

莫比乌斯梯的基于度的拓扑指数计算

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摘要: 早期的实验暗示着化合物的分子结构直接决定它的特性. 化学化合物的拓扑指数是与其分子图相关的数值, 取决于其中存在的对称性, 并且不通过实验就可以描述化学化合物的性质. 作为加法拓扑指数的推广, 乘法拓扑指数同样可以有效地预测化合物的物理化学特性, 并用于制药学或材料工程领域. 基于此, 计算了莫比乌斯梯的基于乘法度的拓扑指数.

关键词: 莫比乌斯梯; 萨格勒布指数; 乘法萨格勒布指数; 度; 图

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Computing Degree-based Topological Indices of Möbius Ladder

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Abstract: Early experiments imply that the molecular structure of a compound directly determines its properties. A topological index of a chemical compound is a numerical number associated with its molecular graph depending on the symmetry present in it and describes properties of chemical compound without performing experiments in lab. As a generalization of the additive topological index, the multiplicative topological index can also effectively predict the physicochemical properties of the compound and used in the field of pharmacy or materials engineering, so that to compute multiplicative degree based topological indices of Möbius Ladder.

Key words: Möbius Ladder; Zagreb index; multiplicative Zagreb index; degree; graph

1 Background Knowledge

Mathematical chemistry is an area of research in chemistry in which mathematical tools are used to solve problems of chemistry. Chemical graph theory is an important area of research in mathematical chemistry which deals with topology of molecular structure such as the mathematical study of isomerism and the development of topological descriptors or indices. Topological indices are real numbers attached to graph networks and graph of chemical compounds with applications in quantitative structure-property relationships. This remains invariant up to graph isomorphism and helps to predict many properties of chemical compounds, networks and nanomaterials, for example, viscosity, boiling points, radius of gyrations, etc., without going to lab.

Another emerging field is Cheminformatics, in which we use QSAR and QSPR relationship to guess biological activity and chemical properties of nanomaterial and networks. In these investigations, some physico-chemical properties and topological indices are utilized to guess the behavior of chemical networks. Like topological indices, polynomials also find considerable applications in network theory and chemistry, for example, Hosoya polynomial, which is also known as Wiener polynomial play an important role in computation of distance-based topological indices. M-polynomial was defined in 2015 and plays a similar role in computation of numerous degree-based

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topological indices. The M-polynomial contains precious information about degree-based topological indices and many topological indices can be computed from this simple algebraic polynomial. The first topological index was defined in 1947 by Wiener while studying boiling point of alkanes. This index is now known as Wiener index. Thus Wiener established the framework of topological indices and the Wiener index is initially the first and most concentrated topological index.

A graph G is an ordered pair (V, E) , where V and E represents vertex set and edge set respectively. A connected graph is a graph in which every two vertices of it are connected with each other. Graph theory is contributing a lion's share in many areas such as chemistry, physics, pharmacy, as well as in industry^[1]. We will start with some preliminary facts.

The first and second multiplicative Zagreb indices^[2] are defined as:

$$\begin{aligned} H_1(G) &= \prod_{u \in V(G)} (d_u)^2; \\ H_2(G) &= \prod_{uv \in E(G)} d_u \times d_v. \end{aligned}$$

respectively.

The Narumi-Katayama index^[3] is defined as:

$$NK(G) = \prod_{u \in V(G)} d_u.$$

Like the Wiener index, these indices are the focus of considerable research in computational chemistry. For example, in 2011^[4] characterized the multiplicative Zagreb indices for trees and determined the unique trees that obtained maximum and minimum values for $M_1(G)$ and $M_2(G)$, respectively. Wang et al^[5] extended Gutman's result to the following index for k -trees,

$$W_1^s(G) = \prod_{u \in V(G)} (d_u)^s.$$

Notice that for $s = 1, 2$, the above defined index is Narumi-Katayama index and Zagreb index, respectively. Based on the successful consideration of multiplicative Zagreb indices, Eliasi et al^[6] continued to define a new multiplicative version of the first Zagreb index as:

$$H_1^*(G) = \prod_{uv \in E(G)} (d_u + d_v).$$

Furthering the concept of indexing with the edge set, the first and second multiplicative hyper-Zagreb indices of a graph^[7] are defined as:

$$\begin{aligned} HII_1(G) &= \prod_{uv \in E(G)} (d_u + d_v)^2; \\ HII_2(G) &= \prod_{uv \in E(G)} (d_u \times d_v)^2. \end{aligned}$$

In Kulli et al^[8] defined the first and second generalized multiplicative Zagreb indices as:

$$\begin{aligned} MZ_1^a(G) &= \prod_{uv \in E(G)} (d_u + d_v)^a; \\ MZ_2^a(G) &= \prod_{uv \in E(G)} (d_u \times d_v)^a. \end{aligned}$$

Multiplicative sum connectivity and multiplicative product connectivity indices^[9] are defined as:

$$\begin{aligned} SCH(G) &= \prod_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}}; \\ PCH(G) &= \prod_{uv \in E(G)} \frac{1}{\sqrt{d_u \times d_v}}. \end{aligned}$$

Multiplicative atomic bond connectivity index and multiplicative Geometric arithmetic index are defined as:

$$\begin{aligned} ABCII(G) &= \prod_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}}; \\ GAI(G) &= \prod_{uv \in E(G)} \frac{2\sqrt{d_u \times d_v}}{d_u + d_v}; \end{aligned}$$

$$GA^a H(G) = \prod_{uv \in E(G)} \left(\frac{2\sqrt{d_u \times d_v}}{d_u + d_v} \right)^a.$$

In this paper we compute multiplicative indices of Möbius Ladder. The Möbius ladder M_n which is a cubic circulant graph with an even number of vertices, formed from an n -cycle by adding edges (called “rungs”) connecting opposite pair of vertices in the cycle. It is so-called because (with the exception of $M_6 = K_{3,3}$) M_n has exactly $n/2$ 4-cycles which link together by their shared edges to form a topological Möbius strip. Möbius ladders can also be viewed as a prism with one twisted edge. The Möbius ladders M_{16} have been shown in Figure 1. Möbius ladders have many applications in chemistry, chemical stereography, electronics and computer science. For our convenience, we view the Möbius ladder M_n which is a cubic circulant graph with an even number of vertices, formed from an n -cycle by adding edges (called “rungs”) connecting the opposite pair of vertices in the cycle.

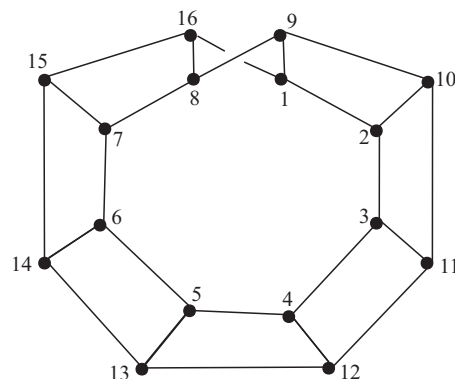


Figure 1 Möbius Ladder M_{16}

2 Computational Results

In this section, we present our computational results.

Theorem 1 Let M_n be the Möbius Ladder. Then

- 1) $MZ_1^a(M_n) = (6)^{3an}$;
- 2) $MZ_2^a(M_n) = (3)^{6an}$;
- 3) $G^a H(M_n) = (1)^{3an} = 1$.

Proof Let M_n be the Möbius Ladder. It is clear that M_n has only one type of vertex set i. e.,

$$V_1(M_n) = \{v \in V(M_n) : d_v = 3\}.$$

The edge set of M_n can be characterize as,

$$E_1(M_n) = \{e = uv \in E(M_n) : d_u = d_v = 3\}.$$

Such that,

$$|E_1(M_n)| = 3n.$$

Now by the definition, we have

$$MZ_1^\alpha(M_n) = \prod_{uv \in E(M_n)} (d_u + d_v)^\alpha = \prod_{u \in E_1(M_n)} (d_u + d_v)^\alpha = (d_u + d_v)^\alpha |E_1(M_n)| = (3 + 3)^{3an} = (6)^{3an};$$

$$MZ_2^\alpha(M_n) = \prod_{uv \in E(M_n)} (d_u \times d_v)^\alpha = \prod_{u \in E_1(M_n)} (d_u \times d_v)^\alpha = (d_u \times d_v)^\alpha |E_1(M_n)| = (3 \times 3)^{\alpha(3n)} = (3)^{6an};$$

$$\begin{aligned} G^\alpha H(M_n) &= \prod_{uv \in E(M_n)} \left(\frac{2\sqrt{d_u \times d_v}}{d_u + d_v} \right)^\alpha = \prod_{uv \in E_1(M_n)} \left(\frac{2\sqrt{d_u \times d_v}}{d_u + d_v} \right)^\alpha \\ &= \left(\frac{2\sqrt{d_u \times d_v}}{d_u + d_v} \right)^\alpha |E_1(M_n)| = \left(\frac{2\sqrt{3 \times 3}}{3 + 3} \right)^{3an} = (1)^{3an} = 1. \end{aligned}$$

Corollary 1 Let M_n be the Möbius Ladder. Then

- 1) $MZ_1(M_n) = H_1^*(M_n) = (6)^{3n}$;
- 2) $MZ_2(M_n) = H_2(M_n) = (3)^{6n}$;
- 3) $GAH(M_n) = (1)^{3n} = 1$.

Proof The proof follows immediately by putting $\alpha = 1$ in Theorem 1.

Corollary 2 Let M_n be the Möbius Ladder. Then

- 1) $H_1(M_n) = (6)^{6n}$;

$$2) \ HII_2(M_n) = (3)^{12n}.$$

Proof The proof follows immediately by putting $\alpha = 2$ in Theorem 1.

Corollary 3 Let M_n be the Möbius Ladder. Then

$$1) \ PCH(M_n) = (1/\sqrt{6})^{3n};$$

$$2) \ SCH(M_n) = (1/3)^{3n}.$$

Proof The proof follows immediately by putting $\alpha = -1/2$ in Theorem 1.

Theorem 2 Let M_n be the Möbius Ladder. Then

$$ABCH(M_n) = (2/3)^{3n}.$$

Proof From the information given in Theorem 1, we have

$$\begin{aligned} ABCH(M_n) &= \prod_{uv \in E(M_n)} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}} = \prod_{uv \in E_1(M_n)} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}} = \left(\sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}} \right)^{|E_1(M_n)|} = \left(\sqrt{\frac{3+3-2}{3 \times 3}} \right)^{3n} \\ &= \left(\sqrt{\frac{4}{9}} \right)^{3n} = \left(\frac{2}{3} \right)^{3n}. \end{aligned}$$

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