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# M-Polynomial and Related Topological Indices of Nanostar Dendrimers

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**Abstract:** Dendrimers are highly branched organic macromolecules with successive layers of branch units surrounding a central core. The M-polynomial of nanotubes has been vastly investigated as it produces many degree-based topological indices. These indices are invariants of the topology of graphs associated with molecular structure of nanomaterials to correlate certain physicochemical properties like boiling point, stability, strain energy, etc. of chemical compounds. In this paper, we first determine M-polynomials of some nanostar dendrimers and then recover many degree-based topological indices.

**Keywords:** degree-based topological indices; Zagreb indices; general Randic index; symmetric division index; M-polynomials; nanostar dendrimers

## 1. Introduction

In the last decade, discrete geometry and graph theory played a synergic role in the area of research of nanomaterials and nanosciences. It conferred chemists with a variety of useful tools like polynomials, eigenvalues and topological indices to predict some properties of the latest synthesized nanomaterials theoretically. To engineer a nanomaterial endowed with a proposed properties, one can control structural sensitive properties like fracture toughness, yield stress, etc. through Cheminformatics. It combines mathematics, chemistry and information science to analyze quantitative structure-activity (QSAR) and structure-property (QSPR) relationships that are used to predict the biological activities and properties of chemical compounds (see [1–3]). A graph-theoretic representation can be given to the physical structure of a nano-material whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. A graph $G(V, E)$ with vertex set V and edge set E is connected, if there exists a connection between any pair of vertices in $G$. A network is simply a connected graph having no multiple edges and no loops. For a graph G, the degree of a vertex v is the number of edges incident with v and denoted by $\deg(v)$. Nanobiotechnology is a rapidly advancing area of scientific and technological opportunity that applies the tools and processes of nano-fabrication to build devices for studying bio-systems. Dendrimers are one of the main objects of this new area of science, see [1,4–8]. Dendrimers are generally synthesized from monomers by iterative growth and activation steps. They are large and complex, with very well-defined chemical structure, and commercially one of the major available nanoscale building blocks. These are nearly perfect mono-disperse macromolecules with a regular and highly branched three-dimensional architecture [4–6]. Their three major architectural components are core, branches and end groups. New branches emitting from a central core are added in steps until a tree-like structure is formed (see Figures 1–4). Nanostar

dendrimer is a part of a new group of macro-particles that appear to be photon funnels just like artificial antennas and are used in the formation of nanotubes, micro and macro-capsules, chemical sensors, colored glasses, and modified electrodes [4,5]. Due to large-scale applications, these compounds are subject matters in both chemistry and mathematics [1,5,6,8]. Polymers are chemical molecules comprised of large numbers of identical substructures, called units, linked together with chemical, or sometimes physical, bonds. The spatial configuration of polymer molecules in an Euclidean space depends on the adjacency of their units. The configuration dependent properties of the so-called Gaussian polymer molecules of different structures can be expressed in terms of graph-theoretical categories and their related topological indices, which depends upon the number of spanning trees, path lengths of these graphs [9]. For detailed insight, see [10–12] and the reference therein.

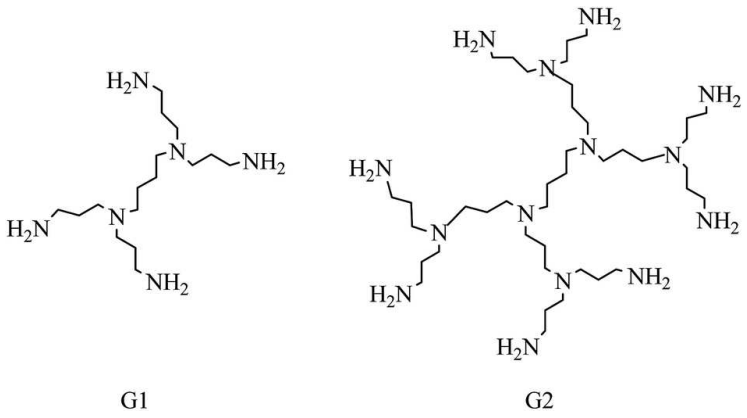


**Figure 1.** $NS_1[1]$ and $NS_1[n]$ polypropylenimine octaamin dendrimer.

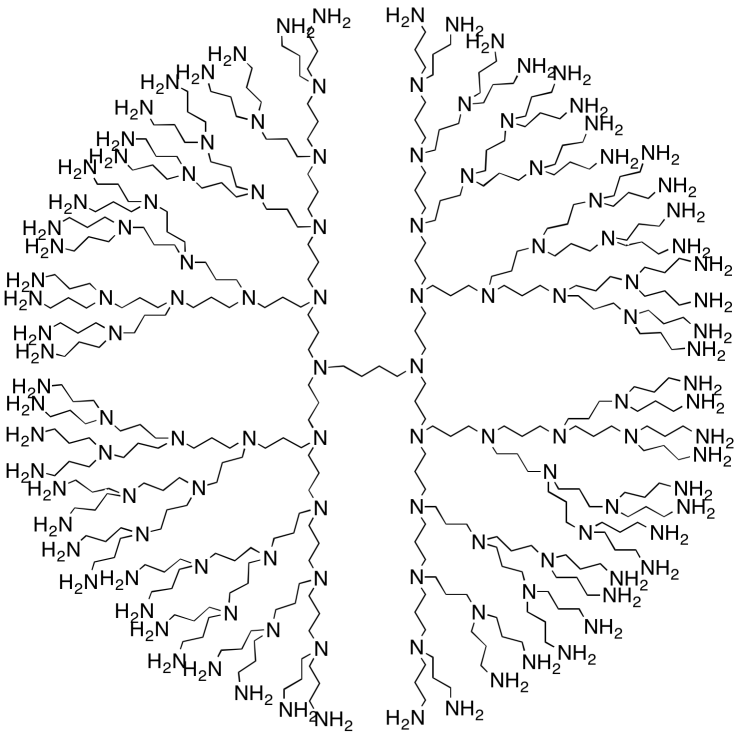

**Figure 2.** $NS_2[n]$ Polypropylenimine octaamin dendrimer.

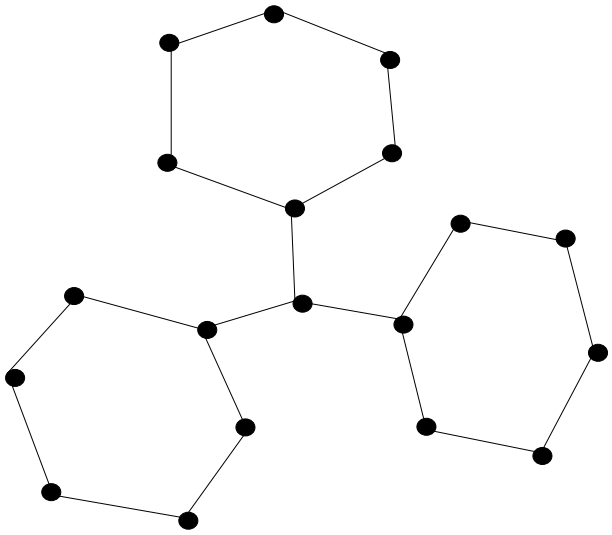

**Figure 3.** The nanostar dendrimer $Dn$ for $n = 1$.

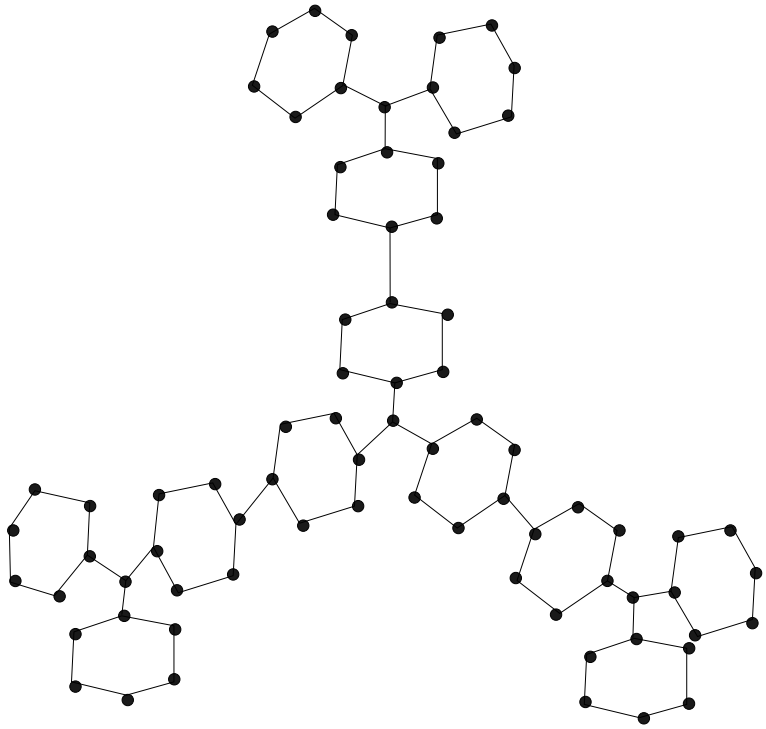

**Figure 4.** The nanostar dendrimer Dn for $n = 2$.

Diudea et al. in [5] computed the Sadhana polynomial of nano-dendrimers, and, in [13], discussed topology of some classes of dendrimers. Recently, in [14], Kamran et al. computed the hyper-Zagreb index, first multiple Zagreb index, second multiple Zagreb index and Zagreb polynomials for some nanostar dendrimers.

A graph invariant is a number, a polynomial, or a matrix that uniquely represents the whole graph [15]. Topological index is a graph invariant that characterizes the topology of the graph and remains invariant under graph automorphism. Degree-based topological indices are of great importance and play a vital role in chemical graph theory (see [13,16,17]). Wiener [18], working on the boiling point of paraffin, introduced the idea of topological index. The Wiener index was originally the first and most studied topological index and is defined as the sum of distances between all pairs of

vertices in $G$, (for more details, see [19–21]). Zagreb indices were introduced 38 years ago by Gutman and Trinajstic [3]. The first Zagreb index $M_1(G)$ is defined as sum of the squares of degrees of a graph $G$ and the second Zagreb $M_2(G)$ is the sum of the product of all degrees corresponding to each edge in $G$ see [3]. The second modified Zagreb index is defined by

$$^{m}M_2(G) = \Sigma_{uv\epsilon E(G)} \frac{1}{d(u)d(v)},$$

where $d(u)$ and $d(v)$ are the degrees of vertices $u$ and $v$, respectively (see [22]). The general Randic index of $G$ is defined as sum of $(d(u)d(v))^{\alpha}$ over all edges $uv$ of $G$, where $d(u)$ denote the degree of vertex $u$ of $G$,

$$R_{\alpha}(G) = \Sigma_{uv\epsilon E(G)}(d(u)d(v))^{\alpha},$$

where $\alpha$ is an arbitrary real number see [23]. Symmetric division index is defined by

$$SDD(G) = \Sigma_{uv\epsilon E(G)}(\frac{min\{d_u, d_v\}}{max\{d_u, d_v\}} + \frac{min\{d_u, d_v\}}{max\{d_u, d_v\}}),$$

where $d_i$ is the degree of vertex $i$ in Graph $G$. These indices can help to characterize the chemical and physical properties of molecules (see [13,14,16–18,22–25]).

In this article, we compute the closed forms of M-polynomials of dendirimers and represent them graphically using Maple 13. As a consequence, we derive some topological degree-based indices easily. However, it is important to remark that we computed different sets of topological indices as those computed in [14]. We start by defining the M-polynomial of a general graph (see [26]).

**Definition 1.** *Let $G$ be a graph, which is a simple molecular connected graph, and $d_v(1 \leq d_v \leq n-1)$ be the degrees of vertices in $G$. We partition the set of vertex $V(G)$ and edge set $E(G)$ of $G$ as follows: $(\forall i,\ j$ and $k$: $\delta \leq i, j, k \leq \triangle)$: $V_k = v\epsilon V(G)|d_v = k$ $E_{i,j} = \{e = uv\epsilon E(G)|d_u = j and d_v = i\}$, where $\delta$ and $\triangle$ are the minimum and maximum of degree of $d_v \forall v\epsilon V(G)$ and $\delta = Min\{d_v|v\epsilon V(G)\}$ and $\triangle = Max\{d_v|v\epsilon V(G)\}$, respectively. Now, let $G = (V, E)$ be a graph and let $m_{ij}$ be the number of degrees $e = uv$ of $G$ such that $\{d_v(G), d_u(G)\} = \{i, j\}$, then the M-polynomial of $G$ define as follows:*

$$M(G, x, y) = \Sigma_{\delta \leq i \leq j \triangle} m_{ij} x^i y^j,$$

*where $d_u, d_v(1 \leq \delta \leq d_u, d_v \leq \triangle \leq |V(G)| - 1)$ are the degrees of vertices $u, v\ \epsilon\ V(G)$.*

We can compute many indices directly from this polynomial [26]. The following Table 1 enlists some standard degree-based topological indices and their derivation from the $M$-polynomial, where $D_x(f(x,y)) = x\frac{\partial f(x,y)}{\partial x}, D_y(f(x,y)) = y\frac{\partial f(x,y)}{\partial y}, S_x(f(x,y)) = \int_0^x \frac{f(t,y)}{t}dt, S_y(f(x,y)) = \int_0^y \frac{f(x,t)}{t}dt$.

**Table 1.** Relations of $M$-polynomial with Topological Indices.

| Topological Index | $f(x,y)$ | Derivation from $M(G,x,y)$ |
|---|---|---|
| First Zagreb | $x+y$ | $(D_x + D_y)(M(G;x,y))\|_{x=y=1}$ |
| Second Zagreb | $xy$ | $(D_xD_y)(M(G;x,y))\|_{x=y=1}$ |
| $^{m}M_2(G)$ | $\frac{1}{xy}$ | $(S_xD_y)(M(G;x,y))\|_{x=y=1}$ |
| General Randić $\alpha\epsilon N$ | $(xy)^{\alpha}$ | $(D_x^{\alpha}D_y^{\alpha})(M(G;x,y))\|_{x=y=1}$ |
| General Randić $\alpha\epsilon N$ | $\frac{1}{xy}^{\alpha}$ | $(S_x^{\alpha}S_y^{\alpha})(M(G;x,y))\|_{x=y=1}$ |
| Symmetric Division Index | $\frac{x^2+y^2}{xy}$ | $(D_xS_y + D_yS_x)(M(G;x,y))\|_{x=y=1}$ |

## 2. Main Results

In this section, we give the M-polynomials of some famous classes of dendirimers and represent them using Maple 13 (Maplesoft, Waterloo, Ontario, Canada). Finally, with the help of the above theorem, we find some topological indices of these nanostructures.

### *2.1. M-Polynomials*

**Theorem 1.** *Let $NS_1[n]$ be a polypropylenimine octaamin dendrimer; then, the M-Polynomial is*

$$M((NS_1[n]), x, y) = 2^{n+1}x^1y^2 + 4(2^n - 1)x^1y^3 + \{12 \times 2^n - 11\}x^2y^2 + 14(2^n - 1)x^2y^3.$$

**Proof.** From the structure of $NS_1[n]$, we can see that there are three partitions $V_{\{1\}} = \{v \epsilon V(NS_1[n])|d_v = 1\}$, $V_{\{2\}} = \{v \epsilon V(NS_1[n])|d_v = 2\}$, and $V_{\{3\}} = \{v \epsilon V(NS_1[n])|d_v = 3\}$. By the definition of $M$-polynomial, we see that the edge set of the $NS_1[n]$ partition is as follows:

$$\begin{aligned}
E_{\{1,2\}} &= \{e = uv \epsilon E(NS_1[n])|d_u = 1 \& d_v = 2\} \rightarrow |E_{\{1,2\}}| = 2^{n+1},\\
E_{\{1,3\}} &= \{e = uv \epsilon E(NS_1[n])|d_u = 1 \& d_v = 3\} \rightarrow |E_{\{1,3\}}| = 4(2^n - 1),\\
E_{\{2,2\}} &= \{e = uv \epsilon E(NS_1[n])|d_u = 2 \& d_v = 2\} \rightarrow |E_{\{2,2\}}| = 12 \times 2^n - 11,\\
E_{\{2,3\}} &= \{e = uv \epsilon E(NS_1[n])|d_u = 2 \& d_v = 3\} \rightarrow |E_{\{2,3\}}| = 14(2^n - 1).
\end{aligned}$$

Thus, the $M$-Polynomial of $(NS_1[n], x, y)$

$$\begin{aligned}
& M(NS_1[n], x, y)\\
= & \sum_{i \leq j} m_{ij}(NS_1[n])x^i y^j\\
= & \sum_{1 \leq 2} m_{12}(NS_1[n])x^1y^2 + \sum_{1 \leq 3} m_{13}(NS_1[n])x^1y^3\\
& + \sum_{2 \leq 2} m_{22}(NS_1[n])x^2y^2 + \sum_{2 \leq 3} m_{23}(NS_1[n])x^2y^3\\
= & \sum_{uv \epsilon E_{\{1,2\}}} m_{12}(NS_1[n])x^1y^2 + \sum_{uv \epsilon E_{\{1,3\}}} m_{13}(NS_1[n])x^1y^3\\
& + \sum_{uv \epsilon E_{\{2,2\}}} m_{22}(NS_1[n])x^2y^2 + \sum_{uv \epsilon E_{\{2,3\}}} m_{23}(NS_1[n])x^2y^3\\
= & |E_{\{1,2\}}|x^1y^2 + |E_{\{1,3\}}|x^1y^3 + |E_{\{2,2\}}|x^2y^2 + |E_{\{2,2\}}|x^2y^3\\
= & 2^{n+1}x^1y^2 + 4(2^n - 1)x^1y^3 + \{12 \times 2^n - 11\}x^2y^2 + 14(2^n - 1)x^2y^3.
\end{aligned}$$

□

**Theorem 2.** *Let $NS_2[n]$ be the polypropylenimine octaamin dendrimer; then, the M-Polynomial is*

$$M((NS_2[n]), x, y) = 2^{n+1}x^1y^2 + \{8 \times 2^n - 5\}|x^2y^2 + 6(2^n - 1)x^2y^3.$$

**Proof.** From the structure of $NS_2[n]$, we can see that there are three partitions $V_{\{1\}} = \{v \epsilon V(NS_2[n])|d_v = 1\}$, $V_{\{2\}} = \{v \epsilon V(NS_2[n])|d_v = 2\}$, and $V_{\{3\}} = \{v \epsilon V(NS_2[n])|d_v = 3\}$. By the definition of $M$-polynomial, we see that the edge set of $NS_2[n]$ partition as follows:

$$\begin{aligned}
E_{\{1,2\}} &= \{e = uv \epsilon E(NS_2[n])|d_u = 1 \& d_v = 2\} \rightarrow |E_{\{1,2\}}| = 2^{n+1},\\
E_{\{2,2\}} &= \{e = uv \epsilon E(NS_2[n])|d_u = 2 \& d_v = 2\} \rightarrow |E_{\{2,2\}}| = 8 \times 2^n - 5,\\
E_{\{2,3\}} &= \{e = uv \epsilon E(NS_2[n])|d_u = 2 \& d_v = 3\} \rightarrow |E_{\{2,3\}}| = 6(2^n - 1).
\end{aligned}$$

Thus, the $M$-Polynomial of $(NS_2[n], x, y)$

$$\begin{aligned} M(NS_2[n], x, y) &= \sum_{i \leq j} m_{ij}(NS_2[n]) x^i y^j \\ &= \sum_{1 \leq 2} m_{12}(NS_2[n]) x^1 y^2 + \sum_{2 \leq 2} m_{22}(NS_2[n]) x^2 y^2 \\ &\quad + \sum_{2 \leq 3} m_{23}(NS_2[n]) x^2 y^3 \\ &= \sum_{uv \epsilon E_{\{1,2\}}} m_{12}(NS_2[n]) x^1 y^2 + \sum_{uv \epsilon E_{\{2,2\}}} m_{22}(NS_2[n]) x^2 y^2 \\ &\quad + \sum_{uv \epsilon E_{\{2,3\}}} m_{23}(NS_2[n]) x^2 y^3 \\ &= |E_{\{1,2\}}| x^1 y^2 + |E_{\{2,2\}}| x^2 y^2 + |E_{\{2,2\}}| x^2 y^3 \\ &= 2^{n+1} x^1 y^2 + \{8 \times 2^n - 5\} | x^2 y^2 + 6(2^n - 1) x^2 y^3. \end{aligned}$$

□

**Theorem 3.** *Let $D_n$ be the nanostar dendrimer; then, the M-Polynomial is*

$$M(D_n, x, y) = 12(2 \times 2^{n-1} - 1) x^2 y^2 + 6(5 \times 2^{n-1} - 4) x^2 y^3 + (12 \times 2^{n-1} - 9) x^3 y^3.$$

**Proof.** From the structure of $D_n$, we can see that there are two partitions $V_{\{2\}} = \{v \epsilon V(D_n) | d_v = 2\}$ *and* $V_{\{3\}} = \{v \epsilon V(D_n) | d_v = 3\}$. By the definition of the $M$-polynomial, we see that the edge set of $D_n$ partition as follows:

$$\begin{aligned} E_{\{2,2\}} &= \{e = uv \epsilon E(D_n) | d_u = 2 \& d_v = 2\} \rightarrow |E_{\{2,2\}}| = 12(2 \times 2^{n-1} - 1), \\ E_{\{2,3\}} &= \{e = uv \epsilon E(D_n) | d_u = 2 \& d_v = 3\} \rightarrow |E_{\{2,3\}}| = 6(5 \times 2^{n-1} - 4), \\ E_{\{3,3\}} &= \{e = uv \epsilon E(D_n) | d_u = 3 \& d_v = 3\} \rightarrow |E_{\{3,3\}}| = 12 \times 2^{n-1} - 9. \end{aligned}$$

Thus, the $M$-Polynomial of $(D_n, x, y)$

$$\begin{aligned} M(D_n, x, y) &= \sum_{i \leq j} m_{ij}(D_n) x^i y^j \\ &= \sum_{2 \leq 2} m_{22}(D_n) x^2 y^2 + \sum_{2 \leq 3} m_{23}(D_n) x^2 y^3 + \sum_{3 \leq 3} m_{33}(D_n) x^3 y^3 \\ &= \sum_{uv \epsilon E_{\{2,2\}}} m_{22}(D_n) x^2 y^2 + \sum_{uv \epsilon E_{\{2,3\}}} m_{23}(D_n) x^2 y^3 + \sum_{uv \epsilon E_{\{3,3\}}} m_{33}(D_n) x^3 y^3 \\ &= |E_{\{2,2\}}| x^2 y^2 + |E_{\{2,3\}}| x^2 y^3 + |E_{\{3,3\}}| x^3 y^3 \\ &= 12(2 \times 2^{n-1} - 1) x^2 y^2 + 6(5 \times 2^{n-1} - 4) x^2 y^3 + (12 \times 2^{n-1} - 9) x^3 y^3. \end{aligned}$$

□

### *2.2. Surfaces Representing M-Polynomials*

We use Maple 13 to represent graphs of $M$-polynomials of the above-mentioned dendrimers. From graphs, it can be seen that the behavior of the polynomials differ along different parameters see Figures 5–7.

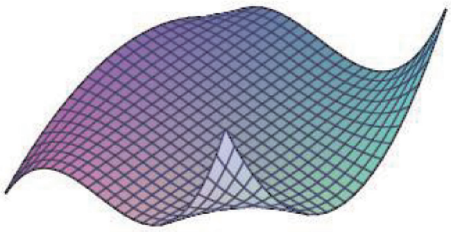

**Figure 5.** *M*-polynomial of $NS_1[n]$ polypropylenimine octaamin dendrimer.

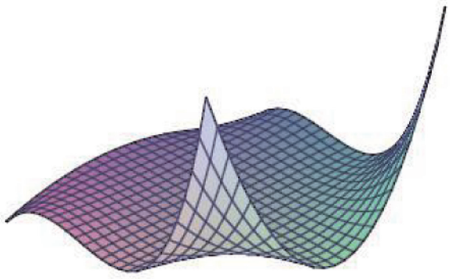

**Figure 6.** *M*-polynomial of $NS_2[n]$ polypropylenimine octaamin dendrimer.

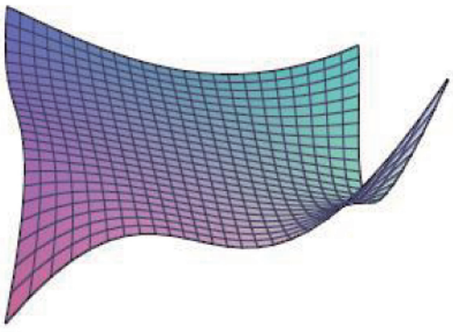

**Figure 7.** *M*-polynomial of $D_n$ polypropylenimine octaamin dendrimer.

*2.3. Some Degree-Based Topological Indices*

In this part, we compute some degree-based topological indices of some classes of dendrimers.

**Theorem 4.** *Let $G = NS_1[n]$ be a polypropylenimine octaamin dendrimer; then,*

1. $M_1(G) = 2(35 \times 2^{n+1} - 53)$
2. $M_2(G) = 1189 \times 2^{2n+2} - 3722 \times 2^{n+1} + 2808$

3. ${}^{m}M_2(G) = 247 \times 2^{2n} - 433 \times 2^n + \frac{2277}{12}$

4. $R_\alpha(G) = (1189 \times 2^{2n+2} - 3722 \times 2^{n+1} + 2808)^\alpha$

5. $R_\alpha(G) = (247 \times 2^{2n} - 433 \times 2^n + \frac{2277}{12})^\alpha$

6. *SDD(G)*= $1156 \times 2^{2n+1} - 1010 \times 2^{n+1} - 1690 \times 2^n + 1482$

**Proof.** Let $f(x,y) = M((NS_1[n]), x, y) = 2^{n+1}x^1y^2 + 4(2^n - 1)x^1y^3 + \{12 \times 2^n - 11\}x^2y^2 + 14(2^n - 1)x^2y^3$

$$D_x(f(x,y)) = 2^{n+1}y^2 + 4(2^n - 1)y^3 + 2(12 \times 2^n - 11)xy^2 + 28(2^n - 1)xy^3$$

$$(D_x f(x,y))(M(NS_1(n); x, y))|_{x=y=1} = 29 \times 2^{n+1} - 54$$

$$D_y(f(x,y)) = 2^{n+2}xy + 12(2^n - 1)xy^2 + 2(12 \times 2^n - 11)x^2y + 42(2^n - 1)x^2y^2$$

$$(D_x f(x,y))(M(NS_1(n); x, y))|_{x=y=1} = 41 \times 2^{n+1} - 52$$

$$S_x f(x,y) = 2^{n+1}xy^2 + 4(2^n - 1)xy^3 + \frac{1}{2}(12 \times 2^n - 1)x^2y^2 + 7(2^n - 1)x^2y^3$$

$$(S_x f(x,y))(M(NS_1(n); x, y))|_{x=y=1} = 19 \times 2^n - \frac{33}{2}$$

$$S_y f(x,y) = 2^n xy^2 + \frac{4}{3}(2^n - 1)xy^3 + \frac{1}{2}(12 \times 2^n - 11)x^2y^2 + \frac{14}{3}(2^n - 1)x^2y^3$$

$$(S_y f(x,y))(M(NS_1(n); x, y))|_{x=y=1} = 13 \times 2^n - \frac{23}{2}.$$

□

**Theorem 5.** *1.* $M_1(G)$*:*

$$(D_x + D_y)f(x,y)(M(NS_1(n); x, y))|_{x=y=1} = 2(35 \times 2^{n+1} - 53).$$

2. $M_2(G)$*:*

$$(D_x D_y)f(x,y)(M(NS_1(n); x, y))|_{x=y=1} = 1189 \times 2^{2n+2} - 3722 \times 2^{n+1} + 2808.$$

3. ${}^{m}M_2(G)$*:*

$$(S_x S_y)f(x,y)(M(NS_1(n); x, y))|_{x=y=1} = 24 \times 2^{2n} - 433 \times 2^n + \frac{2277}{12}.$$

4. $R_\alpha(G)$*:*

$$(D_x D_y)^\alpha f(x,y)(M(NS_1(n); x, y))|_{x=y=1} = (1189 \times 2^{2n+2} - 3722 \times 2^{n+1} + 2808)^\alpha.$$

5. $R_\alpha(G)$*:*

$$(S_x S_y)^\alpha f(x,y)(M(NS_1(n); x, y))|_{x=y=1} = (24 \times 2^{2n} - 433 \times 2^n + \frac{2277}{12})^\alpha.$$

6. $SDD(G)$*:*

$$(D_x S_y + D_y S_x)(M(G; x, y))|_{x=y=1} = 1156 \times 2^{2n+1} - 1010 \times 2^{n+1} - 1690 \times 2^n + 1482,$$

$$M((NS_2[n]), x, y) = 2^{n+1}x^1y^2 + \{8 \times 2^n - 5\}x^2y^2 + 6(2^n - 1)x^2y^3.$$

**Theorem 6.** *Topological Index Derivation from* $M((NS_2[n], x, y)$

1. $M_1(G) = 2(17 \times 2^{n+1} - 25)$
2. $M_2(G) = 285 \times 2^{2n+2} - 838 \times 2^{n+1} + 616$
3. ${}^{m}M_2(G) = 63 \times 2^{2n} - 79 \times 2^n + \frac{99}{4}$
4. $R_\alpha(G) = (285 \times 2^{2n+2} - 838 \times 2^{n+1} + 616)^\alpha$
5. $R_\alpha(G) = (63 \times 2^{2n} - 79 \times 2^n + \frac{99}{4})^\alpha$
6. $SDD(G) = 276 \times 2^{2n+1} - 172 \times 2^{n+1} - 406 \times 2^n + 253$

**Proof.** Let $f(x,y) = M((NS_2[n]), x, y) = 2^{n+1}x^1y^2 + (8 \times 2^n - 5)x^2y^2 + 6(2^n - 1)x^2y^3$,

$$D_x(f(x,y)) = 2^{n+1}y^2 + 2(8 \times 2^n - 5)xy^2 + 12(2^n - 1)xy^3$$
$$(D_x f(x,y))(M(NS_2(n); x, y))|_{x=y=1} = 15 \times 2^{n+1} - 22,$$
$$D_y(f(x,y)) = 2^{n+2}xy + 2(8 \times 2^n - 5)x^2y + 18(2^n - 1)x^2y^2,$$
$$(D_x f(x,y))(M(NS_2(n); x, y))|_{x=y=1} = 19 \times 2^{n+1} - 28,$$
$$S_x f(x,y) = 2^{n+1}xy^2 + \frac{1}{2}(8 \times 2^n - 5)x^2y^2 + 3(2^n - 1)x^2y^3,$$
$$(S_x f(x,y))(M(NS_2(n); x, y))|_{x=y=1} = 9 \times 2^n - \frac{11}{2},$$
$$S_y f(x,y) = 2^n xy^2 + \frac{1}{2}(8 \times 2^n - 5)x^2y^2 + 2(2^n - 1)x^2y^3,$$
$$(S_y f(x,y))(M(NS_2(n); x, y))|_{x=y=1} = 7 \times 2^n - \frac{9}{2}.$$

1. $M_1(G)$:
$$(D_x + D_y)f(x,y)(M(NS_2(n); x, y))|_{x=y=1} = 2(17 \times 2^{n+1} - 25).$$
2. $M_2(G)$:
$$(D_x D_y)f(x,y)(M(NS_2(n); x, y))|_{x=y=1} = 285 \times 2^{2n+2} - 838 \times 2^{n+1} + 616.$$
3. ${}^{m}M_2(G)$:
$$(S_x S_y)f(x,y)(M(NS_2(n); x, y))|_{x=y=1} = 63 \times 2^{2n} - 79 \times 2^n + \frac{99}{4}.$$
4. $R_\alpha(G)$:
$$(D_x D_y)^\alpha f(x,y)(M(NS_2(n); x, y))|_{x=y=1} = (285 \times 2^{2n+2} - 838 \times 2^{n+1} + 616)^\alpha.$$
5. $R_\alpha(G)$:
$$(S_x S_y)^\alpha f(x,y)(M(NS_2(n); x, y))|_{x=y=1} = (63 \times 2^{2n} - 79 \times 2^n + \frac{99}{4})^\alpha.$$
6. $SDD(G)$:
$$(D_x S_y + D_y S_x)(M(NS_2(n); x, y))|_{x=y=1} = 276 \times 2^{2n+1} - 172 \times 2^{n+1} - 406 \times 2^n + 253,$$

□

$$M((D_n, x, y) = 12(2 \times 2^{n-1} - 1)x^2y^2 + 6(5 \times 2^{n-1} - 4)x^2y^3 + (12 \times 2^{n-1} - 9)x^3y^3.$$

**Theorem 7.** *Topological Index Derivation from* $M(D_n, x, y)$

1. $M_1(G) = 2(159 \times 2^{n-1} - 111)$
2. $M_2(G) = 2^{2n+3} \times 783 - 17469 \times 2^n + 12177$
3. ${}^mM_2(G) = 403 \times 2^{2n-1} - 1073 \times 2^{n-1} + 357$
4. $R_\alpha(G) = (2^{2n+3} \times 783 - 17469 \times 2^n + 12177)^\alpha$
5. $R_\alpha(G) = (403 \times 2^{2n-1} - 1073 \times 2^{n-1} + 357)^\alpha$
6. $SDD(G) = 9138 \times 2^{2n-2} - 12489 \times 2^{n-1} + 4266$

**Proof.** Let $f(x,y) = M(D_n; x, y) = 2^{n+1}x^1y^2 + 4(2^n - 1)x^1y^3 + \{12 \times 2^n - 11\}x^2y^2 + 14(2^n - 1)x^2y^3$,

$$D_x(f(x,y)) = 24(2^n - 1)xy^2 + 12(5 \times 2^{n-1} - 4)xy^3 + 9(2^{n+1} - 3)x^2y^3,$$
$$(D_xf(x,y))(M(D_n; x, y))|_{x=y=1} = 9(2^{n+3} - 11),$$
$$D_y(f(x,y)) = 24(2^n - 1)x^2y + 18(5 \times 2^n - 4)x^2y^2 + 9(2^{n+1} - 3)x^3y^2,$$
$$(D_xf(x,y))(M(D_n; x, y))|_{x=y=1} = 174 \times 2^{n-1} - 123,$$
$$S_xf(x,y) = 6(2^n - 1)x^2y^2 + 3(5 \times 2^{n-1} - 4)x^2y^3 + (4 \times 2^{n-1} - 3)x^3y^3,$$
$$(S_xf(x,y))(M(D_n; x, y))|_{x=y=1} = 31 \times 2^{n-1} - 21,$$
$$S_yf(x,y) = 6(2^n - 1)x^2y^2 + 2(5 \times 2^{n-1} - 4)x^2y^3 + (2^{n+1} - 3)x^3y^3,$$
$$(S_yf(x,y))(M(D_n; x, y))|_{x=y=1} = 13 \times 2^n - 17.$$

1. $M_1(G)$:
$$(D_x + D_y)f(x,y)(M(D_n; x, y))|_{x=y=1} = 2(159 \times 2^{n-1} - 111).$$
2. $M_2(G)$:
$$(D_xD_y)f(x,y)(M(D_n; x, y))|_{x=y=1} = 783 \times 2^{2n+3} - 17469 \times 2^n + 12177.$$
3. ${}^mM_2(G)$:
$$(S_xS_y)f(x,y)(M(D_n; x, y))|_{x=y=1} = 403 \times 2^{2n-1} - 1073 \times 2^{n-1} + 357.$$
4. $R_\alpha(G)$:
$$(D_xD_y)^\alpha f(x,y)(M(NS_1(n); x, y))|_{x=y=1} = (783 \times 2^{2n+3} - 17469 \times 2^n + 12177)^\alpha.$$
5. $R_\alpha(G)$:
$$(S_xS_y)^\alpha f(x,y)(M(NS_1(n); x, y))|_{x=y=1} = (403 \times 2^{2n-1} - 1073 \times 2^{n-1} + 357)^\alpha.$$
6. $SDD(G)$:
$$(D_xS_y + D_yS_x)(M(G; x, y))|_{x=y=1} = 9138 \times 2^{2n-2} - 12489 \times 2^{n-1} + 4266.$$

□

## 3. Conclusions

We first determine M-polynomials of some nanostar dendrimers, and then recover many degree-based topological indices. A large amount of chemical experiments requires determining the chemical properties of new compounds and new drugs. Fortunately, the chemical based experiments indicate that there is a strong inherent relationship between the chemical characteristics of chemical compounds and drugs and their molecular structures. Topological indices calculated for these chemical molecular structures can help us to understand the physical features, chemical reactivity, and biological activity. The topological index of a molecule structure can be considered as a non-empirical numerical quantity that quantities the molecular structure and its branching pattern. In this point of view, topological indices can be regarded as a score function that maps each molecular structure to a real number and can also be used as a descriptor of the molecule under testing. These results can also play a vital rule in preparation of new drugs.

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