Research Article

On Computation of Edge Degree-Based Banhatti Indices of a Certain Molecular Network

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Chemical graph theory deals with the basic properties of a molecular graph. In graph theory, we correlate molecular descriptors to the properties of molecular structures. Here, we compute some Banhatti molecular descriptors for water-soluble dendritic unimolecular polyether micelle. Our results prove to be very significant to understand the behaviour of water-soluble dendritic unimolecular polyether micelle as a drug-delivery agent.

1. Introduction

Topological indices are graph invariants associated with numbers that describe the properties of the graph. In chemical graph theory, topological indices play a vital role to explore the structures of different graphs. In 1947, Harold Wiener gave the idea of topological indices [1]. After that, he published a series of papers describe the relation between wiener index and physicochemical properties of carbon-based compounds [2, 3] in 1947 and [4, 5] in 1948. The analysis of topological indices has great importance in nanotechnology and theoretical chemistry. The irregularity of graph was discussed [6] in 1997. In the last decade of the 20th century, a large number of topological indices were introduced that were related to the Wiener index. In the second decade of the 21st century, irregularity topological indices were computed for different chemical structures. In [7], it was shown that Randic and modified Zagreb indices are in one-to-one correspondence for all acyclic molecules which consist of no more than 100 atoms. In [8], the new notion of total irregularity was introduced, and the authors determined the

graphs with maximum total irregularity. In [9–11], the total irregularity of graphs was discussed under the graph operations. In [12], the total irregularity of graphs was discussed to study QSPR. An Indian mathematician Kulli in 2016 [13] introduced some new Banhatti indices such as K Banhatti indices, modified Banhatti indices and, hyper K Banhatti indices. In the last decade, irregular, distance- and degree-based topological indices became hot topics for research in chemical graph theory. Many researchers computed these indices for different chemical graphs to study their biochemical properties. In [14], Zheng et al. computed some eccentricity-based topological indices and polynomials of Poly(EThylene Amido Amine) (PETAA) dendrimers. In [15], Ye et al. worked on the Zagreb connection number index of nanotubes and regular hexagonal lattice. In [16], Fahad et al. studied the topological descriptors of Poly Propyl Ether Imine (PETIM) dendrimers. In [17], Qureshi studied the Zagreb connection index of drug-related chemical structures. In [18], Zhang et al. worked on a newly defined topological index named face index for silicon carbides. In [19], Luo et al. computed lower bounds on the entire Zagreb indices

of trees. In [20], Chu et al. studied the irregular indices for metal organic frameworks and certain 2D lattices. The Zagreb connection index is computed for silicate, hexagonal, honeycomb, and oxide networks in [21] in 2021. In [22], Rao et al. studied some degree-based topological indices of a caboxy-terminated dendritic macromolecule. In [23], the authors computed the face index for Boron triangular nanotubes and for quadrilateral sections cut from a regular hexagonal lattice. In [24], Hussain et al. computed topological indices for new classes of Benes network.

Let $G(V, E)$ be a graph where V is a set of vertices and E is a set of edges. A cardinality of edges associated with a vertex is called the degree of the vertex. Here, we use a special term of $e = st$ as an edge of G where the vertex s and vertex t are linked together by edge e. Let $d_G(e)$ denote the degree of an edge e in G, which is defined by $d_G(e) = d_G(s) + d_G(t) - 2$ with $e = st$. For more details, refer the work of Kulli [25].

The first and second K Banhatti indices were introduced by Kulli in [13] as

$$
\begin{aligned}
B_1(G) &= \sum_{e=st \epsilon E(G)} [d_G(s) + d_G(e)], \\
B_2(G) &= \sum_{e=st \epsilon E(G)} [d_G(s) * d_G(e)].
\end{aligned}
\tag{1}
$$

The first and second K hyper Banhatti index of G were introduced by Kulli in [26] defined as

$$
\begin{aligned}
\mathrm{HB}_1(G) &= \sum_{e=st \epsilon E(G)} [d_G(s) + d_G(e)]^2, \\
\mathrm{HB}_2(G) &= \sum_{e=st \epsilon E(G)} [d_G(s) * d_G(e)]^2.
\end{aligned}
\tag{2}
$$

The first and second modified Banhatti indices of G were introduced by Kulli in [27] as

$$
\begin{aligned}
\mathrm{mB}_1(G) &= \sum_{e=st \epsilon E(G)} \left[\frac{1}{(d_G(s) + d_G(e)) + (d_G(t) + d_G(e))} \right], \\
\mathrm{mB}_2(G) &= \sum_{e=st \epsilon E(G)} \left[\frac{2}{(d_G(s) + d_G(e)) + (d_G(t) + d_G(e))} \right].
\end{aligned}
\tag{3}
$$

The harmonic K-Banhatti index of a graph G was introduced by Kulli in [27] as

$$
H_b(G) = \sum_{e=st \epsilon E(G)} \left[\frac{2}{(d_G(s) + d_G(e)) + (d_G(t) + d_G(e))} \right].
\tag{4}
$$

Let G be a graph of water-soluble dendritic unimolecular polyether micelle. It has $38(2^n) - 4$ number of vertices and $42(2^n) - 5$ number of edges where n is the number of growth of the graph. The graph has $4(2^n)$ number of vertices having degree 1, $22(2^n) - 2$ vertices having degree 2 and $12(2^n) - 2$ vertices having degree 3. The graph has $4(2^n)$ number of edges having degree $(1, 3)$, $8(2^n) + 2$ edges having degree $(2, 2)$, $28(2^n) - 8$ edges having degree $(2, 3)$, and $(2, 3)$ number of edges having degree $(3, 3)$. In Figure 1, the graph G is given for $n = 4$. Dendritic unimolecular micelles play an important role in drug delivery systems. Unimolecular micelles have a unique property of uniform size and high stability. Also, they have attracted increasing attention due to their high functionality in various applications.

In the next section, we will compute the Banhatti indices for the water-soluble dendritic unimolecular polyether micelle.

2. Main Results

Table 1 shows the partition of the edge set for the molecular graph G of water-soluble dendritic unimolecular polyether micelle.

Theorem 1. *Let G be the molecular graph of water-soluble dendritic unimolecular polyether micelle; then, the first K Banhatti index of G is*

$$
B_1(G) = 432(2^n) - 58.
\tag{5}
$$

Proof. By using Table 1 and the definition of the first K Banhatti index, we have

$$
\begin{aligned}
B_1(G) &= \sum_{e=st \epsilon E(G)} [d_G(s) + d_G(e)], \\
&= 4(2^n)[(1 + 2) + (3 + 2)] + (8(2^n) + 2)[(2 + 2) + (2 + 2)] \\
&\quad + (28(2^n) - 8)[(2 + 3) + (3 + 3)] + (2(2^n) + 1)[(3 + 4) + (3 + 4)], \\
&= 32(2^n) + 64(2^n) + 16 + 308(2^n) - 88 + 28(2^n) + 14, \\
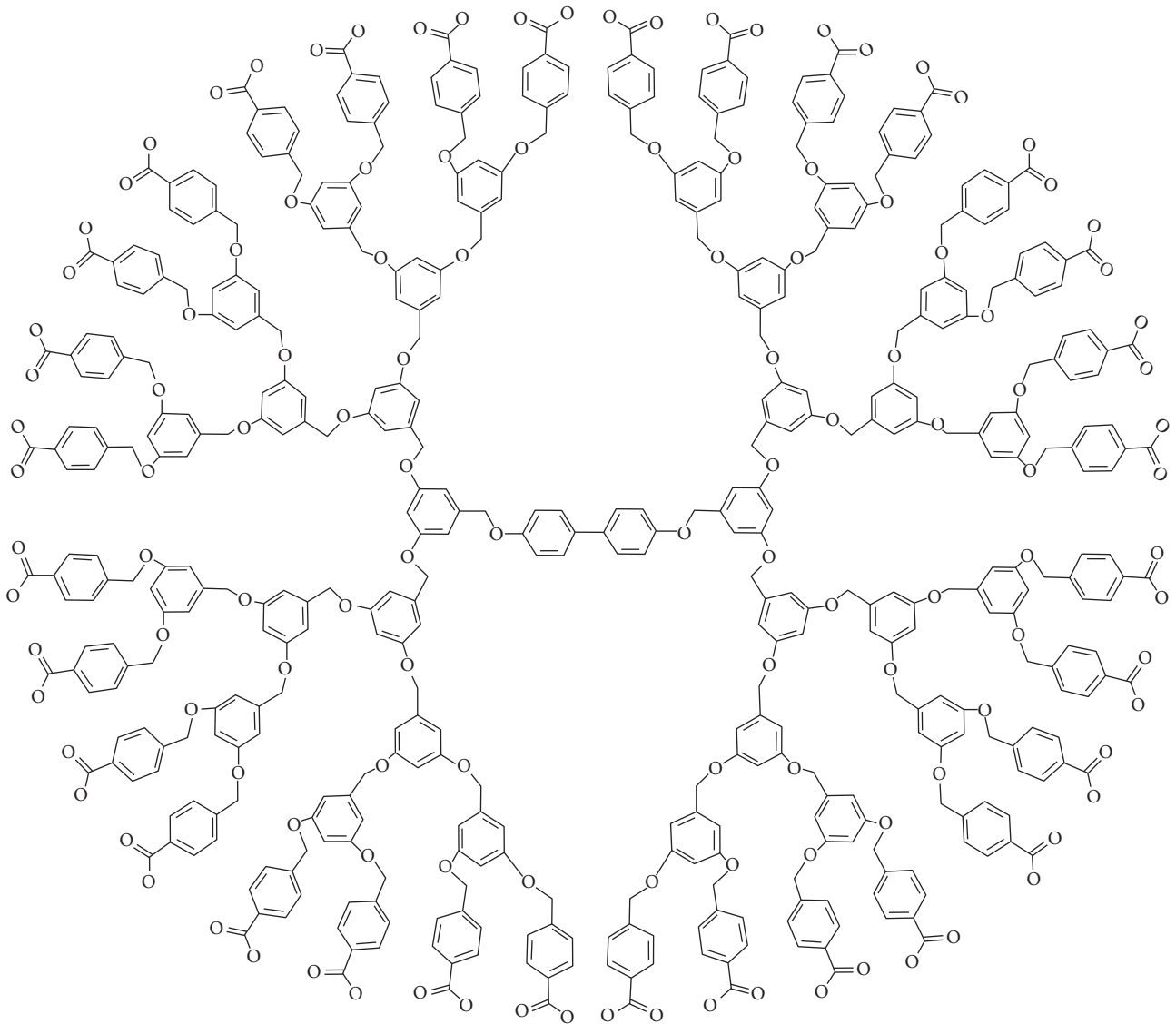&= 432(2^n) - 58.
\end{aligned}
\tag{6}
$$

□

Figure 1: Graph of water-soluble unimolecular polyether micelle for growth four.

Table 1: Edge partition of water-soluble dendritic unimolecular polyether micelle.

$(d_G(s), d_G(t))$, where $st \epsilon E(G)$	$d_G(e)$	Number of edges
$(1,3)$	2	$4(2^n)$
$(2,2)$	2	$8(2^n) + 2$
$(2,3)$	3	$28(2^n) - 8$
$(3,3)$	4	$2(2^n) + 1$

Theorem 2. *Let G be the molecular graph of water-soluble dendritic unimolecular polyether micelle; then, the second K Banhatti index of G is*

$$B_2(G) = 564(2^n) - 80. \tag{7}$$

Proof. To compute the second K Banhatti index, we will use Table 1.

$$
\begin{aligned}
B_2(G) &= \sum_{e=st\epsilon E(G)} [d_G(s) * d_G(e)], \\
&= 4(2^n)[(1*2) + (3*2)] + (8(2^n) + 2)[(2*2) + (2*2)] \\
&\quad + (28(2^n) - 8)[(2*3) + (3*3)] + (2(2^n) + 1)[(3*4) + (3*4)], \\
&= 32(2^n) + 64(2^n) + 16 + 420(2^n) - 120 + 48(2^n) + 24, \\
&= 564(2^n) - 80.
\end{aligned}
\tag{8}
$$

□

Theorem 3. *Let G be the molecular graph of water-soluble dendritic unimolecular polyether micelle; then, the first K hyper Banhatti index of G is*

$$HB_1(G) = 2296(2^n) - 326. \tag{9}$$

Proof. The edge partition given in Table 1 and the definition of the first K hyper Banhatti index give

$$
\begin{aligned}
HB_1(G) &= \sum_{e=st\epsilon E(G)} [d_G(s) + d_G(e)]^2, \\
&= 4(2^n)[(1+2)^2 + (3+2)^2] + (8(2^n) + 2)[(2+2)^2 + (2+2)^2] \\
&\quad + (28(2^n) - 8)[(2+3)^2 + (3+3^2)] + (2(2^n) + 1)[(3+4)^2 + (3+4)^2], \\
&= 136(2^n) + 256(2^n) + 64 + 1708(2^n) - 488 + 196(2^n) + 98, \\
&= 2296(2^n) - 326.
\end{aligned}
\tag{10}
$$

□

Theorem 4. *Let G be the molecular graph of water-soluble dendritic unimolecular polyether micelle; then, the second K hyper Banhatti index of G is*

$$HB_2(G) = 4268(2^n) - 584. \tag{11}$$

Proof. The result follows by using the values from Table 1 and the definition of the second K hyper Banhatti index.

$$
\begin{aligned}
HB_2(G) &= \sum_{e=st\epsilon E(G)} [d_G(s) * d_G(e)]^2, \\
&= 4(2^n)[(1*2)^2 + (3*2)^2] + (8(2^n) + 2)[(2*2)^2 + (2*2)^2] \\
&\quad + (28(2^n) - 8)[(2*3)^2 + (3*3)^2] + (2(2^n) + 1)[(3*4)^2 + (3*4)^2], \\
&= 160(2^n) + 256(2^n) + 64 + 3276(2^n) - 936 + 576(2^n) + 288, \\
&= 4268(2^n) - 584.
\end{aligned}
\tag{12}
$$

□

TABLE 2: Banhatti indices of water-soluble dendritic unimolecular polyether micelle.

Banhatti indices	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
$B_1(G)$	806	1670	3398	6854	13766
$B_2(G)$	1048	2176	4432	8944	17968
$HB_1(G)$	4266	8858	18042	36410	73146
$HB_2(G)$	7952	16488	33560	67704	135992
$mB_1(G)$	7.9709	16.3477	33.1013	66.6085	133.6229
$mB_2(G)$	6.6584	13.5584	27.3584	54.9584	110.1584
$H_b(G)$	15.9416	32.6948	66.2012	133.214	267.2396

Theorem 5. *Let G be the molecular graph of water-soluble dendritic unimolecular polyether micelle; then, the first modified Banhatti index of G is*

$$mB_1(G) = 4.1884(2^n) - 0.4059. \tag{13}$$

Proof. By using the definition of the first modified Banhatti index and Table 1, we have

$$
\begin{aligned}
mB_1(G) &= \sum_{e=st \in E(G)} \left[\frac{1}{(d_G(s) + d_G(e)) + (d_G(t) + d_G(e))} \right], \\
&= 4(2^n)\left[\frac{1}{(1+2)+(3+2)} \right] + (8(2^n)+2)\left[\frac{1}{(2+2)+(2+2)} \right] + \\
&\quad (28(2^n)-8)\left[\frac{1}{(2+3)+(3+3)} \right] + (2(2^n)+1)\left[\frac{1}{(3+4)+(3+4)} \right], \\
&= \frac{2^n}{2} + 2^n + \frac{1}{4} + \frac{28(2^n)}{11} - \frac{8}{11} + \frac{2^n}{7} + \frac{1}{14}, \\
&= 4.1884(2^n) - 0.4059.
\end{aligned}
\tag{14}
$$

□

Theorem 6. *Let G be the molecular graph of water-soluble dendritic unimolecular polyether micelle; then, the second modified Banhatti index of G is*

$$mB_2(G) = 3.45(2^n) - 0.2416. \tag{15}$$

Proof. The second modified Banhatti index can be computed by using Table 1 as

$$
\begin{aligned}
mB_2(G) &= \sum_{e=st \in E(G)} \left[\frac{2}{(d_G(s) + d_G(e)) + (d_G(t) + d_G(e))} \right], \\
&= 4(2^n)\left[\frac{1}{(1 \times 2)+(3 \times 2)} \right] + (8(2^n)+2)\left[\frac{2}{(2 \times 2)+(2 \times 2)} \right] + \\
&\quad (28(2^n)-8)\left[\frac{2}{(2 \times 3)+(3 \times 3)} \right] + (2(2^n)+1)\left[\frac{2}{(3 \times 4)+(3 \times 4)} \right], \\
&= \frac{2^n}{2} + 2^n + \frac{1}{4} + \frac{28(2^n)}{15} - \frac{8}{15} + \frac{2^n}{12} + \frac{1}{24}, \\
&= 3.45(2^n) - 0.2416.
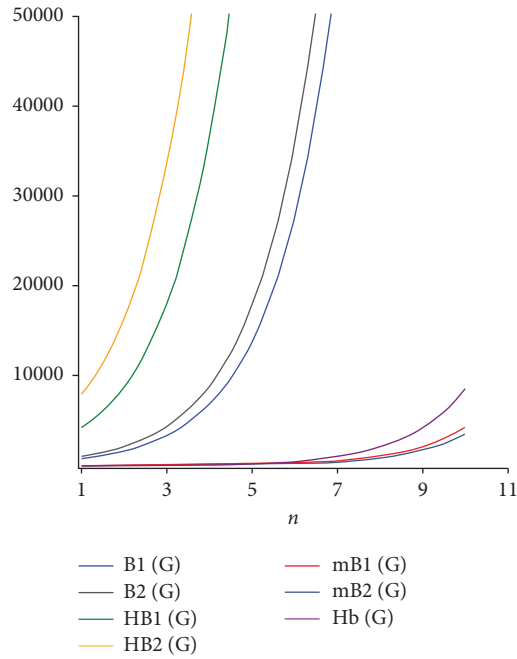\end{aligned}
\tag{16}
$$

□

FIGURE 2: Comparison graph of Banhatti indices of water-soluble unimolecular polyether micelle for growth four.

Theorem 7. *Let G be the molecular graph of water-soluble dendritic unimolecular polyether micelle; then, the harmonic Banhatti index of G is*

$$H_b(G) = 8.3766\,(2^n) - 0.8116. \tag{17}$$

Proof. The result can be obtained as follows by using Table 1 and the definition of the harmonic Banhatti index:

$$
\begin{aligned}
H_b(G) &= \sum_{e=st\epsilon E(G)} \left[\frac{2}{(d_G(s) + d_G(e)) + (d_G(t) + d_G(e))} \right], \\
&= 4\,(2^n) \left[\frac{2}{(1+2)+(3+2)} \right] + (8\,(2^n)+2) \left[\frac{2}{(2+2)+(2+2)} \right] + \\
&\quad (28\,(2^n)-8) \left[\frac{2}{(2+3)+(3+3)} \right] + (2\,(2^n)+1) \left[\frac{2}{(3+4)+(3+4)} \right], \\
&= 2^n + 2\,(2^n) + \frac{1}{2} + \frac{56\,(2^n)}{11} - \frac{16}{11} + \frac{2\,(2^n)}{7} + \frac{2}{14}, \\
&= 8.3766\,(2^n) - 0.8116.
\end{aligned}
\tag{18}
$$

□

3. Graphical Analysis and Conclusions

This section actually provides the summary of this article. Table 2 gives the comparison for the said topological indices of the graph. We can see that $mB_2(G)$ gives the least values for different growths of the graph whereas $HB_2(G)$ gives largest values. In Table 2, we can check the values for some test values of parameter n. Also, the graphical comparison is presented in Figure 2.

Data Availability

No data were used to support for this research.

Conflicts of Interest

The authors declare no conflicts of interest.

Authors' Contributions

All authors contributed equally to the writing of this article.

Acknowledgments

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