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A Consequential Computation of Degree-Based Topological Indices of Triangular Benzenoid

P. Gayathri[1,*] and S. Pavithra[1]

1 PG & Research Department of Mathematics, A.V.C.College (Autonomous), Mannampandal, Tamil Nadu, India.

Abstract: There are various topological indices such as degree-based topological indices, distance based topological indices and counting related topological indices, etc. In this paper, we compute many degree-based topological indices like Randic, Geometric-Arithmetic, Sum-connectivity, Harmonic, First Zagreb, Second Zagreb, Second modified Zagreb, Inverse Sum, Alberston, Atom-Bond Connectivity, Symmetric-Division index and Augmented Zagreb indices for Triangular Benzenoid. Our results are extensions of many existing results.

Keywords: Topological index, Molecular graph, M-polynomial, Triangular Benzenoid.

1. Introduction

A topological index is a numerical parameter mathematically derived from the graph structure. A massive of early drug tests implies that there exist strong inner interaction between the bio-medical and pharmacology characteristics of drugs and their molecular structures. In the past 40 years, scientists have introduced several important indices such as Wiener index, PI index, Zagreb index and eccentric index to measure the characters of drug molecules. In drug, mathematical model, the structure of drug is represented as an undirected graph, where each vertex corresponds to an atom and each edge represents a chemical bond between these atoms. Obviously, the number of vertices and the number of edges are topological index. Triangular Benzenoid is the family of Benzenoid molecular graphs, which is generalizations of Benzene molecule C_6 also the Benzene molecule is a usual molecule in chemistry, physics and nano sciences and is very useful to synthesize aromatic compounds [1–4] usage of topological indices in biology and chemistry began in 1947 when chemist Harold Wiener introduced Wiener index to demonstrate correlations between physicochemical properties of organic compounds and the index of their molecular graphs. The connectivity index introduced in 1975 by Milan Randic who has shown this index to reflect molecular branching. With rapid development of medicine manufacture, a large number of new drugs have been developed each year [5]. Fortunately, many previous studies [6, 7] have pointed that chemical and pharma co dynamics characteristics of drugs and their molecular structures are closely linked. If we calculate indicate indicators of these drugs molecular structures [8–10] in view of defining the topological indices, the medical and pharmaceutical scholars could find it useful to well know their medicinal properties, which can make up the defects of medicine and chemical experiments. From this standpoint, the methods on topological index computation are very suitable and serviceable for developing countries in which they can yield the available biological and medical information of new drugs without chemical experiment hardware. Although there

* *E-mail: pgayathrisundar@gmail.com*

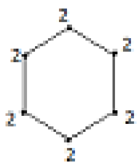
have been several contributions on distance-based indices and degree-based molecular structures [12–15] the researches of topological index for certain special drug structures are still largely limited. Because of these, tremendous academic [16–18] and industrial interest has been attracted to research the topological index of drug molecular structure from a mathematical point of view. In this paper, the degree-based topological indices for the Triangular Benzenoid are computed as expressions in 'n' as a closed formula.

2. M-polynomial

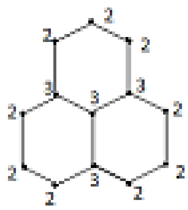
M-polynomial of graph G is defined as if $G = (V,\ E)$ is a graph and $v \in V$, then $d_v\,(G)$ (or d_v) denotes the degree of v. Let G be a graph and let $m_{ij}\,(G)\,,\ i,\ j \geq 1$, be the number of edges $e = uv$ of G such that $\{d_u\,(G)\,,\ \ d_v\,(G)\} = \{i,j\}$. The M-polynomial of G as $M\,(G;x,y) = \sum\limits_{i \leq j} m_{ij}\,(G)\,x^i y^j$. For a graph $G = (V,E)$, a degree-based topological index is a graph invariant of the form $I\,(G) = \sum\limits_{e=uv\in E} f\,(d_u,d_v)$ where $f = f\,(x,y)$ is a function appropriately selected for possible chemical applications.

3. Computational Procedure Using Some Special Cases

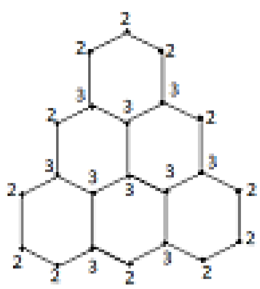
Case 1: Let $T_B\,(n)$ be a Triangular Benzenoid $\Rightarrow$ Number of hexagon $= a = 1$. For $n = 1$ in $T_B\,(1)$, the total number of edges with end degrees (2, 2) is 6.



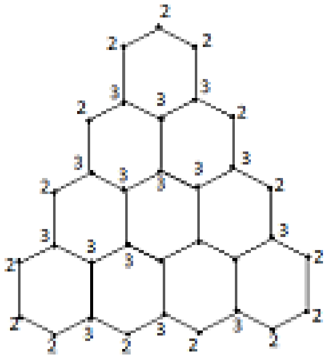
Case 2: Let $T_B\,(n)$ be a Triangular Benzenoid $\Rightarrow$ Number of hexagon $= a = 3$. For $n = 2$ in $T_B\,(2)$, the number of edges with end degrees (2, 2) is 6, the number of edges with end degrees (2, 3) is 6, the number of edges with end degrees (3,3) is 3, the total number of edges for $n = 2$ is 15.



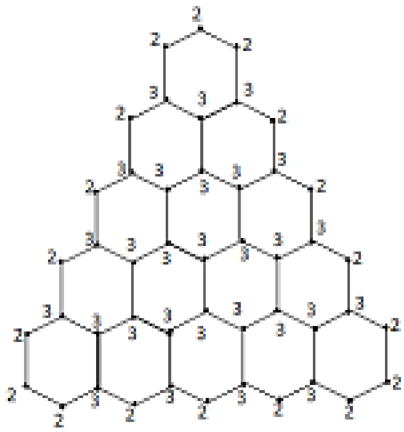
Case 3: Let $T_B\,(n)$ be a Triangular Benzenoid $\Rightarrow$ Number of hexagon $= a = 6$. For $n = 3$ in $T_B\,(3)$, the number of edges with end degrees (2, 2) is 6, the number of edges with end degrees (2, 3) is 12, the number of edges with end degrees (3,3) is 9,the total number of edges for $n = 3$ is 27.



Case 4: Let $T_B\,(n)$ be a Triangular Benzenoid $\Rightarrow$ Number of hexagon $= a = 10$. For $n = 4$ in $T_B\,(4)$, the number of edges with end degrees (2, 2) is 6, the number of edges with end degrees (2, 3) is 18, the number of edges with end degrees (3,3) is 18, the total number of edges for $n = 4$ is 42.



Case 5: Let $T_B\,(n)$ be a Triangular Benzenoid $\Rightarrow$ Number of hexagon $= a = 15$. For $n = 5$ in $T_B\,(5)$, the number of edges with end degrees (2, 2) is 6, the number of edges with end degrees (2, 3) is 24, the number of edges with end degrees (3,3) is 30, the total number of edges for $n = 4$ is 60.



4. Generalization of the Results Obtained for the Molecular Graph of Triangular Benzenoid

Edges (2, 2):

'n' values	**1**	**2**	**3**	**4**	**5**
Result	6	6	6	6	6

Therefore the general form is constant and it is 6.

Edges (2, 3):

'n' values	**1**	**2**	**3**	**4**	**5**
Result	0	6	12	18	24

Therefore the general form is given by $6n - 6$.

Edges (3, 3):

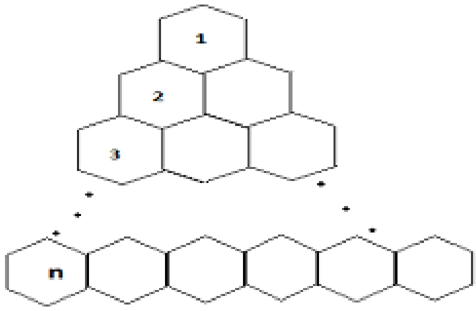
'n' values	1	2	3	4	5
Result	0	3	9	18	30

Therefore the general form is given by $\frac{3n(n-1)}{2}$.

The total number of edges is given in the below table

'n' values	1	2	3	4	5
Result	6	15	27	42	60

Therefore the general form is given by $\frac{3n(n+3)}{2}$.



5. M-Polynomial of Triangular Benzenoid Molecular Graphs

$M[T_B(n)] = 6x^2y^2 + (6n-6)\,x^2y^3 + \left(\frac{3n(n-1)}{2}\right)x^3y^3$, for all $n \geq 1$.

Topological Index	$\{\phi_{ij}\}$	Notation	Topological Index	$\{\phi_{ij}\}$	Notation
Randic	$\frac{1}{\sqrt{ij}}$	$\chi(G)$	Second modified Zagreb	$\frac{1}{ij}$	$M_3(G)$
Geometric-Arithmetic	$\frac{2\sqrt{ij}}{i+j}$	$GA(G)$	Inverse Sum	$\frac{ij}{i+j}$	$IS(G)$
Sum-connectivity	$\frac{1}{\sqrt{i+j}}$	$SCI(G)$	Albertson	$\lvert i-j\rvert$	$Alb(G)$
Harmonic	$\frac{2}{i+j}$	$HI(G)$	Atom-Bond connectivity	$\sqrt{\frac{i+j-2}{ij}}$	$ABC(G)$
First Zagreb	$i+j$	$M_1(G)$	Symmetric Division Index	$\frac{i^2+j^2}{ij}$	$SD(G)$
Second Zagreb	ij	$M_2(G)$	Augmented Zagreb	$\left(\frac{ij}{i+j-2}\right)^3$	$AZI(G)$

Table 1. **Some Important Formulae of degree-based Topological indices**

6. Topological Indices of Triangular Benzenoid Molecular Graphs

Theorem 6.1. *Let n be the number of rows in the Triangular Benzenoid of graph $T_B(n)$, then Randic Index is given by* $\chi(T_B(n)) = \frac{\mathrm{n}^2-\mathrm{n}+2\sqrt{6}\mathrm{n}-2\sqrt{6}+6}{2}$.

Proof. Randic Index is denoted by

$$\begin{aligned}
\chi(T_B(n)) &= \frac{1}{\sqrt{ij}}T_B(n) \\
&= \frac{1}{\sqrt{ij}}\{6\} + \frac{1}{\sqrt{ij}}\{6n-6\} + \frac{1}{\sqrt{ij}}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{1}{\sqrt{2*2}}\{6\} + \frac{1}{\sqrt{2*3}}\{6n-6\} + \frac{1}{\sqrt{3*3}}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{1}{\sqrt{4}}\{6\} + \frac{1}{\sqrt{6}}\{6n-6\} + \frac{1}{\sqrt{9}}\left\{\frac{3n(n-1)}{2}\right\}
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{\sqrt{4}}\{6n+4\} + \frac{1}{\sqrt{6}}\{4n\} + \frac{1}{\sqrt{9}}\{4n-3\} \\
&= \frac{6}{2} + \frac{6n-6}{\sqrt{6}} + \frac{3n(n-1)}{3*2} = 3 + \frac{6(n-1)}{\sqrt{6}} + \frac{3n(n-1)}{6} \\
&= 3 + \frac{\sqrt{6}\sqrt{6}(n-1)}{\sqrt{6}} + \frac{n(n-1)}{2} \\
&= 3 + \sqrt{6}(n-1) + \frac{n(n-1)}{2} \\
&= \frac{n^2 - n + 2\sqrt{6}n - 2\sqrt{6} + 6}{2} \\
&= \frac{n^2 - n + 2\sqrt{6}n - 2\sqrt{6} + 6}{2} \\
\chi(T_B(n)) &= \frac{n^2 - n + 2\sqrt{6}n - 2\sqrt{6} + 6}{2}.
\end{aligned}
$$

□

Theorem 6.2. *Let n be the number of rows in the Triangular Benzenoid of graph $T_B(n)$, then Geometric-Arithmetic is given by $GA(T_B(n)) = \frac{(15n+24\sqrt{6})(n-1)+60}{10}$.*

Proof. Geometric-Arithmetic is denoted by

$$
\begin{aligned}
GA(T_B(n)) &= \frac{2\sqrt{ij}}{i+j} \\
&= \frac{2\sqrt{ij}}{i+j}\{6\} + \frac{2\sqrt{ij}}{i+j}\{6n-6\} + \frac{2\sqrt{ij}}{i+j}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{2\sqrt{2*2}}{2+2}(6) + \frac{2\sqrt{2*3}}{2+3}\{6n-6\} + \frac{2\sqrt{3*3}}{3+3}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{2\sqrt{4}}{4}(6) + \frac{2\sqrt{6}}{5}\{6n-6\} + \frac{2\sqrt{9}}{6}\left\{\frac{3n(n-1)}{2}\right\} \\
&= 6 + \frac{2\sqrt{6}}{5}\{6n-6\} + \frac{3n(n-1)}{2} \\
&= \frac{60 + 24\sqrt{6}(n-1) + 15n(n-1)}{10} \\
&= \frac{\{24\sqrt{6} + 15n\}(n-1) + 60}{10} \\
GA(T_B(n)) &= \frac{\left(15n + 24\sqrt{6}\right)(n-1) + 60}{10}.
\end{aligned}
$$

□

Theorem 6.3. *Let n be the number of rows in the Triangular Benzenoid of graph $T_B(n)$, then Sum-connectivity index is given by $SCI(T_B(n)) = 3 + \frac{6n-6}{\sqrt{5}} + \frac{3n(n-1)}{2\sqrt{6}}$.*

Proof. Sum-connectivity is denoted by

$$
\begin{aligned}
SCI(T_B(n)) &= \frac{1}{\sqrt{i+j}} \\
&= \frac{1}{\sqrt{i+j}}\{6\} + \frac{1}{\sqrt{i+j}}\{6n-6\} + \frac{1}{\sqrt{i+j}}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{1}{\sqrt{2+2}}\{6\} + \frac{1}{\sqrt{2+3}}\{6n-6\} + \frac{1}{\sqrt{3+3}}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{1}{\sqrt{4}}\{6\} + \frac{1}{\sqrt{5}}\{6n-6\} + \frac{1}{\sqrt{3+3}}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{1}{2}\{6\} + \frac{1}{\sqrt{5}}\{6n-6\} + \frac{1}{\sqrt{6}}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{6}{2} + \frac{6n}{\sqrt{5}} + \frac{6}{\sqrt{5}} - \frac{3n(n-1)}{2\sqrt{6}} \\
&= 3 + \frac{6n}{\sqrt{5}} - \frac{6}{\sqrt{5}} + \frac{3n(n-1)}{2\sqrt{6}} \\
SCI(T_B(n)) &= 3 + \frac{6n-6}{\sqrt{5}} + \frac{3n\,(n-1)}{2\sqrt{6}}.
\end{aligned}
$$

□

Theorem 6.4. *Let n be the number of rows in the Triangular Benzenoid of graph $T_B\,(n)$, then harmonic index is given by* $HI(T_B\,(n)) = \frac{5n^2+19n+6}{10}$.

Proof. Harmonic index is denoted by

$$\begin{aligned}
HI(T_B\,(n)) &= \frac{2}{i+j} \\
&= \frac{2}{i+j}\,\{6\} + \frac{2}{i+j}\,\{6n-6\} + \frac{2}{i+j}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{2}{2+2}\,\{6\} + \frac{2}{2+3}\,\{6n-6\} + \frac{2}{3+3}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{2}{4}\,\{6\} + \frac{2}{5}\,\{6n-6\} + \frac{2}{3+3}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{1}{2}\,\{6\} + \frac{2}{5}\,\{6n-6\} + \frac{2}{3+3}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{6}{2} + \frac{12n-12}{5} + \frac{2}{6}\left\{\frac{3n(n-1)}{2}\right\} \\
&= 3 + \frac{12n-12}{5} + \left\{\frac{n(n-1)}{2}\right\} \\
&= \frac{30+24n-24+5n^2-5n}{10} \\
&= \frac{5n^2+19n+6}{10} \\
HI(T_B\,(n)) &= \frac{5n^2+19n+6}{10}.
\end{aligned}$$

□

Theorem 6.5. *Let n be the number of rows in the Triangular Benzenoid of graph $T_B\,(n)$, then First Zagreb is given by* $M_1(T_B\,(n)) = 9n^2 + 21n - 6$.

Proof. First Zagreb is denoted by

$$\begin{aligned}
M_1(T_B\,(n)) &= i+j \\
&= (i+j)\,\{6\} + (i+j)\{6n-6\} + (i+j)\left(\frac{3n(n-1)}{2}\right) \\
&= (2+2)\,\{6\} + (2+3)\{6n-6\} + (3+3)\left(\frac{3n(n-1)}{2}\right) \\
&= (4)\,\{6\} + (5)\{6n-6\} + (3+3)\left(\frac{3n(n-1)}{2}\right) \\
&= 24 + 30n - 30 + 9n^2 - 9n \\
&= 9n^2 + 21n - 6 \\
M_1(T_B\,(n)) &= 9n^2 + 21n - 6.
\end{aligned}$$

□

Theorem 6.6. *Let n be the number of rows in the Triangular Benzenoid of graph $T_B\,(n)$, then Second Zagreb is given by* $M_2(T_B\,(n)) = \frac{3}{2}\left(9n^2 + 15\mathrm{n} - 8\right)$.

Proof. Second Zagreb is denoted by

$$\begin{aligned}
M_2(T_B\,(n)) &= ij \\
&= (ij)\,\{6\} + (ij)\{6n-6\} + (ij)\left(\frac{3n(n-1)}{2}\right) \\
&= (2*2)\,\{6\} + (2*3)\{6n-6\} + (3*3)\left(\frac{3n(n-1)}{2}\right)
\end{aligned}$$

$$
\begin{aligned}
&= (4)\{6\} + (6)\{6n-6\} + (3*3)\left(\frac{3n(n-1)}{2}\right) \\
&= 24 + 36n - 36 + \left(\frac{3n(n-1)}{2}\right) \\
&= 24 + 36n - 36 + \left(\frac{27n(n-1)}{2}\right) \\
&= \frac{48 + 72n - 72 + 27n(n-1)}{2} \\
&= \frac{48 + 72n - 72 + 27n^2 - 27n}{2} \\
&= \frac{27n^2 + 45n - 24}{2} \\
&= \frac{3}{2}(9n^2 + 15n - 8) \\
M_2(T_B(n)) &= \frac{3}{2}\left(9n^2 + 15n - 8\right).
\end{aligned}
$$

□

Theorem 6.7. *Let n be the number of rows in the Triangular Benzenoid of graph $T_B(n)$, then Second Modified Zagreb is given by $M_3(T_B(n)) = \frac{n^2+5n+3}{6}$.*

Proof. Second Modified Zagreb is denoted by

$$
\begin{aligned}
M_3(T_B(n)) &= \frac{1}{ij} \\
&= \frac{1}{ij}\{6\} + \frac{1}{ij}\{6n-6\} + \frac{1}{ij}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{1}{2*2}\{6\} + \frac{1}{2*3}\{6n-6\} + \frac{1}{3*3}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{1}{4}\{6\} + \frac{1}{6}\{6n-6\} + \frac{1}{3*3}\left\{\frac{3n(n-1)}{2}\right\} \\
&= \frac{6}{4} + \frac{6n-6}{6} + \frac{3n(n-1)}{18} \\
&= \frac{3}{2} + (n-1) + \frac{n(n-1)}{6} \\
&= \frac{18 + 12n - 12 + 2n^2 - 2n}{12} \\
&= \frac{2n^2 + 10n + 6}{12} \\
&= \frac{n^2 + 5n + 3}{6} \\
M_3(T_B(n)) &= \frac{n^2 + 5n + 3}{6}.
\end{aligned}
$$

□

Theorem 6.8. *Let n be the number of rows in the Triangular Benzenoid of graph $T_B(n)$, then Inverse Sum is given by $IS(T_B(n)) = .\frac{3}{20}\left(15n^2 + 33n - 8\right)$.*

Proof. Inverse Sum is denoted by

$$
\begin{aligned}
IS(T_B(n)) &= \frac{ij}{i+j} \\
&= \frac{ij}{i+j}\{(6\} + \frac{ij}{i+j}\{6n-6\} + \frac{ij}{i+j}\left(\frac{3n(n-1)}{2}\right) \\
&= \frac{2*2}{2+2}\{6\} + \frac{2*3}{2+3}\{6n-6\} + \frac{3*3}{3+3}\left(\frac{3n(n-1)}{2}\right) \\
&= 6 + \frac{36n}{5} - \frac{36}{5} + \frac{9n(n-1)}{4} \\
&= \frac{120 + 144n - 144 + 45n(n-1)}{20}
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{120+144n-144+45n^2-45n}{20}\\
&= \frac{45n^2-24+99n}{20}\\
&= \frac{3}{20}(15n^2+33n-8)\\
IS(T_B(n)) &= \frac{3}{20}\left(15n^2+33n-8\right).
\end{aligned}
$$

□

Theorem 6.9. *Let n be the number of rows in the Triangular Benzenoid of graph $T_B(n)$, then Albertson is given by $Alb(T_B(n)) = 6n-6$.*

Proof. Albertson is denoted by

$$
\begin{aligned}
Alb(T_B(n)) &= |i-j|\\
&= |i-j|\{6\} + |i-j|\{6n-6\} + |i-j|\left(\frac{3n(n-1)}{2}\right)\\
&= |2-2|\{6\} + |2-3|\{6n-6\} + |3-3|\left(\frac{3n(n-1)}{2}\right)\\
&= 6n-6\\
Alb(T_B(n)) &= 6n-6.
\end{aligned}
$$

□

Theorem 6.10. *Let n be the number of rows in the Triangular Benzenoid of graph $T_B(n)$, then Atom-Bond connectivity is given by $ABC(T_B(n)) = n\left(n+3\sqrt{2}-1\right)$.*

Proof. Atom-Bond connectivity is denoted by

$$
\begin{aligned}
ABC(T_B(n)) &= \sqrt{\frac{i+j-2}{ij}}\\
&= \sqrt{\frac{i+j-2}{ij}}\{6\} + \sqrt{\frac{i+j-2}{ij}}\{6n-6\} + \sqrt{\frac{i+j-2}{ij}}\left(\frac{3n(n-1)}{2}\right)\\
&= \sqrt{\frac{2+2-2}{2*2}}\{6\} + \sqrt{\frac{2+3-2}{2*3}}\{6n-6\} + \sqrt{\frac{3+3-2}{3*3}}\left(\frac{3n(n-1)}{2}\right)\\
&= \sqrt{\frac{2}{4}}\{6\} + \sqrt{\frac{3}{6}}\{6n-6\} + \sqrt{\frac{4}{9}}\left(\frac{3n(n-1)}{2}\right)\\
&= \sqrt{\frac{1}{2}}\{6\} + \sqrt{\frac{1}{2}}\{6n-6\} + \frac{2}{3}\left(\frac{3n(n-1)}{2}\right)\\
&= \sqrt{\frac{1}{2}}\{6\} + \sqrt{\frac{1}{2}}\{6n-6\} + \frac{2}{3}\left(\frac{3n(n-1)}{2}\right)\\
&= \frac{1}{\sqrt{2}}\{6\} + \frac{1}{\sqrt{2}}\{6n-6\} + \frac{2}{3}\left(\frac{3n(n-1)}{2}\right)\\
&= \frac{6}{\sqrt{2}} + \frac{6n-6}{\sqrt{2}} + \frac{6(n(n-1))}{6}\\
&= \frac{6n}{\sqrt{2}} + n(n-1)\\
&= \frac{2\times 3n}{\sqrt{2}} + n(n-1)\\
&= 3\sqrt{2}n + n(n-1)\\
&= n(3\sqrt{2}+n-1)\\
ABC(T_B(n)) &= n\left(n+3\sqrt{2}-1\right).
\end{aligned}
$$

□

Theorem 6.11. *Let n be the number of rows in the Triangular Benzenoid of graph $T_B(n)$, then Symmetric Division Index is given by $SD(T_B(n)) = 3n^2 + 10n - 1$.*

Proof. Symmetric Division Index is denoted by

$$\begin{aligned}
SD(T_B(n)) &= \frac{i^2+j^2}{ij} \\
&= \frac{i^2+j^2}{ij}\{6\} + \frac{i^2+j^2}{ij}\{6n-6\} + \frac{i^2+j^2}{ij}\left(\frac{3n(n-1)}{2}\right) \\
&= \frac{(2)^2+(2)^2}{2*2}\{6\} + \frac{(2)^2+(3)^2}{2*3}\{6n-6\} + \frac{(3)^2+(3)^2}{3*3}\left(\frac{3n(n-1)}{2}\right) \\
&= \frac{4+4}{4}\{6\} + \frac{4+9}{6}\{6n-6\} + \frac{9+9}{9}\left(\frac{3n(n-1)}{2}\right) \\
&= \frac{8}{4}\{6\} + \frac{13(6n-6)}{6} + \frac{18}{9}\left(\frac{3n(n-1)}{2}\right) \\
&= 12 + 13n - 13 + 3n(n-1) \\
&= 3n^2 - 3n + 13n + 12 - 13 \\
&= 3n^2 + 10n - 1 \\
SD(T_B(n)) &= 3n^2 + 10n - 1.
\end{aligned}$$

□

Theorem 6.12. *Let n be the number of rows in the Triangular Benzenoid of graph $T_B(n)$, then Augmented Zagreb is given by $AZI(T_B(n)) = \frac{3n}{128}(729n + 1319)$.*

Proof. Augmented Zagreb is denoted by

$$\begin{aligned}
AZI(T_B(n)) &= \left(\frac{ij}{i+j-2}\right)^3 \\
&= \left(\frac{ij}{i+j-2}\right)^3\{6\} + \left(\frac{ij}{i+j-2}\right)^3\{6n-6\} + \left(\frac{ij}{i+j-2}\right)^3\left(\frac{3n(n-1)}{2}\right) \\
&= \left(\frac{2*2}{2+2-2}\right)^3\{6\} + \left(\frac{2*3}{2+3-2}\right)^3\{6n-6\} + \left(\frac{3*3}{3+3-2}\right)^3\left(\frac{3n(n-1)}{2}\right) \\
&= \left(\frac{4}{2}\right)^3\{6\} + \left(\frac{6}{3}\right)^3\{6n-6\} + \left(\frac{3*3}{4}\right)^3\left(\frac{3n(n-1)}{2}\right) \\
&= (2)^3\{6\} + (2)^3\{6n-6\} + \left(\frac{9}{4}\right)^3\left(\frac{3n(n-1)}{2}\right) \\
&= (8)\{6\} + (8)\{6n-6\} + \left(\frac{9}{4}\right)^3\left(\frac{3n(n-1)}{2}\right) \\
&= 48 + 48n - 48 + \left(\frac{729}{64}\right)\left(\frac{3n(n-1)}{2}\right) \\
&= 48 + 48n - 48 + \left(\frac{729}{64}\right)\left(\frac{3n(n-1)}{2}\right) \\
&= 48n + \left(\frac{729}{64}\right)\left(\frac{3n(n-1)}{2}\right) \\
&= 48n + \frac{2187n^2 - 2187n}{128} \\
&= \frac{6144n + 2187n^2 - 2187n}{128} \\
&= \frac{2187n^2 + 3957n}{128} \\
&= \frac{3n}{128} \\
AZI(T_B(n)) &= \frac{3n}{128}.
\end{aligned}$$

□

7. Conclusion

In this paper, we have computed the degree-based topological indices of molecular graph "Triangular Benzenoid $T_B(n)$". In theoretical chemistry, the topological indices and molecular structure descriptors are used for modelling physic-chemical, toxicological, biological and other properties of chemical compounds. This paper is very useful for pharmaceutical and medical scientists to grasp the biological and chemical characteristics of new drugs.

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