

# 纳米管 $TUC_4C_8(S)$ 和纳米环 $TC_4C_8(S)$ 的拓扑指数<sup>①</sup>

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**摘要:** 化合物、材料和药物的生物化学性质与其分子结构有密切的关联, 通过化学拓扑指数的计算可了解化合物的性质. 作为一类重要的化学参数, Szeged 指数和修改的 Szeged 指数并广泛用于各类化学与制药学工程应用中. 通过边划分方法, 给出纳米管  $TUC_4C_8(S)$  和纳米环  $TC_4C_8(S)$  的若干基于距离的拓扑指数.

**关 键 词:** 理论化学; Szeged 指数; 修改的 Szeged 指数; 纳米管

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近年来, 化学图论作为化学和数学的交叉学科越来越受到广大学者的重视. 其模型是用图结构来表示分子, 原子用顶点来表示, 原子之间的化学键用边来表示. 通过对这些指数的研究, 人们可以在不做任何化学实验的前提下了解化合物或者药物的某种性质. 相关内容可参考文献[1-10]. 设  $G$  是一个图, 用  $V(G)$  和  $E(G)$  来表示它的顶点集合和边集. 本文所考虑的图均为无向、简单、有限图, 文中涉及标记和符号若没有特别定义则与文献[11]一致.

对图中的任意一条边  $e = uv$ , 设

$$\begin{aligned} n_u(e) &= |\{x \mid x \in V(G), d(u, x) < d(v, x)\}| \\ n_v(e) &= |\{x \mid x \in V(G), d(u, x) > d(v, x)\}| \\ m_u(e) &= |\{x \mid x \in E(G), d(u, x) < d(v, x)\}| \\ m_v(e) &= |\{x \mid x \in E(G), d(u, x) > d(v, x)\}| \end{aligned}$$

则, Szeged 指数和边 Szeged 指数分别定义为

$$\begin{aligned} Sz(G) &= \sum_{e=uv} n_u(e)n_v(e) \\ Sz_e(G) &= \sum_{e=uv} m_u(e)m_v(e) \end{aligned}$$

对应的 Szeged 多项式和边 Szeged 多项式分别定义为

$$Sz(G, x) = \sum_{e=uv} x^{n_u(e)n_v(e)}, Sz_e(G, x) = \sum_{e=uv} x^{m_u(e)m_v(e)}$$

再设

$$\begin{aligned} n(e) &= |\{x \mid x \in V(G), d(u, x) = d(v, x)\}| \\ m(e) &= |\{x \mid x \in E(G), d(u, x) = d(v, x)\}| \end{aligned}$$

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从而修改的 Szeged 指数和修改的边 Szeged 指数分别为

$$Sz^*(G) = \sum_{e=uv} \left( n_u(e) + \frac{n(e)}{2} \right) \left( n_v(e) + \frac{n(e)}{2} \right)$$
$$Sz_e^*(G) = \sum_{e=uv} \left( m_u(e) + \frac{m(e)}{2} \right) \left( m_v(e) + \frac{m(e)}{2} \right)$$

Graovac 和 Ghorbani<sup>[12]</sup> 定义了第二类化学键连通指数(atom-bond connectivity index, 简称 ABC 指数):

$$ABC_2(G) = \sum_{e=uv} \sqrt{\frac{n_u(e) + n_v(e) - 2}{n_u(e)n_v(e)}}$$

而第三类化学键连通指数则为

$$ABC_3(G) = \sum_{e=uv} \sqrt{\frac{m_u(e) + m_v(e) - 2}{m_u(e)m_v(e)}}$$

顶点  $PI$  指数和边  $PI$  指数分别为

$$PI_v(G) = \sum_{e=uv} (n_u(e) + n_v(e))$$
$$PI(G) = \sum_{e=uv} (m_u(e) + m_v(e))$$

它们对应的多项式为

$$PI_v(G, x) = \sum_{e=uv} x^{n_u(e) + n_v(e)}$$
$$PI(G, x) = \sum_{e=uv} x^{m_u(e) + m_v(e)}$$

Aouchiche 和 Hansen<sup>[13]</sup> 定义了正则修改的 Szeged 指数为

$$Sz_s^*(G) = \sqrt{\frac{Sz^*(G)}{|E(G)|}}$$

纳米管  $TUC_4C_8(S) = T[p, q]$  和纳米环  $TC_4C_8(S) = S[p, q]$  的结构如图 1 和图 2 所示, 其中  $p, q$  分别表示每一行和每一列中八角形的个数.

易知  $|V(T[p, q])| = |V(S[p, q])| = 8pq$ ,  $|E(T[p, q])| = 12pq - 2p$ ,  $|E(S[p, q])| = 12pq$ . 下面将给出纳米管  $TUC_4C_8(S) = T[p, q]$  和纳米环  $TC_4C_8(S) = S[p, q]$  的若干拓扑指数.

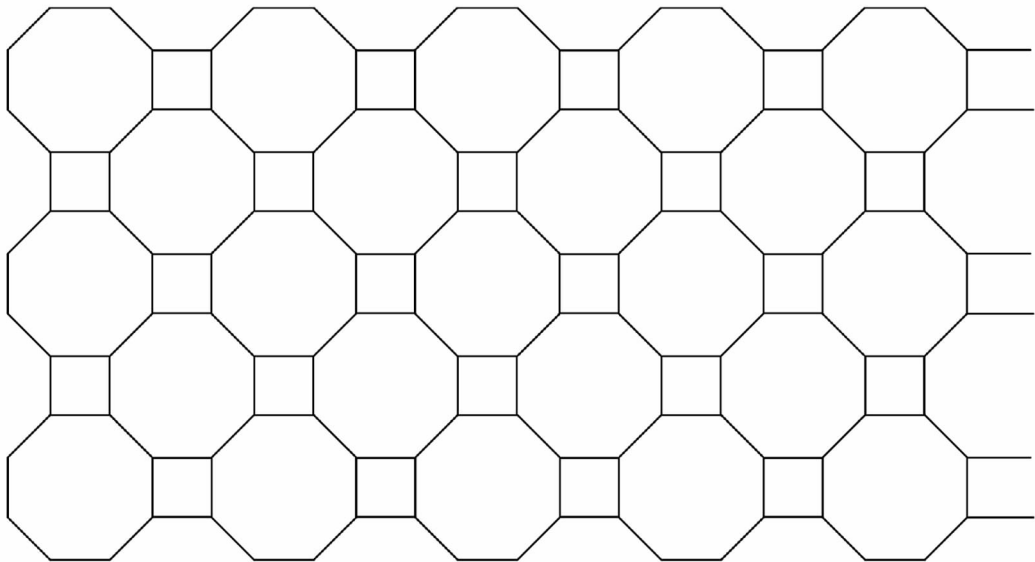
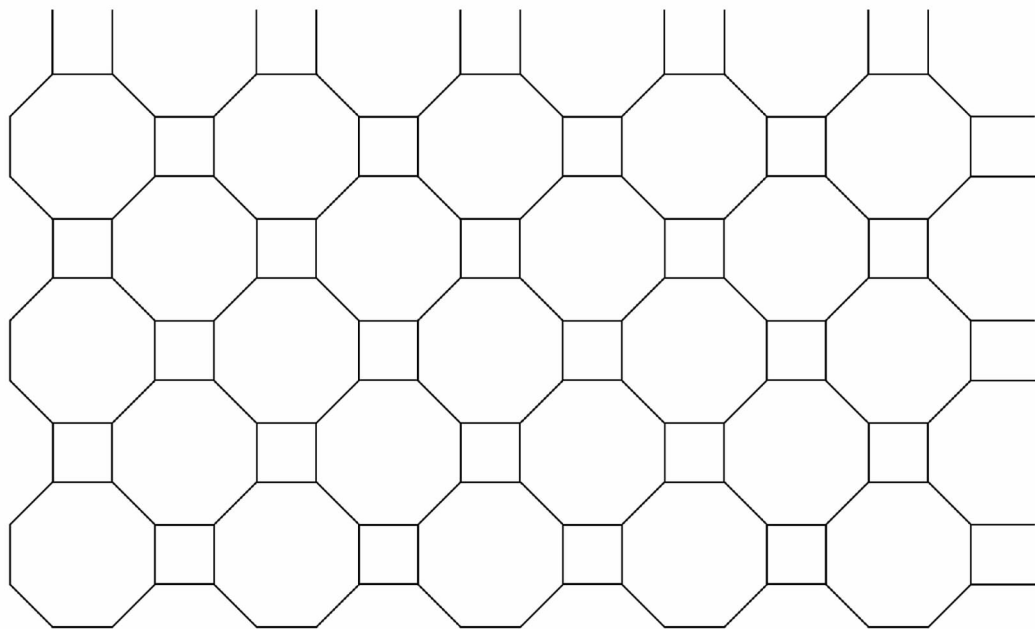


图 1  $p = 5$  和  $q = 3$  时的纳米管  $TUC_4C_8(S)$

图 2  $p = 5$  和  $q = 3$  时的纳米环  $TC_4C_8(S)$ 

主要结论及证明

**定理 1** 设  $TUC_4C_8(S) = T[p, q]$ , 则

$$Sz(T[p, q]) = Sz^*(T[p, q]) = \begin{cases} -4p^4q + \frac{320}{3}p^3q^3 + 16p^3q^2 - \frac{32}{3}p^3q + 32p^2q^3 + 4p^2q \\ + \frac{32}{3}pq^4 - \frac{8}{3}pq^2 - \frac{64}{5}q^5 + \frac{16}{3}q^3 - \frac{8}{5}q & \text{若 } p \leq \frac{q}{2} \\ \frac{320}{3}p^3q^3 - \frac{32}{3}p^3q - \frac{64}{3}q^5 + \frac{16}{3}q^3 & \text{若 } p > \frac{q}{2} \end{cases}$$

$$Sz(T[p, q], x) = \begin{cases} 4pqx^{16p^2q^2} + 2 \sum_{i=1}^{2q} x^{(p+i-1)(p+i)(8pq-(p+i-1)(p+i))} + 2p \sum_{i=1}^{2q-1} x^{4pi(8pq-4pi)} & \text{若 } p \leq \frac{q}{2} \\ 4pqx^{16p^2q^2} + 2 \sum_{i=1}^{2q} x^{(4q^2+2q-4iq)(8pq-(4q^2+2q-4iq))} + 2p \sum_{i=1}^{2q-1} x^{4pi(8pq-4pi)} & \text{若 } p > \frac{q}{2} \end{cases}$$

$$Sz_e(T[p, q], x) = 4pqx^{(6pq-p-q)^2} + \sum_{uv \in E_2(T[p, q])} x^{m_u(e)m_v(e)} + 2p \sum_{i=0}^{2q-2} x^{(4p+6pi)(12pq-8p-6pi)}$$

$$Sz_e^*(T[p, q]) = 4pq(6pq-p)^2 + \sum_{uv \in E_2(T[p, q])} (m_u(e) + \frac{m(e)}{2})(m_v(e) + \frac{m(e)}{2}) +$$

$$2p \sum_{i=0}^{2q-2} (5p+6pi)(12pq-7p-6pi)$$

$$ABC_2(T[p, q]) = \begin{cases} \sqrt{8pq-2} + 2 \sum_{i=1}^{2q} \sqrt{\frac{8pq-2}{(p+i-1)(p+i)(8pq-(p+i-1)(p+i))}} + 2p \sum_{i=1}^{2q-1} \sqrt{\frac{8pq-2}{4pi(8pq-4pi)}}, & \text{若 } p \leq \frac{q}{2} \\ \sqrt{8pq-2} + 2 \sum_{i=1}^{2q} \sqrt{\frac{8pq-2}{(4q^2+2q-4iq)(8pq-(4q^2+2q-4iq))}} + 2p \sum_{i=1}^{2q-1} \sqrt{\frac{8pq-2}{4pi(8pq-4pi)}}, & \text{若 } p > \frac{q}{2} \end{cases}$$

$$ABC_3(T[p, q]) = \frac{4pq}{6pq-p-q} \sqrt{12pq-2p-2q-2} +$$

$$\sum_{uv \in E_2(T[p, q])} \sqrt{\frac{m_u(e) + m_v(e) - 2}{m_u(e)m_v(e)}} + 2p \sum_{i=0}^{2q-2} \sqrt{\frac{12pq-4p-2}{(4p+6pi)(12pq-8p-6pi)}}$$

$$PI_v(T[p, q]) = 96p^2q^2 - 16p^2q$$

$$PI(T[p, q]) = 4pq(24pq - 12p - 2q) + 8p^2 + \sum_{uv \in E_2(T[p, q])} (m_u(e) + m_v(e))$$

$$PI_v(T[p, q], x) = (12pq - 2p)x^{8pq}$$

$$PI(T[p, q], x) = 4pqx^{12pq-2p-2q} + \sum_{uv \in E_2(T[p, q])} x^{m_u(e)+m_v(e)} + 2p(2q-1)x^{12pq-4p}$$

$$Szs^*(T[p, q]) = \begin{cases} ((-4p^4q + \frac{320}{3}p^3q^3 + 16p^3q^2 - \frac{32}{3}p^3q + 32p^2q^3 + 4p^2q + \frac{32}{3}pq^4 \\ - \frac{8}{3}pq^2 - \frac{64}{5}q^5 + \frac{16}{3}q^3 - \frac{8}{5}q)/(12pq - 2p))^{\frac{1}{2}}, & \text{若 } p \leq \frac{q}{2} \\ \sqrt{\frac{\frac{320}{3}p^3q^3 - \frac{32}{3}p^3q - \frac{64}{3}q^5 + \frac{16}{3}q^3}{12pq - 2p}}, & \text{若 } p > \frac{q}{2} \end{cases}$$

**证** 本结论的证明主要运用边划分技术完成. 将  $T[p, q]$  的边集合划分成 3 个子类:  $E_1(T[p, q])$ ,  $E_2(T[p, q]) = \bigcup_{k=1}^{2q} e_{2,k}$ ,  $E_3(T[p, q])$ , 且用  $e_1, e_2, e_3$  来分别代表 3 个边集合中的边. 三类边的定义可见图 3, 图 4 和图 5 中虚线所通过的部分.

因此, 在计算拓扑指数时, 可分别考虑 3 个边子集合中边  $e = uv$  对应的  $n_u(e)$ ,  $n_v(e)$ ,  $m_u(e)$  和  $m_v(e)$ .

1) 对于  $e = uv \in E_1(T[p, q])$ , 有  $n_u(e) = n_v(e) = \frac{|V(T[p, q])|}{2} = 4pq$ ,  $m_u(e) = m_v(e) =$

$$\frac{|E(T[p, q])| - 2q}{2} = 6pq - p - q, n(e) = 0, m(e) = 2q, |E_1(T[p, q])| = 4pq.$$

2) 对于  $e = uv \in E_2(T[p, q])$ . 当  $p \leq \frac{q}{2}$  时, 对每个  $e_{2,i} = uv$  有  $n(e) = 0$ ,  $n_u(e) = (p + i - 1)$

$(p + i)$ ,  $n_v(e) = 8pq - (p + i - 1)(p + i)$ ; 当  $p > \frac{q}{2}$  时, 对每个  $e_{2,i} = uv$  有  $n(e) = 0$ ,  $n_u(e) = 4q^2 +$

$2q - 4iq$ ,  $n_v(e) = 8pq - (4q^2 + 2q - 4iq)$ .

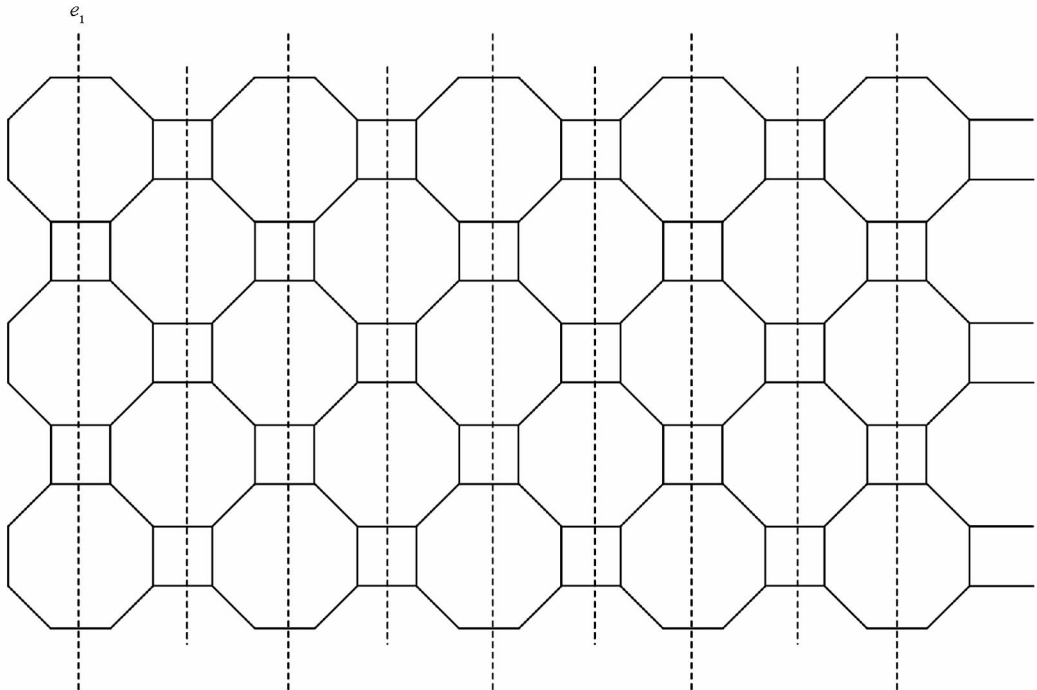


图 3 集合  $E_1(T[p, q])$

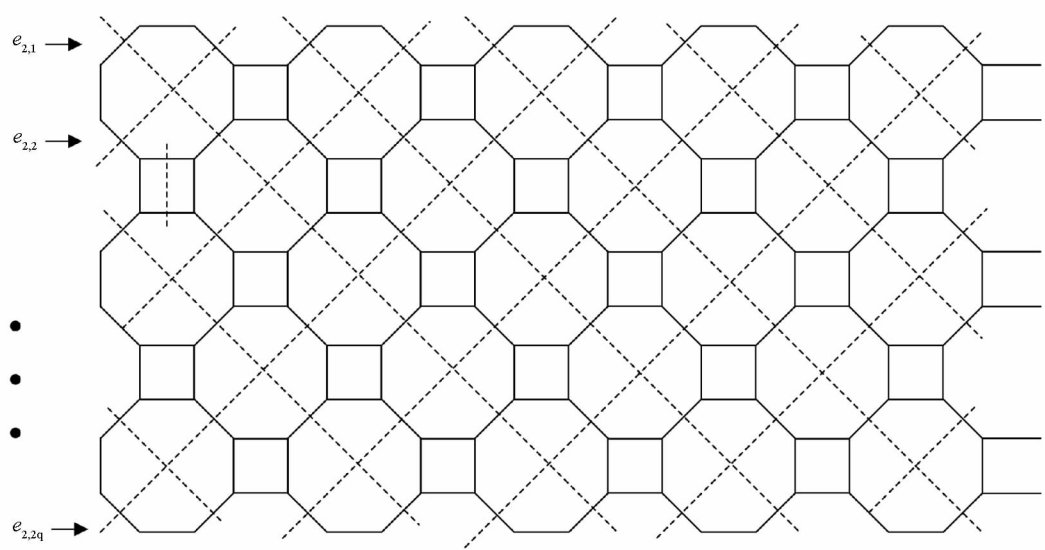


图 4 集合  $E_2(T[p, q])$

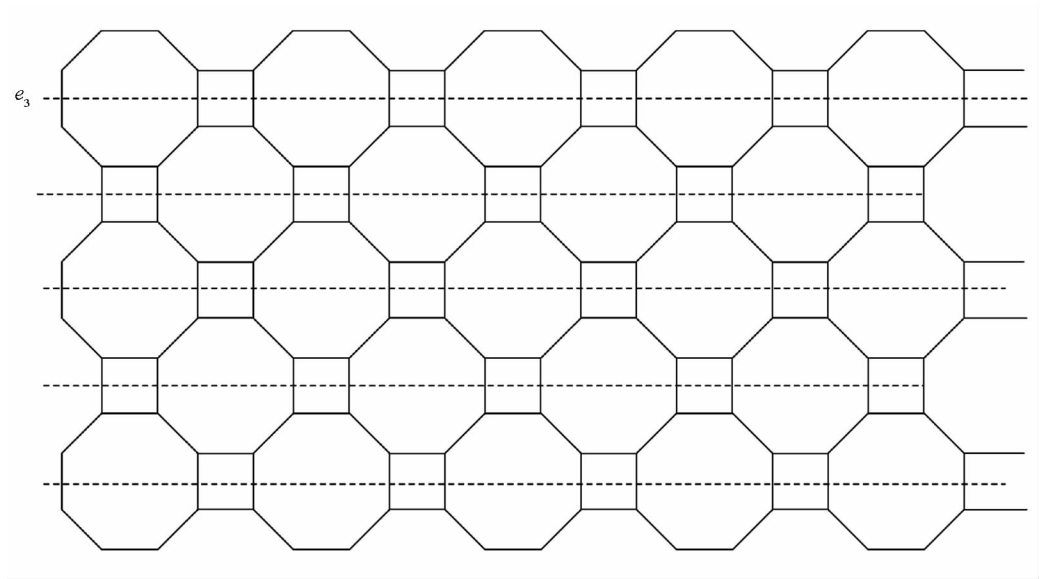


图 5 集合  $E_3(T[p, q])$

若  $i$  为奇数且  $1 \leq i \leq q$ , 则对于  $e_{2,i} = uv$  有

$$m_v(e) = \begin{cases} \left( (p+i-1)2 + \left\lfloor \frac{p^2}{2} \right\rfloor + (i-1)p + \frac{(i-1)^2}{2} \right) & p < 2q - 2 \left\lfloor \frac{i-1}{2} \right\rfloor \\ 6pq - 6q^2 + (6i-4)q - 2p + 2 \left\lfloor \frac{p}{2} \right\rfloor - i + 1 & p \geq 2q - 2 \left\lfloor \frac{i-1}{2} \right\rfloor \end{cases}$$
$$m_u(e) = \begin{cases} (12pq - 2p) - m_v(e) - (2p + 2i - 2) & p < 2q - 2 \left\lfloor \frac{i-1}{2} \right\rfloor \\ (12pq - 2p) - m_v(e) - 4pq & p \geq 2q - 2 \left\lfloor \frac{i-1}{2} \right\rfloor \end{cases}$$
$$m(e) = \begin{cases} 2p + 2i - 2 & p < 2q - 2 \left\lfloor \frac{i-1}{2} \right\rfloor \\ 4pq & p \geq 2q - 2 \left\lfloor \frac{i-1}{2} \right\rfloor \end{cases}$$

若  $i$  为偶数且  $1 \leq i \leq q$ , 则对于  $e_{2,i} = uv$  有

$$m_v(e) = \begin{cases} (p+i-1)2 + \left\lfloor \frac{p^2+1}{2} \right\rfloor + (i-1)p + \frac{i(i-2)}{2} & p < 2q-2 \left\lfloor \frac{i-1}{2} \right\rfloor \\ 6pq - 6q^2 + (6i-4)q - 2p + 2 \left\lfloor \frac{p}{2} \right\rfloor - i & p \geq 2q-2 \left\lfloor \frac{i-1}{2} \right\rfloor \end{cases}$$

$$m_u(e) = \begin{cases} (12pq - 2p) - m_v(e) - (2p + 2i - 2) & p < 2q-2 \left\lfloor \frac{i-1}{2} \right\rfloor \\ (12pq - 2p) - m_v(e) - 4pq & p \geq 2q-2 \left\lfloor \frac{i-1}{2} \right\rfloor \end{cases}$$

$$m(e) = \begin{cases} 2p + 2i - 2 & p < 2q-2 \left\lfloor \frac{i-1}{2} \right\rfloor \\ 4pq & p \geq 2q-2 \left\lfloor \frac{i-1}{2} \right\rfloor \end{cases}$$

3) 对于  $e = uv \in E_3(T[p, q])$ , 可知每一行中这样的边共有  $2p$  条. 对于第  $i$  行中  $E_3(T[p, q])$  的边  $e = uv$ , 有  $n_u(e) = 4pi$ ,  $n_v(e) = 8pq - 4pi$ ,  $n(e) = 0$ ,  $m_u(e) = 4p + 6pi$ ,  $m_v(e) = 12pq - 8p - 6pi$ ,  $m(e) = 2p$ .

最后, 由拓扑指数的定义可得最后的结果.

**定理 2** 设  $TC_4C_8(S) = S[p, q]$ , 则

$$Sz(S[p, q]) = Sz^*(S[p, q]) = 192p^3q^3$$

$$Sz_e(S[p, q]) = 4pq(108p^2q^2 + p^2 + q^2 - 12pq(p+q+3r-1) + (3r-1)^2)$$

$$Sz(S[p, q], x) = 12pqx^{16p^2q^2}$$

$$Sz_e(S[p, q], x) = 4pqx^{(6pq-q)^2} + 4pqx^{(6pq+1-3r)^2} + 4pqx^{(6pq-p)^2}$$

$$Sz_e^*(S[p, q]) = 4pq(108p^2q^2 + p^2 + q^2 + 12pq(p+q+3r-1) + (3r-1)^2)$$

$$ABC_2(S[p, q]) = 3 \sqrt{8pq-2}$$

$$ABC_3(S[p, q]) = \frac{4pq}{6pq-q} \sqrt{12pq-2q-2} + \frac{4pq}{6pq+1-3r} \sqrt{12pq-6r} + \frac{4pq}{6pq-p} \sqrt{12pq-2p-2}$$

$$PI_v(S[p, q]) = 96p^2q^2$$

$$PI(S[p, q]) = 144p^2q^2 - 8pq(p+q+3r-1)$$

$$PI_v(S[p, q], x) = 12pqx^{8pq}$$

$$PI(S[p, q], x) = 4pqx^{12pq-2q} + 4pqx^{12pq+2-6r} + 4pqx^{12pq-2p}$$

$$Sz_s^*(S[p, q]) = 4pq$$

**证** 显然纳米环  $TC_4C_8(S) = S[p, q]$  为二部图, 对于任意  $e = uv \in E(S[p, q])$ , 有  $n_u(e) = n_v(e) = \left\lfloor \frac{V(S[p, q])}{2} \right\rfloor = 4pq$ ,  $n(e) = 0$ . 对于顶点与边的距离的计算, 依然采用边划分方法. 类似定理 1 的证明,

将  $E(S[p, q])$  划分成如图 6 虚线所示 3 个子集.

1) 对于  $e = uv \in E_1(S[p, q])$ , 有  $m_u(e) = m_v(e) = 6pq - q$ ,  $m(e) = 2q$ .

2) 对于  $e = uv \in E_2(S[p, q])$ , 有  $m_u(e) = m_v(e) = 6pq + 1 - 3r$ ,  $m(e) = 6r + 2$ , 其中  $r = \min\{p, q\}$ .

3) 对于  $e = uv \in E_3(S[p, q])$ , 有  $m_u(e) = m_v(e) = 6pq - p$ ,  $m(e) = 2p$ .

进而, 由拓扑指数的定义得到相应的结果.

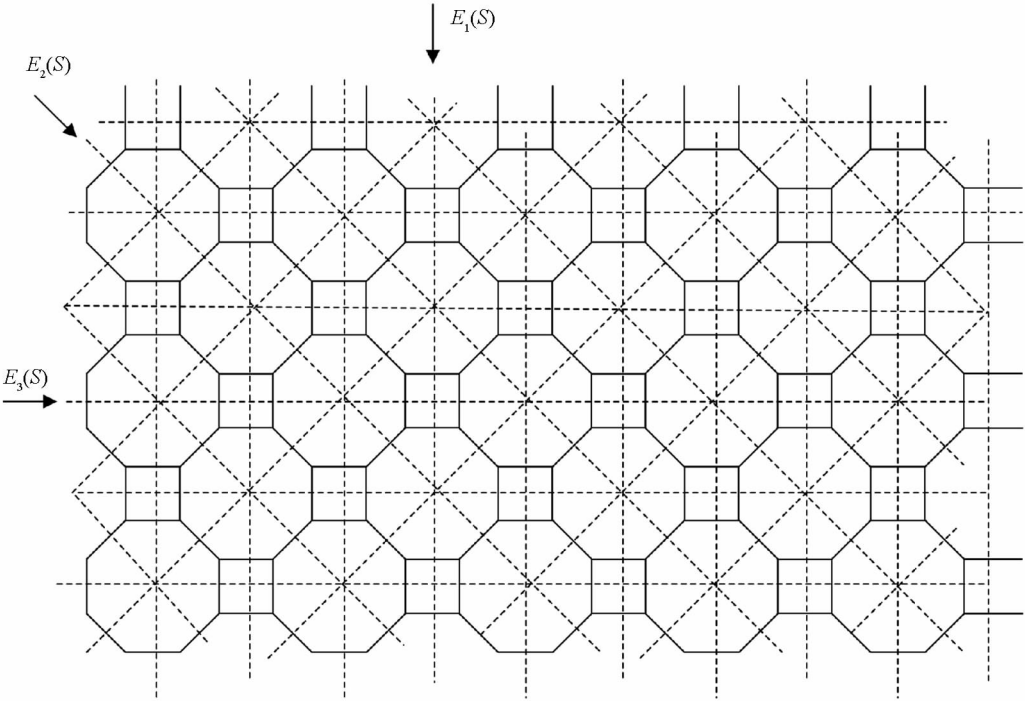


图 6 纳米环  $TC_4C_8(S) = S[p, q]$  的边划分

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## On Topological Index of Nanotube $TUC_4C_8(S)$ and Nanotori $TC_4C_8(S)$

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**Abstract:** The biochemical properties of compounds, materials and drugs are closely related to their molecular structure; thus the properties of the compounds can be learned by the calculation of the chemical topological index. As a class of parameter of chemical, Szeged index and revised Szeged index have been widely used in various chemical and pharmaceutical engineering. The distance—based indices of nanotube  $TUC_4C_8(S)$  and nanotori  $TC_4C_8(S)$  are studied by means of edge dividing method.

**Key words:** Theoretical Chemical; Szeged index; revised Szeged index; Nanostar

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