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REFLECTIONS ON *M*-POLYNOMIAL AND RELATED TOPOLOGICAL INDICES OF NANOSTAR DENDRIMERS

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Abstract

This commentary addresses flaws discovered in Munir et al.'s recent paper [VI] on the M-Polynomial and associated topological descriptors of dendrimers. Our examination reveals inconsistencies in numerous critical aspects of their work. First, the figures representing the nanostar dendrimer formations must be more accurate. This means that the pictures used to depict the production of these molecules need to be revised. Second, flaws exist within the formulae used for the computations. Finally, based on incorrect formulae and figures, the claimed computational findings must be corrected. We suggest a complete correction approach to ensure the correctness of Munir et al.'s [VI] findings on nanostar dendrimers. It includes supplying corrected figures that accurately portray the nanostar dendrimer structures and removing the inconsistencies in the previous images. In addition, we will use revised notations to ensure that all parameters used in computations are explicitly and consistently described to eliminate ambiguities. Furthermore, we will provide the Accurate Formula for the Symmetric Division Index, which is critical for achieving precise results. Finally, all topological indices will be recalculated using these modifications with the revised figures and formulae to represent the genuine values. These corrections are necessary to give the validity of the results and pave the path for future research in this field.

Keywords: Degree-based Topological Indices, M-polynomials, Nanostar Dendrimers

I. Introduction

All the graphs examined here are simple and finite. All the notations and terminologies that are used here, are found in [I], [VI]. Topological descriptors play a crucial part in graph theory to examine the structural characteristics of graphs and are utilized in various disciplines like chemistry, drug discovery, pharmaceutical, and discrete dynamical systems. Dendrimers are the a greatest part of nano-structures that can be incorporated through either divergent or convergent methods. Dendrimers exhibit a chemical structure featuring three primary components: core, branches, and end groups. The branches attached to the core and are added in a stepwise way. Dendrimers have the most significant applications in nano-technology. With the help of these on can construct nanotubes, chemical sensors, micro- and macro-capsules, colored glass, modified electrodes, and photon funnels, including artificial antennas. In this context, the research related to nanostar dendrimers has acquired a significant attraction in the areas of chemical and mathematical.

These corrections of article [VI] are necessary to establish the validity of the findings and paving the path for future advances in this field. Because topological invariants computed for different chemical structures will enhance our understanding of the physical characteristics, chemical reactivity, and biological activity. It's necessary to give the correct results for further research on these dendrimers for researchers.

The relation of degree-based invariants and M-polynomials is shown in Table 1, here D_x, D_y, S_x and S_y are described as: D_x and D_y are the partial derivatives of $f(x,y)$ w.r.t x and y, respectively, S_x (or S_y) is integral from 0 to x (or 0 to y) of $\frac{f(t,y)}{t}$ (or $\frac{f(x,t)}{t}$) w.r.t "t".

Table 1 Formulae of Indices Derived from M-polynomial

Topological Index	$f(x,y)$	Formulae
First Zagreb	$x+y$	$(D_x+D_y)M(H;x,y)\|_{x=y=1}$
second Zagreb	xy	$(D_xD_y)M(H;x,y)\|_{x=y=1}$
Modified second Zagreb	$\frac{1}{xy}$	$(S_xS_y)M(H;x,y)\|_{x=y=1}$
General Randić	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)M(H;x,y)\|_{x=y=1}$
Inverse Randić	$\frac{1}{(xy)^\alpha}$	$(S_x^\alpha S_y^\alpha)M(H;x,y)\|_{x=y=1}$

The authors in [III], and [VI] give the same dendrimers $NS_2[n]$ in Figure 1 and Figure 2, these are only the different generations of $NS_2[n]$. In the caption of Figure 1 the authors write $NS_1[1]$ and $NS_1[n]$, that is incorrect, actually these are Figures of $NS_2[1]$ and $NS_2[2]$. So, we give here the correct figures of $NS_1[1]$ (see fig 1) and $NS_2[n]$ (see fig 2) from [II],[IV], [V].

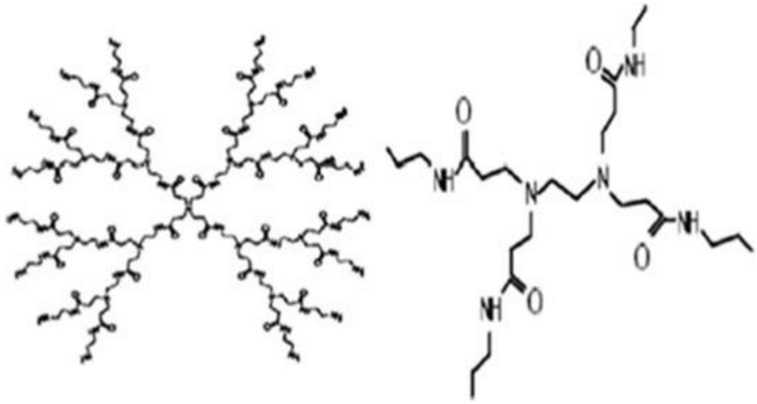

Fig. 1. Polypropylenimine octaamine dendrimer $NS_1[n]$.

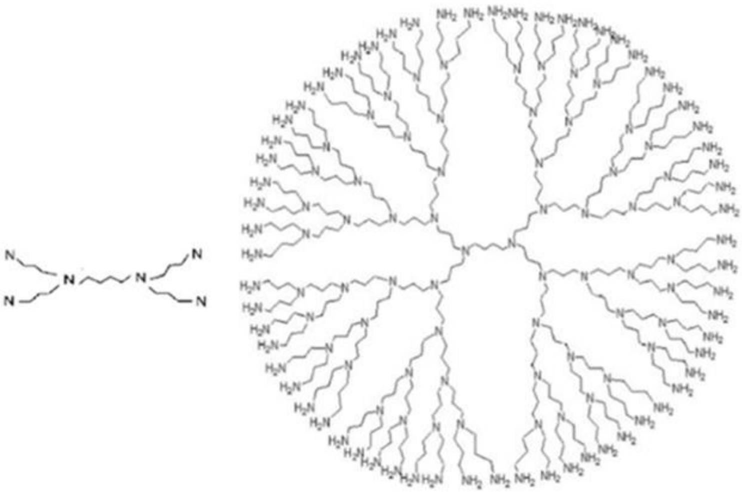

Fig. 2. Polypropylenimine octaamine dendrimer $NS_2[n]$.

Next, we recognized some of the typos mistakes: the notation for the degree of a vertex $u \in V(G)$ is "$d(u)$" and "d_u" have been used interchangeably in [VI], however since the notation "d_u" has been used more frequently in [VI], therefore we suggest that "$d(u)$" should be replaced by "d_u". Also the formula for the symmetric division index is incorrect. Its correct formula is as follows:

$$SDD(H) = \sum_{uv \in E(H)} \left(\frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}} + \frac{\min\{d_u, d_v\}}{\max\{d_u, d_v\}} \right).$$

OR

$$SDD(H) = \sum_{uv \in E(H)} \left(\frac{d_u}{d_v} + \frac{d_v}{d_u} \right).$$

II. Main Results

Now, we correct some erroneous results determined in [VI]. We start with Theorem 4 of [6], in that theorem authors used the wrong formulas for $D_xD_yf(x,y)$, $S_xS_yf(x,y)$, $D_x^{\phi}D_y^{\phi}f(x,y)$, $S_x^{\phi}S_y^{\phi}f(x,y)$, $S_yD_xf(x,y)$ and $S_xD_yf(x,y)$. In the following theorem, we give corrections of formulas and computations of indices.

Theorem 2.1 *Assume $G = NS_1[n]$ is a polypropylenimine octaamin dendrimer. We acquire*

1. $M_1(G) = 2(35 \times 2^{n+1} - 65)$.
2. $M_2(G) = 37 \times 2^{n+2} - 140$.
3. ${}^mM_2(G) = \frac{23}{3} \times 2^n - \frac{77}{12}$.
4. $R_\alpha(G) = 2^\alpha \times 2^{n+1} + 3^\alpha \times 4(2^n - 1) + 4^\alpha(12 \times 2^n - 11) + 6^\alpha \times 14(2^n - 1)$.
5. $RR_\alpha(G) = \frac{1}{2^\alpha} \times 2^{n+1} + \frac{1}{3^\alpha} \times 4(2^n - 1) + \frac{1}{4^\alpha}(12 \times 2^n - 11) + \frac{1}{6^\alpha} \times 14(2^n - 1)$.
6. $SSD(G) = \frac{218}{3} \times 2^n - \frac{197}{3}$.

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

$$D_xf(x,y) = x\frac{\partial f(x,y)}{\partial x} = 2^{n+1}x^1y^2 + 4(2^n - 1)x^1y^3 + 2(12 \times 2^n - 11)x^2y^2 + 28(2^n - 1)x^2y^3.$$

$$D_yf(x,y) = y\frac{\partial f(x,y)}{\partial y} = 2 \times 2^{n+1}x^1y^2 + 12(2^n - 1)x^1y^3 + 2(12 \times 2^n - 11)x^2y^2 + 42(2^n - 1)x^2y^3.$$

$$D_xD_yf(x,y) = x\frac{\partial}{\partial x}D_yf(x,y) = 2 \times 2^{n+1}x^1y^2 + 12(2^n - 1)x^1y^3 + 4(12 \times 2^n - 11)x^2y^2 + 84(2^n - 1)x^2y^3.$$

$$S_xf(x,y) = \int_0^x \frac{f(t,y)}{t} = 2^{n+1}x^1y^2 + 4(2^n - 1)x^1y^3 + \frac{1}{2}(12 \times 2^n - 11)x^2y^2 + 14(2^n - 1)x^2y^3.$$

$$S_y f(x,y) = \int_0^y \frac{f(x,t)}{t} d$$
$$= 2^n x^1 y^2 + \frac{4}{3}(2^n - 1)x^1 y^3 + \frac{1}{2}(12 \times 2^n - 11)x^2 y^2 + \frac{14}{3}(2^n - 1)x^2 y^3.$$

$$S_x S_y f(x,y) = \int_0^x \frac{S_y f(t,y)}{t} dt$$
$$= 2^n x^1 y^2 + \frac{4}{3}(2^n - 1)x^1 y^3 + \frac{1}{4}(12 \times 2^n - 11)x^2 y^2 + \frac{7}{3}(2^n - 1)x^2 y^3.$$

$$D_x^{\phi} D_y^{\phi} f(x,y) = 2^{\alpha} \times 2^{n+1} x^1 y^2 + 4 \times 3^{\alpha}(2^n - 1)x^1 y^3 + 2^{2\alpha}(12 \times 2^n - 11)x^2 y^2 + 6 \times 14^{\alpha}(2^n - 1)x^2 y^3.$$

$$S_x^{\phi} S_y^{\phi} f(x,y) = 2^{-\alpha} \times 2^{n+1} x^1 y^2 + 4 \times 3^{-\alpha}(2^n - 1)x^1 y^3 + \frac{1}{4^{-\alpha}}(12 \times 2^n - 11)x^2 y^2 + 14 \times 6^{-\alpha}(2^n - 1)x^2 y^3.$$

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

$$S_x D_y f(x,y) = 2 \times 2^{n+1} x^1 y^2 + 12(2^n - 1)x^1 y^3 + (12 \times 2^n - 11)x^2 y^2 + 21(2^n - 1)x^2 y^3.$$

Next, putting $x = y = 1$ in all previous results of this theorem to acquire the correct formulae of different topological descriptors.

$$M_1((NS_1[n])) = (D_x + D_y)M((NS_1[n]); x,y)|_{x=y=1} = 2(35 \times 2^{n+1} - 65).$$

$$M_2((NS_1[n])) = (D_x D_y)M((NS_1[n]); x,y)|_{x=y=1} = 37 \times 2^{n+2} - 140.$$

$$^{m}M_2((NS_1[n])) = (S_x S_y)M((NS_1[n]); x,y)|_{x=y=1} = \frac{23}{3} \times 2^n - \frac{77}{12}.$$

$$R_{\alpha}((NS_1[n])) = (D_x^{\alpha} D_y^{\alpha})M((NS_1[n]); x,y)|_{x=y=1}$$
$$= 2^{\alpha} \times 2^{n+1} + 3^{\alpha} \times 4(2^n - 1) + 4^{\alpha}(12 \times 2^n - 11) + 6^{\alpha} \times 14(2^n - 1).$$

$$RR_{\phi}((NS_1[n])) = (S_x^{\phi} S_y^{\phi})M((NS_1[n]); x,y)|_{x=y=1}$$
$$= \frac{1}{2^{\alpha}} \times 2^{n+1} + \frac{1}{3^{\alpha}} \times 4(2^n - 1) + \frac{1}{4^{\alpha}}(12 \times 2^n - 11) + \frac{1}{6^{\alpha}} \times 14(2^n - 1).$$

$$SSD((NS_1[n])) = (D_xS_y + D_yS_x)M((NS_1[n]); x, y)|_{x=y=1} = \frac{218}{3} \times 2^n - \frac{197}{3}.$$

Also in theorems 5 and 6 of [VI], they used wrong formulas for $D_xD_yf(x,y)$, $S_xS_yf(x,y)$, $D_x^{\phi}D_y^{\phi}f(x,y)$, $S_x^{\phi}S_y^{\phi}f(x,y)$, $S_yD_xf(x,y)$ and $S_xD_yf(x,y)$. In the next theorems, we give corrections of formulaes and computations of indices.

Theorem 2.2 *Assume $G = NS_2[n]$ is a polypropylenimine octaamin dendrimer. We acquire*

1. $M_1(G) = 2(17 \times 2^{n+1} - 25)$.
2. $M_2(G) = 72 \times 2^n - 56$.
3. ${}^mM_2(G) = 4 \times 2^n - \frac{9}{4}$.
4. $R_\alpha(G) = 2^\alpha \times 2^{n+1} + 4^\alpha(8 \times 2^n - 5) + 6^\alpha \times 6(2^n - 1)$.
5. $RR_\alpha(G) = \frac{1}{2^\alpha} \times 2^{n+1} + \frac{1}{4^\alpha}(8 \times 2^n - 5) + \frac{1}{6^\alpha} \times 6(2^n - 1)$.
6. $SSD(G) = 34 \times 2^n - 23$.

Theorem 2.3 *Let $G = D_n$ be a nanostar dendrimer; then,*

1. $M_1(G) = 159 \times 2^n - 222$.
2. $M_2(G) = 384 \times 2^{n-1} - 273$.
3. ${}^mM_2(G) = \frac{37}{3} \times 2^{n-1} - 8$.
4. $R_\alpha(G) = 4^\alpha \times 12(2^n - 1) + 6^\alpha \times 6(5 \times 2^{n-1} - 4) + 9^\alpha(12 \times 2^{n-1} - 9)$.
5. $RR_\alpha(G) = \frac{1}{4^\alpha} \times 12(2^n - 1) + \frac{1}{6^\alpha} \times 6(5 \times 2^{n-1} - 4) + \frac{1}{9^\alpha}(12 \times 2^{n-1} - 9)$.
6. $SSD(G) = 137 \times 2^{n-1} - 94$.

III. Verification of our results

In the previous section, we give the correction of the obtained results of [VI] by the use of M. Polynomial. For the further accuracy of our results, here we have also computed the indices by using direct formulas of discussed indices. By the definition of $NS_1[n]$, the edge partitioning (see in [II], [VI]) is as follows:

$$E_{1,2} = \{e = uv \in E(NS_1[n]) | d_u = 1 \ and \ d_v = 2\} \longrightarrow |E_{1,2}| = 2^{n+1},$$

$$E_{1,3} = \{e = uv \in E(NS_1[n]) | d_u = 1 \ and \ d_v = 3\} \longrightarrow |E_{1,3}| = 4(2^n - 1),$$

$$E_{2,2}=\{e=uv\in E(NS_1[n])|d_u=2\ \ and\ \ d_v=2\}\longrightarrow|E_{2,2}|=12\times 2^n-11,$$

$$E_{2,3}=\{e=uv\in E(NS_1[n])|d_u=2\ \ and\ \ d_v=3\}\longrightarrow|E_{2,3}|=14(2^n-1).$$

$$M_1(G)=2^{n+1}(1+2)+4(2^n-1)(1+3)+(12\times 2^n-11)(2+2)+14(2^n-1)(2+3)$$

$$=2(35\times 2^{n+1}-65).$$

$$M_2(G)=2^{n+1}(1\times 2)+4(2^n-1)(1\times 3)+(12\times 2^n-11)(2\times 2)+14(2^n-1)(2\times 3)$$

$$=37\times 2^{n+2}-140.$$

$${}^{m}M_2(G)=\frac{1}{1\times 2}\times 2^{n+1}+\frac{1}{1\times 3}\times 4(2^n-1)+\frac{1}{2\times 2}\times(12\times 2^n-11)+\frac{1}{2\times 3}\times 14(2^n-1)$$

$$=\frac{23}{3}\times 2^n-\frac{77}{12}.$$

$$R_\alpha(G)=(1\times 2)^\alpha\times 2^{n+1}+(1\times 3)^\alpha\times 4(2^n-1)+(2\times 2)^\alpha(12\times 2^n-11)+(2\times 3)^\alpha\times 14(2^n-1)$$

$$=2^\alpha\times 2^{n+1}+3^\alpha\times 4(2^n-1)+4^\alpha(12\times 2^n-11)+6^\alpha\times 14(2^n-1).$$

$$RR_\alpha(G)=\frac{1}{(1\times 2)^\alpha}\times 2^{n+1}+\frac{1}{(1\times 3)^\alpha}\times 4(2^n-1)+\frac{1}{(2\times 2)^\alpha}(12\times 2^n-11)+\frac{1}{(2\times 3)^\alpha}\times 14(2^n-1)$$

$$=\frac{1}{2^\alpha}\times 2^{n+1}+\frac{1}{3^\alpha}\times 4(2^n-1)+\frac{1}{4^\alpha}(12\times 2^n-11)+\frac{1}{6^\alpha}\times 14(2^n-1).$$

$$SSD(G)=2^{n+1}\left(\frac{1}{2}+\frac{2}{1}\right)+4(2^n-1)\left(\frac{1}{3}+\frac{3}{1}\right)+(12\times 2^n-11)\left(\frac{2}{2}+\frac{2}{2}\right)+14(2^n-1)\left(\frac{2}{3}+\frac{3}{2}\right)$$

$$=\frac{218}{3}\times 2^n-\frac{197}{3}.$$

By the definition of $NS_2[n]$, the edge partitioning (see in [II], [VI]) is as follows:

$$E_{1,2}=\{e=uv\in E(NS_2[n])|d_u=1\ \ and\ \ d_v=2\}\longrightarrow|E_{1,2}|=2^{n+1},$$

$$E_{2,2}=\{e=uv\in E(NS_2[n])|d_u=2\ \ and\ \ d_v=2\}\longrightarrow|E_{2,2}|=8\times 2^n-5,$$

$$E_{2,3}=\{e=uv\in E(NS_2[n])|d_u=2\ \ and\ \ d_v=3\}\longrightarrow|E_{2,3}|=6(2^n-1).$$

$M_1(G) = 2^{n+1}(1+2) + (8\times 2^n - 5)(2+2) + 16(2^n - 1)(2+3) = 2(17\times 2^{n+1} - 25).$

$$M_2(G) = 2^{n+1}(1\times 2) + (8\times 2^n - 5)(2\times 2) + 6(2^n - 1)(2\times 3) = 72\times 2^n - 56.$$

$$^{m}M_2(G) = \frac{1}{1\times 2}\times 2^{n+1} + \frac{1}{2\times 2}\times (8\times 2^n - 5) + \frac{1}{2\times 3}\times 6(2^n - 1) = 4\times 2^n - \frac{9}{4}.$$

$$R_\alpha(G) = (1\times 2)^\alpha \times 2^{n+1} + (2\times 2)^\alpha(8\times 2^n - 5) + (2\times 3)^\alpha \times 6(2^n - 1)$$

$$= 2^\alpha \times 2^{n+1} + 4^\alpha(8\times 2^n - 5) + 6^\alpha \times 6(2^n - 1).$$

$$RR_\alpha(G) = \frac{1}{(1\times 2)^\alpha}\times 2^{n+1} + \frac{1}{(2\times 2)^\alpha}(8\times 2^n - 5) + \frac{1}{(2\times 3)^\alpha}\times 6(2^n - 1)$$

$$= \frac{1}{2^\alpha}\times 2^{n+1} + \frac{1}{4^\alpha}(8\times 2^n - 5) + \frac{1}{6^\alpha}\times 6(2^n - 1).$$

$$SSD(G) = 2^{n+1}\left(\frac{1}{2} + \frac{2}{1}\right) + (8\times 2^n - 5)\left(\frac{2}{2} + \frac{2}{2}\right) + 6(2^n - 1)\left(\frac{2}{3} + \frac{3}{2}\right) = 34\times 2^n - 23.$$

By the definition of D_n, the edge partitioning (see in [II], [VI]) is as follows:

$$E_{2,2} = \{e = uv \in E(D_n) | d_u = 2 \ \ and \ \ d_v = 2\} \longrightarrow |E_{2,2}| = 12(2\times 2^{n-1} - 1),$$

$$E_{2,3} = \{e = uv \in E(D_n) | d_u = 2 \ \ and \ \ d_v = 3\} \longrightarrow |E_{2,3}| = 6(5\times 2^{n-1} - 4),$$

$$E_{3,3} = \{e = uv \in E(D_n) | d_u = 3 \ \ and \ \ d_v = 3\} \longrightarrow |E_{3,3}| = 12\times 2^{n-1} - 9.$$

$M_1(G) = 12(2\times 2^{n-1} - 1)(2+2) + 6(5\times 2^{n-1} - 4)(2+3) + (12\times 2^{n-1} - 9)(3+3) = 159\times 2^n - 222.$

$$M_2(G) = 12(2\times 2^{n-1} - 1)(2\times 2) + 6(5\times 2^{n-1} - 4)(2\times 3) + (12\times 2^{n-1} - 9)(3\times 3) = 384\times 2^{n-1} - 273.$$

$$^{m}M_2(G) = 12(2\times 2^{n-1} - 1)\times \frac{1}{2\times 2} + 6(5\times 2^{n-1} - 4)\times \frac{1}{2\times 3} + (12\times 2^{n-1} - 9)\times \frac{1}{3\times 3}$$

$$= \frac{37}{3}\times 2^{n-1} - 8.$$

$$R_\alpha(G) = 12(2\times 2^{n-1}-1)(2\times 2)^\alpha + 6(5\times 2^{n-1}-4)(2\times 3)^\alpha + (12\times 2^{n-1} - 9)(3\times 3)^\alpha$$

$$= 4^\alpha \times 12(2^n-1) + 6^\alpha \times 6(5\times 2^{n-1}-4) + 9^\alpha(12\times 2^{n-1}-9).$$

$$RR_\alpha(G) = 12(2\times 2^{n-1}-1)\times \frac{1}{(2\times 2)^\alpha} + 6(5\times 2^{n-1}-4)\times \frac{1}{(2\times 3)}^\alpha + (12\times 2^{n-1}-9)\times \frac{1}{(3\times 3)^\alpha}$$

$$= \frac{1}{4^\alpha}\times 12(2^n-1) + \frac{1}{6^\alpha}\times 6(5\times 2^{n-1}-4) + \frac{1}{9^\alpha}(12\times 2^{n-1}-9).$$

$$SSD(G) = 12(2\times 2^{n-1}-1)\times\left(\frac{2}{2}+\frac{2}{2}\right) + 6(5\times 2^{n-1}-4)\left(\frac{3}{2}+\frac{2}{3}\right) + (12\times 2^{n-1} - 9)\left(\frac{3}{3}+\frac{3}{3}\right)$$

$$= 137\times 2^{n-1} - 94.$$

IV. Conclusion

Topological invariants computed for different chemical structures will enhance our understanding of the physical characteristics, chemical reactivity, and biological activity. In this article, we discussed the corrections of a recent paper by Munir et al. [VI]. Firstly, the figures of the discussed nanostar dendrimer formed accurately. Secondly, we gave the correct computation of incorrect formulae and figures. We suggest a complete correction approach to ensure the correctness of Munir et al.'s [VI] findings on nanostar dendrimers. In addition, we revised notations to ensure that all parameters used in computations are explicitly and consistently described to eliminate ambiguities. Furthermore, we verified our results by using the direct method for the computation of different indices. These corrections are critical to establishing the validity of the findings and paving the path for future advances in this discipline.

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Conflicts of Interest

The authors declare that they have no conflicts of interest.

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