

# V-苯烯纳米管的逆基于度的拓扑指数

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**摘要:** 在数学化学中, 无需在实验室中进行实验就可以定义几种拓扑指数来推测化合物的性质. 而使用一个单一的拓扑指数则无法描述相关化合物的所有特性, 但是它们一起在某种程度上可起到预测化学性质的作用, 因此总是有空间定义新的索引. 基于此, 引进了一些新的基于度的拓扑指数, 同时利用图分析的方法对 V-苯烯纳米管计算了这些指数.

**关键词:** 数学化学; 拓扑指数; 萨格勒布指数; V-苯烯纳米管

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## Reverse Degree-based Topological Indices for V-Phenylenic Nanotube

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**Abstract:** In mathematical chemistry, several topological indices are defined to guess the properties of chemical compounds without performing experiments in the lab. No single topological index describes all the properties of concerned compound but together they made it, up to some extent, hence there is always space to define new indices. In this paper, we introduce some new degree-based topological indices and compute for V-Phenylenic Nanotubes by means of graph analysis.

**Key words:** mathematical chemistry; Topological index; Zagreb index; V-Phenylenic nanotubes

In mathematical chemistry, the tools of mathematics, for example, polynomials and topological index help researchers to know properties of nanotubes without experiments. These mathematical tools depend on the symmetry of graphs of nanotubes<sup>[1-2]</sup>. It is a well-known fact that most of the properties of nanotubes, for example, heat of formation, boiling point, strain energy, rigidity and fracture toughness of a nanotube are directly connected to its graphical representation and this fact plays a very important role in chemical graph theory.

Many algebraic polynomials have useful applications in the field of chemistry, for instant, Hosoya polynomial help researchers to determine distance-based topological indices. Another algebraic polynomials is the M-polynomial<sup>[3]</sup>, that was introduced in year 2015 have same role as that of Hosoya polynomial for degree-based topological indices<sup>[4-5]</sup>.

The first topological index was introduced by Wiener<sup>[6]</sup> and it was named path number, which is now known as Wiener index. After the success of Wiener index, a series of topological indices has been defined. Due to need of new indices as described in abstract of this paper, reverse first and second Zagreb indices has been defined in [7]. In this paper, we defined reverse modified second Zagreb index, reverse symmetric division index, reverse harmonic index and reverse inverse sum index. Moreover we computed above mentioned topological indices for V-Phenylenic Nanotubes.

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1 Definitions

In this section, we give some definitions of reverse degree-based topological indices.

**Definition 1** (Reverse First Zagreb Index)

For a connected simple graph  $G$ , the reverse first Zagreb index is defined as:

$$CM_1(G) = \sum_{uv \in E(G)} c_u + c_v.$$

**Definition 2** (Reverse Second Zagreb Index)

For a connected simple graph  $G$ , the reverse second Zagreb index is defined as:

$$CM_2(G) = \sum_{uv \in E(G)} c_u \times c_v.$$

**Definition 3** (Reverse Second Modified Zagreb Index)

For a connected simple graph  $G$ , the reverse second modified Zagreb index is defined as:

$$C^m M_2(G) = \sum_{uv \in E(G)} \frac{1}{(c_u \times c_v)}.$$

**Definition 4** (Reverse Symmetric Division Index)

For a connected simple graph  $G$ , the reverse Symmetric division index is defined as:

$$CSDD(G) = \sum_{uv \in E(G)} \left\{ \frac{\min(c_u, c_v)}{\max(c_u, c_v)} + \frac{\max(c_u, c_v)}{\min(c_u, c_v)} \right\}.$$

**Definition 5** (Reverse Harmonic Index)

For a connected simple graph  $G$ , the reverse Harmonic index is defined as:

$$CH(G) = \sum_{uv \in E(G)} \frac{2}{c_u + c_v}.$$

**Definition 6** (Reverse Inverse Sum-Index)

For a connected simple graph  $G$ , the reverse Inverse Sum-index is defined as:

$$CI(G) = \sum_{uv \in E(G)} \frac{c_u \times c_v}{c_u + c_v}.$$

2 Main Results

The molecular graph of V-Pheylenic Nanotube is given in Figure 1.

The edge partition of V-Pheylenic Nanotube based on the degree of end vertices is given in Table 1.

The reverse degree based edge partition of V-Pheylenic Nanotube is given in Table 2, where

$c_v = \Delta(G) - d_v + 1$  and  $\Delta(G)$  is the maximum degree of the graph.

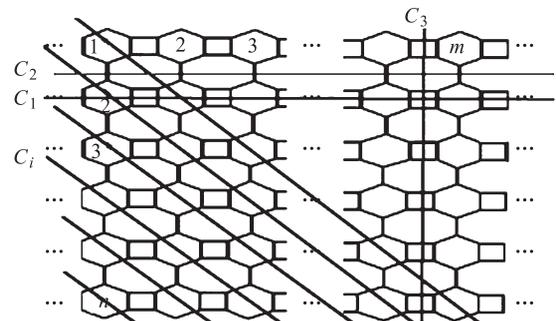


Figure1 Molecular graph of V-Phenylenic Nanotube

Table 1 Degree based edge partition of V-Pheylenic Nanotube

$(d_u, d_v)$ Where $uv \in E(VPHX[m, n])$	Number of Edges
(2,3)	$4m$
(3,3)	$m(9n - 5)$

Table 2 Reverse degree based edge division of V-Pheylenic Nanotube

$(c_u, c_v)$ Where $uv \in E(VPHY[m, n])$	Number of Edges
(2,1)	$4m$
(1,1)	$m(9n - 5)$

**Theorem 1** Let  $VPHX[m, n]$  be V-Pheylenic Nanotube. Then

$$CM(VPHX[m, n], x, y) = 4mx^2y + 9mnxy - 5mxy.$$

**Proof** By using the definition of reverse first Zagreb index and reverse edge partition of V-Phenylenic Nanotube given in Table 2, we have

$$\begin{aligned}
CM(VPHX[m, n], x, y) &= \sum_{uv \in E(VPHX[m, n])} Cm_{ij} x^i y^j \\
&= \sum_{uv \in E_1(VPHX[m, n])} Cm_{ij} x^i y^j + \sum_{uv \in E_2(VPHX[m, n])} Cm_{ij} x^i y^j \\
&= \sum_{uv \in E_1(VPHX[m, n])} x^2 y^1 + \sum_{uv \in E_2(VPHX[m, n])} x^1 y^1 \\
&= |CE_1(VPHX[m, n])| x^2 y^1 + |CE_2(VPHX[m, n])| x^1 y^1 \\
&= (4m)x^2 y + m(9n - 5)xy = 4mx^2 y + 9mnxy - 5mxy.
\end{aligned}$$

**Theorem 2** Let  $VPHX[m, n]$  be V-Pheyleneic Nanotube. Then

$$CM_1(VPHX[m, n]) = 2m(1 + 9n).$$

**Proof** By using the definition of reverse second Zagreb index and reverse edge partition of V-Phenyleneic Nanotube given in Table 2, we have

$$\begin{aligned}
CM_1(VPHX[m, n]) &= \sum_{uv \in E(VPHX[m, n])} (c_u + c_v) \\
&= \sum_{uv \in E_1(VPHX[m, n])} (c_u + c_v) + \sum_{uv \in E_2(VPHX[m, n])} (c_u + c_v) \\
&= \sum_{uv \in E_1(VPHX[m, n])} (2 + 1) + \sum_{uv \in E_2(VPHX[m, n])} (1 + 1) \\
&= 3|CE_1(VPHX[m, n])| + 2|CE_2(VPHX[m, n])| \\
&= 3(4m) + 2(m(9n - 5)) = 2m(1 + 9n).
\end{aligned}$$

**Theorem 3** Let  $VPHX[m, n]$  be V-Pheyleneic Nanotube. Then

$$CM_2(VPHX[m, n]) = 3m(1 + 3n).$$

**Proof** By using the definition of reverse modified second Zagreb index and reverse edge partition of V-Phenyleneic Nanotube given in Table 2, we have

$$\begin{aligned}
CM_2(VPHX[m, n]) &= \sum_{uv \in E(VPHX[m, n])} (c_u \times c_v) \\
&= \sum_{uv \in E_1(VPHX[m, n])} (c_u \times c_v) + \sum_{uv \in E_2(VPHX[m, n])} (c_u \times c_v) \\
&= \sum_{uv \in E_1(VPHX[m, n])} (2 \times 1) + \sum_{uv \in E_2(VPHX[m, n])} (1 \times 1) \\
&= 2|CE_1(VPHX[m, n])| + 1|CE_2(VPHX[m, n])| \\
&= 2(4m) + 1(m(9n - 5)) = 3m(1 + 3n).
\end{aligned}$$

**Theorem 4** Let  $VPHX[m, n]$  be V-Pheyleneic Nanotube. Then

$$C^m M_2(VPHX[m, n]) = 3m(3n - 1).$$

**Proof** By using the definition of reverse modified second Zagreb index and reverse edge partition of V-Phenyleneic Nanotube given in Table 2, we have

$$\begin{aligned}
C^m M_2(VPHX[m, n]) &= \sum_{uv \in E(VPHX[m, n])} \frac{1}{(c_u \times c_v)} \\
&= \sum_{uv \in E_1(VPHX[m, n])} \frac{1}{(c_u \times c_v)} + \sum_{uv \in E_2(VPHX[m, n])} \frac{1}{(c_u \times c_v)} \\
&= \sum_{uv \in E_1(VPHX[m, n])} \frac{1}{2 \times 1} + \sum_{uv \in E_2(VPHX[m, n])} \frac{1}{1 \times 1} \\
&= \frac{1}{2}|CE_1(VPHX[m, n])| + 1|CE_2(VPHX[m, n])| \\
&= \frac{1}{2}(4m) + 1(m(9n - 5)) = 3m(3n - 1).
\end{aligned}$$

**Theorem 5** Let  $VPHX[m, n]$  be V-Pheyleneic Nanotube. Then

$$CH(VPHX[m, n]) = \frac{m}{3}(27n - 7).$$

**Proof** By using the definition of reverse harmonic index and reverse edge partition of V-Phenyleneic Nanotube

given in Table 2, we have

$$\begin{aligned}
 CH(VPHX[m, n]) &= \sum_{uv \in E(VPHX[m, n])} \frac{2}{(c_u + c_v)} \\
 &= \sum_{uv \in E_1(VPHX[m, n])} \frac{2}{(c_u + c_v)} + \sum_{uv \in E_2(VPHX[m, n])} \frac{2}{(c_u + c_v)} \\
 &= \sum_{uv \in E_1(VPHX[m, n])} \frac{2}{2+1} + \sum_{uv \in E_2(VPHX[m, n])} \frac{2}{1+1} \\
 &= \frac{2}{3} |CE_1(VPHX[m, n])| + 1 |CE_2(VPHX[m, n])| \\
 &= \frac{2}{3}(4m) + 1(m(9n - 5)) = \frac{m}{3}(27n - 7).
 \end{aligned}$$

**Theorem 6** Let  $VPHX[m, n]$  be V-Phenylenic Nanotube. Then

$$CI(VPHX[m, n]) = \frac{m}{6}(1 + 27n).$$

**Proof** By using the definition of reverse inverse sum index and reverse edge partition of V-Phenylenic Nanotube given in Table 2, we have

$$\begin{aligned}
 CI(VPHX[m, n]) &= \sum_{uv \in E(VPHX[m, n])} \frac{c_u \times c_v}{(c_u + c_v)} \\
 &= \sum_{uv \in E_1(VPHX[m, n])} \frac{c_u \times c_v}{(c_u + c_v)} + \sum_{uv \in E_2(VPHX[m, n])} \frac{c_u \times c_v}{(c_u + c_v)} \\
 &= \sum_{uv \in E_1(VPHX[m, n])} \frac{2 \times 1}{2+1} + \sum_{uv \in E_2(VPHX[m, n])} \frac{1 \times 1}{1+1} \\
 &= \frac{2}{3} |CE_1(VPHX[m, n])| + \frac{1}{2} |CE_2(VPHX[m, n])| \\
 &= \frac{2}{3}(4m) + \frac{1}{2}(m(9n - 5)) = \frac{m}{6}(1 + 27n).
 \end{aligned}$$

### 3 Concluding Remarks

In this paper we have defined some new indices and computed for V-Phenylenic Nanotube. Our results will be a good addition in the field of chemical graph theory. To define reverse version of other degree based topological indices is an interesting problem.

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