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Computing Y-index of V-phenylenic nanostructures

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Abstract

Topological measures of molecular graph structure according to degree yield valuable tools that facilitate understanding material's characteristics through their structures involving physical, chemical, and biological properties. In this study, we have computed the Y-index and Y – *polynomial* for specific chemical structures, namely V-Phenylenic Nanotube and Nanotorus, as well as their molecular complement graphs. By analyzing the data from the computations using MATLAB, we were able to determine the connection between Y – *index*

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and Υ – *polynomial* describing the V-Phenylenic Nanotube and Nanotorus. This elucidation provided insight into the physicochemical properties inherent to these compounds.

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Keywords: *Y-index, V-Phenylenic nanotubes, V-Phenylenic nanotorus, Molecular graph, Molecular complement graph.*

1. Introduction

Within the field of chemical graph theory, topological indices are crucial molecular descriptors for establishing structure-property and structure-activity relationships that describe the structures of chemical compounds and aid in the prediction of specific physico-chemical properties [1, 2, 3]. These descriptors come in many different varieties, including those based on degree, distance, eigenvalues, matching, and mixed bases. The calculation of degree-based graph-theoretical indices has drawn increasing attention in the present period, highlighting how such indices impact meaningfully the scientific study of matters concerning chemistry. In our study, we have computed the degree-based topological descriptors of a specific nanostructure, utilizing them to provide insight into chemical reactivity and structural information. Thus, in this paper, we expound upon the structural analysis and mathematical derivation necessary to identify the Y-index and Y-polynomial values of the V-Phenylenic Nanotube and Nanotorus. The first and second Zagreb indices, which were originally defined in 1972 by Gutman and Trinajstić [4, 5], represent some of the earliest graph invariants in the field of chemical graph theory. These indices have been the subject of much research and study since their inception and have proven to be valuable tools for understanding the properties of molecular graphs. Specifically, Zagreb indices of order one and two are stipulated for a certain molecular graph Γ as follows:

$$M_1(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} [deg_\Gamma(\mu) + deg_\Gamma(\nu)],$$
$$M_2(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} deg_\Gamma(\mu)\, deg_\Gamma(\nu),$$

Furtula et al. [6] proposed a neglected topological index referred to as the F-index, establishing its formulation as follows:

$$F(\Gamma) = \sum_{\nu\in V(\Gamma)} deg_\Gamma^3(\nu) = \sum_{\mu\nu\in E(\Gamma)} (deg_\Gamma^2(\mu) + deg_\Gamma^2(\nu))$$

In [7, 8], Alameri et al. (2020) introduced the concepts of the Y-index and coindex, respectively, defining them as:

$$Y(\Gamma) = \sum_{\mu\nu\in E(\Gamma)} [deg_\Gamma^3(\mu) + deg_\Gamma^3(\nu)],$$
$$\overline{Y}(\Gamma) = \sum_{\mu\nu\notin E(\Gamma)} [deg_\Gamma^3(\mu) + deg_\Gamma^3(\nu)]$$

And in the same papers, the Y-index and coindex formulas of graph and complement graph Γ are investigated, and defined as:

$$Y(\overline{\Gamma}) = p(p-1)^4 - 8q(p-1)^3 + 6(p-1)^2 M_1(\Gamma) - 4(p-1)F(\Gamma) + Y(\Gamma), \quad (1)$$

$$\overline{Y}(\Gamma) = (p-1)F(\Gamma) - Y(\Gamma), \tag{2}$$

$$\overline{Y}(\overline{\Gamma}) = 4q(p-1)^3 - 3(p-1)^2 M_1(\Gamma) + 3(p-1)F(\Gamma) - Y(\Gamma), \tag{3}$$

The computation of the sadhana polynomial of V-phenylenic nanotubes and nanotori was examined by Ashrafi et al. [9] in 2008. Let the molecular graph of V-Phenylenic Nanotubes be represented as $\mathrm{F} = VPHX[q,p]$ with $|V(\mathrm{F})| = 6qp$ & $E(\mathrm{F})| = 9qp - q$, and let $\Upsilon = VPHY[q,p]$ be the graph of V-Phenylenic Nanotori with $|V(\Upsilon)| = 6qp$ & $|E(\Upsilon)| = 9qp$. ($\forall q,p \in \mathbb{N} - \{1\}$). Farahani et al. [10, 11, 12] computed the Zagreb, Hyper-Zagreb indices of F and Υ (Fig. 1,2) respectively, such as the follows:

$$M_1(\mathrm{F}) = 54qp - 10q, \qquad M_1(\Upsilon) = 54qp, \tag{4}$$

$$M_2(\mathrm{F}) = 81qp + 3q, \qquad M_2(\Upsilon) = 81qp, \tag{5}$$

$$HM(\mathrm{F}) = 4q(81n - 20), \qquad HM(\Upsilon) = 324qp, \tag{6}$$

$$HM_2(\mathrm{F}) = 9q(81n - 29), \qquad HM_2(\Upsilon) = 729qp. \tag{7}$$

Alsharafi and Alameri in [19] have computed $(F - index)$ of V-Phenylenic Nanotube and V-Phenylenic Nanotorus such as:

$$F(VPHX[q,p]) = 162qp - 38q. \qquad F(VPHX[q,p]) = 162qp. \tag{8}$$

Alamian et al. [13] introduced the concept of the PI Polynomial of V-Phenylenic Nanotubes and Nanotori, while Ahmad et al. [14] presented new results on eccentric connectivity indices of V-Phenylenic Nanotube. Other researchers [16, 17, 18, 19, 20] have also contributed to the study of various topological indices of Nano-Structures, including degree-based and distance-based topological descriptors. The importance of these structures in the field of mathematical chemistry is evidenced by the abundance of research articles in this area. Nano-tubes and Nano-torus are instrumental in a variety of applications, including but not limited to, energy storage, bioelectronics, and optoelectronics [15]. In this study, we focus on the Y-index and Y-polynomials of V-Phenylenic Nanotubes and Nanotori, as well as their complement graph structures. For improved illumination of the results, we offer a numerical comparison of our computed results, accompanied by illustrative figures, to enhance the understanding of our findings.

2. Main Results

2.1 *Quantifying Topological Indices for V-Phenylenic Nanotubes: A Study of the Y-Index and Co-Index*

Within this subsection, we undertake the computation of the $Y - index$ for select chemical structures, namely the line graphs of Phenylenic nanotubes denoted as $VPHX[q,p]$ for all q and p belonging to the set of natural numbers excluding 1, as well as their corresponding molecular complement Nano-structure. Additionally, our investigation extends to the examination of $Y - polynomial$ of V-Phenylenic Nanotubes.

Theorem 2.1.1: *Suppose that* $F = VPHX[q,p]$ *(See Fig. 1), then the* $(Y-index)$ *of* F *is given by*

$$Y(\mathrm{F}) = 486qp - 130q.$$

Proof: According to the concept of the Y-Index, we have

$$Y(\mathrm{F}) = \sum_{\mu\nu\in E(\mathrm{F})} [deg^3_{\mathrm{F}}(\mu) + deg^3_{\mathrm{F}}(\nu)],$$

The vertex and edge sets partitions $V(\mathrm{F})$ & $E(\mathrm{F})$ are given in (Table 1.) [12], such that for a connected graph $\mathrm{F} = (V(\mathrm{F}), E(\mathrm{F}))$ with

$$deg = Max[deg(\nu)|\nu \in V(\mathrm{F})] \quad \text{and} \quad deg = Min[deg(\nu)|\nu \in V(\mathrm{F})]$$

For F, its vertex set $V(\mathrm{F})$ and edge set $E(\mathrm{F})$ can be divided into various divisions:

For any $r \in \mathbb{N}$, $2deg(\mathrm{F}) \le r \le 2deg(\mathrm{F})$, let $E_r = \{e = \mu\nu \in E(\mathrm{F}): deg(\mu) + deg(\nu) = r\}$; for any $s \in \mathbb{N}, deg^2(\mathrm{F}) \le s \le deg^2(\mathrm{F})$, let $E^*_s = \{e = \mu\nu \in E(\mathrm{F}): deg(\mu)deg(\nu) = s\}$; for any $t \in \mathbb{N}, deg(\mathrm{F}) \le t \le deg(\mathrm{F})$, let $V_t = \{\nu\nu \in V(\mathrm{F}): deg(\nu) = t\}$; Then, the edge set of $\mathrm{F} = VPHX[q,p]$ is divided into two edge partitions based on the sum of degrees of the end vertices as:

$$E_5(\mathrm{F}) = E^*_6 = \{e = \mu\nu \in E(\mathrm{F}): deg(\mu) = 2, deg(\nu) = 3, deg(\mu)deg(\nu) = 6\},$$

$$E_6(\mathrm{F}) = E^*_9 = \{e = \mu\nu \in E(\mathrm{F}): deg(\mu) = 3, deg(\nu) = 3, deg(\mu)deg(\nu) = 9\},$$

Table 1
The Partitions of Edges and Vertices for Nanotubes Structure $\mathbf{F} = \boldsymbol{VPHX[q,p]}$**.**

Edge partition	$E_5 = E^*_6$	$E_6 = E^*_9$
Cardinality	$4q$	$9qp - 5q$

Vertex partition	V_2	V_3
Cardinality	$q + q$	$6qp - 2q$

Thus:

$$\begin{aligned} Y(\mathrm{F}) = \sum_{\mu\nu\in E(\mathrm{F})} [deg^3_{\mathrm{F}}(\mu) + deg^3_{\mathrm{F}}(\nu)] &= \sum_{\mu\nu\in E^*_6(\mathrm{F})} [deg^3_{\mathrm{F}}(\mu) + deg^3_{\mathrm{F}}(\nu)] \\ &\quad + \sum_{\mu\nu\in E^*_9(\mathrm{F})} [deg^3_{\mathrm{F}}(\mu) + deg^3_{\mathrm{F}}(\nu)] \\ &= 35|E^*_6(\mathrm{F})| + 54|E^*_9(\mathrm{F})| = 486qp - 130q. \end{aligned}$$

Theorem 2.1.2: *The Y topological polynomial of Nanotubes structure* $F = VPHX[q,p]$ *(Fig. 1) is :*

$$Y(\mathrm{F}, x) = q[4x^{35} + [9p-5]x^{54}].$$

Proof: Given that the Y topological polynomial for graph Γ is

$$Y(\Gamma, x) = \sum_{\mu\nu\in E(\Gamma)} x^{[deg^3_\Gamma(\mu) + deg^3_\Gamma(\nu)]}$$

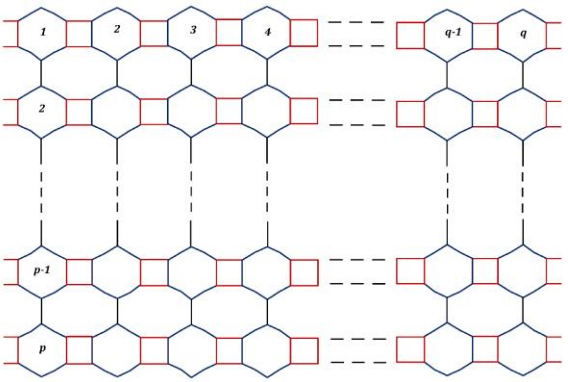

Figure 1
The molecular structure of $\mathbf{F} = \boldsymbol{VPHX[q,p]}$ Nanotubes.

Taking into consideration the partitions of the vertex and edge sets $V(\mathrm{F}), E(\mathrm{F})$ as provided in (Theorem 2.1.1), it consequently follows that:

$$Y(\mathrm{F},x) = \sum_{\mu\nu\in E(\mathrm{F}} x^{[deg^3_{\mathrm{F}}(\mu)+deg^3_{\mathrm{F}}(\nu)]} = \sum_{\mu\nu\in E^*_6(\mathrm{F})} x^{[deg^3_{\mathrm{F}}(\mu)+deg^3_{\mathrm{F}}(\nu)]} + \sum_{\mu\nu\in E^*_9(\mathrm{F})} x^{[deg^3_{\mathrm{F}}(\mu)+deg^3_{\mathrm{F}}(\nu)]}$$
$$= |E^*_6(\mathrm{F})|x^{35} + |E^*_9(\mathrm{F})|x^{54} = 4qx^{35} + [9qp-5q]x^{54}.$$

The Y-index representing F can likewise be obtained by derivative the aforementioned Y-polynomial of F relative to x, giving:

$$Y(\mathrm{F}) = \frac{\partial}{\partial x}Y(\mathrm{F},x)|_{x=1} = \frac{\partial}{\partial x}[4qx^{35} + q[9p-5]x^{54}]|_{x=1} = 486qp - 130q.$$

Corollary 2.1.3: *The descriptor of $Y-index$ of complement graph of Nanotubes $F = VPHX[q,p]$ (Fig. 1) is*

$$Y(\overline{\mathrm{F}}) = 6qp[6qp-1]^4 - 8[9qp-q][6qp-1]^3 + 6[6qp-1]^2[54qp-10q] - 4[6qp-1][162qp-38q] + 486qp - 130q.$$

Proof: By virtue of (Eq. 4, Eq. 8), as well as the partitions ascribed to the vertex and edge sets $|V(\mathrm{F})| = 6qp, \quad |E(\mathrm{F})| = 9qp - m$, given in Theorem (2.1.1), and applying Eq.(1), we get required.

Corollary 2.1.4: *The topological descriptor $Y-coindex$ of Nanotubes $\overline{F} = \overline{VPHX[q,p]}$ is given by*

$$\overline{Y}(\overline{\mathrm{F}}) = 4(9qp-q)[6qp-1]^3 - 3[6qp-1]^2(54qp-10q) + 3[6qp-1](162qp-38q) - 486qp + 130q.$$

Proof: As (Theorem 3.1.1) in [19] $F(\mathrm{F}) = 162qp - 38q$, and $Y(\mathrm{F}) = 486qp - 130q$ given in Theorem (2.1.1) above. and applying Eq.(3), we have

$$\begin{aligned}\overline{Y}(\overline{\mathrm{F}}) &= 4\sum |E(\mathrm{F})|[\sum |V(\mathrm{F})|-1]^3 - 3[\sum |V(\mathrm{F})|-1]^2 M_1(\mathrm{F}) \\ &\quad + 3[\sum |V(\mathrm{F})|-1]F(\mathrm{F}) - Y(\mathrm{F}) \\ &= 4(9qp-q)[6qp-1]^3 - 3[6qp-1]^2(54qp-10q) \\ &\quad + 3[6qp-1](162qp-38q) - 486qp + 130q.\end{aligned}$$

2.2 *Quantifying Topological Indices for V-Phenylenic Nanotorus: A Study of the Y-Index and Co-Index*

In this subsection, we undertake the computation of the $Y-index$ for select chemical structures, namely the line graphs of V-Phenylenic Nanotorus denoted as $VPHY[q,p]$ for all q and p belonging to the set of natural numbers excluding 1, as well as their corresponding molecular complement Nano-structure. Additionally, our investigation extends to the examination of the $Y-polynomial$ of V-Phenylenic Nanotorus.

Theorem 2.2.1: *Let $\Upsilon = VPHX[q,p]$ be V-Phenylenic Nanotorus (See Fig. 2), then the $(Y-index)$ of Υ is given by*

$$Y(\Upsilon) = 486qp.$$

Proof: According to the concept of the Y-Index, we have

$$Y(\Upsilon) = \sum_{\mu\nu\in E(\Upsilon)} [deg^3_{\Upsilon}(\mu) + deg^3_{\Upsilon}(\nu)],$$

The vertex and edge sets partitions $V(\Upsilon), E(\Upsilon)$ of V-Phenylenic nanotorus are given in (Table 2.) [13], such that for a connected graph $\Upsilon = (V(\Upsilon), E(\Upsilon))$ with $deg = Maxdeg(\nu)|\nu \in V(\Upsilon)$ and $deg = Mindeg(\nu)|\nu \in V(\Upsilon)$, its vertex set $V(\Upsilon)$ and edge set $E(\Upsilon)$ are divided into several partitions:

For any $i \in \mathbb{N}$, $2deg(\Upsilon) \le i \le 2deg(\Upsilon)$, let $E_i = \{e = \mu\nu \in E(\Upsilon): deg(\mu) + deg(\nu) = i\}$; for any $j \in \mathbb{N}, deg^2(\Upsilon) \le j \le deg^2(\Upsilon)$, let $E^*_j = \{e = \mu\nu \in E(\Upsilon): deg(u)deg(\nu) = j\}$; for any $k \in \mathbb{N}, deg(G) \le k \le deg(\Upsilon)$, let $V_k = \{\nu\nu \in V(\Upsilon): deg(\nu) = k\}$; Then, the edge set of $\Upsilon = VPHY[q,p]$ have only one type of edges:

$E_6(\Upsilon) = E^*_9 = \{e = \mu\nu \in E(\Upsilon): deg(\mu) = 3, deg(\nu) = 3, deg(\mu)deg(\nu) = 9,$

Table 2
The Partitions of Edges and Vertices for Nanotorus Structure $\Upsilon = VPHY[q,p]$.

Edge partition	$E_6 = E^*_9$
Cardinality	$9qp$

Vertex partition	V_3
Cardinality	$6qp$

Thus:

$$\begin{aligned}Y(\Upsilon) &= \sum_{\mu\nu\in E(\Upsilon)} [deg^3_{\Upsilon}(\mu) + deg^3_{\Upsilon}(\nu)] = \sum_{\mu\nu\in E^*_9(\Upsilon)} [deg^3_{\Upsilon}(\mu) + deg^3_{\Upsilon}(\nu)] \\ &= 54|E^*_9(\Upsilon)| = 486qp.\end{aligned}$$

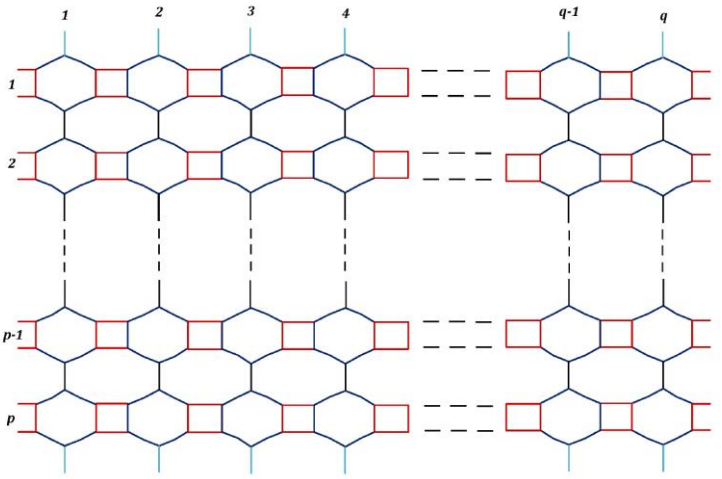

Figure 2
The molecular graph of $VPHY[q,p]$ Nanotorus.

Theorem 2.2.2: *The Y topological polynomial of Nanotorus structure* $\Upsilon = VPHY[q,p]$ *is:*

$$Y(\Upsilon,x) = 9qpx^{54}$$

Proof: Given that the Y topological polynomial for graph Γ is

$$Y(\Gamma,x) = \sum_{\mu\nu\in E(\Gamma)} x^{[deg^3(\mu)+deg^3(\nu)]}$$

Taking into consideration the partitions of the vertex and edge sets $V(\Upsilon), E(\Upsilon)$ as provided in (Theorem 2.2.1), it consequently follows that:

$$Y(\Upsilon,x) = \sum_{\mu\nu\in E(\Upsilon)} x^{[deg^3(\mu)+deg^3(\nu)]} = \sum_{\mu\nu\in E_9^*(\Upsilon)} x^{[deg^3(\mu)+deg^3(\nu)]}$$
$$= |E_9^*(\Upsilon)|x^{54} = 9qpx^{54}.$$

The Y-index representing Υ can likewise be obtained by derivative the aforementioned Y-polynomial of Υ relative to x, giving:

$$Y(\Upsilon) = \frac{\partial}{\partial x}Y(\Upsilon,x)|_{x=1} = \frac{\partial}{\partial x}[9qpx^{54}]|_{x=1} = 486qp.$$

Corollary 2.2.3: *The* $Y-index$ *of complement* $\Upsilon = VPHY[q,p]$ *Nanotorus is given by*

$$Y(\overline{\Upsilon}) = 6qp[6qp-1]^4 - 8[9qp-m][6qp-1]^3$$
$$+ 324qp[6qp-1]^2 - 648qp[6qp-1] + 486qp.$$

Proof: By virtue of (Eq. 4, Eq. 8), as well as the partitions ascribed to the vertex and edge sets $|V(\Upsilon)| = 6qp$, $|E(\Upsilon)| = 9qp$, given in Theorem (2.2.1), and applying Eq.(1), we have

$$\begin{aligned} Y(\overline{\Upsilon}) &= |V(\Upsilon)|[|V(\Upsilon)|-1]^4 - 8|E(\Upsilon)|[|V(\Upsilon)|-1]^3 \\ &\quad + 6[|V(\Upsilon)|-1]^2 M_1(\Upsilon) - 4[|V(\Upsilon)|-1]F(\Upsilon) + Y(\Upsilon) \\ &= 6qp[6qp-1]^4 - 8[9qp-q][6qp-1]^3 \\ &\quad + 324qp[6qp-1]^2 - 648qp[6qp-1] + 486qp. \end{aligned}$$

Corollary 2.2.4: *The $Y-coindex$ of complement $\Upsilon = VPHY[q,p]$ Nanotorus (Fig 2.) is given by*

$$\overline{Y}(\overline{\Upsilon}) = qp[36[6qp-1]^3 - 162[6qp-1]^2 + 486[6qp-2]].$$

Proof: As (Theorem 3.2.1) in [19] $F(\Upsilon) = 162qp$, and $Y(\Upsilon) = 486qp$ given in Theorem (2.2.1)above. and applying Eq.(3), we have

$$\begin{aligned} \overline{Y}(\overline{\Upsilon}) &= 4|E(\Upsilon)|[|V(\Upsilon)|-1]^3 - 3[|V(\Upsilon)|-1]^2 M_1(\Upsilon) \\ &\quad + 3[|V(\Upsilon)|-1]F(\Upsilon) - Y(\Upsilon) \\ &= qp[36[6qp-1]^3 - 162[6qp-1]^2 + 486[6qp-2]]. \end{aligned}$$

3. Numerical and Graphical Representation

In this section, we have presented MATLAB codes that allow the calculation of indices and $Ypolynomials$, for V Phenylenic Nanotube ($VPHX[q,p]$) and V Phenylenic Nanotorus ($VPHY[q,p]$). These indices include the First and Second Zagreb indices, $Yindex$, and First and Second Hyper Zagreb indices.

The numerical values of these indices are shown in Tables 3. and 4. for Nanotubes $VPHX[q,p]$ and Nanotorus $VPHY[q,p]$ respectively. The formulas used to calculate these values are reported in Eq. (4 to 7) and (Theorem 2.1.1) for Nanotubes $VPHX[q,p]$ while Eq. (4 to 7) and (Theorem 2.2.1) are used for the Nanotorus $VPHY[qp]$. These tables clearly demonstrate that all index values increase as the values of q and p increase.

Furthermore, we have provided representations in Figures 3, 4, and 5. Figure 3. compares the $Ypolynomials$ of the V Phenylenic Nanotube with those of the V Phenylenic Nanotorus. Meanwhile, Figures 4. and 5. explore topological descriptor values. It's clear that as the values of q and p increase, in the numbers we can observe an increase in the first and second Zagreb indices, Y index, and first and second Hyper Zagreb indices of the Nanotubes $VPHX[q,p]$ and Nanotorus $VPHY[q,p]$. However, when it comes to capacity to dimension, the first and second Zagreb indices show relatively lower performance compared to the other measures. However, both the first and second Hyper Zagreb indices as well as the Y index show a steeper escalation with increasing dimensions.

Y-polynomial algorithm of V-Phenylenic Nanotorus and Nanotube

```
clear;
 clc;
 syms x;
 m=input('Enter q number of hexagons in the first   row: q= ');
 n=input('Enter p number of hexagons in the first coluqp: p= ');
 a=4*q;
 b=9*q*p;
 c=9*q*p-5*q;
 fprintf('Y(VPHX[q,p];x)=%dx^(35)+%dx^(54)',a,c);
 fprintf('Y(VPHY[q,p];x)=%dx^(54)',b);
```

In these programs, we will use the following shortcuts:

M1: First Zagreb index, M2: 2^{nd} Zagreb index, Y: $Y-index$, $VPHX$: V-Phenylenic Nanotubes $VPHX[q,p]$, $VPHY$: V-Phenylenic Nanotorus $VPHY[q,p]$, HM: hyper Zagreb index, and HM2: 2^{nd} hyper Zagreb index.

Zagreb and Hyper-Zagreb indices and $Y-index$ algorithms of V-Phenylenic Nanotorus and Nanotube

```
clear;
clc;
m=input('Enter q number of hexagons in the first   row: q= ');
n=input('Enter p number of hexagons in the first column: p= ');

M1_VPHX(q,p)=54*q*p-10*q;
M2_VPHX(q,p)=81*q*p+3*q;
Y_VPHX(q,p)=486*q*p-130*q;
HM_VPHX(q,p)=324*q*p-80*q;
HM2_VPHX(q,p)=729*q*p-261*q;


M1_VPHY(q,p)=54*q*p;
M2_VPHY(q,p)=81*q*p;
Y_VPHY(q,p)=486*q*p;
HM_VPHY(q,p)=324*q*p;
HM2_VPHY(q,p)=729*q*p;


fprintf('First Zagreb index, M1(VPHX[q,p])=%d',M1_VPHX(q,p));
fprintf('Second Zagreb index, M2(VPHX[q,p])=%d',M2_VPHX(q,p));
fprintf('Y-index, Y(VPHX[q,p])=%d',Y_VPHX(q,p));
fprintf('Hyper-Zagreb index, HM(VPHX[q,p])=%d',HM_VPHX(q,p));
fprintf('2nd Hyper-Zagreb index,HM2(VPHX[q,p])=%d',HM2_VPHX(q,p));


fprintf('First Zagreb index, M1(VPHY[q,p])=%d',M1_VPHY(q,p));
fprintf('2^nd Zagreb index, M2(VPHY[q,p])=%d',M2_VPHY(q,p));
fprintf('Y-index, Y(VPHY[q,p])=%d',Y_VPHY(q,p));
fprintf('Hyper-Zagreb index, HM(VPHY[q,p])=%d',HM_VPHY(q,p));
fprintf('2nd Hyper-Zagreb index,HM2(VPHY[q,p])=%d',HM2_VPHY(q,p));
```

Table 3
Analytical data of the Zagreb hyper Zagreb indices and Y-index of $\mathrm{F} = \boldsymbol{VPHX}[\boldsymbol{q},\boldsymbol{p}]$ Nanotubes.

q	p	$M_1(\mathrm{F})$	$M_2(\mathrm{F})$	$Y(\mathrm{F})$	$HM(\mathrm{F})$	$HM_2(\mathrm{F})$
2	2	196	330	1684	1136	2394
2	3	304	492	2656	1784	3852
3	2	294	495	2526	1704	3591
3	3	456	738	3984	2676	5778
2	4	412	654	3628	2432	5310
3	4	618	981	5442	3648	7965
4	2	392	660	3368	2272	4788
4	3	608	984	5312	3568	7704
4	4	824	1308	7256	4864	10620
5	5	1300	2040	11500	7700	16920

Table 4
Analytical data of Zagreb, hyper Zagreb indices, and Y-index of $\Upsilon = \boldsymbol{VPHY}[\boldsymbol{q},\boldsymbol{p}]$ Nanotorus.

q	p	$M_1(\Upsilon)$	$M_2(\Upsilon)$	$Y(\Upsilon)$	$HM(\Upsilon)$	$HM_2(\Upsilon)$
2	2	216	324	1944	1296	2916
2	3	324	486	2916	1944	4374
3	2	324	486	2916	1944	4374
3	3	486	729	4374	2916	6561
2	4	432	648	3888	2592	5832
3	4	648	972	5832	3888	8748
4	2	432	648	3888	2592	5832
4	3	648	972	5832	3888	8748
4	4	864	1296	7776	5184	11664
5	5	1350	2025	12150	8100	18225

4. Conclusion

The current study has performed calculations for the $Y - index$ and $Y - polynomial$ of chemical structures of V-Phenylenic Nanotorus and Nanotube, as well as their corresponding molecular complement graphs. In addition, a numerical comparison of the computed results was presented, including graphical representations of the corresponding behavior illustrated in the figures.

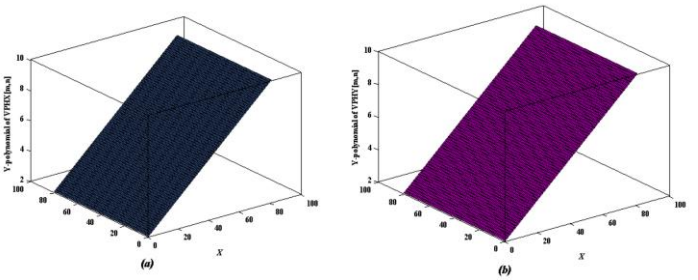

Figure 3
Numerical comparison of (a) Y-polynomial of $VPHX[q,p]$ (b) Y-polynomial of $VPHY[q,p]$ (when p=q=2).

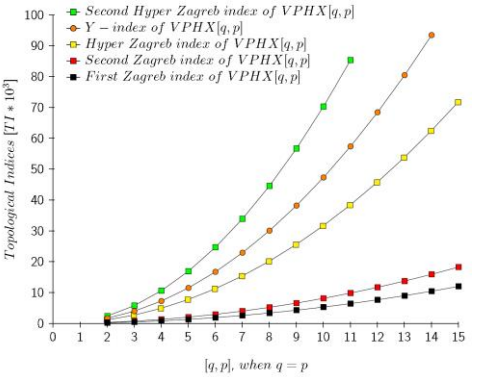

Figure 4
Comparative analysis of Zagreb, hyper Zagreb indices, and Y-index of V-Phenylenic Nanotube.

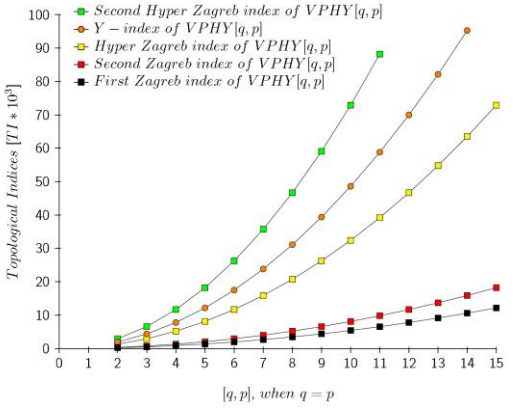

Figure 5
Comparative analysis of Zagreb, hyper Zagreb indices, and Y-index of V-Phenylenic Nanotorus.

References

[1] Y. Kwun, M. Munir, S. A. Bokhary, K. Ali, A. Rehman, and I. N. Cangül, "M-Polynomials and topological indices of V-Phenylenic Nanotubes and Nanotori," *Scientific Reports*, vol. 7, no. 1, p. 8756 (2017).

[2] M. Alsharafi, M. Shubatah, and A. Alameri, "The forgotten index of complement graph operations and its applications of molecular graph," *Open Journal of Discrete Applied Mathematics,* vol. 3, no. 3, pp. 53–61 (2020).

[3] M. Alsharafi, M. Shubatah, and A. Alameri, "The first and second Zagreb index of complement graph and its applications of molecular graph," *Asian Journal of Probability and Statistics,* vol. 8, no. 3, pp. 15–30 (2020).

[4] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, pp. 535–538 (1972).

[5] M. Khalifeh, H. Yousefi-Azari, and A. R. Ashrafi, "The first and second Zagreb indices of some graph operations," *Discrete Applied Mathematics,* vol. 157, no. 4, pp. 804–811 (2009).

[6] B. Furtula and I. Gutman, "A forgotten topological index," *Journal of Mathematical Chemistry,* vol. 53, no. 4, pp. 1184–1190 (2015).

[7] A. Alameri, N. Al-Naggar, M. Al-Rumaima, and M. Alsharafi, "Y-index of some graph operations," *International Journal of Applied Engineering Research*, vol. 15, no. 2, pp. 173–179 (2020).

[8] A. Alameri, M. Al-Rumaima, and M. Almazah, "Y-coindex of graph operations and its applications of molecular descriptors," *Journal of Molecular Structure,* vol. 1221, p. 128754 (2020).

[9] A. R. Ashrafi, M. Ghorbani, and M. Jalali, "Computing sadhana polynomial of V-phenylenic nanotubes and nanotori," *Indian Journal of Chemistry, Sect. A*, vol. 47, pp. 535–537 (2008).

[10] M. R. Farahani, R. P. Kumar, and M. R. Kanna, "First and second Zagreb indices and polynomials of V-phenylenic nanotubes and nanotori," *International Journal of Pharmaceutical Sciences and Research,* vol. 8, no. 1, pp. 330–333 (2017).

[11] M. R. Farahani, M. R. Kanna, and R. P. Kumar, "On the Hyper-Zagreb indices of nano-structures," *Asian Academic Research Journal of Multidisciplinary*, vol. 3, no. 1, pp. 115–123 (2016).

[12] M. R. Farahani and W. Gao, "On multiplicative and redefined version of Zagreb indices of V-phenylenic nanotubes and nanotorus," *BJMCS*, vol. 13, no. 5, pp. 1–8 (2016).

[13] V. Alamian, A. Bahrami, and B. Edalatzadeh, "PI Polynomial of V-phenylenic nanotubes and nanotori," *International Journal of Molecular Sciences*, vol. 9, pp. 229–234 (2008).

[14] Z. Ahmad, M. Naseem, M. K. Jamil, M. K. Siddiquid, and M. F. Nadeemd, "New results on eccentric connectivity indices of V-phenylenic nanotube," *Eurasian Chemical Communications*, vol. 2, pp. 663–671 (2020).

[15] B. Furtula, I. Gutman, and M. Dehmer, "On structure-sensitivity of degree-based topological indices," *Applied Mathematics and Computation*, vol. 219, pp. 8973–8978 (2013).

[16] H. Jiang, M. S. Sardar, K. Ali, S. A. Bokhary, M. Munir, A. Rehman, and I. N. Cangül, "Computing sanskruti index V-phenylenic nanotube and nanotori," *International Journal of Pure and Applied Mathematics*, vol. 115, no. 4, pp. 859–865, 2017).

[17] S. Mondal, A. Bhosale, N. De, and A. Pal, "Topological properties of some nanostructures," *Nanosystems: Physics, Chemistry, Mathematics*, vol. 11, no. 1, pp. 14–24 (2020).

[18] M. Alsharafi, M. Shubatah, and A. Alameri, "The hyper-Zagreb index of some complement graphs," *Advances in Mathematics: Scientific Journal*, vol. 9, no. 6, pp. 3631–3642 (2020).

[19] M. Alsharafi and A. Alameri, "The F-index and coindex of V-phenylenic nanotubes and nanotorus and their molecular complement graphs," *Nanosystems: Physics, Chemistry, Mathematics*, vol. 12, no. 3, pp. 263–270 (2021).

[20] A. Ayache, A. Alameri, M. Alsharafi, and H. Ahmed, "The second Hyper-Zagreb coindex of chemical graphs and some applications," *Journal of Chemistry*, vol. 2021, Article ID 3687533, 8 pages (2021).

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