阿兹特克钻石的 M-多项式和拓扑指数

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摘要：为计算基于度的阿兹特克钻石拓扑指数，通过基本微积分计算了 Aztec 钻石的 M-多项式，并给出 9 类基于度的拓扑指数，即第 1 类萨格勒布指数、第 2 类萨格勒布指数、修正的第 2 类萨格勒布指数、Randić 和逆 Randić 指数、对称分割指数、调和指数、逆和指数和增强的萨格勒布指数.

关键词：阿兹特克钻石；萨格勒布指数；Randić指数；M-多项式

M-Polynomial and Topological Indices for Aztec Diamonds

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Abstract：In order to compute degree based topological indices for Aztec Diamonds, we compute M-polynomial for the Aztec Diamonds by applying fundamental calculus and obtain nine degree-based topological indices namely first Zagreb index, second Zagreb index, modified second Zagreb index, Randić and inverse Randić index, Symmetric division index, harmonic index, inverse sum index and augmented Zagreb index.

Key words：Aztec diamond；Zagreb index；Randić index；M-polynomial

1　Basic Knowledge

Chemical graph theory is a subject which connects Mathematics, chemistry and graph theory. A topological index is a numeric number associated with molecular graph and this number correlate certain physio-chemical properties of chemical compounds. The topological indices such as the Wiener index, first and second Zagreb index, modified Zagreb index, Randić index and symmetric division index, Harmonic index, Invers sum index, Augmented Zagreb index, etc. are useful in prediction of bioactivity of the chemical compounds[1]. These indices capture the overall structure of compound and predict chemical properties such as strain energy, heat of formation, and boiling points etc.

Algebraic polynomials have many useful applications in chemistry. For instance, Hosoya Polynomial (also called Wiener polynomial) plays a vital role in determining distance-based topological indices. M-polynomial[2] introduced in 2015, plays the same role in determining many degree-based topological indices[3-4].

Throughout this paper, G denotes connected graph, $V(G)$ and $E(G)$ denotes the vertex set and the edge set and d_v denotes the degree of a vertex.

Definition 1[2]　The M-polynomial of G is defined as：

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

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

The first well-known topological index in chemistry was introduced by Wiener when he was studying boiling point of paraffin. He named it the path number, which is now known as Wiener index. The first degree based topological index is Randić index denoted by $R_{-1/2}(G)$ and introduced by Milan Randić [5] in 1975. The Randić index is defined as：

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

In 1998, working independently, Bollobas and Erdos[6] and Amic et al. [7] proposed the generalized Randić index and has been studied extensively by both chemist and mathematicians.

The general Randić index defined as：

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

Obviously $R_{-1/2}(G)$ is the particular case of $R_\alpha(G)$ when $\alpha = -1/2$.

Ivan Gutman and Trinajstić introduced first Zagreb index and second Zagreb index, which are defined as： $M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$ and $M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v)$ respectively. The second modified Zagreb index was defined as：

$$^mM_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}.$$

For detail about these indices we refer[8-12] to the readers.

The Symmetric division index is defined as：

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

The following table 1 relates some well-known degree-based topological indices with M-polynoimal[2].

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

Topological Index	Derivation from $M(G; x, y)$
First Zagreb	$(D_x + D_y)(M(G; x, y))\big|_{x=y=1}$
Second Zagreb	$(D_x D_y)(M(G; x, y))\big|_{x=y=1}$
Second Modified Zagreb	$(S_x S_y)(M(G; x, y))\big|_{x=y=1}$
General Randić $\alpha \in N$	$(D_x^\alpha D_y^\alpha)(M(G; x, y))\big|_{x=y=1}$
Symmetric Division Index	$(D_x S_y + S_x D_y)(M(G; x, y))\big|_{x=y=1}$
Harmonic Index	$2S_x J(M(G; x, y))_{x=1}$
Inverse sum Index	$S_x J D_x D_y(M(G; x, y))_{x=1}$
Augmented Zagreb Index	$S_x^3 Q_{-2} J D_x^3 D_y^3(M(G; x, y))_{x=1}$

Here $D_x = x\dfrac{\partial f(x, y)}{\partial x}$, $D_y = y\dfrac{\partial f(x, y)}{\partial y}$, $S_x = \int_0^x \dfrac{f(t, y)}{t}\mathrm{d}t$, $S_y = \int_0^y \dfrac{f(x, t)}{t}\mathrm{d}t$, $J(f(x, y)) = f(x, x)$ and $Q_\alpha(f(x, y)) = x^\alpha f(x, y)$.

In this paper, we will derive M-polynomial of Aztec diamonds and with the help of this polynomial we calculate nine degree-based topological indices.

2 Main Results

Theorem 1 Let $AZ(n)$ be the graph of Aztec Diamonds. Then the M-polynomial of $AZ(n)$ is

$M(AZ(n)；x，y) = 8x^2y^3 + 4x^3y^4 + (8n-8)x^2y^4 + (4n^2-4)x^4y^4.$

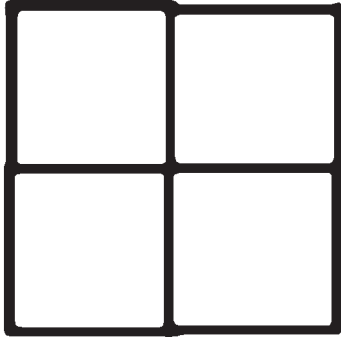**Proof**　Let $AZ(n)$ be the Aztec Diamonds shown in Figure 1，2，3，4.
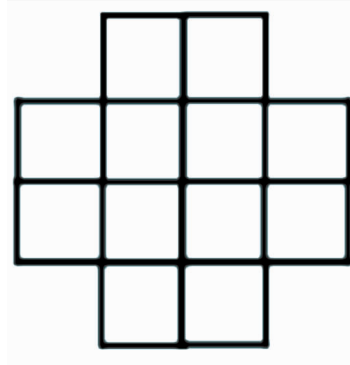

Figure 1　The structure of *AZ*(1)
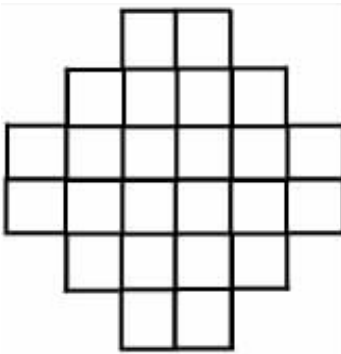

Figure 2　The structure of *AZ*(2)

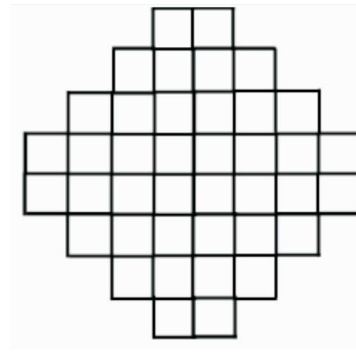**Figure 3　The structure of *AZ*(3)**

Figure 4　The structure of *AZ*(4)

It can be observed easily that the number of vertices in $AZ(n)$ are $2n^2 + 6n + 1$. The total number of edges in $AZ(n)$ are $4n^2 + 8n$ and we have four partitions of the edge set based on degrees of end vertices of each edge：

$$E_1(AZ(n)) = \{uv \in E(AZ(n))；d_u = 2 \text{ and } d_v = 3\};$$
$$E_2(AZ(n)) = \{uv \in E(AZ(n))；d_u = 3 \text{ and } d_v = 4\};$$
$$E_3(AZ(n)) = \{uv \in E(AZ(n))；d_u = 2 \text{ and } d_v = 4\};$$
$$E_4(AZ(n)) = \{uv \in E(AZ(n))；d_u = 4 \text{ and } d_v = 4\}.$$

Then　　$|E_1(AZ(n))| = 8$，$|E_2(AZ(n))| = 4$，$|E_3(AZ(n))| = 8n - 8$ and $|E_4(AZ(n))| = 4n^2 - 4$.

Now，we have

$$
\begin{aligned}
M(AZ(n)；x，y) &= \sum_{\delta \leqslant i \leqslant j \leqslant \Delta} m_{ij}x^iy^j \\
&= \sum_{2 \leqslant 3} m_{23}x^2y^3 + \sum_{3 \leqslant 4} m_{34}x^3y^4 + \sum_{2 \leqslant 4} m_{24}x^2y^4 + \sum_{4 \leqslant 4} m_{44}x^4y^4 \\
&= \sum_{uv \in E_1(AZ(n))} m_{23}x^2y^3 + \sum_{uv \in E_2(AZ(n))} m_{34}x^3y^4 + \sum_{uv \in E_3(AZ(n))} m_{24}x^2y^4 + \sum_{uv \in E_4(AZ(n))} m_{44}x^4y^4 \\
&= |E_1(AZ(n))|x^2y^3 + |E_2(AZ(n))|x^3y^4 + |E_3(AZ(n))|x^2y^4 + |E_4(AZ(n))|x^4y^4 \\
&= 8x^2y^3 + 4x^3y^4 + (8n-8)x^2y^4 + (4n^2-4)x^4y^4.
\end{aligned}
$$

From above M-polynomial we calculate some degree-based topological indices in the following proposition.

Proposition 1　Let $AZ(n)$ be the Aztec Diamonds. Then

$$M_1(AZ(n)) = 32n^2 + 48n - 12，$$
$$M_2(AZ(n)) = 64n^2 + 64n - 56，$$
$$M_2^m(AZ(n)) = \frac{n^2}{4} + n + \frac{5}{12}，$$

$$R_\alpha(AZ(N)) = 8 \times 6^\alpha + 4 \times 12^\alpha + (8n-8) \times 8^\alpha + (4n^2-4)16\alpha,$$

$$SSD\ (AZ\ (N)) = 8 \times n^2 + 20 \times n + \frac{40}{3},$$

$$H(AZ(N)) = n^2 + \frac{8n}{3} + \frac{176}{105},$$

$$I(G) = \frac{n^2-1}{2} + \frac{4(n-1)}{3} + \frac{76}{35},$$

$$A(G) = (2\,038)2^n - 931.$$

Proof　Let $M(AZ\ (n);\ x,\ y) = f(x,\ y) = 8x^2 y^3 + 4x^3 y^4 + (8n-8)x^2 y^4 + (4n^2-4)x^4 y^4.$ Then

$$D_x f(x,\ y) = 16x^2 y^3 + 12x^3 y^4 + 2(8n-8)x^2 y^4 + 4(4n^2-4)x^4 y^4,$$

$$D_y f(x,\ y) = 24x^2 y^3 + 16x^3 y^4 + 4(8n-8)x^2 y^4 + 4(4n^2-4)x^4 y^4,$$

$$D_y D_x f(x,\ y) = 48x^2 y^3 + 12x^3 y^4 + 8(8n-8)x^2 y^4 + 16(4n^2-4)x^4 y^4,$$

$$S_y(f(x,y)) = \frac{8x^2 y^3}{3} + x^3 y^4 + 2(n-1)x^2 y^4 + (n^2-1)x^4 y^4,$$

$$S_x S_y(f(x, KG-*5y)) = \frac{4x^2 y^3}{3} + \frac{x^3 y^4}{3} + (n-1)x^2 y^4 + \frac{(n^2-1)x^4 y^4}{4},$$

$$D_y^\alpha(f(x,y)) = 3^\alpha(8x^2 y^3) + 4^\alpha(4x^3 y^4) + 4^\alpha(8n-8)(x^2 y^4) + 4^\alpha(4n^2-4)(x^2 y^3),$$

$$S_y^\alpha(f(x,y)) = \frac{8x^2 y^3}{3^\alpha} + \frac{4x^3 y^4}{4^\alpha} + \frac{(8n-8)x^2 y^4}{4^\alpha} + \frac{(4n^2-4)x^4 y^4}{4^\alpha},$$

$$S_x^\alpha S_y^\alpha(f(x,y)) = \frac{8x^2 y^3}{6^\alpha} + \frac{4x^3 y^4}{12^\alpha} + \frac{(8n-8)x^2 y^4}{8^\alpha} + \frac{(4n^2-4)x^4 y^4}{16^\alpha},$$

$$S_y D_x(f(x,y)) = \frac{16x^2 y^3}{3} + 3x^3 y^4 + \frac{2(8n-8)x^2 y^4}{2} + (4n^2-4)x^4 y^4,$$

$$S_x D_y(f(x,y)) = 12x^2 y^3 + \frac{16x^3 y^4}{3} + 2(8n-8)x^2 y^4 + (4n^2-4)x^4 y^4,$$

$$Jf(x,y) = 8x^5 + 4x^7 + (8n-8)x^6 + (4n^2-4)x^8,$$

$$S_x Jf(x,y) = \frac{8}{5}x^5 + \frac{4}{7}x^7 + \frac{4(n-1)}{3}x^6 + \frac{(n^2-1)}{2}x^8,$$

$$JD_x D_y f(x,y) = 48x^5 + 48x^7 + 2(8n-8)x^6 + 16(4n^2-4)x^8,$$

$$S_x JD_x D_y f(x,y) = \frac{48x^5}{5} + \frac{48x^7}{7} + \frac{(8n-8)x^6}{3} + 2(4n^2-4)x^8,$$

$$D_y^3 f(x,y) = 216x^2 y^3 + 256x^3 y^4 + 64(8n-8)x^2 y^4 + 64(4n^2-4)x^4 y^4,$$

$$\begin{aligned} D_x^3 D_y^3 f(x,y) &= 3^3 \times 2^3(8x^2 y^3) + 3^3 \times 4^3(4x^3 y^4) + 2^3 \times 4^3(8n-8)(x^2 y^4) + 4^3 \times 4^3(4n^2-4)(x^4 y^4) \\ &= 1\,728(x^2 y^3) + 6\,912(x^3 y^4) + 512(8n-8)(x^2 y^4) + 4\,096(4n^2-4)(x^4 y^4), \end{aligned}$$

$$JD_x^3 D_y^3 f(x,y) = 1\,728x^5 + 6\,912x^7 + 4\,096(n-1)x^6 + 16\,384(n^2-1)x^8,$$

$$Q_{-2} JD_x^3 D_y^3 f(x,y) = 1\,728x^3 + 6\,912x^5 + 4\,096(n-1)x^4 + 16\,384(n^2-1)x^6,$$

$$S_{x^3} Q_{-2} JD_x^3 D_y^3 f(x,y) = 64x^3 + \frac{110\,592x^5}{125} + 64(n-1)x^4 + \frac{2\,048(n^2-1)x^6}{27}.$$

1）First Zagreb Index

$$M_1(G) = (D_x + D_y)f(x,y)\big|_{x=y=1} = 48n + 32n^2 - 12.$$

2）Second Zagreb Index

$$M_2(G) = D_y D_x(f(x,y))\big|_{x=y=1} = 64n^2 + 64n - 68.$$

3）Modified Second Zagreb Index

$$^m M_2(G) = S_x S_y(f(x,y))\big|_{x=y=1} = \frac{n^2}{4} + n + \frac{5}{12}.$$

4）Generalized Randić Index

$$R_\alpha(G) = D_x^\alpha D_y^\alpha(f(x,y))\big|_{x=y=1} = 8\times 6^\alpha + 4\times 12^\alpha + (8n-8)\times 8^\alpha + (4n^2-4)16^\alpha.$$

5）Inverse Randić Index

$$R_\alpha(G) = S_x^\alpha S_y^\alpha(f(x,y))\big|_{x=y=1} = \frac{8}{6^\alpha} + \frac{4}{12^\alpha} + \frac{8n-8}{8^\alpha} + \frac{4n^2-4}{16^\alpha}.$$

6）Symmetric Division Index

$$SSD(G) = (S_y D_x + S_x D_y)(f(x,y))\big|_{x=y=1} = 8n^2 + 20n + \frac{40}{3}.$$

7）Harmonic Index

$$H(G) = 2S_x J(f(x,y))\big|_{x=1} = n^2 + \frac{8n}{3} + \frac{71}{105}.$$

8）Inverse Sum Index

$$I(G) = S_x J D_x D_y(f(x,y))_{x=1} = 8n^2 + \frac{8n}{3} + \frac{608}{105}.$$

9）Augmented Zargreb Index

$$A(G) = S_x^3 Q_{-2} J D_x^3 D_y^3(f(x,y))\big|_{x=1} = \left(\frac{2\,048}{27}\right)n^2 + 64n - \frac{69\,376}{3\,375}.$$

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