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Fourth Order and Fourth Sum Connectivity Indices of Polyphenylene Dendrimers

[1]Nabeel E. Arif, [2]Roslan Hasni and [3]Saeid Alikhani
[1]School of Mathematical Sciences, Universiti Sains Malaysia, 11800, Penang, Malaysia
[2]Department of Mathematics, Faculty of Science and Technology, Universiti Malaysia Terengganu, 21030 Kuala, Terengganu, Malaysia
[3]Department of Mathematics, Yazd University, 89175-741, Yazd, Iran

Abstract: The m-order connectivity index ${}^{m}\chi(G)$ of a graph G is ${}^{m}\chi(G)=\sum_{v_{i_1}v_{i_2}\cdots v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}d_{i_2}\ldots d_{i_{m+1}}}}$, where, $d_{i_1}d_{i_2}\ldots d_{i_{m+1}}$ runs over all paths of length m in G and d_i denotes the degree of vertex v_i. Also ${}^{ms}X(G)=\sum_{v_{i_1}v_{i_2}\cdots v_{i_{m+1}}}\frac{1}{\sqrt{d_{i_1}+d_{i_2}+\ldots+d_{i_{m+1}}}}$ is its m-sum connectivity index. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this study, the 4-connectivity and 4-sum connectivity indices of an infinite family of polyphenylene dendrimer are computed.

Key words: 4-connectivity index, 4-sum connectivity index, dendrimer, graph

INTRODUCTION

A graph G is a finite nonempty set V(G) of objects called vertices together with a (possibly empty) set E(G) of 2-element subsets of V(G) called edges. In a chemical graph, vertices represents atoms and edges represents bonds (Trinajstic, 1983).

A single number which characterizes the graph of a molecular is called a graph theoretical invariant or topological index. The connectivity index is one of the most popular topological indices introduced by (Randic, 1975). This index has been used in a wide spectrum of applications ranging from predicting physicochemical properties such as boiling point and solubility partition. The molecular connectivity index χ provides a quantitative assessment of branching of molecules. Randic (1975) first addressed the problem of relating the physical properties of alkanes to the degree of branching across an isomeric series. The degree of branching of a molecule was quantified using a branching index which subsequently became known as first-order molecular connectivity index χ. Kier and Hall (1986) extended this to higher orders and introduced modifications to account for heteroatoms.

Let G be a simple connected graph of order n. For an integer m = 1, the m-order connectivity index of an organic molecule whose molecule graph G is defined as:

$$ {}^{m}\chi(G)=\sum_{i_1\cdots i_{m+1}}\frac{1}{\sqrt{d_{i_1}\ldots d_{i_{m+1}}}} \quad (1)$$

where, $i_1\cdots i_{m+1}$ (for simplicity) runs over all paths of length m in G and d_i denote the degree of vertex v_i. In particular, 4-order connectivity index is defined as follows:

$$ {}^{4}\chi(G)=\sum_{i_1\cdots i_5}\frac{1}{\sqrt{d_{i_1}d_{i_2}d_{i_3}d_{i_4}d_{i_5}}} \quad (2)$$

Recently, a closely related variant of the Randiæ connectivity index called the sum-connectivity index was introduced by Zhou and Trinajstic (2009, 2010). For a simple connected graph G, its sum-connectivity index X(G) is defined as the sum over all edges of the graph of the terms $(d_u+d_v)^{-1/2}$, that is:

$$ {}^{s}X(G)=\sum_{uv}\frac{1}{\sqrt{d_u+d_v}} \quad (3)$$

where, d_u and d_v are the degrees of the vertices u and v, respectively. It is a graph-based molecular structure descriptor. It has been found that the sum-connectivity index correlates well with π-electronic energy of benzenoid hydrocarbons and it is frequently applied in quantitative structure property and Structure-activity studies (Kier and Hall, 1986; Todeschini and Consonni, 2000).

Corresponding Author: Roslan Hasni, Department of Mathematics, Faculty of Science and Technology, Universiti Malaysia Terengganu, 21030 Kuala, Terengganu, Malaysia

The m-sum connectivity index of G is defined as:

$$ {}^{ms}X(G) = \sum_{i_1 \cdots i_{m+1}} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + \ldots + d_{i_{m+1}}}} \quad (4) $$

where, $i_1i_2 \cdots i_{m+1}$ runs over all paths of length n in G. In particular, 4-sum connectivity index are defined as:

$$ {}^{4s}\chi(G) = \sum_{i_1 \cdots i_5} \frac{1}{\sqrt{d_{i_1} + d_{i_2} + d_{i_3} + d_{i_4} + d_{i5}}} \quad (5) $$

Dendrimers are hyper-branched macromolecules, with a rigorously tailored architecture. They can be synthesized, in a controlled manner, either by a divergent or a convergent procedure. Dendrimers have gained a wide range of applications in supra-molecular chemistry, particularly in host guest reactions and self-assembly processes. Their applications in chemistry, biology and nano-science are unlimited. Recently, some researchers investigated m-order connectivity indices of some dendrimer nanostars, where, m = 2 and 3 (Ashrafi and Nikzad, 2009; Ahmadi and Sadeghimehr, 2009; Chen and Yang, 2011; Madanshekaf and Ghaneei, 2011; Yang *et al*., 2011). In this study, the 4-connectivity and 4-sum connectivity of an infinite families of polyphenylene dendrimers are computed.

FOURTH-ORDER CONNECTIVITY INDEX OF DENDRIMER

We consider polyphenylene dendrimer by construction of dendrimer generations G_n has grown n stages. We denote this graph by $D_4[n]$. Figure 1 shows the generations G_2 has grown 2 stages.

The following theorem gives the fourth-order connectivity index of polyphenylene dendrimer.

Theorem 1: Let $n \in N$. The fourth-order connectivity index of $D_4[n]$ is:

$$ {}^4\chi(D_4[n]) = \frac{1}{27}(438\sqrt{2} + 386\sqrt{3} + 126) + \frac{1}{18}\left(\frac{271\sqrt{2}}{2} + \frac{353\sqrt{3}}{3}\right)(2^{n+1} - 4) $$

Proof: First we compute ${}^4\chi(D_4[n])$. Let $d_{i_1i_2i_3i_4i_5}$ denote the number of 4-paths whose five consecutive vertices are of degree i_1, i_2, i_3, i_4, i_5, respectively. In the same way, we use $d^{(n)}_{i_1i_2i_3i_4i_5}$ to mean $d_{i_1i_2i_3i_4i_5}$ in nth stages. Particularly, $d^{(n)}_{i_1i_2i_3i_4i_5} = d^{(n)}_{i_5i_4i_3i_2i_1}$.

We can see that:

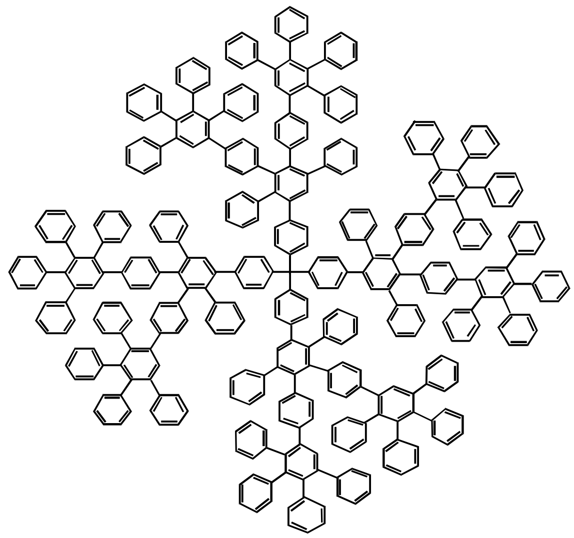

Fig. 1: Polyphenylene dendrimer of generations G_n has grown 2 stages

$$ d^{(1)}_{22222} = 16d, {}^{(1)}_{22223} = 32,\ d^{(1)}_{22232} = 32,\ d^{(1)}_{22233} = 32,\ d^{(1)}_{22322} = 24,\ d^{(1)}_{22332} = 16, $$
$$ d^{(1)}_{22333} = 64,\ d^{(1)}_{23223} = 16,\ d^{(1)}_{23323} = 16,\ d^{(1)}_{23332} = 16,\ d^{(1)}_{23333} = 128,\ d^{(1)}_{32333} = 16, $$
$$ d^{(1)}_{33223} = 8,\ d^{(1)}_{33233} = 16,\ d^{(1)}_{33333} = 32,\ d^{(1)}_{32234} = 8,\ d^{(1)}_{22343} = 24,\ d^{(1)}_{23432} = 24 $$

Therefore, by Eq. 2, we obtain:

$$ {}^4\chi(D_4[1]) = \frac{16}{\sqrt{2\times2\times2\times2\times2}} + \frac{32}{\sqrt{2\times2\times2\times2\times3}} + \frac{32}{\sqrt{2\times2\times2\times3\times2}} + \frac{32}{\sqrt{2\times2\times2\times3\times3}} + \frac{24}{\sqrt{2\times2\times3\times2\times2}} + \frac{16}{\sqrt{2\times2\times3\times3\times2}} + \frac{64}{\sqrt{2\times2\times3\times3\times3}} + \frac{16}{\sqrt{2\times3\times2\times2\times3}} + \frac{16}{\sqrt{2\times3\times3\times2\times3}} + \frac{16}{\sqrt{2\times3\times3\times3\times2}} + \frac{128}{\sqrt{2\times3\times3\times3\times3}} + \frac{16}{\sqrt{3\times2\times3\times3\times3}} + \frac{8}{\sqrt{3\times3\times2\times2\times3}} + \frac{16}{\sqrt{3\times3\times2\times3\times3}} + \frac{32}{\sqrt{3\times3\times3\times3\times3}} + \frac{8}{\sqrt{3\times2\times2\times3\times4}} + \frac{24}{\sqrt{2\times2\times3\times4\times3}} + \frac{24}{\sqrt{2\times3\times4\times3\times2}} $$

Now, we construct the relation between ${}^4\chi(D_4[n])$ and ${}^4\chi(D_4[n\text{-}1])$ for $n \le 2$. By simple reduction, we have:

$$ d^{(n)}_{22222} = d^{(n-1)}_{22222} + 6\times2^n,\ d^{(n)}_{22223} = d^{(n-1)}_{22223} + 12\times2^n,\ d^{(n)}_{22232} = d^{(n-1)}_{22232} + 12\times2^n, $$
$$ d^{(n)}_{22233} = d^{(n-1)}_{22233} + 12\times2^n,\ d^{(n)}_{22322} = d^{(n-1)}_{22322} + 10\times2^n,\ d^{(n)}_{22332} = d^{(n-1)}_{22332} + 8\times2^n, $$
$$ d^{(n)}_{22333} = d^{(n-1)}_{22333} + 32\times2^n,\ d^{(n)}_{23223} = d^{(n-1)}_{23223} + 8\times2^n,\ d^{(n)}_{23323} = d^{(n-1)}_{23323} + 8\times2^n, $$
$$ d^{(n)}_{23332} = d^{(n-1)}_{23332} + 8\times2^n,\ d^{(n)}_{23333} = d^{(n-1)}_{23333} + 64\times2^n,\ d^{(n)}_{32333} = d^{(n-1)}_{32333} + 8\times2^n, $$
$$ d^{(n)}_{33223} = d^{(n-1)}_{33223} + 8\times2^n,\ d^{(n)}_{33233} = d^{(n-1)}_{33233} + 8\times2^n,\ d^{(n)}_{33333} = d^{(n-1)}_{33333} + 16\times2^n $$

and for any:

$(i_1i_2i_3i_4i_5) \neq$ (22222), (22223), (22232), 22322, (22332), (22333), (23223), (23323), (23332), (23333), (32333), (33223), (33333), (32234), (22343), (23432)

we have $d^{(n)}_{i_1i_2i_3i_4i_5} = 0$.

Therefore, by Eq. 2, we have:

$$\begin{aligned}
{}^4\chi(D_4[n]) &= {}^4\chi(D_4[n-1]) + \frac{6\times 2^n}{\sqrt{2\times2\times2\times2\times2}} + \frac{12\times 2^n}{\sqrt{2\times2\times2\times2\times3}} + \\
&\frac{12\times 2^n}{\sqrt{2\times2\times2\times3\times2}} + \frac{12\times 2^n}{\sqrt{2\times2\times2\times3\times3}} + \frac{10\times 2^n}{\sqrt{2\times2\times3\times2\times2}} + \frac{8\times 2^n}{\sqrt{2\times2\times3\times3\times2}} + \\
&\frac{32\times 2^n}{\sqrt{2\times2\times3\times3\times3}} + \frac{8\times 2^n}{\sqrt{2\times3\times2\times2\times3}} + \frac{8\times 2^n}{\sqrt{2\times3\times3\times2\times3}} + \frac{8\times 2^n}{\sqrt{2\times3\times3\times3\times2}} + \\
&\frac{64\times 2^n}{\sqrt{2\times3\times3\times3\times3}} + \frac{8\times 2^n}{\sqrt{3\times2\times3\times3\times3}} + \frac{8\times 2^n}{\sqrt{3\times3\times2\times2\times3}} + \frac{8\times 2^n}{\sqrt{3\times3\times2\times3\times3}} + \\
&\frac{16\times 2^n}{\sqrt{3\times3\times3\times3\times3}} = {}^4\chi(D_4[n-1]) + \frac{1}{18}\left(\frac{271\sqrt{2}}{2} + \frac{353\sqrt{3}}{3}\right)\times 2^n
\end{aligned}$$

From above recursion formula, we have:

$$\begin{aligned}
{}^4\chi(D_4[n]) &= {}^4\chi(D_4[n-1]) + \frac{1}{18}\left(\frac{271\sqrt{2}}{2} + \frac{353\sqrt{3}}{3}\right)\times 2^n \\
&= {}^4\chi(D_4[n-2]) + \frac{1}{18}\left(\frac{271\sqrt{2}}{2} + \frac{353\sqrt{3}}{3}\right)(2^n + 2^{n-1}) \\
&\vdots \\
&= {}^4\chi(D_4[1]) + \frac{1}{18}\left(\frac{271\sqrt{2}}{2} + \frac{353\sqrt{3}}{3}\right)(2^n + 2^{n-1} + \ldots + 2^2) \\
&= \frac{1}{27}(438\sqrt{2} + 386\sqrt{3} + 126) + \frac{1}{18}\left(\frac{271\sqrt{2}}{2} + \frac{353\sqrt{3}}{3}\right)(2^n + 2^{n-1} + \ldots + 2^2) \\
{}^4\chi(D_4[n]) &= \frac{1}{27}(438\sqrt{2} + 386\sqrt{3} + 126) + \frac{1}{18}\left(\frac{271\sqrt{2}}{2} + \frac{353\sqrt{3}}{3}\right)(2^{n+1} - 4)
\end{aligned}$$

The proof is now complete.

FOURTH-SUM CONNECTIVITY INDEX OF DENDRIMER D_4[N]

In this section, we will study the 4-sum connectivity index of the same family of dendrimers as shown in Fig. 1.

The following theorem gives the fourth-sum connectivity index of polyphenylene dendrimers.

Theorem 2: Let $n \in N$. The fourth-sum connectivity index of $D_4[n]$ is:

$$\begin{aligned}
{}^{4s}\chi(D_4[n]) &= \frac{1}{105}(168\sqrt{10} + 840\sqrt{11} + 560\sqrt{12} + 840\sqrt{13} + 1575\sqrt{14} + 224\sqrt{15}) + \\
&\left(\frac{3}{5}\sqrt{10} + \frac{34}{11}\sqrt{11} + \frac{7}{3}\sqrt{12} + \frac{56}{13}\sqrt{13} + \frac{40}{7}\sqrt{14} + \frac{16}{15}\sqrt{15}\right)(2^{n+1} - 4)
\end{aligned}$$

Proof: First we compute ${}^{4S}\chi(D_4[1])$. Let $d_{i_1i_2i_3i_4i_5}$ denote the number of 4-paths whose five consecutive vertices are of degree i_1, i_2, i_3, i_4, i_5, respectively. In the same way, we use $d^{(n)}_{i_1i_2i_3i_4i_5}$ to mean $d_{i_1i_2i_3i_4i_5}$ in nth stages. Particularly, $d^{(n)}_{i_1i_2i_3i_4i_5} = d^{(n)}_{i_5i_4i_3i_2i_1}$.

We note that:

$$\begin{aligned}
&d^{(1)}_{22222} = 16,\ d^{(1)}_{22223} = 32,\ d^{(1)}_{22232} = 32,\ d^{(1)}_{22233} = 32,\ d^{(1)}_{22322} = 24,\ d^{(1)}_{22332} = 16, \\
&d^{(1)}_{22333} = 64,\ d^{(1)}_{23223} = 16,\ d^{(1)}_{23323} = 16,\ d^{(1)}_{23332} = 16,\ d^{(1)}_{23333} = 128,\ d^{(1)}_{32333} = 16, \\
&d^{(1)}_{33223} = 8,\ d^{(1)}_{33233} = 16,\ d^{(1)}_{33333} = 32,\ d^{(1)}_{32234} = 8,\ d^{(1)}_{22343} = 24,\ d^{(1)}_{23432} = 24
\end{aligned}$$

Therefore, by Eq. 5, we have:

$$\begin{aligned}
{}^4\chi(D_4[1]) &= \frac{16}{\sqrt{2+2+2+2+2}} + \frac{32}{\sqrt{2+2+2+2+3}} + \frac{32}{\sqrt{2+2+2+3+2}} + \\
&\frac{32}{\sqrt{2+2+2+3+3}} + \frac{24}{\sqrt{2+2+3+2+2}} + \frac{16}{\sqrt{2+2+3+3+2}} + \\
&\frac{64}{\sqrt{2+2+3+3+3}} + \frac{16}{\sqrt{2+3+2+2+3}} + \frac{16}{\sqrt{2+3+3+2+3}} + \frac{16}{\sqrt{2+3+3+3+2}} + \\
&\frac{128}{\sqrt{2+3+3+3+3}} + \frac{16}{\sqrt{3+2+3+3+3}} + \frac{8}{\sqrt{3+3+2+2+3}} + \\
&\frac{16}{\sqrt{3+3+2+3+3}} + \frac{32}{\sqrt{3+3+3+3+3}} + \frac{8}{\sqrt{3+2+2+3+4}} + \frac{24}{\sqrt{2+2+3+4+3}} + \frac{24}{\sqrt{2+3+4+3+2}}
\end{aligned}$$

Similar to that of Theorem 1, we can find the relation between ${}^{4S}\chi(D_4[n])$ and ${}^{4S}\chi(D_4[n\text{-}1])$ for $n \le 2$.

We have:

$$\begin{aligned}
&d^{(n)}_{22222} = d^{(n-1)}_{22222} + 6\times 2^n,\ d^{(n)}_{22223} = d^{(n-1)}_{22223} + 12\times 2^n,\ d^{(n)}_{22232} = d^{(n-1)}_{22232} + 12\times 2^n, \\
&d^{(n)}_{22233} = d^{(n-1)}_{22233} + 12\times 2^n,\ d^{(n)}_{22322} = d^{(n-1)}_{22322} + 10\times 2^n,\ d^{(n)}_{22332} = d^{(n-1)}_{22332} + 8\times 2^n, \\
&d^{(n)}_{22333} = d^{(n-1)}_{22333} + 32\times 2^n,\ d^{(n)}_{23223} = d^{(n-1)}_{23223} + 8\times 2^n,\ d^{(n)}_{23323} = d^{(n-1)}_{23323} + 8\times 2^n, \\
&d^{(n)}_{23332} = d^{(n-1)}_{23332} + 8\times 2^n,\ d^{(n)}_{23333} = d^{(n-1)}_{23333} + 64\times 2^n,\ d^{(n)}_{32333} = d^{(n-1)}_{32333} + 8\times 2^n, \\
&d^{(n)}_{33223} = d^{(n-1)}_{33223} + 8\times 2^n,\ d^{(n)}_{33233} = d^{(n-1)}_{33233} + 8\times 2^n,\ d^{(n)}_{33333} = d^{(n-1)}_{33333} + 16\times 2^n
\end{aligned}$$

and for any:

$$(i_1i_2i_3i_4i_5) \neq (22222), (22223), (22232), (22322), (22332), (22333), (23223), (23323), (23332), (23333), (32333), (33223), (33233), (33333), (32234), (22343), (23432)$$

we have $d^{(n)}_{i_1i_2i_3i_4i_5} = 0$.

Therefore, by Eq. 5, we obtain:

$$\begin{aligned}
{}^{4s}\chi(D_4[n]) &= {}^{4s}\chi(D_4[n-1]) + \frac{6\times 2^n}{\sqrt{2+2+2+2+2}} + \frac{12\times 2^n}{\sqrt{2+2+2+2+3}} + \frac{12\times 2^n}{\sqrt{2+2+2+3+2}} + \\
&\frac{12\times 2^n}{\sqrt{2+2+2+3+3}} + \frac{10\times 2^n}{\sqrt{2+2+3+2+2}} + \frac{8\times 2^n}{\sqrt{2+2+3+3+2}} + \frac{32\times 2^n}{\sqrt{2+2+3+3+3}} + \\
&\frac{8\times 2^n}{\sqrt{2+3+2+2+3}} + \frac{8\times 2^n}{\sqrt{2+3+3+2+3}} + \frac{8\times 2^n}{\sqrt{2+3+3+3+2}} + \frac{64\times 2^n}{\sqrt{2+3+3+3+3}} + \\
&\frac{8\times 2^n}{\sqrt{3+2+3+3+3}} + \frac{8\times 2^n}{\sqrt{3+3+2+2+3}} + \frac{8\times 2^n}{\sqrt{3+3+2+3+3}} + \frac{16\times 2^n}{\sqrt{3+3+3+3+3}} \\
&= {}^{4s}\chi(D_4[n-1]) + \left(\frac{3}{5}\sqrt{10} + \frac{34}{11}\sqrt{11} + \frac{7}{3}\sqrt{12} + \frac{56}{13}\sqrt{13} + \frac{40}{7}\sqrt{14} + \frac{16}{15}\sqrt{15}\right)\times 2^n
\end{aligned}$$

From above recursion formula, we have:

$$\begin{aligned}
{}^{4s}\chi(D_4[n]) &= {}^{4s}\chi(D_4[n-1]) + \left(\frac{3}{5}\sqrt{10} + \frac{34}{11}\sqrt{11} + \frac{7}{3}\sqrt{12} + \frac{56}{13}\sqrt{13} + \frac{40}{7}\sqrt{14} + \frac{16}{15}\sqrt{15}\right)\times 2^n \\
&= {}^{4s}\chi(D_4[n-2]) + \left(\frac{3}{5}\sqrt{10} + \frac{34}{11}\sqrt{11} + \frac{7}{3}\sqrt{12} + \frac{56}{13}\sqrt{13} + \frac{40}{7}\sqrt{14} + \frac{16}{15}\sqrt{15}\right)(2^n + 2^{n-1}) \\
&\vdots \\
&= {}^{4s}\chi(D_4[1]) + \left(\frac{3}{5}\sqrt{10} + \frac{34}{11}\sqrt{11} + \frac{7}{3}\sqrt{12} + \frac{56}{13}\sqrt{13} + \frac{40}{7}\sqrt{14} + \frac{16}{15}\sqrt{15}\right)(2^n + 2^{n-1} + \ldots + 2^2) \\
&= \frac{1}{105}(168\sqrt{10} + 840\sqrt{11} + 560\sqrt{12} + 840\sqrt{13} + 1575\sqrt{14} + 224\sqrt{15}) + \\
&\left(\frac{3}{5}\sqrt{10} + \frac{34}{11}\sqrt{11} + \frac{7}{3}\sqrt{12} + \frac{56}{13}\sqrt{13} + \frac{40}{7}\sqrt{14} + \frac{16}{15}\sqrt{15}\right)(2^n + 2^{n-1} + \ldots + 2^2) \\
{}^{4s}\chi(D_4[n]) &= \frac{1}{105}(168\sqrt{10} + 840\sqrt{11} + 560\sqrt{12} + 840\sqrt{13} + 1575\sqrt{14} + 224\sqrt{15}) + \\
&\left(\frac{3}{5}\sqrt{10} + \frac{34}{11}\sqrt{11} + \frac{7}{3}\sqrt{12} + \frac{56}{13}\sqrt{13} + \frac{40}{7}\sqrt{14} + \frac{16}{15}\sqrt{15}\right)(2^{n+1} - 4)
\end{aligned}$$

The proof is now complete.

CONCLUSION

In this study, the 4-connectivity and 4-sum connectivity indices for an infinite families of polyphenylene dendrimers were presented. The similar method can be extended to study of the m-connectivity and m-sum connectivity indices of other dendrimers or nano-structures.

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