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碳纳米锥的基于乘法度的拓扑指数

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摘要：纳米锥是各种新型材料中广泛出现的分子结构，在纳米锥的分子图上进行拓扑指数计算有助于理解有关纳米锥的特性，而且萨格勒布乘积指数作为萨格勒布的补充，在化学和其他应用科学领域具有很好的应用前景. 因此，主要利用分子结构图分析方法，计算碳纳米锥的乘法第 1 和第 2 萨格勒布指数的广义形式，同时还计算了碳纳米锥的乘积、连接性和乘积连接性指数.

关键词：拓扑指数；碳纳米锥；萨格勒布指数；分子图
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Multiplicative Degree-based Topological Indices for Carbon Nanocones

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Abstract：Nanocones are the molecular structures widely appearing in various new materials，and topological indices（TIs）computed on the bases of molecular graphs for nanocones are numerical numbers which are helpful to understand properties of concerned nanocones. Multiplicative Zagreb indices，as compensation of Zagreb indices，have outstanding applications in chemistry and other applied sciences. In this paper，using molecular graph analysis，we focused on computing generalized version of multiplicative first and second Zagreb indices for Carbon nanocones. We also computed multiplicative sum connectivity and multiplicative product connectivity indices for Carbon nanocones.

Key words：topological index；Carbon nanocone；Zagreb index；molecular graph

Carbon nanocones have been observed since 1968 or even earlier[1]，on the surface of naturally occurring graphite. Their bases are attached to the graphite and their height varies between 1 and 40 micrometers. Their walls are often curved and are less regular than those of the laboratory made nanocones. Carbon nanostructures have attracted considerable attention due to their potential use in many applications including energy storage，gas sensors，biosensors，nanoelectronic devices and chemical probes[2]. Carbon allotropes such as carbon nanocones and carbon nanotubes have been proposed as possible molecular gas storage devices[3]. More recently，carbon nanocones have gained increased scientific interest due to their unique properties and promising uses in many novel applications such as energy and hydrogen-storage[4]. Figure 1 and figure 2 are carbon nenocones.

The molecular graph of nanocones have conical structures with a cycle of length k at its core and n layers of hexagons placed at the conical surface around its center as shown in following figure 3.

In the present report，we gave closed form of multiplicative versions of some important degree-based TIs.

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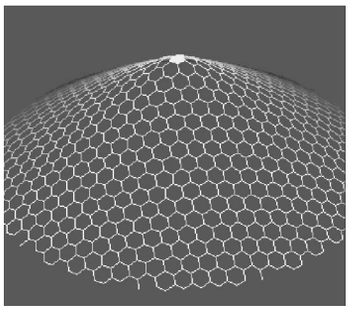

Figure 1　Carbon nenocone

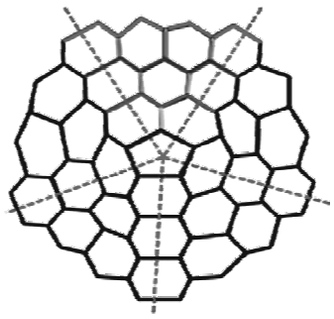

Figure 2　The molecular graph

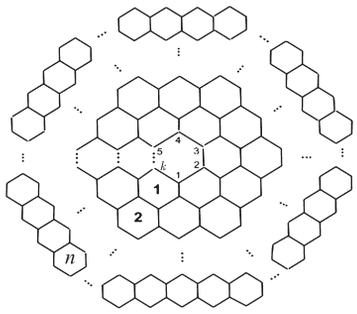

Figure 3　Carbon nenocones

1　Definitions of TIs

In this section, we present definitions of multiplicative versions of TIs.

Definition 1　(First Generalized Multiplication Zagreb Index)

For a connected simple graph G, the first generalized multiplication Zagreb index[5] is defined as:

$$GMZ_1^{\alpha}(G)=\prod_{ij\in E(G)}(d_i+d_j)^{\alpha}.$$

Definition 2　(Second Generalized Multiplication Zagreb Index)

For a connected simple graph G, the second generalized multiplication Zagreb index[5] is defined as:

$$GMZ_2^{\alpha}(G)=\prod_{ij\in E(G)}(d_i\times d_j)^{\alpha}.$$

Definition 3　(First Multiplication Zagreb Index)

For a connected simple graph G, the first multiplication Zagreb index[6] is defined as:

$$MZ_1(G)=\prod_{ij\in E(G)}(d_i+d_j).$$

Definition 4　(Second Multiplication Zagreb Index)

For a connected simple graph G, the second multiplication Zagreb index[6] is defined as:

$$MZ_2(G)=\prod_{ij\in E(G)}(d_i\times d_j).$$

Definition 5　(First Hyper Multiplication Zagreb Index)

For a connected simple graph G, the first hyper multiplication Zagreb index[7] is defined as:

$$MH_1(G)=\prod_{ij\in E(G)}(d_i+d_j)^2.$$

Definition 6　(Second Hyper Multiplication Zagreb Index)

For a connected simple graph G, the second hyper multiplication Zagreb index[7] is defined as:

$$MH_2(G)=\prod_{ij\in E(G)}(d_i\times d_j)^2.$$

Definition 7　(Multiplicative Sum Connectivity Index)

For a connected simple graph G, the multiplicative sum connectivity index[8] is defined as:

$$SCM(G)=\prod_{ij\in E(G)}(d_i+d_j)^{-1/2}.$$

Definition 8　(Multiplicative Product Connectivity Indices)

For a connected simple graph G, the multiplicative product connectivity index[8] is defined as:

$$PCM(G)=\prod_{ij\in E(G)}(d_i\times d_j)^{-1/2}.$$

Definition 9　(Multiplicative Atomic Bond Connectivity Index)

For a connected simple graph G, the multiplicative atomic bond connectivity index[8] is defined as:

$$ABCM(G)=\prod_{ij\in E(G)}\sqrt{\frac{d_i+d_j-2}{d_i\times d_j}}.$$

Definition 10 (Multiplicative Geometric Arithmetic Index)

For a connected simple graph G, the multiplicative geometric arithmetic index[8] is defined as:

$$GAM(G)=\prod_{ij\in E(G)}\frac{2\sqrt{d_i\times d_j}}{d_i+d_j}.$$

2 Computational Results

In this section, we present our results. From figure 3, it can be observed that the edge set molecular graph of Carbon nanocone can be divided into three classes based on the degree of end vertices. The edge partition of molecular graph of Carbon Nanocone is presented in Table 1.

Table 1 Degree based edge partition of *G*

(d_i, d_j) Where $ij\in E(G)$	Number of Edges
(2, 2)	p
(2, 3)	$2pn$
(3, 3)	$\frac{pn}{3}(3n-1)$

Theorem 1 Let G be the molecular graph of Carbon nanocone. Then we have

$$GMZ_1^{\alpha}(G)=2^{2\alpha p+\alpha pn^2-\frac{\alpha pn}{3}}\times 3^{\alpha pn^2-\alpha pn}\times 5^{2\alpha pn}.$$

Proof By the Definition of the generalized first multiplication Zagreb index and using edge partition of molecular graph of Carbon Nanocone, we have following computation:

$$\begin{aligned}GMZ_1^{\alpha}(G)&=\prod_{ij\in E(G)}(d_i+d_j)^{\alpha}\\&=\prod_{ij\in E_1(G)}(d_i+d_j)^{\alpha}\times\prod_{ij\in E_2(G)}(d_i+d_j)^{\alpha}\times\prod_{ij\in E_3(G)}(d_i+d_j)^{\alpha}\\&=\prod_{ij\in E_1(G)}(2+2)^{\alpha}\times\prod_{ij\in E_2(G)}(2+3)^{\alpha}\times\prod_{ij\in E_3(G)}(3+3)^{\alpha}\\&=(4^{\alpha})^{|ij\in E_1(G)|}\times(5^{\alpha})^{|ij\in E_2(G)|}\times(6^{\alpha})^{|ij\in E_3(G)|}\\&=(4^{\alpha})^{p}\times(5^{\alpha})^{2np}\times(6^{\alpha})^{\frac{np}{3}(3n-1)}\\&=2^{2\alpha p+\alpha pn^2-\frac{\alpha pn}{3}}\times 3^{\alpha pn^2-\alpha pn}\times 5^{2\alpha pn}.\end{aligned}$$

Theorem 2 Let G be the molecular graph of Carbon nanocone. Then we have

$$GMZ_2^{\alpha}(G)=2^{2\alpha p(n+1)}\times 3^{2\alpha pn(n+\frac{2}{3})}.$$

Proof By the Definition of the generalized first multiplication Zagreb index and using edge partition of molecular graph of Carbon Nanocone, we have following computation:

$$\begin{aligned}GMZ_2^{\alpha}(G)&=\prod_{ij\in E(G)}(d_i\times d_j)^{\alpha}\\&=\prod_{ij\in E_1(G)}(d_i\times d_j)^{\alpha}\times\prod_{ij\in E_2(G)}(d_i\times d_j)^{\alpha}\times\prod_{ij\in E_3(G)}(d_i\times d_j)^{\alpha}\\&=\prod_{ij\in E_1(G)}(2\times 2)^{\alpha}\times\prod_{ij\in E_2(G)}(2\times 3)^{\alpha}\times\prod_{ij\in E_3(G)}(3\times 3)^{\alpha}\\&=(4^{\alpha})^{|ij\in E_1(G)|}\times(6^{\alpha})^{|ij\in E_2(G)|}\times(9^{\alpha})^{|ij\in E_3(G)|}\\&=(4^{\alpha})^{p}\times(6^{\alpha})^{2np}\times(9^{\alpha})^{\frac{np}{3}(3n-1)}\end{aligned}$$

$$= 2^{2\alpha p(n+1)} \times 3^{2\alpha pn(n+\frac{2}{3})}.$$

Corollary 1　Let G be the molecular graph of Carbon nanocone. Then we have

$$MZ_1(G) = 2^{2p+pn^2-\frac{pn}{3}} \times 3^{pn^2-pn} \times 5^{2pn}.$$

Proof　Taking $\alpha = 1$ in Theorem 1, we get this result immediate.

Corollary 2　Let G be the molecular graph of Carbon nanocone. Then we have

$$MZ_2(G) = 2^{2p(n+1)} \times 3^{2pn(n+\frac{2}{3})}.$$

Proof　Taking $\alpha = 1$ in Theorem 2, we get this result immediate.

Corollary 3　Let G be the molecular graph of Carbon nanocone. Then we have

$$MH_1(G) = 2^{2p(2+n^2-\frac{n}{3})} \times 3^{2pn(n-1)} \times 5^{4pn}.$$

Proof　Taking $\alpha = 2$ in Theorem 1, we get this result immediate.

Corollary 4　Let G be the molecular graph of Carbon nanocone. Then we have

$$MH_2(G) = 2^{4p(n+1)} \times 3^{4pn(n+\frac{2}{3})}.$$

Proof　Taking $\alpha = 2$ in Theorem 2, we get this result immediate.

Corollary 5　Let G be the molecular graph of Carbon nanocone. Then we have

$$SCM(G) = 2^{p(1-\frac{1}{2}n^2+\frac{n}{6})} \times 3^{\frac{1}{2}pn(1-n)} \times 5^{-pn}.$$

Proof　Taking $\alpha = -1/2$ in Theorem 1, we get this result immediate.

Corollary 6　Let G be the molecular graph of Carbon nanocone. Then we have

$$PCM(G) = 2^{-p(n+1)} \times 3^{-pn(n+\frac{2}{3})}.$$

Proof　Taking $\alpha = -1/2$ in Theorem 2, we get this result immediate.

Theorem 3　Let G be the molecular graph of Carbon nanocone. Then we have

$$ABCM(G) = (\frac{1}{2})^{p(n+\frac{1}{2})} \times (\frac{2}{3})^{\frac{pn}{3}(3n-1)}.$$

Proof　By the Definition of the multiplication Atomic bound Connectivity index and using edge partition of molecular graph of Carbon Nanocone, we have following computation:

$$\begin{aligned}
ABCM(G) &= \prod_{ij\in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i \times d_j}} \\
&= \prod_{ij\in E_1(G)} \sqrt{\frac{2+2-2}{2\times 2}} + \prod_{ij\in E_2(G)} \sqrt{\frac{2+3-2}{2\times 3}} + \prod_{ij\in E_3(G)} \sqrt{\frac{3+3-2}{3\times 3}} \\
&= (\frac{1}{\sqrt{2}})^{|ij\in E_1(G)|} \times (\frac{1}{\sqrt{2}})^{|ij\in E_2(G)|} \times (\frac{2}{3})^{|ij\in E_3(G)|} \\
&= (\frac{1}{\sqrt{2}})^{p} \times (\frac{1}{\sqrt{2}})^{2np} \times (\frac{2}{3})^{\frac{pn}{3}(3n-1)} \\
&= (\frac{1}{2})^{p(n+\frac{1}{2})} \times (\frac{2}{3})^{\frac{pn}{3}(3n-1)}.
\end{aligned}$$

Theorem 4　For G, We have

$$GAM(G) = (\frac{2\sqrt{6}}{5})^{2np}.$$

Proof　By the Definition of the multiplication Geometric arithmetic index and using edge partition of molecular graph of Carbon Nanocone, we have following computation:

$$GAM(G) = \prod_{ij\in E(G)} \frac{2\sqrt{d_i \times d_j}}{d_i + d_j}$$

$$= \prod_{ij \in E_1(G)} \frac{2\sqrt{d_i \times d_j}}{d_i + d_j} + \prod_{ij \in E_2(G)} \frac{2\sqrt{d_i \times d_j}}{d_i + d_j} + \prod_{ij \in E_3(G)} \frac{2\sqrt{d_i \times d_j}}{d_i + d_j}$$

$$= \prod_{ij \in E_1(G)} \frac{2\sqrt{2 \times 2}}{2 + 2} + \prod_{ij \in E_2(G)} \frac{2\sqrt{2 \times 3}}{2 + 3} + \prod_{ij \in E_3(G)} \frac{2\sqrt{3 \times 3}}{3 + 3}$$

$$= (1)^{|ij \in E_1(G)|} \times (\frac{2\sqrt{6}}{5})^{|ij \in E_2(G)|} \times (1)^{|ij \in E_3(G)|}$$

$$= (1)^{p} \times (\frac{2\sqrt{6}}{5})^{2np} \times (1)^{\frac{pn}{3}(3n-1)} = (\frac{2\sqrt{6}}{5})^{2np}.$$

3 Conclusion

In this paper, we computed multiplicative versions of several degree-based TIs for molecular graph of Carbon nanocones. Our result can help in understanding topology of concerned nanocone and in guessing its properties. In future, we are interested in computed distance based polynomials and indices for it.

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