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关于 H-Pantancenic 线图的 M-多项式和基于度的拓扑指数

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摘要：管状结构是纳米材料的基本结构之一，从理论的角度研究纳米管的化学性质可以对材料合成和设计提供理论依据. 利用化学分子结构建模和图论的方法，计算 H-Pantancenic 纳米管线图的基于度的拓扑指数，同时也计算了 H-Pantancenic 纳米管线图的 M-多项式，并从中恢复了 9 个基于度的拓扑指数. 得到的理论计算结果在纳米材料学的实际工程应用中有潜在的参考价值.

关键词：度；拓扑指数；线图；亚苯基；H-Pantacenic 纳米管
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M-Polynomial and Degree Based Topological Indices of Line Graph of H-Pantancenic

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Abstract: Tube structure is one of the basic structures of nanomaterials. Studying the chemical properties of nanotubes from a theoretical perspective can provide a theoretical basis for material synthesis and design. In this paper, by means of chemical molecular structure modeling and graph theory, our purpose is to calculate degree based topological indices of line graph of H-Pantancenic Nanotubes. We compute the M-polynomial of line graph of H-Pantancenic Nanotubes and recover nine degree-based topological indices from it. The theoretical calculation results obtained have potential reference value in practical engineering applications of materials science and nanoscience.

Key words: degree; topological index; line graph; phenylenes; H-Pantacenic nanotube

1　Preliminary Knowledge

Chemical graph theory is a branch of graph theory in which a chemical compound is represented by a simple graph called molecular graph in which vertices are atoms of compound and edges are the atomic bounds. A graph is connected if there is atleast one connection between its vertices. Throughout this paper we take G as a connected graph. If a graph does not contain any loop or multiple edges then it is called a network. Between two vertices u and v, the distance is the shortest path between them and is denoted by $d(u,v) = d_G(u,v)$ in graph G. For a vertex v of G the "degree" d_v is the number of vertices attached with it. The edge connecting the vertices u and v will

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be denoted by uv. The degree and valence in chemistry are closely related to each other. We refer to the book[1] for more details. Another emerging field is Cheminformatics, which helps to predict biological activities with the relationship of Structure-property and quantitative structure-activity. Topological indices and Physico-chemical properties are used in the prediction of bioactivity if underlined compounds are used in these studies[2-3].

The number that describe the topology of a graph is called topological index. In 1947, the first and most studied topological index was introduced by Weiner[4].

The M-polynomial of the graph G isgenerally defined as[5]:

$$M(G,x,y) = \sum_{\delta \leqslant i \leqslant j \leqslant \Delta} m_{ij}(G) x^i y^j. \tag{1}$$

Where $\delta = \mathrm{Min}\{d_v \mid v \in V(G)\}$, $\Delta = \mathrm{Max}\{d_v \mid v \in V(G)\}$, and $m_{ij}(G)$ is the edge $vu \in E(G)$ such that $\{d_v, d_u\} = \{i, j\}$.

Topological indices are graph invariants and presently play important role in the field of mathematical chemistry, so many useful topological indices have been introduced. In 1975, Milan Randic introduced the Randic index[6], which is defined as

$$R_{-1/2}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

The generalized Randic index was introduced by Bollobas and Erdos[7] and Amic et al.[8] while working in 1998. The general Randic index is defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha,$$

The inverse Randic index is defined as

$$RR_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)^\alpha}.$$

The modify Randic and sum connectivity index are defined as

$$R'(G) = \sum_{uv \in E(G)} \frac{1}{\mathrm{Max}\{d_u, d_v\}}.$$

The first Zagreb index $M_1(G)$ and second Zagreb index $M_2(G)$ are proposed by Gutman and Trinajstic′ which are $M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$ and $M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v)$. Thesecond modified Zagreb index is defined as[9-10]:

$${}^{m}M_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}.$$

The augmented Zagreb index is

$$A(G) = \sum_{vu \in E(G)} \left\{\frac{d_u d_v}{d_u + d_v - 2}\right\}^3.$$

The Symmetric division index is

$$SDD(G) = \sum_{uv \in E(G)} \left\{\frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)}\right\}.$$

Harmonic index is another variant form of randic index:

$$H(G) = \sum_{vu \in E(G)} \frac{2}{d_u + d_v}.$$

The Inverse-sum index is

$$I(G) = \sum_{vu \in E(G)} \frac{d_u d_v}{d_u + d_v}.$$

For more details about degree based topological indices please see[11-15].

Some well-known degree-based topological indices are closely related to the M-polynomial[5]; in Table 1 you can see such relations.

Tab. 1　Derivation of some degree-based topological indices from M-polynomial

Topological Index	Derivation from $M(G;\ x,\ y)$
First Zagreb $M_1(G)$	$(D_x+D_y)(M(G;x,y))_{x=y=1}$
Second Zagreb $M_2(G)$	$(D_xD_y)(M(G;x,y))_{x=y=1}$
Second Modified Zagreb ${}^mM_2(G)$	$(S_xS_y)(M(G;x,y))_{x=y=1}$
Inverse Randic $RR_\alpha(G)$	$(D_x^\alpha D_y^\alpha)(M(G;x,y))_{x=y=1}$
General Randic $R_\alpha(G)$	$(S_x^\alpha S_y^\alpha)(M(G;x,y))_{x=y=1}$
Symmetric Division Index $SDD(G)$	$(D_xS_y+S_xD_y)(M(G;x,y))_{x=y=1}$
Harmonic Index $H(G)$	$2S_xJ(M(G;x,y))_{x=1}$
Inverse sum Index $I(G)$	$S_xJD_xD_y(M(G;x,y))_{x=1}$
Augmented Zagreb Index $A(G)$	$S_x{}^3Q_{-2}JD_x{}^3D_y{}^3(M(G;x,y))_{x=1}$

Here

$$D_x = x\frac{\partial(f(x,y)}{\partial x},$$

$$D_y = y\frac{\partial(f(x,y)}{\partial y},$$

$$S_x = \int_0^x \frac{f(t,y)}{t}\mathrm{d}t,$$

$$S_y = \int_0^y \frac{f(x,t)}{t}\mathrm{d}t,$$

$$J(f(x,y)) = f(x,x),$$

$$Q_\alpha(f(x,y)) = x^\alpha f(x,y).$$

Lemma 1　Let G be a graph of order p and size q. Then the line graph $L(G)$ of G is a graph of order p and size $\frac{1}{2}M_1(G)-q$.

In this report we compute some degree based topological indices of line graph of H-Pantacenic nanotube. The graph of H-Pantacenic nanotube are given in figure 1, and the line graph of H-Pantacenic nanotube is given in figure 2.

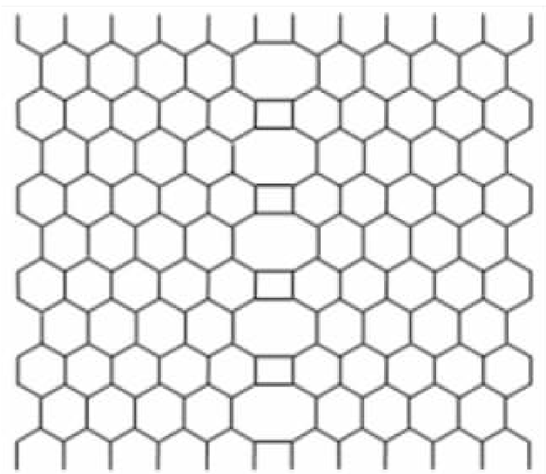

Fig.1　The H-Pantacenic nanotube $K[p,q]$

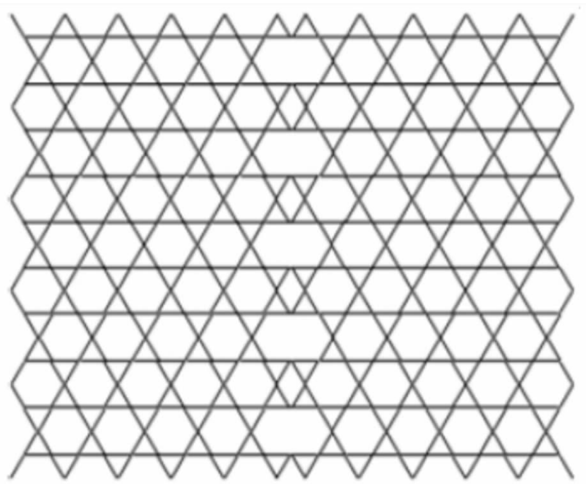

Fig.2　The line graph of H-Pantacenic nanotube $K[p,q]$

In this paper, we calculate M-polynomial of the Line Graphs of H-Pantacenic Nanotubes. From this M-polynomial we recover many degree based topological indices of the Line Graphs of H-Pantacenic and V-Pantacenic Nanotubes.

2 Computational Results

Theorem 1 Let $G=L(K[p,q])$ be a line graph of H-Pantacenic nanotube. Then

$$M(G,x,y)=4qx^2y^3+8qx^3y^4+66pqx^4y^4-20qx^4y^4.$$

Proof The line graph of H-Pantancenic Nanotubes is shown in figure 2. It can be observed from the figure 2 and lemma 1 that

$$|V(G)|=33pq-2q,$$
$$|E(G)|=66pq-8q.$$

We can divide the edge set of the line graph of H-Pantacenic Nanotube into the following three classes depending on the degree of end vertices of each edge:

$$E_{\{2,3\}}(G)=\{e=uv\in E(G);d_u=2,d_v=3\},$$
$$E_{\{3,4\}}(G)=\{e=uv\in E(G);d_u=3,d_v=4\},$$

and

$$E_{\{4,4\}}(G)=\{e=uv\in E(G);d_u=4,d_v=4\}.$$

Now

$$|E_{\{2,3\}}(G)|=4q,$$
$$|E_{\{3,4\}}(G)|=8q,$$
$$|E_{\{4,4\}}(G)|=66pq-20q.$$

From the definition of M-polynomial, we have

$$\begin{aligned}M(G,x,y)&=\sum_{\delta\leqslant i\leqslant j\leqslant\Delta}m_{ij}x^iy^j\\&=\sum_{uv\in E_{\{2,3\}}(G)}m_{23}x^2y^3+\sum_{uv\in E_{\{3,4\}}(G)}m_{34}x^3y^4+\sum_{uv\in E_{\{4,4\}}(G)}m_{44}x^4y^4\\&=|E_{\{2,3\}}(G)|x^2y^3+|E_{\{3,4\}}(G)|x^3y^4+|E_{\{4,4\}}(G)|x^4y^4\\&=4qx^2y^3+8qx^3y^4+(66pq-20q)x^4y^4.\end{aligned}$$

Corollary 1 For the line graph of H-Pantacenic G, the first Zagreb index is

$$M_1(G)=528pq-84q.$$

Proof Let

$$f(x,y)=M(G,x,y)=4qx^2y^3+8qx^3y^4+66pqx^4y^4-20qx^4y^4.$$

Then

$$D_x(f(x,y))=8qx^2y^3+24qx^3y^4+264pqx^4y^4-80qx^4y^4,$$
$$D_y(f(x,y))=12qx^2y^3+32qx^3y^4+264pqx^4y^4-80qx^4y^4.$$

From the M-polynomial (theorem 1) and table 1

$$\begin{aligned}M_1(G)&=(D_x+D_y)(f(x,y))_{x=y=1}\\&=(20qx^2y^3+56qx^3y^4+528pqx^4y^4-160qx^4y^4)_{x=y=1}\\&=528pq-84q.\end{aligned}$$

Corollary 2 For the line graph of H-Pantacenic G, the second Zagreb index is

$$M_2(G)=1\,056pq-200q.$$

Proof Here

$$D_xD_y(f(x,y))=24qx^2y^3+96qx^3y^4+1\,056pqx^4y^4-320qx^4y^4.$$

From the M-polynomial (theorem 1) and table 1

$$\begin{aligned} M_2(G) &= (D_xD_y)(f(x,y))_{x=y=1} \\ &= (24qx^2y^3 + 96qx^3y^4 + 1\,056pqx^4y^4 - 320qx^4y^4)_{x=y=1} \\ &= 24q + 96q + 1\,056pq - 320q \\ &= 1\,056pq - 200q. \end{aligned}$$

Corollary 3　For the line graph of H-Pantacenic G, the second modified Zagreb index is

$$^mM_2(G) = \frac{165}{8}pq - \frac{19}{12}q.$$

Proof

$$S_y(f(x,y)) = \frac{4}{3}qx^2y^3 + 2qx^3y^4 + \frac{33}{2}pqx^4y^4 - 5qx^4y^4,$$

$$S_xS_y(f(x,y)) = \frac{2}{3}qx^2y^3 + \frac{2}{3}qx^3y^4 + \frac{33}{8}pqx^4y^4 - \frac{5}{4}x^4y^4.$$

From the M-polynomial (theorem 1) and table 1

$$\begin{aligned} ^mM_2(G) &= (S_x S_y)(f(x,y))\big|_{x=y=1} \\ &= \frac{2}{3}q + \frac{2}{3}q + \frac{33}{8}pq - \frac{5}{4}q \\ &= \frac{165}{8}pq - \frac{19}{12}q. \end{aligned}$$

Corollary 4　For the line graph of H-Pantacenic G, the inverse Randic index is

$$RR_\alpha(G) = 4\times 3^\alpha \times 2^\alpha q + 8\times 4^\alpha \times 3^\alpha q + 66\times 4^\alpha \times 4^\alpha pq - 20\times 4^\alpha \times 4^\alpha q.$$

Proof　Here

$$D_y^{\alpha}(f(x,y)) = (4\times 3^\alpha qx^2y^3 + 8\times 4^\alpha qx^3y^4 + 66\times 4^\alpha pqx^4y^4 - 20\times 4^\alpha qx^4y^4).$$

$$\begin{aligned} D_x^{\alpha} D_y^{\alpha}(f(x,y)) = (&4\times 3^\alpha \times 2^\alpha qx^2y^3 + 8\times 4^\alpha \times 3^\alpha \times 3qx^3y^4 + 66\times 4^\alpha \\ &\times 4^\alpha pqx^4y^4 - 20\times 4^\alpha \times 4^\alpha qx^4y^4). \end{aligned}$$

From the M-polynomial (theorem 1) and table 1

$$\begin{aligned} RR_\alpha(G) &= (D_x^\alpha D_y^\alpha)(f(x,y))\big|_{x=y=1} \\ &= (4\times 3^\alpha \times 2^\alpha qx^2y^3 + 8\times 4^\alpha \times 3^\alpha qx^3y^4 + 66\times 4^\alpha \times 4^\alpha pqx^4y^4 - 20\times 4^\alpha \times 4^\alpha qx^4y^4)_{x=y=1} \\ &= 4\times 3^\alpha \times 2^\alpha q + 8\times 4^\alpha \times 3^\alpha q + 66\times 4^\alpha \times 4^\alpha pq - 20\times 4^\alpha \times 4^\alpha q. \end{aligned}$$

Corollary 5　For the line graph of H-Pantacenic G, the general Randic index is

$$R_\alpha(G) = \frac{4q}{2^\alpha 3^\alpha} + \frac{8q}{3^\alpha 4^\alpha} + \frac{66pq}{4^\alpha 4^\alpha} - \frac{20q}{4^\alpha 4^\alpha}.$$

Proof

$$S_y^{\alpha}(f(x,y)) = \left(\frac{4qx^2y^3}{3^\alpha} + \frac{8qx^3y^4}{4^\alpha} + \frac{66pqx^4y^4}{4^\alpha} - \frac{20qx^4y^4}{4^\alpha}\right),$$

$$S_x^{\alpha} S_y^{\alpha}(f(x,y)) = \left(\frac{4qx^2y^3}{2^\alpha 3^\alpha} + \frac{8qx^3y^4}{3^\alpha 4^\alpha} + \frac{66pqx^4y^4}{4^\alpha 4^\alpha} - \frac{20qx^4y^4}{4^\alpha 4^\alpha}\right).$$

From the M-polynomial (theorem 1) and table 1

$$\begin{aligned} R_\alpha(G) &= (S_x^\alpha S_y^\alpha)(f(x,y))\big|_{x=y=1} \\ &= \left(\frac{4qx^2y^3}{2^\alpha 3^\alpha} + \frac{8qx^3y^4}{3^\alpha 4^\alpha} + \frac{66pqx^4y^4}{4^\alpha 4^\alpha} - \frac{20qx^4y^4}{4^\alpha 4^\alpha}\right)_{x=y=1} \\ &= \frac{4q}{2^\alpha 3^\alpha} + \frac{8q}{3^\alpha 4^\alpha} + \frac{66pq}{4^\alpha 4^\alpha} - \frac{20q}{4^\alpha 4^\alpha}. \end{aligned}$$

Corollary 6　For the line graph of H-Pantacenic G, the symmetric division index is

$$SDD(G) = -\frac{44}{3}q + 132pq.$$

Proof

$$D_xS_y(f(x,y)) = \frac{8}{3}qx^2y^3 + 6qx^3y^4 + 66pqx^4y^4 - 20qx^4y^4.$$

$$D_yS_x(f(x,y)) = 6qx^2y^3 + \frac{32}{3}qx^3y^4 + 66pqx^4y^4 - 20qx^4y^4.$$

From the M-polynomial (theorem 1) and table 1

$$\begin{aligned} SDD(G) &= (D_xS_y + S_xD_y)(f(x,y))\big|_{x=y=1} \\ &= \left(\frac{26}{3}qx^2y^3 + \frac{50}{3}qx^3y^4 + 132pqx^4y^4 - 40qx^4y^4\right)\Big|_{x=y=1} \\ &= \frac{26}{3}q + \frac{50}{3}q + 132pq - 40q \\ &= 132pq - \frac{44}{3}q. \end{aligned}$$

Corollary 7 For the line graph of H-Pantacenic G, the harmonic index is

$$H(G) = -81q + \frac{33}{2}pq.$$

Proof

$$J(f(x,y)) = 4qx^5 + 8qx^7 + 66pqx^8 - 20qx^8.$$

$$2S_xJ(f(x,y)) = \frac{8}{5}qx^5 + \frac{16}{7}qx^7 + \frac{33}{2}pqx^8 - \frac{5}{2}qx^8.$$

From the M-polynomial (theorem 1) and table 1

$$\begin{aligned} H(G) &= 2SJ(f(x,y))\big|_{x=1} \\ &= \left(\frac{8}{5}qx^5 + \frac{16}{7}qx^7 + \frac{33}{2}pqx^8 - \frac{5}{2}qx^8\right)\Big|_{x=1} \\ &= \frac{8}{5}q + \frac{16}{7}q + \frac{33}{2}pq - \frac{5}{2}q \\ &= -81q + \frac{33}{2}pq. \end{aligned}$$

Corollary 8 For the line graph of H-Pantacenic G, the Inverse sum-index is

$$I(G) = -752q + 13pq.$$

Proof

$$JD_xD_y(f(x,y)) = 24qx^5 + 96qx^7 + 1\,056pqx^8 - 320qx^8,$$

$$S_xJD_xD_y(f(x,y)) = \frac{24}{5}qx^5 + \frac{96}{7}qx^7 + \frac{1056}{8}pqx^8 - \frac{320}{8}qx^8.$$

From the M-polynomial (theorem 1) and table 1

$$\begin{aligned} I(G) &= S_xJD_xD_y(f(x,y))\big|_{x=y=1} \\ &= \left(\frac{24}{5}qx^5 + \frac{96}{7}qx^7 + \frac{1\,056}{8}pqx^8 - \frac{320}{8}qx^8\right)\Big|_{x=1} \\ &= \frac{24}{5}q + \frac{96}{7}q + 132pq - 40q \\ &= -752q + 13pq. \end{aligned}$$

Corollary 9 For the line graph of H-Pantacenic G, the augmented index is

$$A(G) = \frac{11\,264}{9}pq - \frac{798\,752}{3\,375}q.$$

Proof

$$D_x\,D_y(f(x,y)) = 2\times3\times4qx^2\,y^3 + 3\times4\times8qx^3\,y^4 + 4\times4\times66pqx^4\,y^4 - 4\times4\times20qx^4\,y^4,$$

$$D_x^3\,D_y^3(f(x,y)) = 2^3\times3^3\times4qx^2\,y^3 + 3^3\times4^3\times8qx^3\,y^4 + 4^3\times4^3\times66pqx^4\,y^4 - 4^3\times4^3\times20qx^4\,y^4,$$

$$JD_x^3\,D_y^3(f(x,y)) = 2^3\times3^3\times4qx^5 + 3^3\times4^3\times8qx^7 + 4^3\times4^3\times66pqx^8 - 4^3\times4^3\times20qx^8,$$

$$Q_{-2}\,JD_x^3\,D_y^3(f(x,y)) = 2^3\times3^3\times4qx^3 + 3^3\times4^3\times8qx^5 + 4^3\times4^3\times66pqx^6 - 4^3\times4^3\times20qx^6,$$

$$S_x^3 Q_{-2} J D_x^3 D_y^3(f(x,y)) = \frac{2^3\times 3^3\times 4}{3^3}qx^3 + \frac{3^3\times 4^3\times 8}{5^3}qx^5 + \frac{4^3\times 4^3\times 66}{6^3}pqx^6 - \frac{4^3\times 4^3\times 20}{6^3}qx^6 .$$

Now from the M-polynomial and table 1, we have

$$\begin{aligned} A(G) &= S_x Q_{-2} J D_x^3 D_y^3(f(x,y))\big|_{x=1} \\ &= \left(\frac{2^3\times 3^3\times 4}{3^3}qx^3 + \frac{3^3\times 4^3\times 8}{5^3}qx^5 + \frac{4^3\times 4^3\times 66}{6^3}pqx^6 - \frac{4^3\times 4^3\times 20}{6^3}qx^6\right)\Bigg|_{x=1} \\ &= \frac{11\ 264}{9}pq - \frac{798\ 752}{3\ 375}q. \end{aligned}$$

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