Molecular Descriptors of Certain Classes of Nanotubes

P. Seenuvasan

Department of Mathematics, Government Polytechnic College, Thirukovilur, India

Abstract

A *molecular structure descriptor* is a numerical value associatedwith chemical constitution for correlation of chemical structure/network with various physical properties,chemical reactivity or biological activity. Quantitative structure-activity and structure-propertyrelationships of chemical networks require expressions for the topological properties of these networks.Topological indices provide those expressions of topological properties. Valency-based topological descriptorsare the oldest and most successful class of descriptors so far. A chemical graph isa representation of the structural formula of a chemical compound whose vertices correspond to theatoms of the compound and edges correspond to chemical bonds.In this paper, we study for some degree based molecular descriptorsof certain type of nanotubes.

1. Introduction

Quantitative structure-activity relationship models (*QSAR* models) are regression or classification models used in the chemical and biological sciences and control system engineering. One of the first historical *QSAR* chemical applications was to predict boiling points. Those numerical quantities which transform a chemical structure to a numerical number called the topological descriptors/indices. In *QSAR* study, chemical graph theory plays an important role in modelling of organic chemical structures to hydrogendepleted graphs in which vertices correspond to atoms and edges correspond the bonds in the underlying
chemical compounds.

Chemical graph theory is the topological branch of mathematical chemistry which applies graph theoryto mathematical modelling of chemical phenomena. The adherents of the theory maintain the propertiesof a chemical graph, that is, a graph-theoretical representation of a molecule gives valuable insights into thechemical phenomena. Molecules and molecular compounds are often modelled by molecular graph. Topological indices are the useful tools provided by graph theory for theoretical study of chemical compounds. Topological indices play an important

role in studying certain topological properties of chemical compoundsespecially organic materials i.e. carbon containing molecular structures.

Studying topologicalproperties of fullerenes, nanotubes, nanocones, nanostars etc. are emerging topics in nanotechnology, theoretical chemistry and mathematical chemistry. Hundreds of papers have been published in the field oftopological indices of these nanostructures to study their topologies using mathematical or more preciselygraph-theoretic tools.Degree-based molecular descriptors provide a better correlation for certain physico-chemical propertiesof chemical compounds.In this paper, we study for some degree based molecular descriptorsof certain type of nanotubes

2. Preliminaries

A chemical graph is a simple graph in which the vertices correspond to theatoms and the edges correspond to the bonds between them in a chemical compound. The degree*d(u)* of a vertex *u*in a graph *G*is the number of vertices adjacent to *u*in *G*.
The first degree-based molecular descriptor that were defined by Gutman and Trinajstic[22] in 1972. They obtained the structure-dependency of total π electron energy and obtained by anapproximate formula in which the following terms appeared.

$M_1(G) = \sum_{u\in V(G)}(d_G(u))^2 = \sum_{u,v\in E(G)}(d_G(u)+d_G(v))$ and $M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)$.

Another well-known connectivity topological descriptor is *geometric-arithmetic index*which was introduced by Vukicevic et al. [20] in 2009 and it is defined for a connected graph *G*as

$$GA(G) = \sum_{i=1}^{|E(G)|}\sigma_i \text{ where } \sigma_i = \sum_{u,v\in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}.$$

For certain physico-chemical properties, the predictive power of the *GA* index is somewhat better thanthe predictive power of the Randic connectivity index. Certain mathematical properties of the *GA* indexhave been studied by Yuan et al. [31].

One of the well-known degree based molecular index is an*atom- bond connectivityindex(ABC)*which is proposed by Estrada et al.[26] in 1998. The *ABC* index provides a good model for the stability of linear andbranched alkanes as well as the strain energy of cycloalkanes.It is defined for a connected graph *G*as

$$ABC(G) = \sum_{i=1}^{|E(G)|}\beta_i. \text{ where } \beta_i = \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}.$$

It has been shown that the *ABC* index correlates certain thermodynamic properties of alkanes specificallytheir heats of formation. Estrada [27] provided with a theoretical explanation for this fortunatecharacteristic of the *ABC* index.

Inspired by work on the *ABC* index, Furtula etal. [17] in proposed the following modified versionof the *ABC* index and called it as *augmented Zagreb index* (*AZI*) which is defined for a connected graph *G* as

$$AZI(G)=\sum_{i=1}^{|E(G|}\theta_i,\ \text{where}\ \theta_i=\sum_{u,v\in E(G)}\left(\frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)-2}\right)^3.$$

Only ABC_4 and GA_5 indices can be computed if we are able to find the edge partition of these interconnection networks based on sum of the degrees of end vertices of each edge in these graphs. The*fifth geometric-arithmeticindex*was consideredby Graovac et al.[21] in 2011 and is defined for a graph *G*as

$$GA_5(G)=\sum_{i=1}^{|E(G)|}\sigma_i^{'}\ ,\text{where}\ \sigma_i^{'}=\sum_{u,v\in E(G)}\frac{2\sqrt{S_uS_v}}{S_u+S_v-2}.$$

Later on the fourth member of the class of *ABC*index was introduced by Ghorbani et al. [18] in the following way

$$ABC_4(G)=\sum_{i=1}^{|E(G|}\beta_i^{'},\text{where}\ \beta_i^{'}=\sum_{u,v\in V(G)}\sqrt{\frac{S_u+S_v-2}{S_uS_v}}$$

Motivated by the previous research on topological descriptors and their applications, Hosamani [19] proposed a new index of a molecular graph *G* called *Sanskruti indexS* (*G*) which is defined for a connected graph *G* as

$$S(G)=\sum_{i=1}^{|E(G)|}\theta_i^{'},\ \text{where}\ \theta_i^{'}=\sum_{u,v\in E(G)}\left(\frac{S_uS_v}{S_u+S_v-2}\right)^3.$$

2.Main results

In this section, we study the certain molecular descriptors forH-Naphtalenicnano tubes(*NPHX[m,n]*)and Nano tubes covered by C_4 ($TUC_4[m, n]$).

2.1*H*-Naphtalenic Nanotubes

In this section, we compute the certain topological indices for *H*-Naphtalenic nanotubes. This nanotube is a trivalent decoration having sequence of C_6,C_6,C_4, C_6,C_6,C_4,… in first row and a sequence of C_6,C_8,C_6,C_8,...in other row. In other words, the whole lattice is a plane tiling ofC_4, C_6 and C_8 and this type of tiling can either cover a cylinder or a torus. These nanotubes usually symbolized as *NPHX[m,n]*, in which *m* is the number of pairs of hexagons in first row and *n* is the number of alternative hexagons in a column[15], see Figure 3. Other forms and description are given for example in the Refs. [1, 3, 9, 12] and [14]. From the

structure of *NPHX*[*m*, *n*], we have |*V*(*NPHX*[*m*, *n*])| = 10*mn* and |*E*(*NPHX*[*m*, *n*])| = 15*mn* − 2*m*.

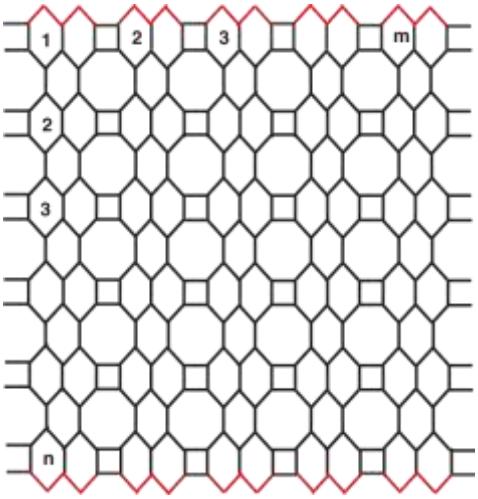

Figure 3. 2D-lattice of *H*-Naphtalenic Nanotubes

The following table gives types of edges, their numbers and amount of σ_i , β_i , θ_i of *NPHX*[*m*, *n*].

Numbers of edges	σ_i	β_i	θ_i	Types of edges
8m	$\frac{2\sqrt{6}}{5}$	$\sqrt{\frac{1}{2}}$	8	(2,3)
15mn-10n	1	$\frac{2}{3}$	$\left(\frac{9}{4}\right)^3$	(3,3)

Table 5.

Let *G* = *NPHX*[*m*, *n*] nanotubes. Then the following results are obtained by using the definitions of indices and Table 5 and 6.

Result 5.

$$(i).GA(G) = m\left(\frac{16\sqrt{6}}{5} - 10\right) + 15m.$$

$$(ii).ABC(G) = 8m\left(8\sqrt{\frac{1}{2} - \frac{20}{3}}\right) + 10mn.$$

$$(iii).AZI(G) = m\left(16 - 10\left(\frac{9}{4}\right)^3\right) + 15mn\left(\frac{9}{4}\right)^3.$$

Number of edges	$\sigma_i^{'}$	$\beta_i^{'}$	$\theta_i^{'}$	Types of edges
4m	$\frac{2\sqrt{42}}{13}$	$\sqrt{\frac{11}{42}}$	$\left(\frac{42}{11}\right)^3$	(6,7)
4m	$\frac{4\sqrt{3}}{7}$	$\sqrt{\frac{1}{4}}$	4^3	(6,8)
2m	1	$\sqrt{\frac{7}{32}}$	$\left(\frac{32}{7}\right)^3$	(8,8)
2m	$\frac{3\sqrt{7}}{8}$	$\sqrt{\frac{14}{63}}$	$\left(\frac{63}{14}\right)^3$	(7,9)
4m	$\frac{12\sqrt{2}}{17}$	$\sqrt{\frac{15}{72}}$	$\left(\frac{72}{15}\right)^3$	(8,9)
15mn-18m	1	$\frac{4}{6}$	$\left(\frac{81}{16}\right)^3$	(9,9)

Table 6. Types of edges, their numbers and amount of $\sigma_i^{'}$, $\beta_i^{'}$, $\theta_i^{'}$ of NPHX[m, *n*].

Result 6.

$$(i).GA_5(G) = 2m\left(\frac{4\sqrt{42}}{13}+\frac{8\sqrt{3}}{7}+\frac{24\sqrt{2}}{17}+\frac{3\sqrt{7}}{8}-8\right)+15mn.$$

$$(ii).ABC_4(G) = 2m\left(2\left(\sqrt{\frac{11}{42}}+\sqrt{\frac{15}{72}}\right)+\sqrt{\frac{7}{32}}+\sqrt{\frac{14}{63}}-3\right)+\frac{20}{3}mn.$$

$$(iii).S(G) = 2m\left(2\left(\frac{42}{11}\right)^3+\left(\frac{72}{15}\right)^3+\left(\frac{32}{7}\right)^3+\left(\frac{63}{14}\right)^3-9\left(\frac{81}{16}\right)^3+128\right)+15mn\left(\frac{81}{16}\right)^3.$$

2.2Nanotubes Covered by C_4

In this section, we compute certain topological indices of nanotubes covered only by C_4. The 2*D* lattice of this family of nanotubes is a plane tiling of C_4. This tessellation of C_4 can either cover acylinder or a torus. This family of nanotubes is denoted by $TUC_4[m,n]$, in which *m* is the number of squares in a row and *n* is the number of squares in a column [15]. One can observe that $|V(TUC4[m, n])|= (n + 1)(m + 1)$ and $|E(TUC4[m, n])| = (2n + 1)(m + 1)$.

Numbers of edges	σ_i	β_i	θ_i	Types of edges
2m+2	1	$\frac{2}{3}$	$\left(\frac{9}{4}\right)^3$	(3,3)
2m+2	$\frac{4\sqrt{3}}{7}$	$\sqrt{\frac{5}{12}}$	$\left(\frac{12}{5}\right)^3$	(3,4)
(m+2)(2n-3)	$\frac{3\sqrt{7}}{8}$	$\sqrt{\frac{3}{8}}$	$\left(\frac{8}{3}\right)^3$	(4,4)

Table 7. Types of edges, their numbers and amount of σ_i , β_i , θ_i of *TUC*$_4$[*m*, *n*].

Let $G = TUC_4[m, n]$ nanotubes. By using Table 7 and 8, we obtain the following results.

Result 7.

$$(i).GA(G) = 2mn - m + 2n + \frac{8\sqrt{3}}{7}(m+1) - 1.$$

$$(ii).ABC(G) = (m+1)\left((2n-3)\sqrt{\frac{3}{8}} + \frac{4}{3} + \sqrt{\frac{5}{3}}\right).$$

$$(iii).AZI(G) = (m+1)\left((2n-3)\left(\frac{8}{3}\right)^3 + 2\left(\left(\frac{9}{4}\right)^3 + \left(\frac{12}{5}\right)^3\right)\right).$$

Number of edges	σ_i'	β_i'	θ_i'	Types of edges
2m+2	1	$\sqrt{\frac{12}{49}}$	$\left(\frac{49}{12}\right)^3$	(7,7)
2m+2	$\frac{\sqrt{105}}{11}$	$\sqrt{\frac{4}{29}}$	$\left(\frac{21}{4}\right)^3$	(7,15)
2m+2	1	$\frac{\sqrt{28}}{15}$	$\left(\frac{225}{28}\right)^3$	(15,15)
2m+2	$\frac{8\sqrt{15}}{31}$	$\frac{1}{4}\sqrt{\frac{29}{15}}$	$\left(\frac{240}{29}\right)^3$	(15,16)
(m+1)(2n-7)	1	$\frac{\sqrt{30}}{16}$	$\left(\frac{128}{15}\right)^3$	(16,16)

Table 8. Types of edges, their numbers and amount of σ_i' , β_i' , θ_i' of *TUC*$_4$[*m*, *n*].

Result 8.

$$(i).GA_5(G) = (m+1)\left(2\left(\frac{\sqrt{105}}{11}+\frac{8\sqrt{15}}{31}+n\right)-3\right).$$

$$(ii).ABC_4(G) = (m+1)\left((2n-7)\frac{\sqrt{30}}{16}+\frac{4\sqrt{3}}{7}+\frac{4}{\sqrt{21}}+\frac{4\sqrt{7}}{15}+\frac{1}{2}\sqrt{\frac{29}{15}}\right).$$

$$(iii).S(G) = (m+1)\left((2n-7)\left(\frac{128}{15}\right)^3+2\left(\left(\frac{49}{12}\right)^3+\left(\frac{21}{4}\right)^3+\left(\frac{225}{28}\right)^3+\left(\frac{240}{29}\right)^3\right)\right).$$

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