

TOPOLOGICAL CHARACTERIZATION OF CELLULOSE NETWORK

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Abstract

Cellulose is one of the natural biopolymers which is the key ingredient for textile products, biofuel, food, cosmetics and pharmaceuticals. We studied its topological aspects through various closed form formulae (topological indices) using Chemical graph theory. Topological indices are graph invariants which associate molecular graph to a numeric value. These invariants having crucial role in Quantitative Structure Property Relationship (QSPR) as well as Quantitative Structure Property Relationship (QSAR) models which infer about the bioactivities and physio-chemical properties of materials. In this work, we computed geometric arithmetic, atom bond connectivity, Sanskruti, general Randić, generalized sum-connectivity and some other well-known indices of cellulose network. We used Mathematica professional software pack for computation and validation of results. These numerical results are potential applications like as, to assist topological characterization of Cellulose to enable its emerging use in pharmaceuticals, food and textile products.

Keywords: Biopolymers; Cellulose; Topological indices; Drug delivery.

Mathematics Subject Classification: 2020 : 06F35, 05C92

1. Introduction

Chem-informatics is comparatively the latest area of information technology which comprise of chemistry, mathematics and other informational sciences that concentrate on gathering, storage, treatment and examination of chemical data. In this work we make approach to structural properties of an important biopolymers cellulose network [9]. It belongs to a polysaccharide class of carbohydrates. Plant stems, leaves, and branches rigidity and strength is mainly depending on it, approximately 40-50% of plant material is cellulose [5]. The strong bonds between molecules of cellulose make it very hard. Chemically it is the most abundant organic compound found on the earth with the general formula $(C_6H_{10}O_5)_n$ consisting of over 3,000 D-glucose units joined by $\beta(1 \rightarrow 4)$ glycosidic bonds. It is a straight chain polymer. The three-dimensional structure of these micro-fibrils is cellulose network CL_n^k , where n is the number of cellulose units in one chain and $k = 6q - 2$, where q represents the number of chains joined together to form CL_n^k . One unit $(C_6H_{10}O_5)$ and two units $(C_6H_{10}O_5)_2$ of these micro-fibrils shown in 1.1 [18]. The figure 1.2 is the molecular representation of cellulose network consisting 6 chains of cellulose joined for $n = 6$. We studied topological aspects of cellulose network CL_n^k through topological indices. Topological indices are the descriptor which characterizes the group topology of graph and invariants

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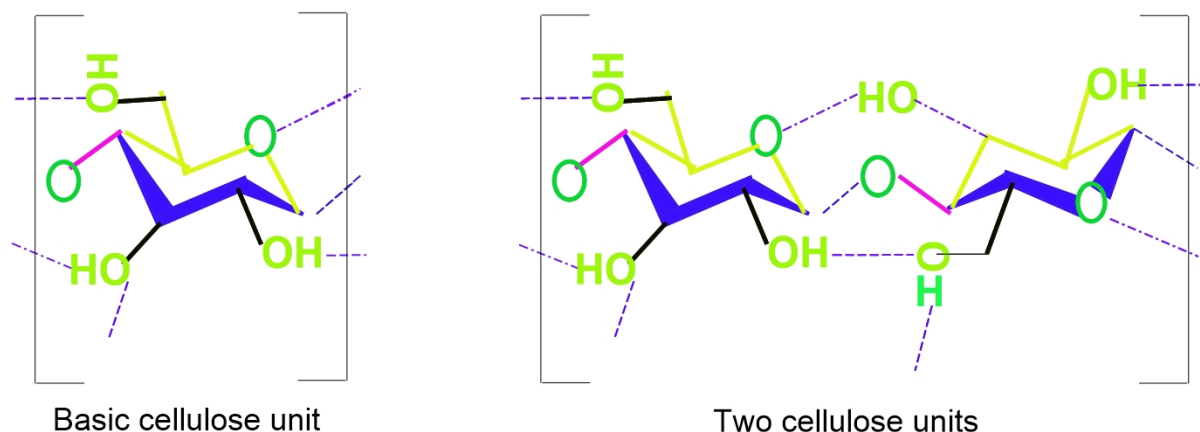


Figure 1.1: Molecular representation of basic cellulose units CL_1^4 and CL_2^4

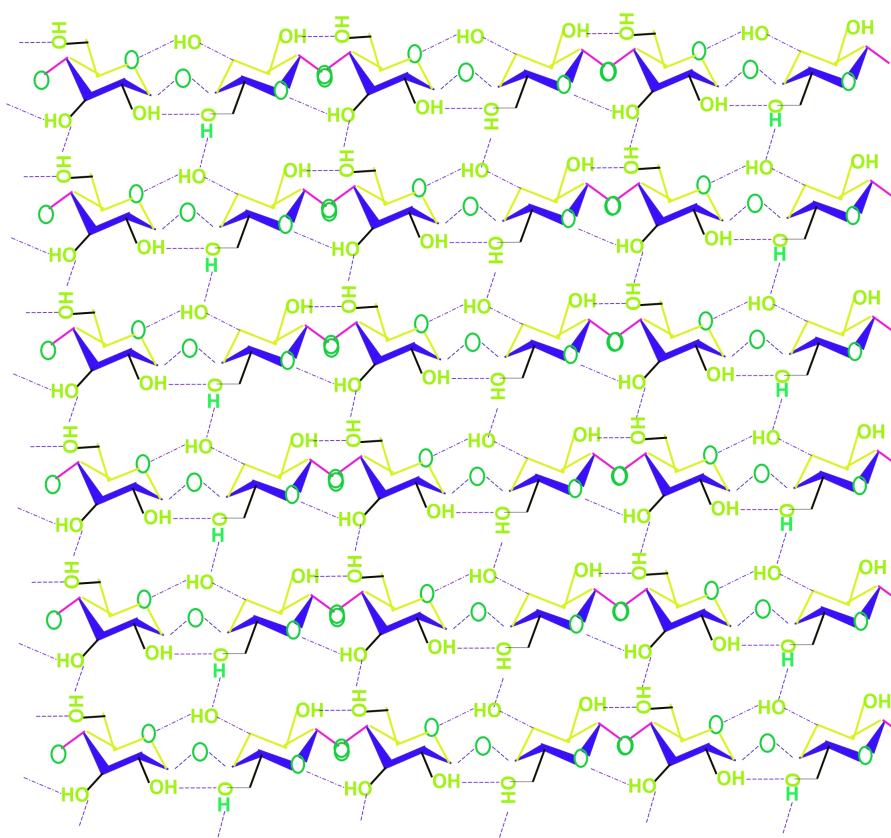


Figure 1.2: Molecular representation of CL_n^k for $k = 34$ and $n = 6$.

under graph isomorphism or equivalently topological indices associate a numerical value with the molecular graph of chemical compound. Among topological indices vertex degree-based indices are the most important and play a vital role in chemical graph theory.

1.1. Materials and method

For mathematical investigation of cellulose network, we used graph theory techniques: edge and vertex segment strategy, degree tallying strategy and degrees of neighbor's vertices listing technique as adopted in [17, 13, 12, 1, 2] for edge and vertex partition according to the values assigned to the vertices of associated graph of CL_n^k . Based on such partition, we computed topological indices of CL_n^k . For computation and verification of computed results we used Wolfram Mathematica Professional Pack. Throughout this work, we use standard notations as used in [10, 15], Γ for simple, finite and connected graph, $E(\Gamma)$ for edge

set, $V(\Gamma)$ for vertex set, d_i for degree of vertex i and S_i for the sum of degree of vertices adjacent to the vertex i , i.e., $S_i = \sum_{j \in N_\Gamma(i)} d_j$ where $N_\Gamma(i) = \{j \in \Gamma : ij \in E(\Gamma)\}$. The Randić index is the most studied vertex degree based topological index among others indices [14]. The numerical elements of Randić index encompass its amalgamation with the Laplacian framework. For a molecular graph Γ , it's defined as

$$R(\Gamma) = \sum_{ij \in E(\Gamma)} \frac{1}{\sqrt{d_i \times d_j}} \quad (1.1)$$

CHEN, et al. [4] purposed generalized sum-connectivity index defined as,

$$\chi_\alpha(\Gamma) = \sum_{ij \in E(\Gamma)} [d_i + d_j]^\alpha, \quad \alpha \in \mathbb{R}^+. \quad (1.2)$$

The Atom-bond connectivity index studied in [6] defined as follow,

$$ABC(\Gamma) = \sum_{ij \in E(\Gamma)} \sqrt{\frac{d_i + d_j - 2}{d_i \times d_j}}, \quad (1.3)$$

Geometric-Arithmetic index GA [16] given as

$$GA(\Gamma) = \sum_{ij \in E(\Gamma)} \frac{2\sqrt{d_i \times d_j}}{d_i + d_j}. \quad (1.4)$$

The fourth version of Atom-bond connectivity index ABC_4 invented in [7], fifth version of geometric-arithmetic index GA_5 introduced in [8] and Sanskruti index $S(\Gamma)$ in [11] are based on the associated value S_i of the vertices of graphs. Their closed form formulas are given as

$$ABC_4(\Gamma) = \sum_{ij \in E(\Gamma)} \sqrt{\frac{S_i + S_j - 2}{S_i \times S_j}}, \quad (1.5)$$

$$GA_5(\Gamma) = \sum_{ij \in E(\Gamma)} \frac{2\sqrt{S_i \times S_j}}{S_i + S_j}, \quad (1.6)$$

and

$$S(\Gamma) = \sum_{ij \in E(\Gamma)} \left(\frac{S_i \times S_j}{S_i + S_j - 2} \right)^3. \quad (1.7)$$

In this work we study structural properties of an important biopolymers CL_n^k . Our focus is to compute closed form formula for topological indices of CL_n^k . In the following section before computation, we describe the construction of planner graph of CL_n^k .

2. Results and discussion

Basic building unit of CL_n^k is $CL_1^4 = C_6H_{10}O_5$ as shown in figure 1.1 consists hexagons with pendant OH, one at upper side and one at lower side. The pendant OH and oxygen atoms connect cellulose units side by side to form straight chains CL_n^4 . These straight chains joined together through hydrogen bonding and forms CL_n^k network, where $k = 6q - 2$, q be the number of chains and $p = 2n - 1$ is the hexagons in one chain. CL_n^k planner graph is the combination of hexagons, octagons and decagons shown in the figure

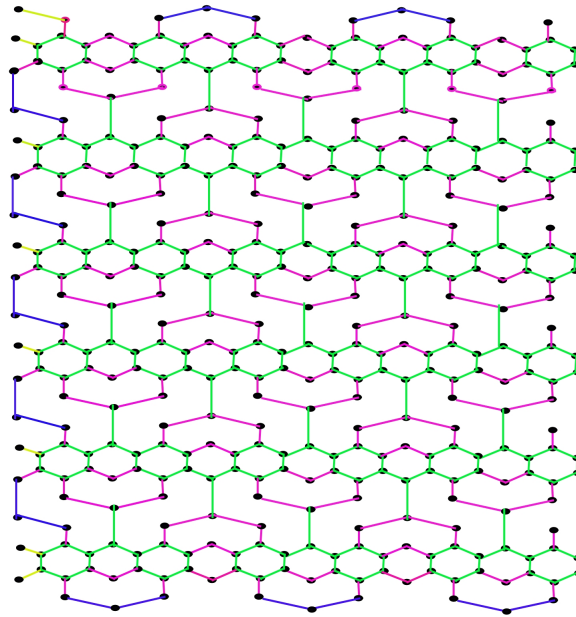


Figure 2.1: Planner graph representation of CL_n^k for.

Table 1: Edge partition table of CL_n^k based on end vertex degrees of the edges

$E_{(i,j)}(\Gamma)$	$e_{i,j}$	$E_{(i,j)}(\Gamma)$	$e_{i,j}$
$E_{(2,1)}(\Gamma)$	1	$E_{(2,2)}(\Gamma)$	$3q + p - 3$
$E_{(3,1)}(\Gamma)$	$2q + 1$	$E_{(3,2)}(\Gamma)$	$3pq + q - 1$
$E_{(3,3)}(\Gamma)$	$\frac{9pq - 3p - 3q + 3}{2}$		

2.1 for $q = 6, n = 6$. The total number of vertices in CL_n^k are $\frac{(11pq+11q)}{6}$ and total number of edges are $\frac{15pq+9q-p-1}{2}$. The set of edges $E(\Gamma)$ partitioned into subsets $E_{(i,j)}(\Gamma)$, on the base of end vertex degrees of the edges of Γ as $i = d_{v_i}$ and $j = d_{v_j}$ and let $|E_{(i,j)}(\Gamma)| = e_{i,j}$. For CL_n^k the set of degrees of vertex is $F = \{1, 2, 3\}$ and $\{(i, j)\} = \{(j, i)\}$ are singleton subset of $F \times F$. Table 1 is the edge partition of $E(\Gamma)$ on the base of end vertex degree of edges. Using table 1, we prove the following theorem for degree based topological indices.

Theorem 2.1. Let $\Gamma = CL_n^k$, then

$$\begin{aligned}
 R(\Gamma) &= \frac{1}{2}(3 + \sqrt{6})pq + \frac{1}{6}(4\sqrt{3} + \sqrt{6} + 6)q + \frac{1}{2}(3\sqrt{2} + 2\sqrt{3} - \sqrt{6} - 6) \\
 F(\Gamma) &= 120pq - 19p + 30q + 5 \\
 GA(\Gamma) &= \frac{3}{10}(15 + 4\sqrt{6})pq + \frac{1}{10}(10\sqrt{3} + 4\sqrt{6} + 15)q - \frac{p}{2} + \frac{1}{30}(20\sqrt{2} + 15\sqrt{3} - 12\sqrt{6} - 45) \\
 ABC(\Gamma) &= \frac{3}{2}(\sqrt{2} + 2)pq + \frac{1}{3}(6\sqrt{2} + 2\sqrt{6} - 3)q + \frac{1}{2}(\sqrt{2} - 2)p + \frac{1}{6}(-9\sqrt{2} + 2\sqrt{6} + 6) \\
 R_\alpha(\Gamma) &= 4^\alpha(p + 3q - 3) + \frac{1}{2}9^\alpha(9pq - 3p - 3q + 3) + 6^\alpha(3pq + q - 1) + 3^\alpha(2q + 1) + 2^\alpha \\
 X_\alpha(\Gamma) &= \frac{3n + 2k - 2}{3} \times 2^{2\alpha} + \frac{kn + 2n - 4}{2} \times 5^\alpha + \frac{3kn - 6k - 4}{4} \times 6^\alpha
 \end{aligned}$$

Proof. Let Γ be the graph of cellulose network CL_n^k . The total number of vertices in CL_n^k are $\frac{11pq+11q}{6}$ and total number of edges are $\frac{15pq+9q-p-1}{2}$. By using table 1 we compute; The Randić index defined as

$$R(\Gamma) = \sum_{ij \in E(\Gamma)} \frac{1}{\sqrt{d_i \times d_j}}$$

$$R(\Gamma) = e_{1,2} \times \frac{1}{\sqrt{1 \times 2}} + e_{2,2} \times \frac{1}{\sqrt{2 \times 2}} + e_{1,3} \times \frac{1}{\sqrt{1 \times 3}} + e_{2,3} \times \frac{1}{\sqrt{2 \times 3}} + e_{3,3} \times \frac{1}{\sqrt{d_i \times d_j}}$$

By using the value of $e_{i,j}$

$$R(\Gamma) = \frac{1}{2}(3 + \sqrt{6})pq + \frac{1}{6}(4\sqrt{3} + \sqrt{6} + 6)q + \frac{1}{2}(3\sqrt{2} + 2\sqrt{3} - \sqrt{6} - 6). \quad (2.1)$$

The forgotten index defined as

$$\begin{aligned} F(\Gamma) &= \sum_{ij \in E(\Gamma)} [d_i^2 + d_j^2] \\ &= e_{1,2} \times [1^2 + 2^2] + e_{2,2} \times [2^2 + 2^2] + e_{1,3} \times [1^2 + 3^2] + e_{2,3} \times [2^2 + 3^2] + e_{3,3} \times [3^2 + 3^2] \end{aligned}$$

By using the value of $e_{i,j}$

$$\begin{aligned} F(\Gamma) &= 1 \times [1^2 + 2^2] + (p + 3q - 3) \times [2^2 + 2^2] + (2q + 1) \times [1^2 + 3^2] \\ &\quad + (3pq + q - 1) \times [2^2 + 3^2] + \frac{(-3p + 9pq - 3q + 3)}{2} \times [3^2 + 3^2] \end{aligned}$$

$$F(\Gamma) = 120pq - 19p + 30q + 5 \quad (2.2)$$

The Geometric Arithmetic index $GA(\Gamma)$ defined as

$$\begin{aligned} GA(\Gamma) &= \sum_{ij \in E(\Gamma)} \frac{2\sqrt{d_i \times d_j}}{d_i + d_j} \\ &= e_{1,2} \times \frac{2\sqrt{1 \times 2}}{1 + 2} + e_{1,3} \times \frac{2\sqrt{1 \times 3}}{1 + 3} + e_{2,2} \times \frac{2\sqrt{2 \times 2}}{2 + 2} + e_{2,3} \times \frac{2\sqrt{2 \times 3}}{2 + 3} \\ &\quad + e_{3,3} \times \frac{2\sqrt{3 \times 3}}{3 + 3} \end{aligned}$$

By using the value of $e_{i,j}$ we get

$$\begin{aligned} GA(\Gamma) &= \frac{3}{10}(15 + 4\sqrt{6})pq + \frac{1}{10}(10\sqrt{3} + 4\sqrt{6} + 15)q - \frac{p}{2} + \frac{1}{30}(20\sqrt{2} \\ &\quad + 15\sqrt{3} - 12\sqrt{6} - 45). \end{aligned} \quad (2.3)$$

The Atomic bond connectivity $ABC(\Gamma)$ index is defined as

$$\begin{aligned} ABC(\Gamma) &= \sum_{ij \in E(\Gamma)} \sqrt{\frac{d_i + d_j - 2}{d_i \times d_j}} \\ &= e_{1,2} \times \sqrt{\frac{1 + 2 - 2}{1 \times 2}} + e_{1,3} \times \sqrt{\frac{1 + 3 - 2}{1 \times 3}} + e_{2,2} \times \sqrt{\frac{2 + 2 - 2}{2 \times 2}} + e_{2,3} \times \sqrt{\frac{2 + 3 - 2}{2 \times 3}} \\ &\quad + e_{3,3} \times \sqrt{\frac{3 + 3 - 2}{3 \times 3}} \end{aligned}$$

By using the value of $e_{i,j}$ we get

$$\begin{aligned} ABC(\Gamma) &= \frac{3}{2}(\sqrt{2} + 2)pq + \frac{1}{3}(6\sqrt{2} + 2\sqrt{6} - 3)q + \frac{1}{2}(\sqrt{2} - 2)p \\ &\quad + \frac{1}{6}(-9\sqrt{2} + 2\sqrt{6} + 6) \end{aligned} \quad (2.4)$$

The general Randic index defined as

$$\begin{aligned} R_\alpha(\Gamma) &= \sum_{ij \in E(\Gamma)} (d_i \times d_j)^\alpha \\ &= e_{1,2} \times (1 \times 2)^\alpha + e_{1,3} \times (1 \times 3)^\alpha + e_{2,2} (2 \times 2)^\alpha + e_{2,3} (2 \times 3)^\alpha + e_{3,3} (3 \times 3)^\alpha \end{aligned}$$

By using the value of $e_{i,j}$ we get

$$\begin{aligned} R_\alpha(\Gamma) &= 4^a(p+3q-3) + \frac{1}{2}9^a(9pq-3p-3q+3) + 6^a(3pq+q-1) \\ &\quad + 3^a(2q+1) + 2^a. \end{aligned} \quad (2.5)$$

$X_\alpha(\Gamma)$ defined as

$$\begin{aligned} X_\alpha(\Gamma) &= \sum_{ij \in E(i,j)} [d_i + d_j]^\alpha \\ &= e_{1,2} \times [1+2]^\alpha + e_{1,3} \times [1+3]^\alpha + e_{2,2} \times [2+2]^\alpha + e_{2,3} \times [2+3]^\alpha + e_{3,3} \times [3+3]^\alpha \end{aligned}$$

By using the value of $e_{i,j}$ we get

$$X_\alpha(\Gamma) = 4^a(p+5q-2) + \frac{1}{2}6^a(9pq-3p-3q+3) + 5^a(3pq+q-1) + 3^a. \quad (2.6)$$

Equation 2.1, 2.2, 2.3, 2.4, 2.5, 2.6 completes the proof. $\square$

The 2.2 is graphical illustration of computed results in theorem 2.1.

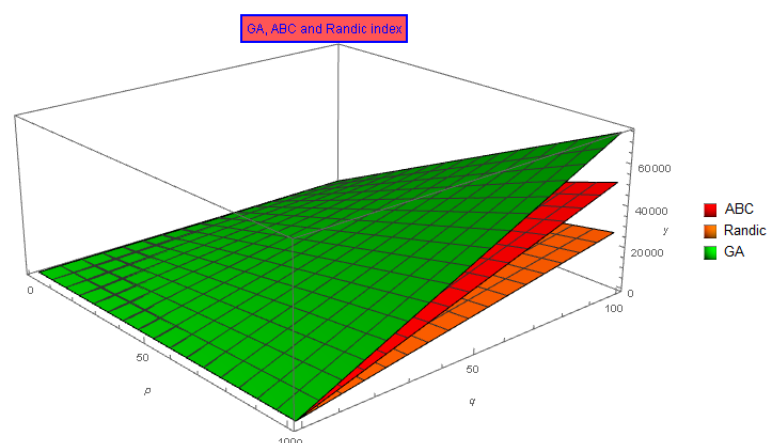


Figure 2.2: Comparison of $ABC(\Gamma)$, $R(\Gamma)$ and $GA(\Gamma)$

The table 2 is the partition of the edge set $E(\Gamma)$ of $G = CL_n^k$ into subsets $E_{(i,j)}(\Gamma)$ on the basis of sum of degrees of vertices at unit distance from end vertices of each edge. Take $e_{i,j} = |E_{(i,j)}(\Gamma)|$. On the basis of table 2 edge partition the following theorems 2.2 to be proved.

Table 2: (S_i, S_j) edge partition table of CL_n^k

(S_i, S_j)	$e_{i,j} = E_{(i,j)}(\Gamma) $	(S_i, S_j)	$e_{i,j} = E_{(i,j)}(\Gamma) $
(2, 4)	1	(6, 7)	$pq - p$
(3, 6)	q	(6, 8)	$2pq - 3q + 3$
(3, 7)	$q + 1$	(6, 9)	$q - 1$
(4, 5)	$p + 2q - 3$	(7, 7)	1
(4, 8)	1	(7, 8)	$3q$
(5, 5)	q	(7, 9)	$\frac{pq - p - q + 1}{2}$
(5, 6)	q	(8, 8)	$pq + 2p - q - 4$
(5, 7)	$q + 1$	(8, 9)	$2pq - 2p - 3q + 3$
(5, 8)	$p + 2q - 4$	(9, 9)	$pq - p - q + 1$

Theorem 2.2. Let cellulose network $\Gamma = CL_n^k$, then

$$\begin{aligned}
ABC_4(\Gamma) &= \left(\frac{1}{6}\sqrt{2} + \frac{1}{8}\sqrt{14} + \frac{1}{6}\sqrt{30} + \frac{1}{42}\sqrt{462} + \frac{13}{9}\right)pq + \left(\frac{-1}{6}\sqrt{2} + \frac{1}{4}\sqrt{14} - \frac{1}{6}\sqrt{30} + \frac{1}{10}\sqrt{35}\right. \\
&\quad + \frac{1}{20}\sqrt{110} - \frac{1}{42}\sqrt{462} - \frac{4}{9}\right)p + \left(\frac{7}{30}\sqrt{2} + \frac{31}{168}\sqrt{14} - \frac{3}{20}\sqrt{30} + \frac{1}{5}\sqrt{35} + \frac{2}{21}\sqrt{42}\right. \\
&\quad + \frac{1}{18}\sqrt{78} + \frac{1}{10}\sqrt{110} + \frac{3}{28}\sqrt{182} - \frac{35}{18}\right)q + \frac{2}{3}\sqrt{2} + \frac{2}{7}\sqrt{3} + \frac{1}{4}\sqrt{5} - \frac{5}{14}\sqrt{14} + \frac{1}{4}\sqrt{30} \\
&\quad - \frac{3}{10}\sqrt{35} + \frac{2}{21}\sqrt{42} - \frac{1}{18}\sqrt{78} - \frac{1}{5}\sqrt{110} + \frac{35}{18} \\
GA_5(\Gamma) &= \left(\frac{24}{17}\sqrt{2} + \frac{8}{7}\sqrt{3} + \frac{3}{16}\sqrt{7} + \frac{2}{13}\sqrt{42} + 2\right)pq + \left(\frac{-24}{17}\sqrt{2} + \frac{4}{9}\sqrt{5} - \frac{3}{16}\sqrt{7} + \frac{4}{13}\sqrt{10}\right. \\
&\quad - \frac{2}{13}\sqrt{42} + 1\right)p + \left(\frac{-74}{51}\sqrt{2} - \frac{12}{7}\sqrt{3} + \frac{8}{9}\sqrt{5} + \frac{2}{5}\sqrt{6} - \frac{3}{16}\sqrt{7} + \frac{8}{13}\sqrt{10} + \frac{4}{5}\sqrt{14} + \frac{1}{5}\sqrt{21}\right. \\
&\quad + \frac{2}{11}\sqrt{30} + \frac{1}{6}\sqrt{35} - 1\right)q + \frac{176}{51}\sqrt{2} + \frac{12}{7}\sqrt{3} - \frac{4}{3}\sqrt{5} - \frac{2}{5}\sqrt{6} + \frac{3}{16}\sqrt{7} - \frac{16}{13}\sqrt{10} + \frac{1}{5}\sqrt{21} \\
&\quad + \frac{1}{6}\sqrt{35} - 2 \\
S(\Gamma) &= \frac{157939036549489}{233744896000}pq - \frac{44337066373489}{233744896000}p - \frac{2701095909052663799}{13865513485824000}q \\
&\quad + \frac{2118453776540577631}{13865513485824000}
\end{aligned}$$

Proof. Let $\Gamma = CL_n^k$. The set of edges $E(\Gamma)$ partitioned into subsets $E_{(i,j)}(\Gamma)$ on the basis of sum of degrees of vertices at unit distance from end vertices of each edge as in the table 2. Take $e_{i,j} = |E_{(i,j)}(\Gamma)|$. The $ABC_4(\Gamma)$ defined as

$$ABC_4(\Gamma) = \sum_{ij \in E(\Gamma)} \sqrt{\frac{S_i + S_j - 2}{S_i \times S_j}}$$

$$\begin{aligned}
ABC_4(CL_n^k) = & e_{2,4}\sqrt{\frac{2+4-2}{2 \times 4}} + e_{3,6}\sqrt{\frac{3+6-2}{3 \times 6}} + e_{3,7}\sqrt{\frac{3+7-2}{3 \times 7}} + e_{4,5}\sqrt{\frac{4+5-2}{4 \times 5}} \\
& + e_{4,8}\sqrt{\frac{4+8-2}{4 \times 8}} + e_{5,5}\sqrt{\frac{5+5-2}{5 \times 5}} + e_{5,6}\sqrt{\frac{5+6-2}{5 \times 6}} + e_{5,7}\sqrt{\frac{5+7-2}{5 \times 7}} \\
& + e_{5,8}\sqrt{\frac{5+8-2}{5 \times 8}} + e_{6,7}\sqrt{\frac{6+7-2}{6 \times 7}} + e_{6,8}\sqrt{\frac{6+8-2}{6 \times 8}} + e_{6,9}\sqrt{\frac{6+9-2}{6 \times 9}} \\
& + e_{7,7}\sqrt{\frac{7+7-2}{7 \times 7}} + e_{7,8}\sqrt{\frac{7+8-2}{7 \times 8}} + e_{7,9}\sqrt{\frac{7+9-2}{7 \times 9}} + e_{8,8}\sqrt{\frac{8+8-2}{8 \times 8}} \\
& + e_{8,9}\sqrt{\frac{8+9-2}{8 \times 9}} + e_{9,9}\sqrt{\frac{9+9-2}{9 \times 9}}
\end{aligned}$$

Using the values of $e_{i,j}$ from table 2 we get,

$$\begin{aligned}
ABC_4(\Gamma) = & \left(\frac{1}{6}\sqrt{2} + \frac{1}{8}\sqrt{14} + \frac{1}{6}\sqrt{30} + \frac{1}{42}\sqrt{462} + \frac{13}{9}\right)pq + \left(-\frac{1}{6}\sqrt{2} + \frac{1}{4}\sqrt{14} - \frac{1}{6}\sqrt{30} + \frac{1}{10}\sqrt{35}\right. \\
& + \frac{1}{20}\sqrt{110} - \frac{1}{42}\sqrt{462} - \frac{4}{9}\Big)p + \left(\frac{7}{30}\sqrt{2} + \frac{31}{168}\sqrt{14} - \frac{3}{20}\sqrt{30} + \frac{1}{5}\sqrt{35} + \frac{2}{21}\sqrt{42}\right. \\
& + \frac{1}{18}\sqrt{78} + \frac{1}{10}\sqrt{110} + \frac{3}{28}\sqrt{182} - \frac{35}{18}\Big)q + \frac{2}{3}\sqrt{2} + \frac{2}{7}\sqrt{3} + \frac{1}{4}\sqrt{5} - \frac{5}{14}\sqrt{14} + \frac{1}{4}\sqrt{30} \\
& - \frac{3}{10}\sqrt{35} + \frac{2}{21}\sqrt{42} - \frac{1}{18}\sqrt{78} - \frac{1}{5}\sqrt{110} + \frac{35}{18}.
\end{aligned} \tag{2.7}$$

The $GA_5(\Gamma)$ defined as

$$GA_5(\Gamma) = \sum_{ij \in E(\Gamma)} \frac{2\sqrt{S_i \times S_j}}{S_i + S_j}$$

$$\begin{aligned}
GA_5(\Gamma) = & e_{2,4}\frac{2\sqrt{2 \times 4}}{2+4} + e_{3,6}\frac{2\sqrt{3 \times 6}}{3+6} + e_{3,7}\frac{2\sqrt{3 \times 7}}{3+7} + e_{4,5}\frac{2\sqrt{4 \times 5}}{4+5} + e_{4,8}\frac{2\sqrt{4 \times 8}}{4+8} + e_{5,5}\frac{2\sqrt{5 \times 5}}{5+5} \\
& + e_{5,6}\frac{2\sqrt{5 \times 6}}{5+6} + e_{5,7}\frac{2\sqrt{5 \times 7}}{5+7} + e_{5,8}\frac{2\sqrt{5 \times 8}}{5+8} + e_{6,7}\frac{2\sqrt{6 \times 7}}{6+7} + e_{6,8}\frac{2\sqrt{6 \times 8}}{6+8} + e_{6,9}\frac{2\sqrt{6 \times 9}}{6+9} \\
& + e_{7,7}\frac{2\sqrt{7 \times 7}}{7+7} + e_{7,8}\frac{2\sqrt{7 \times 8}}{7+8} + e_{7,9}\frac{2\sqrt{7 \times 9}}{7+9} + e_{8,8}\frac{2\sqrt{8 \times 8}}{8+8} + e_{8,9}\frac{2\sqrt{8 \times 9}}{8+9} + e_{9,9}\frac{2\sqrt{9 \times 9}}{9+9}
\end{aligned}$$

by using the values of $e_{i,j}$ from the table.1 we get.

$$\begin{aligned}
GA_5(\Gamma) = & \left(\frac{24}{17}\sqrt{2} + \frac{8}{7}\sqrt{3} + \frac{3}{16}\sqrt{7} + \frac{2}{13}\sqrt{42} + 2\right)pq + \left(-\frac{24}{17}\sqrt{2} + \frac{4}{9}\sqrt{5} - \frac{3}{16}\sqrt{7} + \frac{4}{13}\sqrt{10}\right. \\
& - \frac{2}{13}\sqrt{42} + 1\Big)p + \left(-\frac{74}{51}\sqrt{2} - \frac{12}{7}\sqrt{3} + \frac{8}{9}\sqrt{5} + \frac{2}{5}\sqrt{6} - \frac{3}{16}\sqrt{7} + \frac{8}{13}\sqrt{10} + \frac{4}{5}\sqrt{14} + \frac{1}{5}\sqrt{21}\right. \\
& + \frac{2}{11}\sqrt{30} + \frac{1}{6}\sqrt{35} - 1\Big)q + \frac{176}{51}\sqrt{2} + \frac{12}{7}\sqrt{3} - \frac{4}{3}\sqrt{5} - \frac{2}{5}\sqrt{6} + \frac{3}{16}\sqrt{7} - \frac{16}{13}\sqrt{10} + \frac{1}{5}\sqrt{21} \\
& + \frac{1}{6}\sqrt{35} - 2
\end{aligned} \tag{2.8}$$

The Sanskruti index $S(\Gamma)$ defined as

$$S(\Gamma) = \sum_{ij \in E(\Gamma)} \left(\frac{S_i \times S_j}{S_i + S_j - 2}\right)^3.$$

$$\begin{aligned}
S(\Gamma) = & e_{2,4} \left(\frac{2 \times 4}{2+4-2} \right)^3 + e_{3,6} \left(\frac{3 \times 6}{3+6-2} \right)^3 + e_{3,7} \left(\frac{3 \times 7}{3+7-2} \right)^3 + e_{4,5} \left(\frac{4 \times 5}{4+5-2} \right)^3 \\
& + e_{4,8} \left(\frac{4 \times 8}{4+8-2} \right)^3 + e_{5,5} \left(\frac{5 \times 5}{5+5-2} \right)^3 + e_{5,6} \left(\frac{5 \times 6}{5+6-2} \right)^3 + e_{5,7} \left(\frac{5 \times 7}{5+7-2} \right)^3 \\
& + e_{5,8} \left(\frac{5 \times 8}{5+8-2} \right)^3 + e_{6,7} \left(\frac{6 \times 7}{6+7-2} \right)^3 + e_{6,8} \left(\frac{6 \times 8}{6+8-2} \right)^3 + e_{6,9} \left(\frac{6 \times 9}{6+9-2} \right)^3 \\
& + e_{7,7} \left(\frac{7 \times 7}{7+7-2} \right)^3 + e_{7,8} \left(\frac{7 \times 8}{7+8-2} \right)^3 + e_{7,9} \left(\frac{7 \times 9}{7+9-2} \right)^3 + e_{8,8} \left(\frac{8 \times 8}{8+8-2} \right)^3 \\
& + e_{8,9} \left(\frac{8 \times 9}{8+9-2} \right)^3 + e_{9,9} \left(\frac{9 \times 9}{9+9-2} \right)^3
\end{aligned}$$

Using the values of $e_{i,j}$ from table 2 we get.

$$\begin{aligned}
S(\Gamma) = & \frac{157939036549489}{233744896000}pq - \frac{44337066373489}{233744896000}p - \frac{2701095909052663799}{13865513485824000}q \\
& + \frac{2118453776540577631}{13865513485824000}.
\end{aligned}$$

□

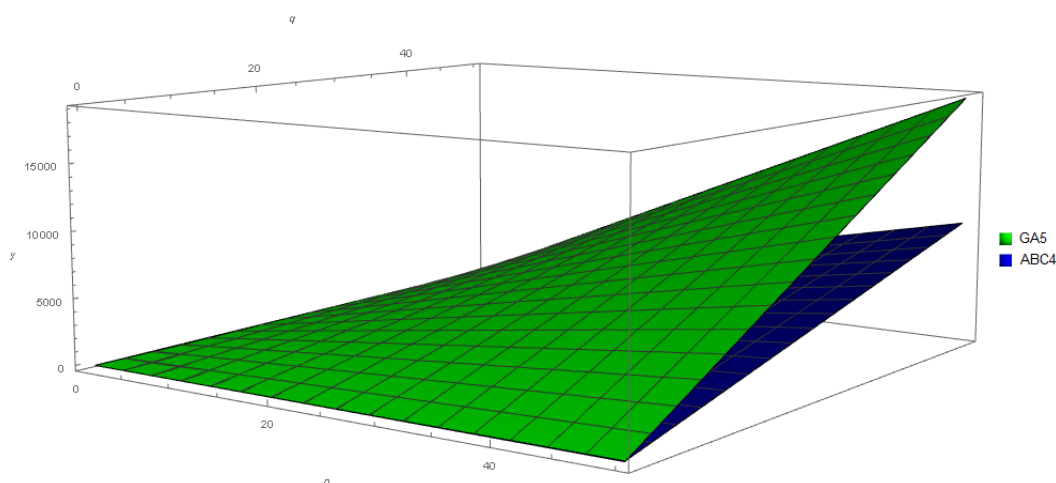


Figure 2.3: Graphical illustration of $ABC_4(\Gamma)$ and $GA_5(\Gamma)$

3. Conclusion

One of the main applications of topological indices is predictions of certain physio-chemical properties of molecules. The CL_n^k is one of the natural biopolymer have a solid impact in cosmetics and pharmaceuticals [3]. For the first time, we compute randić index, forgotten index, Geometric arithmetic index, fifth version of Geometric index, atom-based connectivity index, fourth version of Atom based connectivity index, Sanskruti index, General randić index, generalized Sum-connectivity of CL_n^k . These results can be used for insight learning of CL_n^k according to the interest.

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