Multiplicative Degree Based Topological Indices of Nanostar Dendrimers

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Abstract: A topological index is a numerical quantity connected with a graph describing the molecular topology of the graph. It can predict different physicochemical properties such as boiling point, entropy, acentric factor etc. of chemical compounds. Dendrimers are highly branched nanostructures that are regarded as a building block in nanotechnology having wide applications. In this paper, multiplicative degree-based topological indices are computed for some nanostar dendrimers. The derived results have the potential for implementation in the chemical, biological, and pharmaceutical sciences.

Keywords: Graph; Degree; Topological indices; Molecular graph; Nanostar dendrimers.

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1. Introduction

Throughout this paper, we consider the molecular graph [1]. By molecular graph, we mean a simple connected graph whose nodes are supposed to be an atom, and edges are bonds between them. Let $V(G)$ and $E(G)$ be the vertex and edge sets of a graph $G$, respectively. For the degree of a vertex $v \in V(G)$, we consider $d(v)$. Chemical graph theory is one of the well-nurtured areas of Graph theory. In Chemical graph theory, the topological index is used to better understand the molecular structure. The topological index is a mapping from the collection of molecular graphs to the real numbers, which remain unchanged under graph isomorphism. It is widely used in various fields of chemistry, biochemistry, and nanotechnology in isomer discrimination, QSAR, QSPR, and pharmaceutical medication plan, and so forth. The topological index was first introduced by Wiener [2] in 1947 to model boiling points of paraffin. Initially, it was known as path number, which had been given the name wiener index later on. Since it is beginnings, this index has been generalized to a multitude of constructions as well as used in regression models of QSAR [3-5]. Some indices related to Wiener’s work are the first and second multiplicative Zagreb indices [6], and the Narumi-Katayama index [7] which are defined as,

$$ \Pi_1(G) = \prod_{u \in V(G)} (d(u))^2, $$

$$ \Pi_2(G) = \prod_{u \in V(G)} (d(u) \cdot d(v)), $$

$$ NK(G) = \prod_{u \in V(G)} d(u), $$

respectively. Gutman [8] studied the multiplicative Zagreb indices for trees and fixed the unique trees that attained maximum and minimum values for $\Pi_1(G)$ and $\Pi_2(G)$, respectively. Wang et al. [9] then extended Gutman’s result to the following index for k-trees,
\[ W^s_G = \prod_{u \in V(G)} (d(u))^s. \] (1)

Where \( s \) is a real number. Based on the successful evaluation of these indices, Eliasi \textit{et al.} [10] defined a new multiplicative version of the first Zagreb index as follows:
\[ \Pi_{1}^{*}(G)=\Pi_{uvu}(G)(d(u) + d(v)). \]

Continuing the concept of indexing on the edge set, the first and second hyper Zagreb indices [11] are defined as,
\[ H \Pi_{1}(G) = \Pi_{uvu}(G)(d(u) + d(v))^2 \text{ and } H \Pi_{2}(G) = \Pi_{uvu}(G)(d(u) \cdot d(v))^2, \]
respectively. To generalize these indices Kulli \textit{et al.} [12] presented first and second generalized multiplicative Zagreb indices, which are defined as follows:
\[ MZ_{1}^{a}(G) = \Pi_{uvu}(G)(d(u) + d(v))^a, \]
\[ MZ_{2}^{a}(G) = \Pi_{uvu}(G)(d(u) \times d(v))^a. \] (2)

Where \( a \) is a real number.

Multiplicative sum connectivity and multiplicative product connectivity indices [13] are defined as,
\[ S C I(\Pi)(G) = \Pi_{uvu}(G)(d(u) + d(v))^{-\frac{1}{2}} \text{ and } P C(\Pi)(G) = \Pi_{uvu}(G)(d(u) \cdot d(v))^{-\frac{1}{2}}, \]
respectively. The Multiplicative atomic bond connectivity index and multiplicative Geometric arithmetic index [14] are defined respectively as follows:
\[ A B C(G) = \prod_{uvu}(G) \sqrt{\frac{d(u) + d(v) - 2}{d(u) \cdot d(v)}} \text{ and } G A H(G) = \prod_{uvu}(G) \frac{2 \sqrt{d(u) \cdot d(v)}}{d(u) + d(v)}. \]

Nanobiotechnology is a novel area of science and technology that uses nanofabrication instruments and procedures to construct equipment for biosystem study. Dendrimers [15-20] are one of the significant objects of this region. Iterative development and activation steps usually synthesize dendrimers from monomers. The chemical structure of dendrimers is well-defined. They consist of three significant architectural components, namely the core, interior branches, and surface groups. New branches emitted from a central core are added in steps until a tree-like structure is created. Its general structure is depicted in Figure 1. The red color is used for the core; green, blue, and yellow for interior branches; cyan for the end groups.

\[ \text{Figure 1. The structure of dendrimers.} \]
Dendrimers are regarded to be one of the most significant, commercially accessible construction blocks in nanotechnology. Dendrimers are used in the formation of nanotubes, nanolatex, chemical sensors, micro and macro capsules, colored glass, modified electrodes, and photon funnels such as artificial antennas. Due to its large scale application in different applied fields, researchers put their attention to investigate the underlying topology of the nanostar dendrimers. De et al. [21] have computed the F-index of nanostar dendrimers. Siddiqui et al. [22] have studied the topological properties of some nanostar dendrimers in terms of Zagreb indices. For more discussion related to this field, readers are referred to [23–42]. The goal of this report is to derive the above mentioned multiplicative degree-based topological indices for some nanostar dendrimers.

2. Materials and Methods

Our main outcomes include the computation of some multiplicative topological indices for some nanostar dentrimer. To compute our results, we used the method of combinatorial computing, vertex partition method, edge partition method, graph-theoretical tools, analytic techniques, and degree counting method. First of all, we associated the graphs of polypropylenimine octaamine dendrimers (NS_1[n] and NS_2[n]), polymer dendrimers (NS_3[n] and NS_5[n]) and fullerene dendrimer (NS_4[n]) where atoms and bonds are represented by nodes and edges, respectively. Then by using the symmetry of the molecular structures, vertex partitions and the edge partitions based on the degree of end vertices are obtained. Using those partitions, we computed some general expressions of topological indices from equations (1)-(3). Assigning particular values to the parameters appear in equations (1)-(3), we derived different well established multiplicative indices. We used Latex software to draw the molecular graphs.

3. Results and Discussion

In this section, we derived multiplicative degree-based indices for five classes of nanostar dendrimers namely NS_1[n], NS_2[n], NS_3[n], NS_4[n], and NS_5[n]. We start with NS_1[n].

**Theorem 1.** Let G be NS_1[n]. Then we have

(i) \( W_1^s(G) = 2^s(20.2^n), 3^s(2^n-1) \),

(ii) \( MZ_1^s(G) = 3^a(2^{n+1}), 4^n(16.2^n-15), 5^1 a(2^n-1) \),

(iii) \( MZ_2^s(G) = 2^a(2^{n+1}), 3^a(2^{n-1}), 4^n(12.2^{n-1}), 6^1 a(2^n-1) \),

(iv) \( ABC(G) = \frac{1}{\sqrt{2}}(26.2^n-23), \sqrt{\frac{3}{2}}(4^n-1) \),

(v) \( GAH(G) = \frac{2\sqrt{3}}{3}(2^{n+1}), \frac{\sqrt{5}}{2}(4^n-1), \frac{2\sqrt{6}}{5}(14.2^n-14) \).

**Proof.** To construct the vertex and edge partitions, we consider the following notations.

\( E_{(i,j)} = \{uv \in E(G) : d(u) = i, d(v) = j\} \), \( V_i = \{v \in V(G) : d(v) = i\} \).

The vertex and edge partitions of NS_1[n] are as follows. The structure of NS_1[n] is shown in Figure 2.
Now, in Table 1 and Table 2 are presented the formulation of multiplicative topological indices, we derive the following results.

\[ W_1^s(G) = \prod_{uv \in V(G)} (d(u))^s \]

\[ = \prod_{uv \in E_1} (d(u))^s \times \prod_{uv \in E_2} (d(u))^s \times \prod_{uv \in E_3} (d(u))^s \]

\[ = 1^s(6.2^n-76) \times 2^s(6.2^n-6) \times 3^s(6.2^n-6) \]

\[ = 2^s(5.2^n+2) \times 3^s(2^n-1). \]

\[ MZ_1^a(G) = \prod_{uv \in E(G)} (d(u) + d(v))^a \]

\[ = \prod_{uv \in E_1} (d(u) + d(v))^a \times \prod_{uv \in E_2} (d(u) + d(v))^a \times \prod_{uv \in E_3} (d(u) + d(v))^a \]

\[ = [3^a]^{(2^n+1)} \times [4^a]^2 \times [12.2^n-11]^2 \times [5^a]^{(14.2^n-14)} \]

\[ = 2^2a(16.2^n-15) \times 3^a(2^n+1) \times 5^a(2^n-1). \]

\[ MZ_2^a(G) = \prod_{uv \in E(G)} (d(u) + d(v))^a \]

\[ = \prod_{uv \in E_1} (d(u) + d(v))^a \times \prod_{uv \in E_2} (d(u) + d(v))^a \times \prod_{uv \in E_3} (d(u) + d(v))^a \]

\[ = [2^a]^{(2^n+1)} \times [3^a]^4 \times [12.2^n-11]^2 \times [6^a]^{(14.2^n-14)} \]

\[ = 2^2a(5.2^n+2-18) \times 3^a(2^n-1). \]

\[ ABC (G) = \prod_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u) \times d(v)}} \]

\[ = \prod_{uv \in E_1} \sqrt{\frac{d(u)+d(v)-2}{d(u) \times d(v)}} \times \prod_{uv \in E_2} \sqrt{\frac{d(u)+d(v)-2}{d(u) \times d(v)}} \times \prod_{uv \in E_3} \sqrt{\frac{d(u)+d(v)-2}{d(u) \times d(v)}} \]

\[ = \left( \frac{1}{\sqrt{2}} \right)^{(2^n+1)} \times \left( \frac{1}{\sqrt{2}} \right)^4 \times \left( \frac{1}{\sqrt{2}} \right)^{(12.2^n-11)} \times \left( \frac{1}{\sqrt{2}} \right)^{(14.2^n-14)} \]

\[ = \left( \frac{1}{\sqrt{2}} \right)^{(26.2^n-23)} \times \left( \frac{1}{\sqrt{2}} \right)^{4(2^n-1)}. \]

\[ GAH (G) = \prod_{uv \in E(G)} \left( \frac{2 \sqrt{d(u)+d(v)}}{d(u)+d(v)} \right) \]

\[ = \prod_{uv \in E_1} \left( \frac{2 \sqrt{d(u)+d(v)}}{d(u)+d(v)} \right) \times \prod_{uv \in E_2} \left( \frac{2 \sqrt{d(u)+d(v)}}{d(u)+d(v)} \right) \times \prod_{uv \in E_3} \left( \frac{2 \sqrt{d(u)+d(v)}}{d(u)+d(v)} \right) \]

\[ = \left( \frac{2 \sqrt{3}}{3} \right)^{(2^n+1)} \times \left( \frac{2 \sqrt{5}}{5} \right)^4 \times \left( \frac{2 \sqrt{5}}{5} \right)^{(14.2^n-14)} \]

\[ = \left( \frac{2 \sqrt{3}}{3} \right)^{(2^n+1)} \times \left( \frac{2 \sqrt{5}}{5} \right)^4 \times \left( \frac{2 \sqrt{5}}{5} \right)^{(14.2^n-14)}. \]
Hence the proof.

![Polypropyleneimine octaamine dendrimer \(NS_1[n]\).](https://biointerfaceresearch.com/)

Putting \(s = 1, 2\), \(a = 1, 2, -1/2\), in theorem 1, we obtain the following corollary.

**Corollary 1.** Different multiplicative degree-based indices of \(NS_1[n]\) are given by,

(i) \(NK(G) = 2^{(20.2^n)} \cdot 3^{6(2^n-1)}\),
(ii) \(\Pi_1(G) = 2^{40.2^n} \cdot 3^{12(2^n-1)}\),
(iii) \(\Pi_1'(G) = 3^{2^{n+1} \cdot 4^{16.2^n-15}} \cdot 5^{14(2^n-1)}\),
(iv) \(\Pi_2(G) = 3^{4.2^n} \cdot 4^{2(16.2^n-15)} \cdot 5^{28(2^n-1)}\),
(v) \(SCI\Pi(G) = \left(\frac{1}{\sqrt{3}}\right)^{2^{n+1}} \cdot \left(\frac{1}{2}\right)^{16.2^n-15} \cdot \left(\frac{1}{\sqrt{3}}\right)^{14(2^n-1)}\),
(vi) \(\Pi_2(G) = 2^{2^{n+1} \cdot 3^{4(2^n-1)} \cdot 4^{12.2^n-11} \cdot 6^{14(2^n-1)}\),
(vii) \(\Pi_2(G) = 4^{2^{n+1} \cdot 9^{4(2^n-1)} \cdot 16^{(12.2^n-11)} \cdot 36^{14(2^n-1)}\),
(viii) \(PCI\Pi(G) = \left(\frac{1}{\sqrt{2}}\right)^{2^{n+1}} \cdot \left(\frac{1}{\sqrt{3}}\right)^{4(2^n-1)} \cdot \left(\frac{1}{2}\right)^{12.2^n-11} \cdot \left(\frac{1}{\sqrt{6}}\right)^{14(2^n-1)}\).

Now we consider the nanostar \(NS_2[n]\). The structure of \(NS_2[n]\) is shown in Figure 3.

**Theorem 2:** Let \(G\) be \(NS_2[n]\). Then we have

(i) \(W_f(G) = 2^{3(12.2^n-43)} \cdot 3^{28(2^n-1)}\),
(ii) \(MZ_1(G) = 3^{\alpha \cdot 2^{n+1} \cdot 2^{16\alpha} \cdot (2^n-5) \cdot (5)^{\alpha} \cdot 6(2^n-1)}\),
(iii) \(MZ_2(G) = 2^{2^n \cdot (12.2^n-43)} \cdot (3)^{6\alpha} \cdot (2^n-1)\),
(iv) \(ABC(G) = \left(\frac{1}{\sqrt{2}}\right)^{(15.2^n-44)}\),
(v) \(GAH(G) = \left(\frac{2\sqrt{2}}{3}\right)^{(2^{n+1})} \cdot \left(\frac{2\sqrt{6}}{5}\right)^{6(2^n-1)}\).

**Proof.** To construct the vertex and edge partitions, we consider the same notations as the previous proof, and we use the same for the rest of the paper. The vertex and the edge partitions of \(NS_2[n]\) are as follows:

| Partition of V(G) | \(V_1\) | \(V_2\) | \(V_3\) |
|-------------------|--------|--------|--------|
| Frequency | \(2^{n+1}\) | \(3 \cdot 2^{n+2} - 43\) | \(2(2^n - 1)\) |

| Partition of E(G) | \(E_{(1,2)}\) | \(E_{(2,2)}\) | \(E_{(2,3)}\) |
|-------------------|--------|--------|--------|
| Frequency | \(2^{n+1}\) | \(8 \cdot (2^n - 5)\) | \((6.2^n - 6)\) |
Now, using Table 3 and Table 4 on the definitions of multiplicative topological indices, the required results are obtained as follows:

\[ W_1^s(G) = \prod_{u \in V(G)} (d(u))^s \]
\[ = \prod_{u \in V(G)} (d(u))^s \times \prod_{u \in V(G)} (d(u))^s \times \prod_{u \in V(G)} (d(u))^s \]
\[ = 2^{(12.2^n - 43)} \cdot 3^{2s(2^n - 1)}. \]

\[ MZ_1^a (G) = \prod_{u \in V(G)} (d(u) + d(v))^a \]
\[ = [3^a]^{(2^n+1)} \cdot [4^a]^{8(2^n-5)} \cdot [5^a]^{6(2^n-1)} \]
\[ = 2^{16a(2^n-5)} \cdot 3^{a+2n+1} \cdot 5^{6a(2^n-1)}. \]

\[ MZ_2^a (G) = \prod_{u \in V(G)} (d(u) \cdot d(v))^a \]
\[ = [2^a]^{(2^n+1)} \cdot [4^a]^{8(2^n-5)} \cdot [6^a]^{6(2^n-1)} \]
\[ = 2^{2a(12.2^n - 43)} \cdot 3^{6a(2^n - 1)}. \]

\[ ABC (G) = \prod_{u \in V(E)} \sqrt{\frac{d(u)+d(v)-2}{d(u) \times d(v)}} \]
\[ = \left( \frac{1}{\sqrt{2}} \right)^{(2^n+1)} \cdot \left( \frac{1}{\sqrt{2}} \right)^{8(2^n-5)} \cdot \left( \frac{1}{\sqrt{2}} \right)^{6(2^n-1)} \]
\[ = \left( \frac{1}{\sqrt{2}} \right)^{(15.2^n - 44)}. \]

\[ GAH (G) = \prod_{u \in V(E)} \frac{2\sqrt{d(u) \times d(v)}}{d(u)+d(v)} \]
\[ = \left( \frac{2\sqrt{2}}{3} \right)^{(2^n+1)} \cdot \left( \frac{2\sqrt{2}}{3} \right)^{6(2^n-1)}. \]

Hence the proof.

Putting \( s = 1, 2, \ a = 1, 2, -1/2, \) in theorem 2, we obtain the following corollary.

**Corollary 2.** Different multiplicative degree-based indices of \( NS_2[n] \) are given by

(i) \( NK (G) = 2^{(12.2^n - 43)} \cdot 3^{2(2^n - 1)}, \)

(ii) \( I_1(G) = 2^{2(12.2^n - 43)} \cdot 3^{4(2^n - 1)}, \)

(iii) \( I_1'(G) = 2^{16(2^n - 5)} \cdot 3^{2n+1} \cdot 5^{(2^n - 1)}, \)

Figure 3. Polypropylenimine octaamine dendrimer (\( NS_2[n] \)).
Corollary 3. Different multiplicative degree-based indices of $NS_3[n]$ are given by
### Proof.

The vertex and the edge partitions of $\text{NS}_4[n]$ are described below.

#### Table 7. Vertex partition of $\text{NS}_4[n]$.

| Partition of V(G) | $V_1$ | $V_2$ | $V_3$ | $V_4$ |
|------------------|-------|-------|-------|-------|
| Frequency        | $4(2^n+30)$ | $10.2^n - 27$ | $6.2^n + 70$ | $\frac{9^9}{4^{8^8}}$ |

#### Table 8. Edge partition of $\text{NS}_4[n]$.

| Partition of E(G) | $E_{(1,3)}$ | $E_{(2,2)}$ | $E_{(2,3)}$ | $E_{(3,3)}$ | $E_{(3,4)}$ | $E_{(4,3)}$ |
|-------------------|-------------|-------------|-------------|-------------|-------------|-------------|
| Frequency         | $2^n + 1$   | $2^n + 2$   | $32.2^n - 8$ | $86$       | $6$         | $3$         |

Now using Table 7 and Table 8 on the definitions of multiplicative topological indices, the required result can be obtained easily like previous.

### Figure 5. Fullerene dendrimer ($\text{NS}_4[n]$).
Corollary 4. Different multiplicative degree-based indices of $NS_4[n]$ are given by

(i) $NK(G) = 2^{(10.2^n-\sqrt{n})} \cdot 3^{2(3.2^n+35)}$,

(ii) $\Pi_1(G) = 2^{(10.2^n-\sqrt{n})} \cdot 3^{4(3.2^n+35)}$,

(iii) $\Pi_1^2(G) = 2^{(2n^3+99)} \cdot 3^{8(2n^1+1)} \cdot 7^n$,

(iv) $H\Pi_1^3(G) = 2^{(2n^3+99)} \cdot 3^{172} \cdot 5^{16}(2n^1+1) \cdot 7^{12}$,

(v) $SCI\Pi(G) = \left(\frac{1}{\sqrt{5}}\right)^{16.2^n-8} \cdot \left(\frac{1}{2}\right)^{2(2n^1+1)} \cdot \left(\frac{1}{\sqrt{5}}\right)^{86} \cdot \left(\frac{1}{\sqrt{5}}\right)^{6} \cdot \left(\frac{1}{4}\right)^3$.

(vi) $\Pi_2(G) = 2^{20(2n^1+1)} \cdot 3^{2(9.2^n+85)}$,

(vii) $H\Pi_2(G) = 2^{40(2n^1+1)} \cdot 3^{4(9.2^n+85)}$.

Finally, we consider $NS_5[n]$ nanostar. The structure of $NS_5[n]$ is shown in Figure 6.

Theorem 5. Let $G$ be $NS_5[n]$ nanostar. Then we have

(i) $W_1^5(G) = 2^{3s(10.2^n+1)} \cdot 3^{3s(6.2^n+5)}$,

(ii) $MZ_1^5(G) = 2^{6s(42.2^n+13)} \cdot 3^{24s} \cdot 5^{6}(48.2^n-6)$,

(iii) $MZ_2^5(G) = 2^{6s(10.2^n+1)} \cdot 3^{9s(6.2^n+5)}$,

(iv) $ABC(G) = \left(\frac{1}{\sqrt{2}}\right)^{54.2^n} \cdot \left(\frac{5}{3}\right) \cdot \left(\frac{1}{\sqrt{3}}\right)^{2(2n^1+1)}$,

(v) $GAH(G) = \left(\frac{2\sqrt{5}}{5}\right)^{6(2n^3+1)} \cdot \left(\frac{2}{3}\right)^{3(2n^1+1)}$.

Proof. The vertex and the edge partitions of $NS_5[n]$ are as follows:

| Partition of V(G) | $V_1$ | $V_2$ | $V_3$ |
|-------------------|-------|-------|-------|
| Frequency         | 3(2.2^n-1) | 3(10.2^n+1) | 3(6.2^n+5) |

| Partition of E(G) | $E_{(1,3)}$ | $E_{(2,2)}$ | $E_{(2,3)}$ | $E_{(3,3)}$ |
|-------------------|-------------|-------------|-------------|-------------|
| Frequency         | 3.(2^n+1)   | 6.(2^n+1)   | 24          | 3.(2^n+1)   |

Now putting the vertex (Table 9) and edge partitions (Table 10) of $NS_5[n]$ on the definitions of multiplicative topological indices, the required result can be obtained easily.

Figure 6. The polymer dendrimer ($NS_5[n]$).
Putting \( s = 1, 2, \ a = 1, 2, -1/2 \), in theorem 5, we obtain the following corollary.

**Corollary 5.** Different multiplicative degree-based indices of \( NS_3[n] \) are given by

1. \( \text{NK}(G) = 2^{3(10.2^n+1)} \cdot 3^{3(6.2^n+5)} \),
2. \( \Pi_1(G) = 2^{6(10.2^n+1)} \cdot 3^{6(6.2^n+5)} \),
3. \( \Pi_2(G) = 2^{6(42.2^n+13)} \cdot 3^{24} \cdot 5^{(48.2^n-6)} \),
4. \( H\Pi_1(G) = 2^{(42.2^n+13)} \cdot 3^{48} \cdot 5^{(12(2^n+2)-1)} \),
5. \( S\Pi_1(G) = \left( \frac{1}{\sqrt{3}} \right)^{48.2^n-6} \cdot \left( \frac{1}{2} \right)^{3(42.2^n+3)} \cdot \left( \frac{1}{\sqrt{6}} \right)^{24} \),
6. \( \Pi_2(G) = 2^{6(10.2^n+1)} \cdot 3^{9(6.2^n+5)} \),
7. \( H\Pi_2(G) = 2^{12(10.2^n+1)} \cdot 3^{18}(6.2^n+5) \),
8. \( \text{PCII}(G) = \left( \frac{1}{\sqrt{6}} \right)^{6(2^n+3)-1} \cdot \left( \frac{1}{2} \right)^{6(2^n+1)} \cdot \left( \frac{1}{3} \right)^{24} \cdot \left( \frac{1}{\sqrt{3}} \right)^{3(2^n+1)+1} \).

4. Conclusions

In this work, we consider five families of nano star dendrimers namely \( NS_1[n], NS_2[n], NS_3[n], NS_4[n], \) and \( NS_5[n] \). We have obtained exact expressions of multiplicative degree-based topological indices for these nanostar dendrimers. These results can be utilized in molecular data mining. These results can also play a key role in pharmaceutical drug design. In the future, we want to study these indices for some chemical networks and models, which will be useful to understand their underlying topologies.

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**Conflicts of Interest**

The authors declare no conflict of interest.

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