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丙基醚亚胺 PETIM 树状聚合物的逆指数和逆多项式

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摘要：树状聚合物可用于药物的重要结构研究，掌握其性质具有重要意义. 由于有时会受到实验条件的限制，有许多研究树枝状聚合物性质的实验几乎不可能在实验室完成. 而拓扑指数在这方面能够提供帮助，即研究人员无须进行实验则可预测树状聚合物的性质. 因此，运用拓扑指数对最重要的树状聚合物结构之一，即（丙基）醚亚胺 PETIM 树状聚合物的性质进行研究，同时计算了该聚合物的几个逆指数以及第 1 和第 2 逆萨格勒布多项式.

关键词：树枝状聚合物；拓扑指数；萨格勒布多项式；萨格勒布指数
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Reverse Indices and Polynomials of (Propyl) Ether Imine PETIM Dendrimer

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Abstract: Dendrimers that are useful in medications are important structures research. To understand the properties of dendrimers is an important task. it is almost impossible to study properties of dendrimers in lab due to the limits of experimental conditions. But Topological indices provide help so researchers can predict properties of dendrimers without performing experiments. In this paper, we study one of the most important dendrimer structure namely (propyl) Ether Imine PETIM dendrimer and compute several reverse indices and first and second reverse Zagreb polynomials for (propyl) Ether Imine PETIM dendrimer.
Key words: dendrimer; topological index; Zagreb polynomial; Zagreb index

The research field in which graph theoretical techniques are used to solve the problems of chemistry is known as chemical graph theory. In these studies we associate numbers with the molecular graphs of chemical compounds that remains invariant upto graph isomorphism and are called topological indices (TIs). TIs help us in guessing the properties of concerned chemical compound without performing experiments in the wet lab. An important field of research is Cheminformatics in which QSAR and QSPR together with TIs are used to know about the properties of different chemical structures[1-3].

In recent years, many researchers defined and computed several TIs and correlate them with the properties of chemical compounds[4-5] and more than 150 TIs are present in literature. But the reality is, no single TI can give all properties of a chemical compound. Hence researchers are always interested to define new TIs, for example, reverse TIs, redefined Zagreb indices (ZIs), etc.

A graph G is connected, if all vertices of G are connected with each other. The length of smallest path between

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any two vertices is call distance between them. The degree of a vertex v is the number of vertices that are at distance one from v. Throughout this paper, we consider only simple connected graphs.

The aim of this paper is to compute several reverse degree-based indices and first and second reverse Zagreb polynomials for (propyl) Ether Imine PETIM dendrimer.

1 Definitions of Reverse Topological Indices

In this section, we give definitions of topological indices and polynomials.

Definition 1 (Reverse First ZI)

The reverse first ZI is defined as:

$$CM_1(G) = \sum_{uv \in E(G)} c_u + c_v.$$

Definition 2 (Reverse Second ZI)

The reverse second ZI is defined as:

$$CM_2(G) = \sum_{uv \in E(G)} c_u \times c_v.$$

Definition 3 (Reverse First Hyper ZI)

The reverse first hyper ZI is defined as:

$$CHM_1(G) = \sum_{uv \in E(G)} (c_u + c_v)^2.$$

Definition 4 (Reverse Second Hyper ZI)

The reverse second hyper ZI is defined as:

$$CHM_2(G) = \sum_{uv \in E(G)} (c_u \times c_v)^2.$$

Definition 5 (Reverse Second Modified ZI)

The reverse second modified ZI is defined as:

$$C^m M_2(G) = \sum_{uv \in E(G)} \frac{1}{(c_u \times c_v)}.$$

Definition 6 (Reverse Harmonic Index (HI))

The reverse HI is defined as:

$$CH(G) = \sum_{uv \in E(G)} \frac{2}{c_u + c_v}.$$

Definition 7 (Reverse Inverse Sum-Index (ISI))

The reverse ISI is defined as:

$$CI(G) = \sum_{uv \in E(G)} \frac{c_u \times c_v}{c_u + c_v}.$$

Definition 8 (Reverse Augmented ZI)

The reverse augmented ZI is defined as:

$$CA(G) = \sum_{uv \in E(G)} \left(\frac{c_u \times c_v}{c_u + c_v - 2}\right)^3.$$

Definition 9 (Reverse first Zagreb Polynomial)

The reverse first Zagreb polynomial is defined as:

$$CM_1(G) = \sum_{uv \in E(G)} x^{(c_u + c_v)}.$$

Definition 10 (Reverse Second Zagreb Polynomial)

The reverse second Zagreb polynomial is defined as:

$$CM_2(G) = \sum_{uv \in E(G)} x^{(c_u \times c_v)}.$$

Definition 11 (Reverse first Multiplication ZI)

The reverse first multiplicative ZI is defined as:

$$CPM_1(G) = \prod_{uv \in E(G)} (c_u + c_v).$$

Definition 12 (Reverse Second Multiplication ZI)

The reverse second multiplicative ZI is defined as:

$$CPM_2(G) = \prod_{uv \in E(G)} (c_u \times c_v).$$

Definition 13 (Reverse Randic Index)

The reverse Randic index is defined as:

$$CR_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{(c_u \times c_v)^\alpha}.$$

Definition 14 (Reverse inverse Randic Index)

The reverse inverse Randic index is defined as:

$$CRR_\alpha(G) = \sum_{uv \in E(G)} (c_u \times c_v)^\alpha.$$

Definition 15 (Reverse Symmetric division Index (SDI))

The reverse SDI is defined as:

$$CSDD(G) = \sum_{uv \in E(G)} \left\{ \frac{\min(c_u, c_v)}{\max(c_u, c_v)} + \frac{\max(c_u, c_v)}{\min(c_u, c_v)} \right\}.$$

Definition 16 (Reverse Atomic Bond Connectivity Index (ABC))

The reverse ABC is defiend as:

$$CABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{c_u + c_v - 2}{c_u \times c_v}}.$$

Definition 17 (Reverse Geometric Arithmatic Index (GA))

The reverse GA is defined as:

$$CGA(G) = \sum_{uv \in E(G)} \frac{\sqrt{c_u \times c_v}}{\frac{1}{2}(c_u + c_v)}.$$

Definition 18 (Reverse Sum-connectivity Index (SCI))

The reverse SCI is defined as:

$$C\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{c_u + c_v}}.$$

Definition 19 (Reverse Modified Randic Index)

The reverse modified Randic index is defined as:

$$CR'(G) = \sum_{uv \in E(G)} \frac{1}{\max(c_u, c_v)}.$$

Definition 20 (Reverse Arithmatic Geometric Index (AG))

The reverse AG is defined as:

$$CAG(G) = \sum_{uv \in E(G)} \frac{c_u + c_v}{2\sqrt{c_u \times c_v}}.$$

Definition 21 (Reverse Shigehalli & Kanabur Indices)

The reverse Shigehalli & Kanabur indices are defined as:

$$CSK(G) = \sum_{uv \in E(G)} \frac{c_u + c_v}{2};\ CSK_1(G) = \sum_{uv \in E(G)} \frac{c_u \times c_v}{2};$$

$$CSK_2(G) = \sum_{uv \in E(G)} \left(\frac{c_u + c_v}{2}\right)^2.$$

2　Main Results

In this section, we compute some reverse degree based topological indices of (propyl) Ether Imine PETIM dendrimer. Throughout this section, G denotes (propyl) Ether Imine PETIM dendrimer.

The molecular graph G is given in Figure 1. The edge partition of G based on the degree of end vertices is given in Table 1. The reverse degree based edge partition of G is given in Table 2.

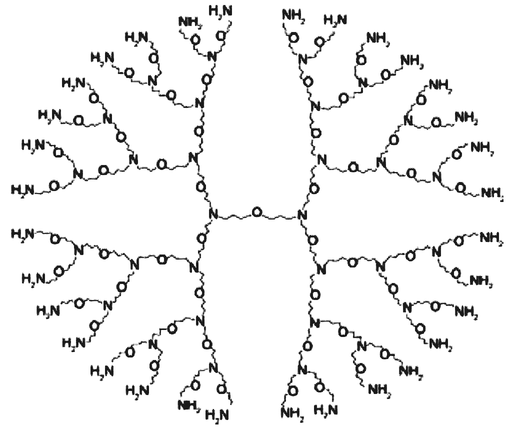

Figure 1　Graph of (Propyl) Ether Imine PETIM Dendrimer

Table 1　Degree Based Edge Partition of G

(d_u, d_v) Where $uv \in E(G)$	Number of Edges
(1, 2)	$2^n + 1$
(2, 2)	$2^{n+4} - 18$
(2, 3)	$6 \times 2^n - 6$

Table 2　Reverse Degree Based Edge Division of G

(c_u, c_v) Where $uv \in E(G)$	Number of Edges
(3, 2)	$2^n + 1$
(2, 2)	$2^{n+4} - 18$
(2, 1)	$6 \times 2^n - 6$

Theorem 1　For G, We have $CM_1(G) = 46(2^{n+1}) - 24$.

Proof　By definition of reverse first ZI, we have

$$\begin{aligned} CM_1(G) &= \sum_{uv \in E(G)} (c_u + c_v) \\ &= \sum_{uv \in E_1(G)} (3+2) + \sum_{uv \in E_2(G)} (2+2) + \sum_{uv \in E_3(G)} (2+1) \\ &= 5\,|CE_1(G)| + 4\,|CE_2(G)| + 3\,|CE_3(G)| \\ &= 5(2^{n+1}) + 4(2^{n+4} - 18) + 3(6 \times 2^n - 6) \\ &= 46(2^{n+1}) - 24. \end{aligned}$$

Theorem 2　For G, We have $CM_2(G) = 44(2^{n+1}) - 84$.

Proof　By definition of reverse second ZI, we have

$$\begin{aligned} CM_2(G) &= \sum_{uv \in E(G)} (c_u \times c_v) \\ &= \sum_{uv \in E_1(G)} (3 \times 2) + \sum_{uv \in E_2(G)} (2 \times 2) + \sum_{uv \in E_3(G)} (1 \times 1) \\ &= 6\,|CE_1(G)| + 4\,|CE_2(G)| + 1\,|CE_3(G)| \\ &= 6(2^{n+1}) + 4(2^{n+4} - 18) + 1(6 \times 2^n - 6) \\ &= 44(2^{n+1}) - 84. \end{aligned}$$

We skipped the proofs of the reaming theorem because they follow similarly as that of Theorem 1 and Theorem 2.

Theorem 3　For G, We have $HCM_1(G) = 180(2^{n+1}) - 342$.

Theorem 4　For G, We have $HCM_2(G) = 176(2^{n+1}) - 312$.

Theorem 5　For G, We have $C^m M_2(G) = \frac{10}{3} 2^n + 2^{n-1} - \frac{15}{2}$.

Theorem 6 For G, We have $CH(G)=\frac{1}{5}2^{n}-13$.

Theorem 7 For G, We have $CI(G)=\frac{7}{5}2^{n+4}-22$.

Theorem 8 For G, We have $CA(G)=96(2^{n+1}-2)$.

Theorem 9 For G, We have $CM_1(G)=(x^5+8x^4+3x^3)2^{n+1}-18x^4-6x^3$.

Theorem 10 For G, We have $CM_2(G)=(x^6+8x^4+3x^2)2^{n+1}-18x^4-6x^2$.

Theorem 11 For G, We have $CPM_1(G)=5^{2^{n+1}}\times 4^{2^{n+4}-18}\times 3^{6\times 2^{n}-6}$.

Theorem 12 For G, We have $CPM_2(G)=6^{2^{n+1}}\times 4^{2^{n+4}-18}\times 2^{6\times 2^{n}-6}$.

Theorem 13 For G, We have $CR_\alpha(G)=\left(\frac{1}{6^\alpha}+\frac{8}{4^\alpha}+\frac{3}{2^\alpha}\right)2^{n+1}-\frac{18}{2^\alpha}-\frac{6}{2^\alpha}$.

Theorem 14 For G, We have $CRR_\alpha(G)=(6^\alpha+8\times 4^\alpha+3\times 2^\alpha)\,2^{n+1}-6\times 2^\alpha(3\times 2^\alpha-1)$.

Theorem 15 For G, We have $CSDD(G)=\frac{77}{3}(2^{n+1})-51$.

Theorem 16 For G, We have $CABC(G)=12\sqrt{2}\,(2^{n}-1)$.

Theorem 17 For G, We have $CGA(G)=\frac{1}{5}(2^{n+1})(2\sqrt{6}+40+10\sqrt{2})-6(3+\sqrt{2})$.

Theorem 18 For G, We have $C\chi(G)=\left(\frac{1}{\sqrt{5}}+\frac{3}{\sqrt{3}}+4\right)2^{n+1}-\left(9+\frac{6}{\sqrt{3}}\right)$.

Theorem 19 For G, We have $CR'(G)=\left(\frac{35}{6}\right)2^{n+1}-12$.

Theorem 20 For G, We have $CAG_1(G)=\left(\frac{5}{2\sqrt{6}}+\frac{45}{4}\right)2^{n+1}-\frac{45}{2}$.

Theorem 21 For G, We have

$CSK(G)=(23)\,2^{n+1}-45$; $CSK_1(G)=(22)\,2^{n+1}-42$; $CSK_2(G)=(45)\,2^{n+1}-\frac{171}{2}$.

3 Conclusions

Dendrimers are artificial chemical structures that are buildup to manufacture new medicines. To avoid lab cast, TIs are used to know about different structural and chemical properties of dendrimers. In this paper, we presented several TIs and some polynomials for (propyl) Ether Imine PETIM dendrimer. Our results can help to understand the topology of concerned dendrimer structure and may help to enhance pharmaceutical industry.

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