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Investigating the topological properties of porphyrin-based dendrimers using discrete Adriatic indices

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Abstract

Topological indices serve as molecular structure descriptors that characterize the topology of a molecule while remaining invariant under graph isomorphism. Discrete Adriatic indices, explored by Vukičević and Gašperov in 2010, are a significant category of topological indices that have demonstrated strong predictive capabilities in assessments implemented by the International Academy of Mathematical Chemistry. Some of the most effective discrete Adriatic indices include the max-min sdeg index, misbalance indeg index, symmetric division deg index, and variable sum exdeg index, all of which have been proposed as potentially useful measures with better quality compared to some existing measures. This paper aims to explore these descriptors for several infinite families of porphyrin-based dendrimers using the edge partition technique.

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1. Introduction

In the field of chemical graph theory, a *molecular graph*–also known as *chemical graph*–represents a chemical structure using a labeled graph, where the vertices represent different atoms and the edges represent the chemical bonds connecting those atoms within the molecule. Topological indices are numerical measures that capture certain graph's characteristics and stay invariant under graph isomorphism [1,2]. These indices are instrumental in studying the relationships between the structures of chemical compounds and their physicochemical properties or biological activities, commonly referred to as Quantitative Structure–Activity Relationships [3].

Some topological indices are *bond additive*, expressed as the sum of contributions from edges. The *discrete Adriatic indices*, a significant category of bond additive topological indices, were explored by Vukičević and Gašperov [4] in 2010. This category comprises 148 discrete Adriatic indices that have proven to possess strong predictive abilities in tests done by the International Academy of Mathematical Chemistry. These indices are straightforward to program and can be readily integrated into current chemical modeling programs. Included in these indices are the *max-min sdeg index* (*MmS* index), *misbalance indeg index* (*MI* index), and *symmetric division deg index* (*SDD* index), each defined for a molecular graph G as follows:

$$MmS(G) = \sum_{j\ell \in E(G)} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2,$$

$$MI(G) = \sum_{j\ell \in E(G)} \left|\frac{1}{d_j} - \frac{1}{d_\ell}\right| = \sum_{j\ell \in E(G)} \frac{|d_j - d_\ell|}{d_j d_\ell},$$

$$SDD(G) = \sum_{j\ell \in E(G)} \left(\frac{d_j}{d_\ell} + \frac{d_\ell}{d_j}\right) = \sum_{j\ell \in E(G)} \frac{d_j^2 + d_\ell^2}{d_j d_\ell},$$

where $E(G)$ shows the edge set of G, while d_j is the degree of vertex j in G (see [5]). It has been demonstrated in [4] that, the *MmS* index can effectively predict the log water activity coefficient for polychlorobiphenyls. Additionally, the *MI* index serves as a reliable tool for the standard enthalpy of vaporization for octane isomers, while the *SDD* index stands out as the most precise predictor for estimating the total surface area of polychlorobiphenyls. In addition, these indices were proposed as potentially useful measures having better quality compared to some previously-introduced measures (see, for example, [6,7]).

In 2011, Vukičević [8] proposed another topological index namely *variable sum exdeg index* (*VSE* index) which was formulated for a molecular graph G as

$$SEI_q(G) = \sum_{j\ell \in E(G)} \left(q^{d_j} + q^{d_\ell}\right) = \sum_{j \in V(G)} d_j q^{d_j},$$

in which $V(G)$ denotes the vertex set of G and $q \in (0,1) \cup (1, +\infty)$ is a variable parameter. It was shown that for certain values of t, the SEI_t index effectively predicts the octanol-water partition coefficient for octane isomers. See, for example, [9-11] for some mathematical properties of *VSE* index.

Dendrimers are hugely branched polymeric substances with dimensions on the nanometer-scale [12]. They consist of three main structural elements: a central core, an inner dendritic branching framework, and an outer surface decorated with functional groups. The central core is usually an atom or a molecule with more than one similar chemical functional group. The branches are the iterated parts of dendrimers, which start from the central core. The geometric repetition of the branches leads to the formation of radially centric layers named generations. The terminal functional groups which are important factors in determining properties of the dendrimers are stationed at the periphery of the dendrimer structure. Dendrimers have gained vast applications such as enhancing drug solubility, stability, and bioavailability. Investigating the mathematical and topological properties of dendrimers has been the focus of numerus studies in mathematical chemistry and chemical graph theory (see, for example, [13-24]).

Porphyrin-cored dendrimers (PC dendrimers) [25,26] represent a prominent group of dendrimers, known for their wide range of uses in fields including light harvesting, electron transfer, and host-guest recognition [27,28].

In this paper, we are concerned with computing the aforementioned discrete Adriatic indices for some infinite families of PC dendrimers.

2. Main results and discussion

Our aim is to calculate the discrete Adriatic indices listed in Section 1 for four types of PC dendrimers by applying the edge-partition technique. The technique is based on dividing the set of edges of the chemical graph corresponding to the respective PC dendrimer to certain proper subsets such that the end-vertex degrees of every edge lying in the same subset are equal. Then by computing the order of any subset as well as the edge contribution of any subset to the considered graph invariant, multiplying these quantities to each other and adding the resulting expressions, we arrive at the amount of the considered graph invariant for the respective dendrimer. The remainder of this section will include four subsections, each dedicated to one of the dendrimer groups under investigation.

2.1 $\mathcal{PC}_a(\mathcal{s})$ *dendrimer*

Let $\mathcal{PC}_a(\mathcal{s})$ stand for the molecular graph of the first $\mathcal{PC}$ dendrimer in such a way that $\mathcal{s}$ represents the steps of growth (see Figure 1). Manifestly, $|V(\mathcal{PC}_a(\mathcal{s})\,)| = 136 \times 2^{\mathcal{s}} - 15$ and $|E(\mathcal{PC}_a(\mathcal{s})| = 152 \times 2^{\mathcal{s}} - 12$. The edges of $\mathcal{PC}_a(\mathcal{s})$ is partitioned into the five subsets $E_1(\mathcal{PC}_a(\mathcal{s}))$, $E_2(\mathcal{PC}_a(\mathcal{s}))$, $E_3(\mathcal{PC}_a(\mathcal{s}))$, $E_4(\mathcal{PC}_a(\mathcal{s}\,))$ and $E_5(\mathcal{PC}_a(\mathcal{s}))$, where

$$E_1(\mathcal{PC}_a(\mathcal{s})) = \{j\ell \in E(\mathcal{PC}_a(\mathcal{s})) : d(j) = d(\ell) = 2\},$$
$$E_2(\mathcal{PC}_a(\mathcal{s})) = \{j\ell \in E(\mathcal{PC}_a(\mathcal{s})) : d(j) = 2, d(\ell) = 3\},$$
$$E_3(\mathcal{PC}_a(\mathcal{s})) = \{j\ell \in E(\mathcal{PC}_a(\mathcal{s})) : d(j) = 1, d(\ell) = 3\},$$
$$E_4(\mathcal{PC}_a(\mathcal{s})) = \{j\ell \in E(\mathcal{PC}_a(\mathcal{s})) : d(j) = d(\ell) = 3\},$$
$$E_5(\mathcal{PC}_a(\mathcal{s})) = \{j\ell \in E(\mathcal{PC}_a(\mathcal{s})) : d(j) = 3, d(\ell) = 4\}.$$

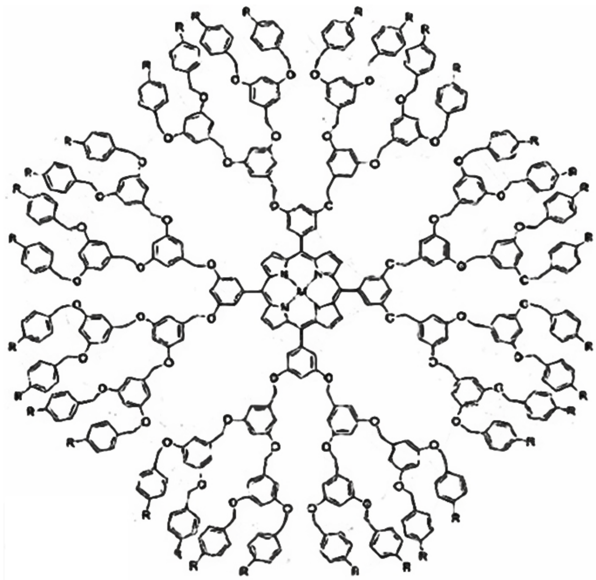

Figure 1
The molecular graph of $\mathcal{PC}_a(4)$ dendrimer.

It can be seen that, $|E_1(\mathcal{PC}_a(s))| = 2^{s+5} - 4$, $|E_2(\mathcal{PC}_a(s))| = 7 \times 2^{s+4} - 32$, $|E_3(\mathcal{PC}_a(s))| = 2^{s+3}$, $|E_4(\mathcal{PC}_a(s))| = 20$ and $|E_5(\mathcal{PC}_a(s))| = 4$.

Theorem 1: *The MmS index of $\mathcal{PC}_a(s)$ satisfies the following identity:*

$$MmS\big(\mathcal{PC}_a(s)\big) = 89 \times 2^{s+2} - \frac{440}{9}.$$

Proof: Applying the definition of the *MmS* index yields:

$$MmS\big(\mathcal{PC}_a(s)\big) = \sum_{j\ell \in E(\mathcal{PC}_a(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2$$

$$= \sum_{j\ell \in E_1(\mathcal{PC}_a(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2$$

$$+ \sum_{j\ell \in E_2(\mathcal{PC}_a(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2$$

$$+ \sum_{j\ell \in E_3(\mathcal{PC}_a(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2$$

$$+ \sum_{j\ell \in E_4(\mathcal{PC}_a(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2$$

$$+ \sum_{j\ell \in E_5(\mathcal{PC}_a(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2$$

$$= |E_1(\mathcal{PC}_a(s))| \left(\frac{2}{2}\right)^2 + |E_2(\mathcal{PC}_a(s))| \left(\frac{3}{2}\right)^2$$

$$+|E_3(\mathcal{PC}_a(\mathscr{s}))|\left(\frac{3}{1}\right)^2+|E_4(\mathcal{PC}_a(\mathscr{s}))|\left(\frac{3}{3}\right)^2$$
$$+|E_5(\mathcal{PC}_a(\mathscr{s}))|\left(\frac{4}{3}\right)^2$$
$$=(2^{\mathscr{s}+5}-4)(1)+(7\times 2^{\mathscr{s}+4}-32)\left(\frac{9}{4}\right)$$
$$+(2^{\mathscr{s}+3})(9)+(20)(1)+(4)\left(\frac{16}{9}\right)$$
$$=89\times 2^{\mathscr{s}+2}-\frac{440}{9}.$$

Theorem 2: *The MI index of $\mathcal{PC}_a(\mathscr{s})$ satisfies the following identity:*
$$MI\big(\mathcal{PC}_a(\mathscr{s})\big)=3\times 2^{\mathscr{s}+3}-5.$$

Proof: Based on the *MI* index definition,
$$MI\big(\mathcal{PC}_a(\mathscr{s})\big)=\sum_{j\ell\in E(\mathcal{PC}_a(\mathscr{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right|$$
$$=\sum_{j\ell\in E_1(\mathcal{PC}_a(\mathscr{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right|+\sum_{j\ell\in E_2(\mathcal{PC}_a(\mathscr{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right|$$
$$+\sum_{j\ell\in E_3(\mathcal{PC}_a(\mathscr{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right|+\sum_{j\ell\in E_4(\mathcal{PC}_a(\mathscr{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right|$$
$$+\sum_{j\ell\in E_5(\mathcal{PC}_a(\mathscr{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right|$$
$$=\big|E_1\big(\mathcal{PC}_a(\mathscr{s})\big)\big|\left|\frac{1}{2}-\frac{1}{2}\right|+\big|E_2\big(\mathcal{PC}_a(\mathscr{s})\big)\big|\left|\frac{1}{2}-\frac{1}{3}\right|$$
$$+\big|E_3\big(\mathcal{PC}_a(\mathscr{s})\big)\big|\left|\frac{1}{1}-\frac{1}{3}\right|+|E_4(\mathcal{PC}_a(\mathscr{s}))|\left|\frac{1}{3}-\frac{1}{3}\right|$$
$$+|E_5(\mathcal{PC}_a(\mathscr{s}))|\left|\frac{1}{4}-\frac{1}{3}\right|$$
$$=(2^{\mathscr{s}+5}-4)(0)+(7\times 2^{\mathscr{s}+4}-32)\left(\frac{1}{6}\right)$$
$$+(2^{\mathscr{s}+3})\left(\frac{2}{3}\right)+(20)(0)+(4)\left(\frac{1}{12}\right)$$
$$=3\times 2^{\mathscr{s}+3}-5.$$

Theorem 3: *The SDD index for the $\mathcal{PC}_a(\mathscr{s})$ dendrimer is expressed as*
$$SDD\big(\mathcal{PC}_a(\mathscr{s})\big)=\left(\frac{125}{3}\right)2^{\mathscr{s}+3}-\frac{87}{3}.$$

Proof: From the *SDD* index definition,
$$SDD\big(\mathcal{PC}_a(\mathscr{s})\big)=\sum_{j\ell\in E(\mathcal{PC}_a(\mathscr{s}))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$
$$=\sum_{j\ell\in E_1(\mathcal{PC}_a(\mathscr{s}))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$
$$+\sum_{j\ell\in E_2(\mathcal{PC}_a(\mathscr{s}))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$

$$+\sum_{j\ell\in E_3(\mathcal{PC}_a(s))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$
$$+\sum_{j\ell\in E_4(\mathcal{PC}_a(s))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$
$$+\sum_{j\ell\in E_5(\mathcal{PC}_a(s))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$
$$=\left|E_1\left(\mathcal{PC}_a(s)\right)\right|\left(\frac{2}{2}+\frac{2}{2}\right)$$
$$+\left|E_2\left(\mathcal{PC}_a(s)\right)\right|\left(\frac{3}{2}+\frac{2}{3}\right)+\left|E_3\left(\mathcal{PC}_a(s)\right)\right|\left(\frac{3}{1}+\frac{1}{3}\right)$$
$$+\left|E_4\left(\mathcal{PC}_a(s)\right)\right|\left(\frac{3}{3}+\frac{3}{3}\right)+\left|E_5(\mathcal{PC}_a(s))\right|\left(\frac{3}{4}+\frac{4}{3}\right)$$
$$=(2^{s+5}-4)(2)+(7\times 2^{s+4}-32)\left(\frac{13}{6}\right)$$
$$+(2^{s+3})\left(\frac{10}{3}\right)+(20)(2)+(4)\left(\frac{25}{12}\right)$$
$$=\left(\frac{125}{3}\right)2^{s+3}-\frac{87}{3}.$$

Theorem 4: *The VSE index of* $\mathcal{PC}_a(s)$ *is given by*

$$SEI_q\left(\mathcal{PC}_a(s)\right)=2^{s+3}q+(2^{s+6}+7\times 2^{n+4}-40)q^2$$
$$+(7\times 2^{s+4}+2^{n+3}+12)q^3+4q^4.$$

Proof: Using the definition of the *VSE* index,

$$SEI_q\left(\mathcal{PC}_a(s)\right)=\sum_{j\ell\in E(\mathcal{PC}_a(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$=\sum_{j\ell\in E_1(\mathcal{PC}_a(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$+\sum_{j\ell\in E_2(\mathcal{PC}_a(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$+\sum_{j\ell\in E_3(\mathcal{PC}_a(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$+\sum_{j\ell\in E_4(\mathcal{PC}_a(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$+\sum_{j\ell\in E_5(\mathcal{PC}_a(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$=\left|E_1\left(\mathcal{PC}_a(s)\right)\right|(q^2+q^2)+\left|E_2\left(\mathcal{PC}_a(s)\right)\right|(q^2+q^3)$$
$$+\left|E_3\left(\mathcal{PC}_a(s)\right)\right|(q^1+q^3)+\left|E_4\left(\mathcal{PC}_a(s)\right)\right|(q^3+q^3)$$
$$+\left|E_5(\mathcal{PC}_a(s))\right|(q^3+q^4)$$
$$=(2^{s+5}-4)(2q^2)+(7\times 2^{s+4}-32)(q^2+q^3)$$
$$+(2^{s+3})(q^1+q^3)+(20)(2q^3)+(4)(q^3+q^4)$$
$$=2^{s+3}q+(2^{s+6}+7\times 2^{s+4}-40)q^2$$
$$+(7\times 2^{s+4}+2^{s+3}+12)q^3+4q^4.$$

3.2 $\mathcal{PC}_{\ell}(s)$ *dendrimer*

Let $\mathcal{PC}_{\ell}(s)$ stand for the molecular graph of the second $\mathcal{PC}$ dendrimer in such a way that s represents the steps of growth (see Figure 2). Manifestly, $|V(\mathcal{PC}_{\ell}(s))| = 256 \times 2^{s} - 63$ and $|E(\mathcal{PC}_{\ell}(s))| = 288 \times 2^{s} - 68$. The edges of $\mathcal{PC}_{\ell}(s)$ is partitioned into the five subsets $E_1(\mathcal{PC}_{\ell}(s))$, $E_2(\mathcal{PC}_{\ell}(s))$, $E_3(\mathcal{PC}_{\ell}(s))$, $E_4(\mathcal{PC}_{\ell}(s))$ and $E_5(\mathcal{PC}_{\ell}(s))$, where

$E_1(\mathcal{PC}_{\ell}(s)) = \{j\ell \in E(\mathcal{PC}_{\ell}(s)) : d(j) = d(\ell) = 2\}$,

$E_2(\mathcal{PC}_{\ell}(s)) = \{j\ell \in E(\mathcal{PC}_{\ell}(s)) : d(j) = 2, d(\ell) = 3\}$,

$E_3(\mathcal{PC}_{\ell}(s)) = \{j\ell \in E(\mathcal{PC}_{\ell}(s)) : d(j) = 1, d(\ell) = 3\}$,

$E_4(\mathcal{PC}_{\ell}(s)) = \{j\ell \in E(\mathcal{PC}_{\ell}(s)) : d(j) = d(\ell) = 3\}$,

$E_5(\mathcal{PC}_{\ell}(s)) = \{j\ell \in E(\mathcal{PC}_{\ell}(s)) : d(j) = 3, d(\ell) = 4\}$.

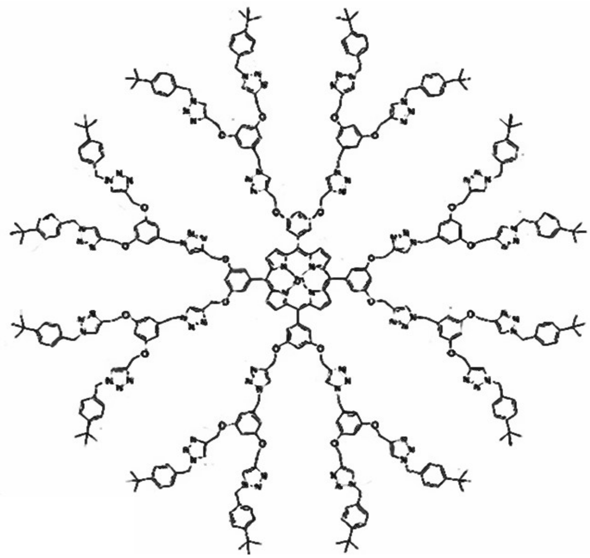

Figure 2

The molecular graph of $\mathcal{PC}_{\ell}(2)$ dendrimer.

It can be seen that, $|E_1(\mathcal{PC}_{\ell}(s))| = 3 \times 2^{s+4} - 12$, $|E_2(\mathcal{PC}_{\ell}(s))| = 13 \times 2^{s+4} - 80$, $|E_3(\mathcal{PC}_{\ell}(s))| = 3 \times 2^{s+3}$, $|E_4(\mathcal{PC}_{\ell}(s))| = 2^{s+3} + 20$ and $|E_5(\mathcal{PC}_{\ell}(s))| = 4$.

Theorem 5: *The MmS index of $\mathcal{PC}_{\ell}(s)$ is given by*

$$MmS(\mathcal{PC}_{\ell}(s)) = 185 \times 2^{s+2} - \frac{1484}{9}.$$

Proof: Using the *MmS* index definition,

$$MmS(\mathcal{PC}_{\ell}(s)) = \sum_{j\ell \in E(\mathcal{PC}_{\ell}(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2$$

$$= \sum_{j\ell \in E_1(\mathcal{PC}_{\ell}(s))} \left(\frac{max\{d_j,d_\ell\}}{min\{d_j,d_\ell\}}\right)^2$$
$$+ \sum_{j\ell \in E_2(\mathcal{PC}_{\ell}(s))} \left(\frac{max\{d_j,d_\ell\}}{min\{d_j,d_\ell\}}\right)^2$$
$$+ \sum_{j\ell \in E_3(\mathcal{PC}_{\ell}(s))} \left(\frac{max\{d_j,d_\ell\}}{min\{d_j,d_\ell\}}\right)^2$$
$$+ \sum_{j\ell \in E_4(\mathcal{PC}_{\ell}(s))} \left(\frac{max\{d_j,d_\ell\}}{min\{d_j,d_\ell\}}\right)^2$$
$$+ \sum_{j\ell \in E_5(\mathcal{PC}_{\ell}(s))} \left(\frac{max\{d_j,d_\ell\}}{min\{d_j,d_\ell\}}\right)^2$$
$$= |E_1(\mathcal{PC}_{\ell}(s))| \left(\frac{2}{2}\right)^2 + |E_2(\mathcal{PC}_{\ell}(s))| \left(\frac{3}{2}\right)^2$$
$$+|E_3(\mathcal{PC}_{\ell}(s))| \left(\frac{3}{1}\right)^2 + |E_4(\mathcal{PC}_{\ell}(s))| \left(\frac{3}{3}\right)^2$$
$$+|E_5(\mathcal{PC}_{\ell}(s))| \left(\frac{4}{3}\right)^2$$
$$= (3 \times 2^{s+4} - 12)(1) + (13 \times 2^{s+4} - 80)\left(\frac{9}{4}\right)$$
$$+(3 \times 2^{s+3})(9) + (2^{s+3} + 20)(1) + (4)\left(\frac{16}{9}\right)$$
$$= 185 \times 2^{s+2} - \frac{1484}{9}.$$

Theorem 6: *The MI index of $\mathcal{PC}_{\ell}(s)$ is given by*

$$MI(\mathcal{PC}_{\ell}(s)) = \left(\frac{19}{3}\right) \times 2^{s+3} - 13.$$

Proof: The definition of the *MI* index yields,

$$MI(G) = \sum_{j\ell \in E(\mathcal{PC}_{\ell}(s))} \left|\frac{1}{d_j} - \frac{1}{d_\ell}\right|$$
$$= \sum_{j\ell \in E_1(\mathcal{PC}_{\ell}(s))} \left|\frac{1}{d_j} - \frac{1}{d_\ell}\right| + \sum_{j\ell \in E_2(\mathcal{PC}_{\ell}(s))} \left|\frac{1}{d_j} - \frac{1}{d_\ell}\right|$$
$$+ \sum_{j\ell \in E_3(\mathcal{PC}_{\ell}(s))} \left|\frac{1}{d_j} - \frac{1}{d_\ell}\right| + \sum_{j\ell \in E_4(\mathcal{PC}_{\ell}(s))} \left|\frac{1}{d_j} - \frac{1}{d_\ell}\right|$$
$$+ \sum_{j\ell \in E_5(\mathcal{PC}_{\ell}(s))} \left|\frac{1}{d_j} - \frac{1}{d_\ell}\right|$$
$$= |E_1(\mathcal{PC}_{\ell}(s))| \left|\frac{1}{2} - \frac{1}{2}\right| + |E_2(\mathcal{PC}_{\ell}(s))| \left|\frac{1}{2} - \frac{1}{3}\right|$$
$$+|E_3(\mathcal{PC}_{\ell}(s))| \left|\frac{1}{1} - \frac{1}{3}\right| + |E_4(\mathcal{PC}_{\ell}(s))| \left|\frac{1}{3} - \frac{1}{3}\right|$$
$$+|E_5(\mathcal{PC}_{\ell}(s))| \left|\frac{1}{4} - \frac{1}{3}\right|$$
$$= (3 \times 2^{s+4} - 12)(0) + (13 \times 2^{s+4} - 80)\left(\frac{1}{6}\right)$$

$$+(3 \times 2^{\mathscr{s}+3})\left(\frac{2}{3}\right) + (2^{\mathscr{s}+3} + 20)(0) + (4)\left(\frac{1}{12}\right)$$
$$= \left(\frac{19}{3}\right) \times 2^{\mathscr{s}+3} - 13.$$

Theorem 7: *The SDD index of $\mathcal{PC}_{\mathscr{b}}(\mathscr{s})$ satisfies that following equality:*

$$SDD(\mathcal{PC}_{\mathscr{b}}(\mathscr{s})) = \left(\frac{241}{3}\right) 2^{\mathscr{s}+3} - 149.$$

Proof: Based on the *SDD* index's definition,

$$SDD(\mathcal{PC}_{\mathscr{b}}(\mathscr{s})) = \sum_{j\ell \in E(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))} \left(\frac{d_j}{d_\ell} + \frac{d_\ell}{d_j}\right)$$
$$= \sum_{j\ell \in E_1(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))} \left(\frac{d_j}{d_\ell} + \frac{d_\ell}{d_j}\right)$$
$$+ \sum_{j\ell \in E_2(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))} \left(\frac{d_j}{d_\ell} + \frac{d_\ell}{d_j}\right)$$
$$+ \sum_{j\ell \in E_3(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))} \left(\frac{d_j}{d_\ell} + \frac{d_\ell}{d_j}\right)$$
$$+ \sum_{j\ell \in E_4(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))} \left(\frac{d_j}{d_\ell} + \frac{d_\ell}{d_j}\right)$$
$$+ \sum_{j\ell \in E_5(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))} \left(\frac{d_j}{d_\ell} + \frac{d_\ell}{d_j}\right)$$
$$= |E_1(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))|\left(\frac{2}{2} + \frac{2}{2}\right) + |E_2(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))|\left(\frac{3}{2} + \frac{2}{3}\right)$$
$$+|E_3(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))|\left(\frac{3}{1} + \frac{1}{3}\right) + |E_4(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))|\left(\frac{3}{3} + \frac{3}{3}\right)$$
$$+|E_5(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))|\left(\frac{3}{4} + \frac{4}{3}\right)$$
$$= (3 \times 2^{\mathscr{s}+4} - 12)(2) + (13 \times 2^{\mathscr{s}+4} - 80)\left(\frac{13}{6}\right)$$
$$+(3 \times 2^{\mathscr{s}+3})\left(\frac{10}{3}\right) + (2^{\mathscr{s}+3} + 20)(2) + (4)\left(\frac{25}{12}\right)$$
$$= \left(\frac{241}{3}\right) 2^{\mathscr{s}+3} - 149.$$

Theorem 8: *The VSE index of $\mathcal{PC}_{\mathscr{b}}(\mathscr{s})$ is given by*

$$SEI_{q}(\mathcal{PC}_{\mathscr{b}}(\mathscr{s})) = 3 \times 2^{\mathscr{s}+3} q + (3 \times 2^{\mathscr{s}+5} + 13 \times 2^{\mathscr{s}+4} - 104) q^2$$
$$+(14 \times 2^{\mathscr{s}+4} + 3 \times 2^{n+3} - 36) q^3 + 4 q^4.$$

Proof: Using the definition of the *VSE* index,

$$SEI_{q}(\mathcal{PC}_{\mathscr{b}}(\mathscr{s})) = \sum_{j\ell \in E(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))} (q^{d_j} + q^{d_\ell})$$
$$= \sum_{j\ell \in E_1(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))} (q^{d_j} + q^{d_\ell})$$
$$+ \sum_{j\ell \in E_2(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))} (q^{d_j} + q^{d_\ell})$$
$$+ \sum_{j\ell \in E_3(\mathcal{PC}_{\mathscr{b}}(\mathscr{s}))} (q^{d_j} + q^{d_\ell})$$

$$+\sum_{j\ell\in E_4(\mathcal{PC}_b(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$+\sum_{j\ell\in E_5(\mathcal{PC}_b(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$=|E_1(\mathcal{PC}_b(s))|(q^2+q^2)+\left|E_2\left(\mathcal{PC}_b(s)\right)\right|(q^2+q^3)$$
$$+|E_3(\mathcal{PC}_b(s))|(q^1+q^3)+|E_4(\mathcal{PC}_b(s))|(q^3+q^3)$$
$$+|E_5(\mathcal{PC}_b(s))|(q^3+q^4)$$
$$=(3\times 2^{s+4}-12)(2q^2)+(13\times 2^{s+4}-80)(q^2+q^3)$$
$$+(3\times 2^{s+3})(q^1+q^3)+(2^{n+3}+20)(2q^3)$$
$$+4(q^3+q^4)$$
$$=3\times 2^{s+3}q+(3\times 2^{s+5}+13\times 2^{s+4}-104)q^2$$
$$+(14\times 2^{s+4}+3\times 2^{s+3}-36)q^3+4q^4.$$

3.3 $\mathcal{PC}_c(s)$ *dendrimer*

Let $\mathcal{PC}_c(s)$ stand for the molecular graph of the third $\mathcal{PC}$ dendrimer (also referred to as Proteo-dendrimers) in such a way that s represent the steps of growth (see Figure 3). Manifestly, $|V(\mathcal{PC}_c(s))|=154\times 2^s-62$ and $|E(\mathcal{PC}_c(s))|=168\times 2^s$. The edges of $\mathcal{PC}_c(s)$ is partitioned into the six subsets $E_1(\mathcal{PC}_c(s))$, $E_2(\mathcal{PC}_c(s))$, $E_3(\mathcal{PC}_c(s))$, $E_4(\mathcal{PC}_c(s)\,)$, $E_5(\mathcal{PC}_c(s)\,)$ and $E_6(\mathcal{PC}_c(s))$, where

$$E_1(\mathcal{PC}_c(s))=\{j\ell\in E(\mathcal{PC}_c(s)):d(j)=1,d(\ell)=2\},$$
$$E_2(\mathcal{PC}_c(s))=\{j\ell\in E(\mathcal{PC}_c(s)):d(j)=d(\ell)=2\},$$
$$E_3(\mathcal{PC}_c(s))=\{j\ell\in E(\mathcal{PC}_c(s)):d(j)=2,d(\ell)=3\},$$
$$E_4(\mathcal{PC}_c(s))=\{j\ell\in E(\mathcal{PC}_c(s)):d(j)=1,d(\ell)=3\},$$

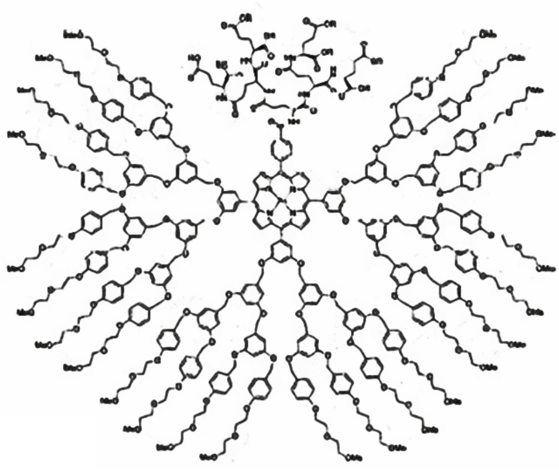

Figure 3
The molecular graph of $\mathcal{PC}_c(s)$ dendrimer.

$$E_5(\mathcal{PC}_c(s)) = \{j\ell \in E(\mathcal{PC}_c(s)) : d(j) = d(\ell) = 3\},$$
$$E_6(\mathcal{PC}_c(s)) = \{j\ell \in E(\mathcal{PC}_c(s)) : d(j) = 3, d(\ell) = 4\}.$$

It can be seen that, $|E_1(\mathcal{PC}_c(s))| = 3 \times 2^{s+1}$, $|E_2(\mathcal{PC}_c(s))| = 7 \times 2^{s+3} - 1$, $|E_3(\mathcal{PC}_c(s))| = 49 \times 2^{s+1} - 22$, $|E_4(\mathcal{PC}_c(s))| = 3 \times 2^{s+1} - 1$, $|E_5(\mathcal{PC}_c(s))| = 2^{s+1} + 20$ and $|E_6(\mathcal{PC}_c(s))| = 4$.

Theorem 9: *The MmS index of $\mathcal{PC}_c(s)$ is given by*

$$MmS(\mathcal{PC}_c(s)) = 713 \times 2^{s-1} - \frac{583}{18}.$$

Proof: Using the definition of the *MmS* index,

$$\begin{aligned}
Mms(\mathcal{PC}_c(s)) &= \sum_{j\ell \in E(\mathcal{PC}_c(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2 \\
&= \sum_{j\ell \in E_1(\mathcal{PC}_c(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2 \\
&+ \sum_{j\ell \in E_2(\mathcal{PC}_c(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2 \\
&+ \sum_{j\ell \in E_3(\mathcal{PC}_c(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2 \\
&+ \sum_{j\ell \in E_4(\mathcal{PC}_c(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2 \\
&+ \sum_{j\ell \in E_5(\mathcal{PC}_c(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2 \\
&+ \sum_{j\ell \in E_6(\mathcal{PC}_c(s))} \left(\frac{max\{d_j, d_\ell\}}{min\{d_j, d_\ell\}}\right)^2 \\
&= |E_1(\mathcal{PC}_c(s))| \left(\frac{2}{1}\right)^2 + |E_2(\mathcal{PC}_c(s))| \left(\frac{2}{2}\right)^2 \\
&+ |E_3(\mathcal{PC}_c(s))| \left(\frac{3}{2}\right)^2 + |E_4(\mathcal{PC}_c(s))| \left(\frac{3}{1}\right)^2 \\
&+ |E_5(\mathcal{PC}_c(s))| + |E_6(\mathcal{PC}_c(s))| \left(\frac{4}{3}\right)^2 \\
&= (3 \times 2^{s+1})(4) + (7 \times 2^{s+3} - 1)(1) \\
&+ (49 \times 2^{s+1} - 22)\left(\frac{9}{4}\right) + (3 \times 2^{s+1} - 1)(9) \\
&+ (2^{s+1} + 20)(1) + (4)\left(\frac{16}{9}\right) \\
&= 713 \times 2^{s-1} - \frac{583}{18}.
\end{aligned}$$

Theorem 10: *The MI index of $\mathcal{PC}_c(s)$ is given by*

$$MI(\mathcal{PC}_c(s)) = \left(\frac{35}{3}\right) \times 2^{n+1} - 4.$$

Proof: By definition of the *MI* index,

$$MI(\mathcal{PC}_c(\mathcal{s})) = \sum_{j\ell\in E(\mathcal{PC}_c(\mathcal{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right|$$

$$= \sum_{j\ell\in E_1(\mathcal{PC}_c(\mathcal{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right| + \sum_{j\ell\in E_2(\mathcal{PC}_c(\mathcal{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right|$$

$$+ \sum_{j\ell\in E_3(\mathcal{PC}_c(\mathcal{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right| + \sum_{j\ell\in E_4(\mathcal{PC}_c(\mathcal{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right|$$

$$+ \sum_{j\ell\in E_5(\mathcal{PC}_c(\mathcal{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right|$$

$$+ \sum_{j\ell\in E_6(\mathcal{PC}_c(\mathcal{s}))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right|$$

$$= \left|E_1(\mathcal{PC}_c(\mathcal{s}))\right|\left|\frac{1}{1}-\frac{1}{2}\right| + \left|E_2(\mathcal{PC}_c(\mathcal{s}))\right|\left|\frac{1}{2}-\frac{1}{2}\right|$$

$$+\left|E_3(\mathcal{PC}_c(\mathcal{s}))\right|\left|\frac{1}{2}-\frac{1}{3}\right| + |E_4(\mathcal{PC}_c(\mathcal{s}))|\left|\frac{1}{1}-\frac{1}{3}\right|$$

$$+|E_5(\mathcal{PC}_c(\mathcal{s}))|\left|\frac{1}{3}-\frac{1}{3}\right| + |E_6(\mathcal{PC}_c(\mathcal{s}))|\left|\frac{1}{4}-\frac{1}{3}\right|$$

$$= (3\times 2^{n+1})\left(\frac{1}{2}\right) + (7\times 2^{n+3}-1)(0)$$

$$+(49\times 2^{n+1}-22)\left(\frac{1}{6}\right) + (3\times 2^{n+1}-1)\left(\frac{2}{3}\right)$$

$$+(2^{n+1}+20)(0) + (4)\left(\frac{1}{12}\right)$$

$$= \left(\frac{35}{3}\right)\times 2^{n+1} - 4.$$

Theorem 11: *The SDD index of $\mathcal{PC}_c(\mathcal{s})$ satisfies the following identity:*

$$SDD(\mathcal{PC}_c(\mathcal{s})) = \left(\frac{545}{3}\right)2^{\mathcal{s}+1} - \frac{14}{3}.$$

Proof: Application of the *SDD* index yields,

$$SDD(\mathcal{PC}_c(\mathcal{s})) = \sum_{j\ell\in E(\mathcal{PC}_c(\mathcal{s}))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$

$$= \sum_{j\ell\in E_1(\mathcal{PC}_c(\mathcal{s}))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$

$$+ \sum_{j\ell\in E_2(\mathcal{PC}_c(\mathcal{s}))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$

$$+ \sum_{j\ell\in E_3(\mathcal{PC}_c(\mathcal{s}))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$

$$+ \sum_{j\ell\in E_4(\mathcal{PC}_c(\mathcal{s}))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$

$$+ \sum_{j\ell\in E_5(\mathcal{PC}_c(\mathcal{s}))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$

$$+ \sum_{j\ell\in E_6(\mathcal{PC}_c(\mathcal{s}))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$

$$= \left|E_1\left(\mathcal{PC}_c(s)\right)\right|\left(\frac{1}{2}+\frac{2}{1}\right)+\left|E_2\left(\mathcal{PC}_c(s)\right)\right|\left(\frac{2}{2}+\frac{2}{2}\right)$$
$$+\left|E_3\left(\mathcal{PC}_c(s)\right)\right|\left(\frac{3}{2}+\frac{2}{3}\right)+|E_4(\mathcal{PC}_c(s))|\left(\frac{3}{1}+\frac{1}{3}\right)$$
$$+|E_5(\mathcal{PC}_c(s))|\left(\frac{3}{3}+\frac{3}{3}\right)+|E_6(\mathcal{PC}_c(s))|\left(\frac{3}{4}+\frac{4}{3}\right)$$
$$=(3\times 2^{s+1})\left(\frac{5}{2}\right)+(7\times 2^{s+3}-1)(2)$$
$$+(49\times 2^{s+1}-22)\left(\frac{13}{6}\right)+(3\times 2^{s+1}-1)\left(\frac{10}{3}\right)$$
$$+(2^{s+1}+20)(2)+(4)\left(\frac{25}{12}\right)$$
$$=\left(\frac{545}{3}\right)2^{s+1}-\frac{14}{3}.$$

Theorem 12: *The VSE index of $\mathcal{PC}_c(s)$ is given by*

$$SEI_q(\mathcal{PC}_c(s)) = (49\times 2^{s+1}-22)q$$
$$+(7\times 2^{s+3}+3\times 2^{s+2}-1)q^2$$
$$+(7\times 2^{s+3}+3\times 2^{s+2}+50\times 2^{s+1}-1)q^3$$
$$+(2^{s+1}+4)q^4.$$

Proof: Using the definition of the *VSE* index,

$$SEI_q(\mathcal{PC}_c(s)) = \sum_{j\ell\in E(\mathcal{PC}_c(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$=\sum_{j\ell\in E_1(\mathcal{PC}_c(s))} q^{d_j}+q^{d_\ell}$$
$$+\sum_{j\ell\in E_2(\mathcal{PC}_c(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$+\sum_{j\ell\in E_3(\mathcal{PC}_c(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$+\sum_{j\ell\in E_4(\mathcal{PC}_c(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$+\sum_{j\ell\in E_5(\mathcal{PC}_c(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$+\sum_{j\ell\in E_6(\mathcal{PC}_c(s))}\left(q^{d_j}+q^{d_\ell}\right)$$
$$=\left|E_1\left(\mathcal{PC}_c(s)\right)\right|(q^1+q^2)+\left|E_2\left(\mathcal{PC}_c(s)\right)\right|(q^2+q^2)$$
$$+\left|E_3\left(\mathcal{PC}_c(s)\right)\right|(q^1+q^3)+|E_4(\mathcal{PC}_c(s))|(q^2+q^3)$$
$$+|E_5(\mathcal{PC}_c(s))|(q^3+q^3)+|E_6(\mathcal{PC}_c(s))|(q^3+q^4)$$
$$=(3\times 2^{s+1})(2q^2)+(7\times 2^{s+3}-1)(q^2+q^3)$$
$$+(49\times 2^{s+1}-22)(q^1+q^3)+(3\times 2^{s+1}-1)(2q^3)$$
$$+(2^{s+1}+20)(q^3+q^4)+4(q^3+q^4)$$
$$=(49\times 2^{s+1}-22)q$$
$$+(7\times 2^{s+3}+3\times 2^{s+2}-1)q^2$$
$$+(7\times 2^{s+3}+3\times 2^{s+2}+50\times 2^{s+1}-1)q^3$$
$$+(2^{s+1}+4)q^4.$$

3.4 $\mathcal{PC}_d(s)$ *Dendrimer*

Let $\mathcal{PC}_d(s)$ stand for the chemical graph of the fourth $\mathcal{PC}$ dendrimer (also known as dendritic iron (II) porphyrin) in such a way that s represents the steps of growth (see Figure 4). Manifestly, $|V(\mathcal{PC}_d(s))| = 154 \times 2^s - 62$ and $|E(\mathcal{PC}_d(s))| = 168 \times 2^s$. The edges of $\mathcal{PC}_d(s)$ is partitioned into the six subsets $E_1(\mathcal{PC}_d(s))$, $E_2(\mathcal{PC}_d(s))$, $E_3(\mathcal{PC}_d(s))$, $E_4(\mathcal{PC}_d(s))$, $E_5(\mathcal{PC}_d(s))$ and $E_6(\mathcal{PC}_d(s))$, where

$$E_1(\mathcal{PC}_d(s)) = \{j\ell \in E(\mathcal{PC}_d(s)): d(j) = 1, d(\ell) = 2\},$$
$$E_2(\mathcal{PC}_d(s)) = \{j\ell \in E(\mathcal{PC}_d(s)): d(j) = d(\ell) = 2\},$$
$$E_3(\mathcal{PC}_d(s)) = \{j\ell \in E(\mathcal{PC}_d(s)): d(j) = 2, d(\ell) = 3\},$$
$$E_4(\mathcal{PC}_d(s)) = \{j\ell \in E(\mathcal{PC}_d(s)): d(j) = 1, d(\ell) = 3\},$$
$$E_5(\mathcal{PC}_d(s)) = \{j\ell \in E(\mathcal{PC}_d(s)): d(j) = d(\ell) = 3\},$$
$$E_6(\mathcal{PC}_d(s)) = \{j\ell \in E(\mathcal{PC}_d(s)): d(j) = 3, d(\ell) = 4\}.$$

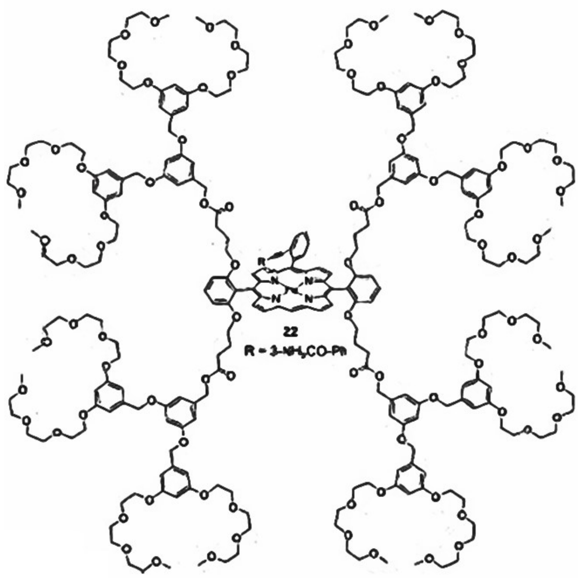

Figure 4
The chemical graph of $\mathcal{PC}_d(1)$.

It can be seen that, $|E_1(\mathcal{PC}_d(s))| = 2^{s+3}$, $|E_2(\mathcal{PC}_d(s))| = 23 \times 2^{s+2} - 5$, $|E_3(\mathcal{PC}_d(s))| = 5 \times 2^{s+4} - 28$, $|E_4(\mathcal{PC}_d(s))| = 2^{s+2} - 3$, $|E_5(\mathcal{PC}_d(s))| = 22$ and $|E_6(\mathcal{PC}_d(s))| = 8$.

Theorem 13: *The MmS index of $\mathcal{PC}_d(s)$ is given by*

$$MmS(\mathcal{PC}_d(s)) = 85 \times 2^{s+2} - \frac{529}{9}.$$

Proof: Using the definition of the *MmS* index,

$$Mms(\mathcal{PC}_d(\mathcal{s})) = \sum_{j\ell\in E(\mathcal{PC}_d(\mathcal{s}))}\left(\frac{max\{d_j,d_\ell\}}{min\{d_j,d_\ell\}}\right)^2$$

$$= \sum_{j\ell\in E_1(\mathcal{PC}_d(\mathcal{s}))}\left(\frac{max\{d_j,d_\ell\}}{min\{d_j,d_\ell\}}\right)^2$$

$$+\sum_{j\ell\in E_2(\mathcal{PC}_d(\mathcal{s}))}\left(\frac{max\{d_j,d_\ell\}}{min\{d_j,d_\ell\}}\right)^2$$

$$+\sum_{j\ell\in E_3(\mathcal{PC}_d(\mathcal{s}))}\left(\frac{max\{d_j,d_\ell\}}{min\{d_j,d_\ell\}}\right)^2$$

$$+\sum_{j\ell\in E_4(\mathcal{PC}_d(\mathcal{s}))}\left(\frac{max\{d_j,d_\ell\}}{min\{d_j,d_\ell\}}\right)^2$$

$$+\sum_{j\ell\in E_5(\mathcal{PC}_d(\mathcal{s}))}\left(\frac{max\{d_j,d_\ell\}}{min\{d_j,d_\ell\}}\right)^2$$

$$+\sum_{j\ell\in E_6(\mathcal{PC}_d(\mathcal{s}))}\left(\frac{max\{d_j,d_\ell\}}{min\{d_j,d_\ell\}}\right)^2$$

$$= |E_1(\mathcal{PC}_d(\mathcal{s}))|\left(\frac{2}{1}\right)^2 + |E_2(\mathcal{PC}_d(\mathcal{s}))|\left(\frac{2}{2}\right)^2$$

$$+|E_3(\mathcal{PC}_d(\mathcal{s}))|\left(\frac{3}{2}\right)^2 + |E_4(\mathcal{PC}_d(\mathcal{s}))|\left(\frac{3}{1}\right)^2$$

$$+|E_5(\mathcal{PC}_d(\mathcal{s}))|\left(\frac{3}{3}\right)^2 + |E_6(\mathcal{PC}_d(\mathcal{s}))|\left(\frac{4}{3}\right)^2$$

$$= (2^{\mathcal{s}+3})(4) + (23\times 2^{\mathcal{s}+2} - 5)(1)$$

$$+(5\times 2^{\mathcal{s}+4} - 28)\left(\frac{9}{4}\right) + (2^{\mathcal{s}+2} - 3)(9)$$

$$+(22)(1) + (8)\left(\frac{16}{9}\right)$$

$$= 85\times 2^{\mathcal{s}+2} - \frac{529}{9}.$$

Theorem 14: *The MI index of $\mathcal{PC}_d(\mathcal{s})$ is given by*

$$MI(\mathcal{PC}_d(\mathcal{s})) = 5\times 2^{\mathcal{s}+2} - 6.$$

Proof: Based on the *MI* index definition,

$$MI(\mathcal{PC}_d(\mathcal{s})) = \sum_{j\ell\in E(\mathcal{PC}_d(\mathcal{s}))}\left|\frac{1}{d_j} - \frac{1}{d_\ell}\right|$$

$$= \sum_{j\ell\in E_1(\mathcal{PC}_d(\mathcal{s}))}\left|\frac{1}{d_j} - \frac{1}{d_\ell}\right| + \sum_{j\ell\in E_2(\mathcal{PC}_d(\mathcal{s}))}\left|\frac{1}{d_j} - \frac{1}{d_\ell}\right|$$

$$+\sum_{j\ell\in E_3(\mathcal{PC}_d(\mathcal{s}))}\left|\frac{1}{d_j} - \frac{1}{d_\ell}\right| + \sum_{j\ell\in E_4(\mathcal{PC}_d(\mathcal{s}))}\left|\frac{1}{d_j} - \frac{1}{d_\ell}\right|$$

$$+\sum_{j\ell\in E_5(\mathcal{PC}_d(\mathcal{s}))}\left|\frac{1}{d_j} - \frac{1}{d_\ell}\right|$$

$$+\sum_{j\ell\in E_6(\mathcal{PC}_d(s))}\left|\frac{1}{d_j}-\frac{1}{d_\ell}\right|$$
$$=\left|E_1(\mathcal{PC}_d(s))\right|\left|\frac{1}{1}-\frac{1}{2}\right|+\left|E_2(\mathcal{PC}_d(s))\right|\left|\frac{1}{2}-\frac{1}{2}\right|$$
$$+\left|E_3(\mathcal{PC}_d(s))\right|\left|\frac{1}{2}-\frac{1}{3}\right|+\left|E_4(\mathcal{PC}_d(s))\right|\left|\frac{1}{1}-\frac{1}{3}\right|$$
$$+\left|E_5(\mathcal{PC}_d(s))\right|\left|\frac{1}{3}-\frac{1}{3}\right|+\left|E_6(\mathcal{PC}_d(s))\right|\left|\frac{1}{4}-\frac{1}{3}\right|$$
$$=(2^{s+3})\left(\frac{1}{2}\right)+(23\times 2^{s+2}-5)(0)$$
$$+(5\times 2^{s+4}-28)\left(\frac{1}{6}\right)+(2^{s+2}-3)\left(\frac{2}{3}\right)$$
$$+(22)(0)+(8)\left(\frac{1}{12}\right)$$
$$=5\times 2^{s+2}-6.$$

Theorem 15: *The SDD index of $\mathcal{PC}_d(s)$ satisfies the following identity:*
$$SDD(\mathcal{PC}_d(s))=\left(\frac{293}{3}\right)2^{s+2}-20.$$

Proof: Applying the definition of the *SDD* index, we obtain
$$SDD(\mathcal{PC}_d(s))=\sum_{j\ell\in E(\mathcal{PC}_d(s))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$
$$=\sum_{j\ell\in E_1(\mathcal{PC}_d(s))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$
$$+\sum_{j\ell\in E_2(\mathcal{PC}_d(s))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$
$$+\sum_{j\ell\in E_3(\mathcal{PC}_d(s))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$
$$+\sum_{j\ell\in E_4(\mathcal{PC}_d(s))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$
$$+\sum_{j\ell\in E_5(\mathcal{PC}_d(s))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$
$$+\sum_{j\ell\in E_6(\mathcal{PC}_d(s))}\left(\frac{d_j}{d_\ell}+\frac{d_\ell}{d_j}\right)$$
$$=\left|E_1(\mathcal{PC}_d(s))\right|\left(\frac{1}{2}+\frac{2}{1}\right)+\left|E_2(\mathcal{PC}_d(s))\right|\left(\frac{2}{2}+\frac{2}{2}\right)$$
$$+\left|E_3(\mathcal{PC}_d(s))\right|\left(\frac{3}{2}+\frac{2}{3}\right)+\left|E_4(\mathcal{PC}_d(s))\right|\left(\frac{3}{1}+\frac{1}{3}\right)$$
$$+\left|E_5(\mathcal{PC}_d(s))\right|\left(\frac{3}{3}+\frac{3}{3}\right)+\left|E_6(\mathcal{PC}_d(s))\right|\left(\frac{3}{4}+\frac{4}{3}\right)$$
$$=(2^{s+3})\left(\frac{5}{2}\right)+(23\times 2^{s+2}-5)(2)$$
$$+(5\times 2^{s+4}-28)\left(\frac{13}{6}\right)+(2^{s+2}-3)\left(\frac{10}{3}\right)$$
$$+(22)(2)+(8)\left(\frac{25}{12}\right)$$
$$=\left(\frac{293}{3}\right)2^{s+2}-20.$$

Theorem 16: *The VSE index of $\mathcal{PC}_d(s)$ is given by*

$$SEI_q(\mathcal{PC}_d(s)) = (2^{s+3} + 2^{n+2} - 3)q + (17 \times 2^{s+4} - 38)q^2$$
$$+(5 \times 2^{s+4} + 2^{s+2} + 21)q^3 + 8q^4.$$

Proof: Using the definition of the *VSE* index,

$$SEI_q(\mathcal{PC}_d(s)) = \sum_{j\ell \in E(\mathcal{PC}_d(s))}(q^{d_j} + q^{d_\ell})$$
$$= \sum_{j\ell \in E_1(\mathcal{PC}_d(s))}(q^{d_j} + q^{d_\ell})$$
$$+\sum_{j\ell \in E_2(\mathcal{PC}_d(s))}(q^{d_j} + q^{d_\ell})$$
$$+\sum_{j\ell \in E_3(\mathcal{PC}_d(s))}(q^{d_j} + q^{d_\ell})$$
$$+\sum_{j\ell \in E_4(\mathcal{PC}_d(s))}(q^{d_j} + q^{d_\ell})$$
$$+\sum_{j\ell \in E_5(\mathcal{PC}_d(s))}(q^{d_j} + q^{d_\ell})$$
$$+\sum_{j\ell \in E_6(\mathcal{PC}_d(s))}(q^{d_j} + q^{d_\ell})$$
$$= |E_1(\mathcal{PC}_d(s))|(q^1 + q^2) + |E_2(\mathcal{PC}_d(s))|(q^2 + q^2)$$
$$+|E_3(\mathcal{PC}_d(s))|(q^2 + q^3) + |E_4(\mathcal{PC}_d(s))|(q^1 + q^3)$$
$$+|E_5(\mathcal{PC}_d(s))|(q^3 + q^3) + |E_6(\mathcal{PC}_d(s))|(q^3 + q^4)$$
$$= (2^{s+3})(q^1 + q^2) + (23 \times 2^{s+2} - 5)(q^2 + q^2)$$
$$+(5 \times 2^{s+4} - 28)(q^2 + q^3)$$
$$+(2^{s+2} - 3)(q^1 + q^3) + 22(q^3 + q^3)$$
$$+8(q^3 + q^4)$$
$$= (2^{s+3} + 2^{s+2} - 3)q + (17 \times 2^{s+4} - 38)q^2$$
$$+(5 \times 2^{s+4} + 2^{s+2} + 21)q^3 + 8q^4.$$

3. Conclusion

This paper focuses on computing certain discrete Adriatic indices, namely the max-min sdeg index, misbalance indeg index, symmetric division deg index, and variable sum exdeg index for four families of PC dendrimers. The selected indices have shown strong predictive properties in prior studies implemented by the International Academy of Mathematical Chemistry, indicating their relevance in the analysis of molecular structures. Future studies could expand on this work by exploring additional dendrimer families and topological indices, further enriching the understanding of their applications in chemistry and related areas.

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Conflict of interest

The authors state that they have no conflicts of interest related to this work.

References

[1] N. Trinajstić, *Chemical Graph Theory*. 2nd ed. Boca Raton, FL, USA: CRC Press (1992), doi: 10.1201/9781315139111.

[2] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*. Weinheim, Germany: Wiley-VCH (Sep. 2000), doi: 10.1002/9783527613106.

[3] M. V. Diudea, QSPR/QSAR Studies by Molecular Descriptors. Huntingdon, NY, USA: Nova Science (2001).

[4] D. Vukičević and M. Gašperov, "Bond additive modeling 1. Adriatic indices," *Croat. Chem. Acta*, vol. 83, no. 3, pp. 243–260 (Oct. 2010).

[5] G.-C. Lau, W. C. Shiu, H.-K. Ng, Z.-B. Gao, and K. Schaffer, "On k-super graceful graphs with extremal maximum vertex degree," *J. Discrete Math. Sci. Cryptogr.*, vol. 27, no. 6, pp. 1765–1783 (Oct. 2024), doi: 10.47974/JDMSC-1722.

[6] B. Furtula, K. C. Das, and I. Gutman, "Comparative analysis of symmetric division deg index as potentially useful molecular descriptor," *Int. J. Quantum Chem.*, vol. 118, Art. no. e25659 (Jul. 2018), doi: 10.1002/qua.25659.

[7] A. Ali, I. Gutman, I. Redžepović, A. M. Albalahia, Z. Raza, and A. E. Hamza, "Symmetric division deg index: Extremal results and bounds," *MATCH Commun. Math. Comput. Chem.*, vol. 90, pp. 263–299 (Oct. 2023), doi: 10.46793/match.90-2.263A.

[8] D. Vukičević, "Bond additive modeling 5. Mathematical properties of the variable sum exdeg index," *Croat. Chem. Acta*, vol. 84, no. 1, pp. 93–101 (Jan. 2011), doi: 10.5562/cca1667.

[9] A. Ali, E. Milovanović, M. Matejić, and I. Milovanović, "On the variable sum exdeg index/coindex of graphs," *MATCH Commun. Math. Comput. Chem.*, vol. 87, no. 1, pp. 133–146 (Apr. 2022), doi: 10.46793/match.87-1.133A.

[10] M. Javaid, A. Ali, I. Milovanović, and E. Milovanović, "On the extremal cactus graphs for variable sum exdeg index with a fixed number of cycles," *AKCE Int. J. Graphs Comb.*, vol. 17, no. 3, pp. 920–923 (Sep. 2020), doi: 10.1016/j.akcej.2019.08.007.

[11] M. Rizwan, A. A. Bhatti, M. Javaid, and Y. Shang, "Conjugated tricyclic graphs with maximum variable sum exdeg index," *Heliyon,* vol. 9, no. 5, Art. no. e15706 (May 2023), doi: 10.1016/j.heliyon.2023.e15706.

[12] G. R. Newcome, C. N. Moorefield, and F. Vögtle, Dendritic Macromolecules: Concepts, Syntheses, Perspectives, Weinheim, Germany: VCH (1996), doi: 10.1002/9783527614875.fmatter.

[13] A. Bharali, A. Pegu, J. Buragohain, and B. Deka, "Generalized ISI index of certain families of nanostar dendrimers," *J Interdiscip. Math.,* vol. 24, no. 7, pp. 2021–2034 (Sep. 2021), doi: 10.1080/09720502.2021.1995181.

[14] J. B. Liu, D. A. Xavier, E. S. Varghese, A. Baby, and D. Mathew, "Computing molecular descriptors of polyphenylene dendrimer," *Polycycl. Aromat. Compd.,* vol. 44, no. 4, pp. 2775–2790 (May 2024), doi: 10.1080/10406638.2023.2222457.

[15] N. H. A. M. Saidi, M. N. Husin, and N. B. Ismail, "On the Zagreb indices of the line graphs of polyphenylene dendrimers," *J. Discret. Math. Sci. Cryptogr.,* vol. 23, no. 6, pp. 1239–1252 (Dec. 2020), doi: 10.1080/09720529.2020.1822041.

[16] T. R. Krishnasamy and M. Angamuthu, "Neighborhood-based descriptors for porphyrin dendrimers," *Biointerface Res. Appl. Chem.,* vol. 12, no. 5, pp. 6297–6307 (Sep. 2020), doi: 10.33263/BRIAC125.62976307.

[17] S. Mondal, N. De, and A. Pal, "Neighborhood degree sum-based molecular descriptors of fractal and Cayley tree dendrimers," *Eur. Phys. J. Plus,* vol. 136, Art. no. 303 (Apr. 2021), doi: 10.1140/epjp/s13360-021-01292-4.

[18] A. Amin, A. U. R. Virk, M. Rehman, and N. A. Shah, "Analysis of dendrimer generation by Sombor indices," *J. Chem.,* vol. 2021, Art. no. 930645 (2021), doi: 10.1155/2021/9930645.

[19] C. G. Huo, F. Azhar, A. U. R. Virk, and T. Ismaeel, "Investigation of dendrimer structures by means of K-Banhatti invariants," *J Math.,* vol. 2022, Art. no. 4451899 (2022), doi: 10.1155/2022/4451899.

[20] S. Zaman, A. Ullah, and A. Shafaqat, "Structural modeling and topological characterization of three kinds of dendrimer networks," *Eur. Phys. J. E. Soft Matter,* vol. 46, no. 5, Art. no. 36 (May 2023), doi: 10.1140/epje/s10189-023-00297-4.

[21] M. Azari and A. Iranmanesh, "Dendrimer graphs as thorn graphs and their topological edge properties," *Natl. Acad. Sci. Lett.,* vol. 39, no. 6, pp. 455–460 (Nov.–Dec. 2016), doi: 10.1007/s40009-016-0514-5.

[22] M. Azari, A. Iranmanesh, and M. V. Diudea, "Vertex-eccentricity descriptors in dendrimers," Studia Univ Babes Bolyai Chem., vol. 62, no. 1, pp. 129–142 (Jan. 2017), doi: 10.24193/subbchem.2017.1.11.

[23] F. Falahati-Nezhad and M. Azari, "Some bond-additive topological indices of four types of dendrimers," *Eur. Phys. J. Plus*, vol. 138, no. 10, Art. no. 892 (Oct. 2023), doi: 10.1140/epjp/s13360-023-04513-0.

[24] J. Ramezani Tousi and M. Ghods, "Some polynomials and degree-based topological indices of molecular graph and line graph of Titanium dioxide nanotubes," *J. Inform. Optim. Sci.,* vol. 45, no. 1, pp. 95–106 (Jan. 2024), doi: 10.47974/JIOS-1284.

[25] W. Maes and W. Dehaen, "Synthetic aspects of porphyrin dendrimers," *Eur. J. Org. Chem.*, vol. 2009, no. 28, pp. 4719–4752 (Jul. 2009), doi: 10.1002/ejoc.200900512.

[26] Y. Kim, M. F. Mayer, and S. C. Zimmerman, "A new route to organic nanotubes from porphyrin dendrimers," *Angew Chem. Int. Ed. Engl.,* vol. 42, no. 10, pp. 1121–1126 (Mar. 2023), doi: 10.1002/anie.200390295.

[27] S. Thyagarajan, T. Leiding, S. P. Arskold, A. V. Cheprakov, and S. A. Vinogradov, "Highly non-planar dendritic porphyrin for pH sensing: observation of porphyrin monocation," *Inorg Chem.,* vol. 49, no. 21, pp. 9909–9920 (Nov. 2010) doi: 10.1021/ic100968p.

[28] L. L. Li and E. W. G. Diau, "Porphyrin-sensitized solar cells," *Chem. Soc. Rev.*, vol. 42, no. 1, pp. 291–304 (Jan. 2013), doi: 10.1039/c2cs35257e.

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