IARJSET

ISSN (Online) 2393-8021
ISSN (Print) 2394-1588

International Advanced Research Journal in Science, Engineering and Technology
Vol. 8, Issue 6, June 2021

DOI: 10.17148/IARJSET.2021.8622

Chromatic Topological Indices of VPH(m,n) and Nanotorus

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Abstract: Nanotechnology stands a vital role in the science research and technology development. Carbon Nanotubes (CNTs) is one among the most promising materials in the field of nanotechnology. Mathematically, topological indices are real numbers invariant under graph isomorphism. In QSAR/QSPR study topological indices are utilized to analyze the physical properties of chemical compounds such as boiling point, melting point, heat capacities, molecular refraction, total surface area, etc. Chromatic topological indices of a graph G is a term that has recently been coined [3] to designate a new coloring version to these indices which embrace both proper coloring and topological indices. In this paper we investigate the different types of Zagreb indices for V -Phenylenic nanotube and Phenylenic nanotorus.

Keywords: Zagreb Indices, Phenylenic nanotorus, V-Phenylenic nanotube.

I. INTRODUCTION

The chemical graph theory is an important branch of mathematical chemistry. A chemical graph is a model of a chemical system, used to characterize the interactions among its components: atoms, bonds, groups of atoms or molecules. A structural formula of a chemical compound can be represented by a molecular graph, its vertices being atoms while edges correspond to covalent bonds; hydrogen atoms are often omitted. A single number representing a chemical structure in graph theoretical terms is called a topological index. Topological indices were successfully employed in developing a suitable correlation between chemical structure and physical activity by translating chemical structures into numerical descriptors. In the past years, nanostructures involving carbon have been the focus of an intense research activity which is driven to a large extent by the quest for new materials with specific applications. Carbon nanotubes are nano objects that have raised great expectations in a number of different applications, including field emission, energy storage, molecular electronics, atomic force microscopy and many others. The use of topological indices as structural descriptors is important in the proper and optimal nanostructure design. The present authors [2,5,6,7] derived some exact formulae for topological indices of some graphs. The main purpose of this paper is to find effect of chromatic topological indices in the physical properties of nanostructures. In this paper we compute the chromatic Zagreb indices of phenylenic nanotube and nanotorus.

II. THE ZAGREB INDICES

A topological index or a molecular structure descriptor is a numerical value associated with chemical structures with various physical properties. The connectivity index and its variants are used more frequently than any other topological index in QSPR and QSAR.

J.Kok et. al. found the general formulae of chromatic Zagreb indices for certain graphs such as tree, caterpillar, etc., [3]. Let $C = \{c_1, c_2, \ldots, c_l\}$ be the proper coloring of any graph G. Since $|C| = l$, G has $l!$ minimum parameter colorings. Denote these colorings as $\phi_t(G), 1 \le t \le l!$.

Definition 2.1

[3] Let G be a graph and let $C = \{c_1, c_2, \ldots, c_l\}$ be the proper coloring of G such that $\phi(v_i) = c_s$, $1 \le i \le n, 1 \le s \le l$. Then for $1 \le t \le l!$,

- The *first chromatic Zagreb index* of G is defined as

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$$M_1^{\phi_t}(G) = \sum_{i=1}^{n} c(v_i)^2$$
$$= \sum_{j=1}^{l} \theta(c_j)\cdot j^2, c_j \in C$$

- The *second chromatic Zagreb index* of *G* is defined as

$$M_2^{\phi_t}(G) = \sum_{i=1}^{n-1}\sum_{j=2}^{n} (c(v_i)\cdot c(v_j)), v_i v_j \in E(G)$$
$$= \sum_{\substack{t<s \\ 1\le t,s\le l}} (t\cdot s)\eta_{ts}$$

- The *third chromatic Zagreb index* of *G* is defined as

$$M_3^{\phi_t}(G) = \sum_{i=1}^{n-1}\sum_{j=2}^{n} |c(v_i) - c(v_j)|, v_i v_j \in E(G)$$
$$= \sum_{\substack{t<s \\ 1\le t,s\le l}} |t-s|\eta_{ts}$$

Here η_{ts} is the number of edges $e(=uv)$ in *G* such that $c(u)=t$ and $c(v)=s$.

III. CHROMATIC ZAGREB INDICES OF PHENYLENIC NANOSTRUCTURES

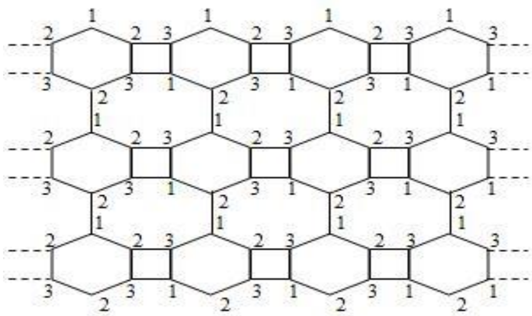
Phenylenic nanostructures $VPH(m, n)$, $TPH(m, n)$ are molecular graphs that are covered by C_6, C_4 and C_8[1]. In the phenylenic nanostructure *n* represents the number of rows and *m* rep- resents the number of columns. The number of vertices in V-phenylenic nanotube is $6mn$. The edges of V-phenylenic nanotube can be divided into 4 types namely horizontal, vertical, acute and obtuse edges. Molecular graphs *V* -phenylenic nanotubes(VPH) and nanotorus(TPH) are two families of nanostructures that their structures consist of cycles with length four, six, and eight by different compound. Chemical structures *V* -Phenylenic nanotubes and *V* -Phenylenic nanotorus are widely used in medical science and pharmaceutical field.

Theorem 3.1

Let *G* be a *V*- phenylenic nanotube *VPH(m,n),* then

$$M_1^{\phi^-}(G) = 28mn$$
$$M_2^{\phi^-}(G) = 33mn - 2m - 3n$$
$$M_3^{\phi^-}(G) = 12mn - m - 2n$$

Proof: The chromatic number of a *V*- phenylenic nanotube is 3. Consider the ϕ^- coloring then $\theta(c_1)=\theta(c_2)=\theta(c_3)=2mn$. From the definition of η_{ts} we found that $\eta_{12}=3mn-m, \eta_{13}=3mn-n$ and $\eta_{23}=3mn.$



ϕ^- & ϕ^+ Coloring of the molecular structure of VPH(4,3)

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$$M_1^{\phi^-}(G) = \sum_{j=1}^{l} \theta(c_j) \cdot j^2, c_j \in C$$

$$= 1(2mn) + 4(2mn) + 9(2mn) = 28mn$$

$$M_2^{\phi^-}(G) = \sum_{1 \le t,s \le l}^{t<s} (t \cdot s)\eta_{ts}$$

$$= 2\eta_{12} + 3\eta_{13} + 6\eta_{23}$$

$$= 2(3mn - m) + 3(3mn - n) + 6(3mn)$$

$$= 33mn - 2m - 3n$$

$$M_3^{\phi^-}(G) = \sum_{1 \le t,s \le l}^{t<s} |t - s| \eta_{ts}$$

$$= 1\eta_{12} + 2\eta_{13} + 1\eta_{23}$$

$$= 1(3mn - m) + 2(3mn - n) + 1(3mn)$$

$$= 12mn - m - 2n.$$

Theorem 3.2

Let G be a V- phenylenic nanotube *VPH(m,n)*, then

$$M_1^{\phi^+}(G) = 28mn$$

$$M_2^{\phi^+}(G) = 33mn - 6m - 3n$$

$$M_3^{\phi^+}(G) = 12mn - m - 2n$$

Proof: The chromatic number of a V- phenylenic nanotube is 3. Consider the ϕ^+ coloring then $\theta(c_1) = \theta(c_2) = \theta(c_3) = 2mn$. From the definition of η_{ts} we found that $\eta_{12} = 3mn, \eta_{13} = 3mn - n$ and $\eta_{23} = 3mn - m.$

$$M_1^{\phi^+}(G) = \sum_{j=1}^{l} \theta(c_j) \cdot j^2, c_j \in C$$

$$= 1(2mn) + 4(2mn) + 9(2mn) = 28mn$$

$$M_2^{\phi^+}(G) = \sum_{1 \le t,s \le l}^{t<s} (t \cdot s)\eta_{ts}$$

$$= 2\eta_{12} + 3\eta_{13} + 6\eta_{23}$$

$$= 2(3mn) + 3(3mn - n) + 6(3mn - m)$$

$$= 33mn - 6m - 3n$$

$$M_3^{\phi^+}(G) = \sum_{1 \le t,s \le l}^{t<s} |t - s| \eta_{ts}$$

$$= 1\eta_{12} + 2\eta_{13} + 1\eta_{23}$$

$$= 1(3mn) + 2(3mn - n) + 1(3mn - m)$$

$$= 12mn - m - 2n.$$

Theorem 3.3

Let G be a phenylenic nanotorus *TPH(m,n)*, then

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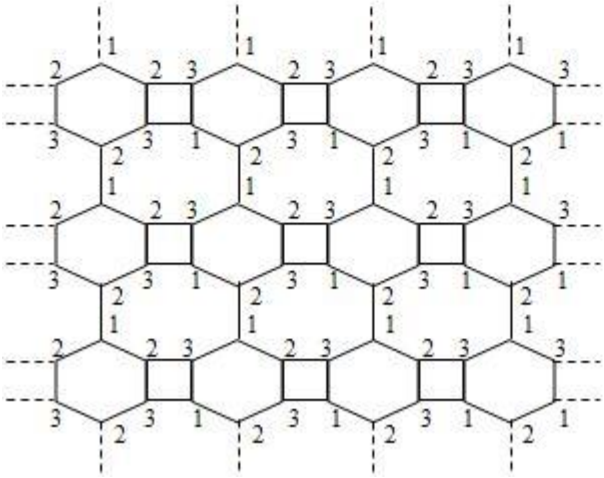
$$M_1^{\phi^-}(G) = M_1^{\phi^+}(G) = 28mn$$
$$M_2^{\phi^-}(G) = M_2^{\phi^+}(G) = 33mn - 3n$$
$$M_3^{\phi^-}(G) = M_3^{\phi^+}(G) = 12mn - 2n$$



ϕ^- & ϕ^+ **Coloring of the molecular structure of TPH (4, 3)**

Proof: The chromatic number of a *V*- phenylenic nanotube is 3. Consider the ϕ^- coloring then $\theta(c_1) = \theta(c_2) = \theta(c_3) = 2mn$. From the definition of η_{ts} we found that $\eta_{12} = 3mn, \eta_{13} = 3mn - n$ and $\eta_{23} = 3mn.$

$$M_1^{\phi^-}(G) = \sum_{j=1}^{l} \theta(c_j) \cdot j^2, c_j \in C$$
$$= 1(2mn) + 4(2mn) + 9(2mn) = 28mn$$

$$M_2^{\phi^-}(G) = \sum_{1 \le t,s \le l}^{t<s} (t \cdot s)\eta_{ts}$$
$$= 2\eta_{12} + 3\eta_{13} + 6\eta_{23}$$
$$= 2(3mn) + 3(3mn - n) + 6(3mn)$$
$$= 33mn - 3n$$

$$M_3^{\phi^-}(G) = \sum_{1 \le t,s \le l}^{t<s} |t - s| \eta_{ts}$$
$$= 1\eta_{12} + 2\eta_{13} + 1\eta_{23}$$
$$= 1(3mn) + 2(3mn - n) + 1(3mn)$$
$$= 12mn - 2n.$$

Similarly, consider the ϕ^+ coloring then $\theta(c_1) = \theta(c_2) = \theta(c_3) = 2mn$. From the definition of η_{ts} we found that $\eta_{12} = 3mn, \eta_{13} = 3mn - n$ and $\eta_{23} = 3mn$ which is similar as ϕ^- coloring. Hence

$$M_1^{\phi^-}(G) = M_1^{\phi^+}(G)$$
$$M_2^{\phi^-}(G) = M_2^{\phi^+}(G)$$
$$M_3^{\phi^-}(G) = M_3^{\phi^+}(G)$$

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IV. RESULT

The Chromatic Zagreb index computed for the nanostructures is given in the following table.

Coloring	Molecular Structure	M_1	M_2	M_3
ϕ^- Coloring	*VPH(m,n)*	*28mn*	*33mn-2m-3n*	*12mn-m-2n*
	TPH(m,n)	*28mn*	*33mn-3n*	*12mn-2n*
ϕ^+ Coloring	*VPH(m,n)*	*28mn*	*33mn-6m-3n*	*12mn-m-2n*
	TPH(m,n)	*28mn*	*33mn-3n*	*12mn-2n*

V. CONCLUSION

Our study is important due o the following reasons. The nanostructures that are studied are one of the fundamental and commonly used nanostructures and the topological index that is computed in this paper, the Chromatic Zagreb index, plays an important role in analyzing the boiling and melting points. Thus, our study has promising application for medical, chemical and nanosciences.

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