)(22i-11)(22d+12-22i)} + \sum_{i=1}^{d} x^{(2+3)(22i-10)(22d+11-22i)} \\ &+ \sum_{i=1}^{d} x^{(3+2)(22i+18-22i)(22i-17)} + \sum_{i=1}^{d} x^{(2+3)(22d+17-22i)(22i-16)} \\ &+ \sum_{i=1}^{d} x^{(2+3)22(i-1)(22d+1-22(i-1))} + \sum_{i=1}^{d} x^{(3+2)(22(i-1)+1)(22d-22(i-1))} \\ &= 2dx^{5(44d-2)} + \sum_{i=1}^{d} x^{5(484(di-i^2)+352i+330(i-d)-240)} + 2\sum_{i=1}^{d} x^{5(484(di-i^2)+374i+352(i-d)-272)} \\ &+ \sum_{i=1}^{d} x^{5(484(id-i^2)+264i+242(i-d)-132)} + \sum_{i=1}^{d} x^{5(484(id-i^2)+242i+220(i-d)-110))} \\ &+ \sum_{i=1}^{d} x^{5(484(di-i^2)+374(i-d)+396i-306)} + \sum_{i=1}^{d-1} x^{5(22((22d+1)(i-1)-22(i-1)^2))} \end{aligned}$$

$$+\sum_{i=1}^{d-1} x^{5(22d((22(i-1)+1))-(22(i-1)+1)(i-1))}$$
$$= 2dx^{5(44d-2)} + \sum_{i=1}^{d} \Big(x^{5(484(di-i^2)+352i+330(i-d)-240)}$$
$$+ 2\left(x^{5(484(di-i^2)+374i+352(i-d)-272)}\right) + x^{5(484(id-i^2)+264i+242(i-d)-132)}$$
$$+ x^{5(484(id-i^2)+242i+220(i-d)-110)} + x^{5(484(di-i^2)+374(i-d)+396i-306)}$$
$$+\sum_{i=1}^{d-1} x^{5(22((22d+1)(i-1)-22(i-1)^2))} + \sum_{i=1}^{d-1} x^{5(22d((22(i-1)+1))-(22(i-1)+1)(i-1))}\Big)$$

For edge partition E_4:

$$\sum_{e=ab\epsilon E_4(CL_d)} x^{(\wedge_a(ab|CL_d)+\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)}$$
$$= 3\sum_{i=1}^{d} x^{(3+3)(22i-16)(22d+17-22i)} + \sum_{i=1}^{d} x^{(3+3)(22i-15)(22d+16-22i)}$$
$$+ 3\sum_{i=1}^{d} x^{(3+3)(22i-5)(22i+6-22i)} + \sum_{i=1}^{d} x^{(3+3)(22i-4)(22d+5-22i)}$$
$$= 3\sum_{i=1}^{d} x^{6(484(di-i^2)+374i+352(d-i)-272)}$$
$$+\sum_{i=1}^{d} x^{6(484(di-i^2)+352i+330(i-d)-240)} + 3\sum_{i=1}^{d} x^{6(484(di-i^2)+132i+110(i-d)-30)}$$
$$+\sum_{i=1}^{d} x^{6(484(di-i^2)+110i+88(i-d)-20)}$$
$$= \sum_{i=1}^{d} \Big(3\left(x^{6(484(di-i^2)+374i+352(d-i)-272)}\right)$$
$$+ x^{6(484(di-i^2)+352i+330(i-d)-240)} + 3\left(x^{6(484(di-i^2)+132i+110(i-d)-30)}\right)$$
$$+x^{6(484(di-i^2)+110i+88(i-d)-20)}\Big)$$

Hence by summarizing these values obtained here for E_1, E_2,E_3 and E_4, we have

$$Sz_A(CL_d, x) = 2dx^{3(22d)} + (4d+2)x^{4(22d)} + 2dx^{5(44d-2)}$$
$$+\sum_{i=1}^{d} \Big(x^{5(484(di-i^2)+352i+330(i-d)-240)} + 2\left(x^{5(484(di-i^2)+374i+352(i-d)-272)}\right)$$
$$+ x^{5(484(id-i^2)+264i+242(i-d)-132)} + x^{5(484(id-i^2)+242i+220(i-d)-110)}$$
$$+ x^{5(484(di-i^2)+374(i-d)+396i-306)} + 3\left(x^{6(484(di-i^2)+374i+352(i-d)-272)}\right)$$
$$+ x^{6(484(di-i^2)+352i+330(i-d)-240)} + 3\left(x^{6(484(di-i^2)+132i+110(i-d)-30)}\right)$$

$$+x^{6(484(di-i^2)+110i+88(i-d)-20)}\Big) + \sum_{i=1}^{d-1} x^{5(22((22d+1)(i-1)-22(i-1)^2))}$$
$$+\sum_{i=1}^{d-1} x^{5(22d((22(i-1)+1)-(22(i-1)+1)(i-1)))}$$

Hence the theorem. □

Theorem 3.6. *Let CL_d be the chemical graph of cellulose,*

$$\begin{aligned}
Sz_M(CL_d,x) &= 2dx^{2(22d)} + (4d+2)x^{3(22d)} + 2dx^{6(44d-2)}\\
&+\sum_{i=1}^{d}\Big(x^{6(484(di-i^2)+352i+330(i-d)-240)} + 2\Big(x^{6(484(di-i^2)+374i+352(i-d)-272)}\Big)\\
&+x^{6(484(id-i^2)+264i+242(i-d)-132)} + x^{6(484(id-i^2)+242i+220(i-d)-110}\\
&+x^{6(484(di-i^2)+374(i-d)+396i-306)} + 3\Big(x^{9(484(di-i^2)+374i+352(i-d)-272)}\Big)\\
&+x^{9(484(di-i^2)+352i+330(i-d)-240)} + 3\Big(x^{9(484(di-i^2)+132i+110(i-d)-30)}\Big)\\
&+x^{9(484(di-i^2)+110i+88(i-d)-20)}\Big) + \sum_{i=1}^{d-1} x^{6(22((22d+1)(i-1)-22(i-1)^2))}\\
&+\sum_{i=1}^{d-1} x^{6(22d((22(i-1)+1))-(22(i-1)+1)(i-1))}
\end{aligned}$$

Proof. To obtained the Multiplicatively weighted szeged polynomial of CL_d, by the definition of Multiplicatively weighted szeged polynomial and from the Table 1., we have

$$\begin{aligned}
Sz_M(CL_d,x) &= \sum_{e=ab\epsilon E(CL_d)} x^{(\wedge_a(ab|CL_d).\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)}\\
Sz_M(CL_d,x) &= \sum_{e=ab\epsilon E_1(CL_d)} x^{(\wedge_a(ab|CL_d).\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)}\\
&+ \sum_{e=ab\epsilon E_2(CL_d)} x^{(\wedge_a(ab|CL_d).\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)}\\
&+ \sum_{e=ab\epsilon E_3(CL_d)} x^{(\wedge_a(ab|CL_d).\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)}\\
&+ \sum_{e=ab\epsilon E_4(CL_d)} x^{(\wedge_a(ab|CL_d).\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)}
\end{aligned}$$

For convenient, we have calculated each summation separately to the corresponding edge partition as mentioned early.
For edge partition E_1:

$$\begin{aligned}
\sum_{e=ab\epsilon E_1(CL_d)} x^{(\wedge_a(ab|CL_d).\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} &= \sum_{e=ab\epsilon E_1(CL_d)} x^{(1.2)22d}\\
&= 2dx^{(2)22d}
\end{aligned}$$

For edge partition E_2:

$$\sum_{e=ab\epsilon E_2(CL_d)} x^{(\wedge_a(ab|CL_d).\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)} = \sum_{e=ab\epsilon E_2(CL_d)} x^{(1.3)22d}$$
$$= (4d+2)x^{(3)22d}$$

For edge partition E_3:

$$\sum_{e=ab\epsilon E_3(CL_d)} x^{(\wedge_a(ab|CL_d).\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)}$$

$$= 2dx^{(2.3)(44d-2)} + \sum_{i=1}^{d} x^{(3.2)(22i-15)(22d+16-22i)} + \sum_{i=1}^{d} x^{(2.3)(22i-16)(22d+17-22i)}$$
$$+ \sum_{i=1}^{d} x^{(3.2)(22i-11)(22d+12-22i)} + \sum_{i=1}^{d} x^{(2.3)(22i-10)(22d+11-22i)}$$
$$+ \sum_{i=1}^{d} x^{(3.2)(22i+18-22i)(22i-17)} + \sum_{i=1}^{d} x^{(2.3)(22d+17-22i)(22i-16)}$$
$$+ \sum_{i=1}^{d-1} x^{(2.3)22(i-1)(22d+1-22(i-1))} + \sum_{i=1}^{d-1} x^{(3+2)(22(i-1)+1)(22d-22(i-1))}$$
$$= 2dx^{6(44d-2)} + \sum_{i=1}^{d} x^{6(484(di-i^2)+352i+330(i-d)-240)} + 2\sum_{i=1}^{d} x^{5(484(di-i^2)+374i+352(i-d)-272)}$$
$$+ \sum_{i=1}^{d} x^{6(484(id-i^2)+264i+242(i-d)-132)} + \sum_{i=1}^{d} x^{6(484(id-i^2)+242i+220(i-d)-110))}$$
$$+ \sum_{i=1}^{d} x^{6(484(di-i^2)+374(i-d)+396i-306)} + \sum_{i=1}^{d-1} x^{6(22((22d+1)(i-1)-22(i-1)^2))}$$
$$+ \sum_{i=1}^{d-1} x^{6(22d((22(i-1)+1))-(22(i-1)+1)(i-1))}$$
$$= 2dx^{6(44d-2)} + \sum_{i=1}^{d} \Big(x^{6(484(di-i^2)+352i+330(i-d)-240)} + 2\left(x^{6(484(di-i^2)+374i+352(i-d)-272)}\right)$$
$$+ x^{6(484(id-i^2)+264i+242(i-d)-132)} + x^{6(484(id-i^2)+242i+220(i-d)-110)}$$
$$+ x^{6(484(di-i^2)+374(i-d)+396i-306)} + \sum_{i=1}^{d-1} x^{6(22((22d+1)(i-1)-22(i-1)^2))}$$
$$+ \sum_{i=1}^{d-1} x^{6(22d((22(i-1)+1))-(22(i-1)+1)(i-1))} \Big)$$

For edge partition E_4:

$$\sum_{e=ab\epsilon E_4(CL_d)} x^{(\wedge_a(ab|CL_d).\wedge_b(ab|CL_d))\aleph_a(ab|CL_d)\aleph_b(ab|CL_d)}$$

$$= 3\sum_{i=1}^{d} x^{(3.3)(22i-16)(22d+17-22i)} + \sum_{i=1}^{d} x^{(3.3)(22i-15)(22d+16-22i)}$$

$$+3\sum_{i=1}^{d} x^{(3.3)(22i-5)(22i+6-22i)} + \sum_{i=1}^{d} x^{(3.3)(22i-4)(22d+5-22i)}$$

$$= 3\sum_{i=1}^{d} x^{9(484(di-i^2)+374i+352(d-i)-272)} + \sum_{i=1}^{d} x^{9(484(di-i^2)+352i+330(i-d)-240)}$$

$$+3\sum_{i=1}^{d} x^{9(484(di-i^2)+132i+110(i-d)-30)} + \sum_{i=1}^{d} x^{9(484(di-i^2)+110i+88(i-d)-20)}$$

$$= \sum_{i=1}^{d} \Big(3\left(x^{9(484(di-i^2)+374i+352(d-i)-272)}\right) + x^{9(484(di-i^2)+352i+330(i-d)-240)}$$

$$+3\left(x^{9(484(di-i^2)+132i+110(i-d)-30)}\right) + x^{9(484(di-i^2)+110i+88(i-d)-20)}\Big)$$

Hence by summarizing these values obtained here for E_1, E_2,E_3 and E_4, we have

$$Sz_M(CL_d, x) = 2dx^{2(22d)} + (4d+2)x^{3(22d)} + 2dx^{6(44d-2)}$$

$$+\sum_{i=1}^{d} \Big(x^{6(484(di-i^2)+352i+330(i-d)-240)} + 2\left(x^{6(484(di-i^2)+374i+352(i-d)-272)}\right)$$

$$+ x^{6(484(id-i^2)+264i+242(i-d)-132)} + x^{6(484(id-i^2)+242i+220(i-d)-110}$$

$$+ x^{6(484(di-i^2)+374(i-d)+396i-306)} + 3\left(x^{9(484(di-i^2)+374i+352(i-d)-272)}\right)$$

$$+ x^{9(484(di-i^2)+352i+330(i-d)-240)} + 3\left(x^{9(484(di-i^2)+132i+110(i-d)-30)}\right)$$

$$+x^{9(484(di-i^2)+110i+88(i-d)-20)}\Big) + \sum_{i=1}^{d-1} x^{6(22(22d+1)(i-1)-22(i-1)^2)}$$

$$+\sum_{i=1}^{d-1} x^{6(22d(22(i-1)+1)-(22(i-1)+1)(i-1))}$$

Hence the theorem. □

Using the results obtained here, the following remarks are easy to observe.

Remark 3.7. *$Sz'(CL_d, 1) = Sz(CL_d)$ and $Sz(CL_d, 1) = |E(CL_d)|$.*

Remark 3.8. *$Sz'_A(CL_d, 1) = Sz_A(CL_d)$ and $Sz_A(CL_d, 1) = |E(CL_d)|$.*

Remark 3.9. *$Sz'_M(CL_d, 1) = Sz_M(CL_d)$ and $Sz_M(CL_d, 1) = |E(CL_d)|$.*

The following corollaries shows the relationship between szeged index, Additively weigted szeged index and Multiplicatively weigted szeged index for cellulose.

Corollary 3.10. *$Sz_A(CL_d) = 5Sz(CL_d) - 2Sz(E_1) - Sz(E_2) + Sz(E_4)$.*

Corollary 3.11. *$Sz_M(CL_d) = 6Sz(CL_d) - 4Sz(E_1) - 3Sz(E_2) + 3Sz(E_4)$.*

Corollary 3.12. *$Sz(CL_d) < Sz_A(CL_d) < Sz_M(CL_d)$.*

4. PADMAKAR-IVAN INDEX AND ITS POLYNOMIAL

In this section, we compute another interesting topological indices based on distance called the Padmakar-Ivan index and its polynomial. Observe that for any edge $e = ab$ of cellulose CL_d has no equidistant vertices, thus we have $\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d) = |V(CL_d)|$.

Theorem 4.1. *Let CL_d be the chemical graph of cellulose, then* $PI(CL_d) = 24d(22d + 1)$.

Proof. To obtained the Padmakar-Ivan index of the CL_d, by the definition of PI index and from the Table 1., we have

$$\begin{aligned} PI(CL_d) = &\sum_{e=ab\epsilon E(CL_d)} (\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) \\ = &\sum_{e=ab\epsilon E_1(CL_d)} (\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) + \sum_{e=ab\epsilon E_2(CL_d)} (\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) \\ + &\sum_{e=ab\epsilon E_3(CL_d)} (\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) + \sum_{e=ab\epsilon E_4(CL_d)} (\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) \end{aligned}$$

Since there is no equidistant vertices exist in CL_d, thus we have

$$\begin{aligned} PI(CL_d) &= 2d(22d + 1) + (4d + 2)(22d + 1) + (10d - 2)(22d + 1) + 8d(22d + 1) \\ &= (2d + 4d + 2 + 10d - 2 + 8d)(22d + 1) \\ &= 24d(22d + 1) \end{aligned}$$

Hence the theorem. □

Theorem 4.2. *Let CL_d be the chemical graph of cellulose, then* $PI_A(CL_d) = (120d - 2)(22d + 1)$.

Proof. To obtained the Additively weighted Padmakar-Ivan index of the CL_d, by the definition of Additively weighted PI index and from the Table 1., we have

$$\begin{aligned} PI_A(CL_d) = &\sum_{e=ab\epsilon E(CL_d)} (\wedge_a(ab|CL_d) + \wedge_b(ab|CL_d))(\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) \\ = &\sum_{e=ab\epsilon E_1(CL_d)} (1 + 2)(\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) + \sum_{e=ab\epsilon E_2(CL_d)} (1 + 3)(\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) \\ + &\sum_{e=ab\epsilon E_3(CL_d)} (2 + 3)(\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) + \sum_{e=ab\epsilon E_4(CL_d)} (3 + 3)(\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) \\ = &\, 2d(1 + 2)|V(CL_d)| + (4d + 2)(1 + 3)|V(CL_d)| + (10d - 2)(2 + 3)|V(CL_d)| \\ + &\, (8d)(3 + 3)|V(CL_d)| \\ = &\, (6d + 16d + 8 + 50d - 10 + 48d)|V(CL_d)| \\ = &\, (120d - 2)|V(CL_d)|, \text{ since } |V(CL_d)| = 22d + 1 \\ = &\, (22d + 1)(120d - 2) \end{aligned}$$

Hence the theorem. □

It should be noted that a similar method can also be used in the study of more general Gaussian-type indices see [5] on generalized distance Gaussian Estrada index of graph.

Theorem 4.3. *Let CL_d be the chemical graph of cellulose, then* $PI_M(CL_d) = (148d - 6)(22d + 1)$.

Proof. To obtained the Multiplicatively weighted Padmakar-Ivan index of the CL_d, by the definition of Multiplicatively weighted PI index and from the Table 1., we have

$$\begin{aligned}
PI_M(CL_d) &= \sum_{e=ab\epsilon E(CL_d)} (\wedge_a(ab|CL_d). \wedge_b (ab|CL_d))(\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) \\
&= \sum_{e=ab\epsilon E_1(CL_d)} (1.2)(\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) + \sum_{e=ab\epsilon E_2(CL_d)} (1.3)(\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) \\
&+ \sum_{e=ab\epsilon E_3(CL_d)} (2.3)(\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) + \sum_{e=ab\epsilon E_4(CL_d)} (3.3)(\aleph_a(ab|CL_d) + \aleph_b(ab|CL_d)) \\
&= 2d(2)|V(CL_d)| + (4d+2)(3)|V(CL_d)| + (10d-2)(6)|V(CL_d)| + (8d)(9)|V(CL_d)| \\
&= (4d + 12d + 6 + 60d - 12 + 72d)|V(CL_d)| \\
&= (148d - 6)|V(CL_d)|, \text{ since } |V(CL_d)| = 22d + 1 \\
&= (148d - 6)(22d + 1)
\end{aligned}$$

Hence the theorem. □

The relationships between the Padmakar-Ivan index, Additively weighted Padmakar-Ivan index, and Multiplicatively weighted Padmakar-Ivan index for the cellulose graphs are shown in the following corollaries.

Corollary 4.4. $PI_A(CL_d) = 4PI(CL_d) + |V(CL_d)||E(CL_d)| - 2|V(CL_d)|$.

Corollary 4.5. $PI_M(CL_d) = 3PI(CL_d) + 2(38d - 3)|V(CL_d)|$.

Corollary 4.6. $PI(CL_d) < PI_A(CL_d) < PI_M(CL_d)$.

Example 4.7. *One can check the above corollaries for, d = 3, with* $|V(CL_3)| = 67$, $|E(CL_3)| = 72$, $PI(CL_3) = 4824$, $PI_A(CL_3) = 23986$, $PI_M(CL_3) = 29346$.

One may generalize the above corollaries for any molecular structure. To the continuity of the above result, now we derive the PI related polynomial's of cellulose.

Theorem 4.8. *Let* CL_d *be the chemical graph of cellulose, then* $PI(CL_d, x) = 24dx^{(22d+1)}$.

Proof. To obtained the Padmakar-Ivan polynomial of the CL_d, by the definition of Padmakar-Ivan polynomial and from the Table 1., we have

$$\begin{aligned}
PI(CL_d, x) &= \sum_{e=ab\epsilon E(ab|CL_d)} x^{(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} \\
&= \sum_{e=ab\epsilon E_1(CL_d)} x^{(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} + \sum_{e=ab\epsilon E_2(CL_d)} x^{(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} \\
&+ \sum_{e=ab\epsilon E_3(CL_d)} x^{(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} + \sum_{e=ab\epsilon E_4(CL_d)} x^{(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} \\
&= 2dx^{|V(CL_d)|} + (4d+2)x^{|V(CL_d)|} + (10d-2)x^{|V(CL_d)|} + 8dx^{|V(CL_d)|} \\
&= (2d + 4d + 2 + 10d - 2 + 8d)x^{(22d+1)}, \text{ since } |V(CL_d)| = 22d + 1
\end{aligned}$$

$= 24dx^{(22d+1)}$

Hence the theorem. $\square$

In this connection now we can obtained the weighted PI related polynomial using the Table 1.

Theorem 4.9. *Let CL_d be the chemical graph of cellulose, then* $PI_A(CL_d, x) = 2dx^{3(22d+1)} + (4d+2)x^{4(22d+1)} + (10d-2)x^{5(22d+1)} + (8d)x^{6(22d+1)|}$.

Proof. To obtained the Additively weighted PI polynomial of the CL_d, by the definition of Additively weighted PI polynomial and from the Table 1., we have

$$\begin{aligned}
PI_A(CL_d, x) &= \sum_{e=ab\epsilon E(CL_d)} x^{(\wedge_a(ab|CL_d)+\wedge_b(ab|CL_d))(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} \\
&= \sum_{e=ab\epsilon E_1(CL_d)} x^{(1+2)(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} + \sum_{e=ab\epsilon E_2(CL_d)} x^{(1+3)(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} \\
&+ \sum_{e=ab\epsilon E_3(CL_d)} x^{(2+3)(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} + \sum_{e=ab\epsilon E_4(CL_d)} x^{(3+3)(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} \\
&= 2dx^{(1+2)|V(CL_d)|} + (4d+2)x^{(1+3)|V(CL_d)|} + (10d-2)x^{(2+3)|V(CL_d)|} + (8d)x^{(3+3)|V(CL_d)|}, \\
&\text{since } |V(CL_d)| = 22d+1 \\
&= 2dx^{3(22d+1)} + (4d+2)x^{(4(22d+1)} + (10d-2)x^{(5(22d+1)} + 8dx^{6(22d+1)}
\end{aligned}$$

Hence the theorem. $\square$

Theorem 4.10. *Let CL_d be the chemical graph of cellulose, then* $PI_M(CL_d, x) = 2dx^{2(22d+1)} + (4d+2)x^{3(22d+1)} + (10d-2)x^{6(22d+1)} + (8d)x^{9(22d+1)}$.

Proof. To obtained the Multiplicatively weighted PI polynomial of the CL_d, by the definition of Multiplicatively weighted PI polynomial and from the Table 1., we have

$$\begin{aligned}
PI_M(CL_d, x) &= \sum_{e=ab\epsilon E(CL_d)} x^{(\wedge_a(ab|CL_d).\wedge_b(ab|CL_d))(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} \\
&= \sum_{e=ab\epsilon E_1(CL_d)} x^{(1.2)(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} + \sum_{e=ab\epsilon E_2(CL_d)} x^{(1.3)(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} \\
&+ \sum_{e=ab\epsilon E_3(CL_d)} x^{(2.3)(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} + \sum_{e=ab\epsilon E_4(CL_d)} x^{(3.3)(\aleph_a(ab|CL_d)+\aleph_b(ab|CL_d))} \\
&= 2dx^{(2)|V(CL_d)|} + (4d+2)x^{(3)|V(CL_d)|} + (10d-2)x^{(6)|V(CL_d)|} + (8d)x^{(9)|V(CL_d)|}, \\
&\text{since } |V(CL_d)| = 22d+1 \\
&= 2dx^{2(22d+1)} + (4d+2)x^{3(22d+1)} + (10d-2)x^{6(22d+1)} + (8d)x^{9(22d+1)}
\end{aligned}$$

Hence the theorem. $\square$

Finally we observe the following remarks, which follows easily from the results discussed here.

Remark 4.11. $PI^{'}(CL_d, 1) = PI(CL_d)$ *and* $PI(CL_d, 1) = |E(CL_d)|$.

Remark 4.12. $PI^{'}_A(CL_d, 1) = PI_A(CL_d)$ *and* $PI_A(CL_d, 1) = |E(CL_d)|$.

Remark 4.13. $PI^{'}_M(CL_d, 1) = PI_M(CL_d)$ *and* $PI_M(CL_d, 1) = |E(CL_d)|$.

5. CONCLUSION

In this study, we primarily calculate the bond-additive based indices such as szeged, PI, weighted Szeged, weighted PI and their polynomials of cellulose graphs using chemical graph analysis are distance calculation. Our theoretical formulations demonstrate the great potential for practical implementation in pharmacy and chemical engineering. As directed networks often predict complex dynamical behaviors more faithfully than undirected networks, it is desirable to bring directness to higher-order structures in the future.

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