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Computation of Topological Indices of HA ($C_5c_6c_7$) Nanotube

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ABSTRACT

Chemical graph theory is a branch of Mathematics in where we can combine Mathematics and chemistry which go hand in hand with each other. Topological index which is popularly known as molecular index which is a category of molecular structure descriptor that is formulated on the molecular graph, named as a structure of a chemical compound. It is simply a numerical quantity which relates chemical structure with physical and chemical properties. The relation between Atom - Bond Connectivity, Geometric - Arithmetic Index, Randic index is well described with the help of chemical graph theory. In nanotechnology topological indices play a huge role in finding the value of the nanoparticles. In this paper structure of the nanotube is investigated and the Atom Bond Connectivity, Geometric Arithmetic Index and Randic Index are computed. The carbon nanotubes are tube like structures whose measurements are made in nanometers has vast range of applications in day-today-life.

Keywords
Atom Bond Connectivity(ABC),Geometric Arithmetic (GA) index, Sum Connectivity Index(SCI), Randic index, Nanotubes.

Introduction

“Chemical graph theory which is one of the branches of mathematics where we tend to apply graph theory to the mathematical model of chemical phenomenon.” Graph theory has a major branch called topological indices where we correlate and discuss certain physio-chemical properties of the corresponding chemical compound. “In the upcoming years chemical graph theory has a huge impact on the development of chemical sciences and medical field.” Topological index most commonly referred as connectivity index is a category of molecular structure descriptor where the end result is based on the molecular structure of a chemical compound. Mainly topological indices are applied in the evolution of Quantity Structure Activity Relationship (QSAR) where biological structure and activity of certain properties and constraints of molecules are linked with their chemical structure as a result , its application is vast not only in biology but also in pharma and medical field.

Nanotechnology is an area of research concerning the nanostructure between 1 to 100 nanometres and it mainly deals with atoms and molecules. “Nanosheet is nothing but a sheet of material whose thickness ranges from of 1 to 100 nanometres and the best example is graphene.” It has a wide range of applications [1] in medicine for treating disease, in industry its applications mainly in materials, electrical and electronics where nanowire and nano rod plays a huge role in this category, for surface coatings carbon nanotubes are preferred. It is no doubt that it is going to show a bright future in the 21^{st} century starting from space to communication, it has a huge impact and it would be part and parcel of our life.

“The two-dimensional lattice graph also known as grid graph is the cartesian product of path graph of m and n vertices named as 2-D lattice.” The carbon nanotubes popularly known as CNTs are cylindrical tube in nature with regard to its structure is made up of graphite sheets. These materials are very strong and possess an excellent thermal conductivity. Carbon nanotubes are relatively thin whose diameter is 10000 times smaller when compared to a human hair. The length of the carbon nanotube ranges from less than 100 nm to 0.5m. There are two types of nanotubes. Single walled nanotube (SWNT) which comprises of only one graphite sheet whereas comprising of more than one nanotube called multi-walled nanotube (MWNT). Carbon nanotube plays a huge role in scientific community not only because of its allure physio-chemical properties but also because of its special application in chemical sciences.

Harold Wiener's work on paraffine to determine its boiling point in 1947 gave rise to the concept of topological index. He named this index as path number which was renamed as Wiener Index.[2]

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The Randic index, abbreviated R (G), was introduced by Milan Randic in 1975 and is the first and oldest degree-based topological index. [3]

The Atom-Bond Connectivity (ABC) index introduced by Estrada et al.in[4] is one of the popular topological index.

Next topological index, Geometric-Arithmetic index is introduced by Vukicevic and Furtula.[5]
The Sum Connectivity Index ($SCI(G)$)being introduced by Zhou and Trinajstic.[6]

Preliminaries

Let G be a connected molecular graph with the vertex and edge sets denoted by V (G) and E (G), respectively. The distance between two vertices a and b are denoted by d (a, b), which is defined as the number of edges in the shortest path connecting a and b.

Definition 1.1

"Let G be a graph. Then the Wiener Index of G is defined as

$$W\ (G) = \frac{1}{2}\sum_{(u,v)\in E(G)} d_G(u,v)$$

Where $(u\ ,v)$ is any ordered pair of vertices in G and d_G(a, b) is a-b geodesic (which is the shortest path).

The very first and oldest degree based topological index is Randic index denoted by R_α(G) introduced by Milan Randic in 1975.[3]

Definition 1.2

Let G be a graph. Then the Randic Index of G is defined as

$$R_\alpha(\mathrm{G}) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u\ d_v}}$$

One of the well-known connectivity topological index is atom-bond connectivity (ABC) index introduced by Estrada et al.in.

Definition 1.3

For a graph G,ABC Index is defined as

$$ABC\ (G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

Another topological index, Geometric_ Arithmetic index is introduced by Vukicevic and Furtula.

Definition 1.4

Consider a graph, then its Geometric Index popularly known as GA index is defined as

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u\ d_v}}{(d_u + d_{v)}}$$

The Sum Connectivity Index $SCI(G)$ was invented by Zhou and Trinajstic.

Definition 1.5

The Sum Connectivity Index $SCI(G)$ is a topological index of a molecular graph G is defined as

$$SCI(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

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Here we discuss certain degree based topological indices of 2-D lattice of HA$C_5C_6C_7$[m,n] , with m=4,n=2 and 2-D graph of lattice T∪ $C_4C_6C_8$[3,4].

These topological indices are used to correlate the molecular structure and physio-chemical properties of these nanotubes.”

Main Results

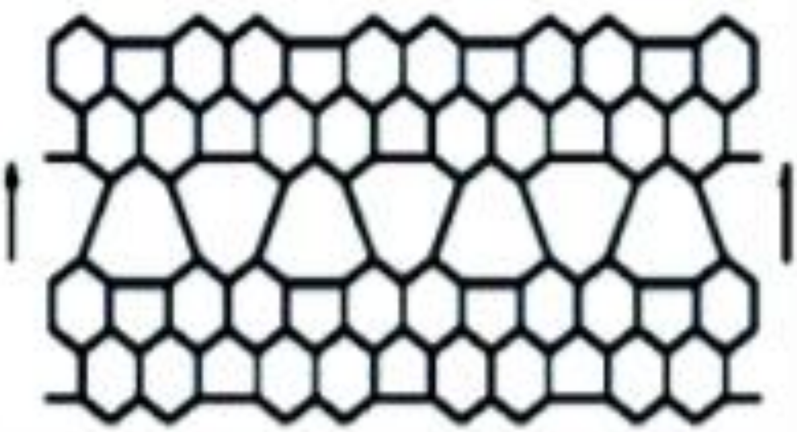
This paper deals with the structural property and specific indications are made on each topological index depending on the nanotubes. “In this article we compute RandicIndex,Atom Bond Connectivity, Geometric Arithmetic and Sum-Connectivity Index.”

“Here the notations are denoted in which p is the number of pentagons in one row, and the first three rows of vertices and edges are repeated alternately, the number of repetitions is denoted by q.”

“The HA$C_5C_6C_7$[p,q] nanotube is a $C_5C_6C_7$ net which is constructed by alternating C_5 , C_6 *and* C_7 giving a trivalent combination.”

The 2-D lattice of HA$C_5C_6C_7$[p,q] with p=4 and q=2 is shown in the figure.[10]

2-D Lattice of HA $C_5C_6C_7$ with p = 4 and q = 2



Lemma 1.1

Let G be a graph of 2-D lattice of nanotubes with (p,q$>$ 1) then its edge set cardinality is
$|E(G)|$ = 24pq-2p

Results

In the edge partition of co-ordination nanosheet c[p,q], here we take two values $E_1$and E_2 for $HAC_5C_6C_7[p,q]$ and is denoted in the tabular column.

d_u,d_v where uv∈ $E(G)$	Total no of edges
E_1(2,3)	8p
E_2(3,3)	24pq-10p

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Theorem 1

In the graph G of HA$C_5C_6C_7$[p,q] , the Randic index of G is defined as

R_α(HA$C_5C_6C_7$[p,q] = $\frac{8p}{\sqrt{6}} + \frac{(24pq-10p)}{3}$.

Proof

The Randic index is expressed as,

$$R_\alpha(\text{HA}C_5C_6C_7[p,q]) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u\ d_v}}$$

$$= \sum_{uv\in E(2,3)} \frac{1}{\sqrt{d_u\ d_v}} + \sum_{uv\in E(3,3)} \frac{1}{\sqrt{d_u\ d_v}}$$

$$= 8p\,\frac{1}{\sqrt{2\times 3}} + (24pq-10p)\frac{1}{\sqrt{3\times 3}}$$

$$= \frac{8p}{\sqrt{6}} + \frac{(24pq-10p)}{3}.$$

Hence the proof.

Theorem 2

In the graph HA$C_5C_6C_7$[p,q] , the Atom Bond Connectivity is given by
ABC (HA$C_5C_6C_7$[p,q]) = $\frac{4}{3}$ p($3\sqrt{2}$ – 5)+16pq.

Proof

The Atom Bond Connectivity index is given by,

$$\text{ABC}(\text{HA}C_5C_6C_7[p,q]) = \sum_{uv\in E(G)} \sqrt{\frac{d_u+d_v-2}{d_ud_v}}$$

$$= \sum_{uv\in E(2,3)} \sqrt{\frac{d_u+d_v-2}{d_ud_v}} + \sum_{uv\in E(3,3)} \sqrt{\frac{d_u+d_v-2}{d_ud_v}}$$

$$= 8p\sqrt{\frac{2+3-2}{2\times 3}} + (24pq-10p)\sqrt{\frac{3+3-2}{3\times 3}}$$

$$= 4\sqrt{2}\,p + \frac{4}{3}(12pq-5p)$$

$$= 4\sqrt{2}\,p - \frac{20}{3}p + 16pq$$

$$= \frac{4}{3}p(3\sqrt{2}-5)+16pq.$$

Hence the proof.

Theorem 3

In the graph G of HA$C_5C_6C_7$[p,q] ,here the Sum Connectivity Index is calculated as
(SCI HA$C_5C_6C_7$[p,q]) = $\left(\frac{8}{\sqrt{5}} - 5\sqrt{\frac{2}{3}}\right)$p + $12\sqrt{\frac{2}{3}}\,pq$.

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Proof

The Sum Connectivity Index is given by,

$$SCI(HAC_5C_6C_7[p,q]) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u+d_v}}.$$

$$= \sum_{uv\in E(2,3)} \frac{1}{\sqrt{d_u+d_v}} + \sum_{uv\in E(3,3)} \frac{1}{\sqrt{d_u+d_v}}$$

$$= 8p\,\frac{1}{\sqrt{2+3}} + (24pq - 10p)\,\frac{1}{\sqrt{3+3}}$$

$$= \frac{8}{\sqrt{5}}\,p + \sqrt{\frac{2}{3}}\,(12pq\text{-}5p)$$

$$= \left(\frac{8}{\sqrt{5}} - 5\sqrt{\frac{2}{3}}\right)p + 12\sqrt{\frac{2}{3}}\,pq$$

Hence the proof

Theorem 4

In the graph G of $HAC_5C_6C_7[p,q]$,the geometric index is given as
$GA\,(HAC_5C_6C_7[p,q]) = 16\,\frac{\sqrt{6}}{5}\,p + 24pq - 10$

Proof

The Geometric Index is given by,

$$GA\,(HAC_5C_6C_7[p,q]) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u\,d_v}}{(d_u+d_v)}$$

$$= \sum_{uv\in E(2,3)} \frac{2\sqrt{d_u\,d_v}}{(d_u+d_v)} + \sum_{uv\in E(3,3)} \frac{2\sqrt{d_u\,d_v}}{(d_u+d_v)}$$

$$= 8\,p \times \frac{\sqrt{2\times3}}{2+3} + (24pq\text{-}10p) \times 2\,\frac{\sqrt{3\times3}}{3+3}$$

$$= 16\,\frac{\sqrt{6}}{5}\,p + 2(12pq\text{-}5)$$

$$= 16\,\frac{\sqrt{6}}{5}\,p + 24pq - 10.$$

Hence the proof.

Conclusion

The aim of topological indices is to transform a molecular graph into a numerical digit [7]. It is understood that new distance can be computed for any indices with the aid of the structure. Topological indices reckoned here can be used to learn the physiochemical properties of nanosheets using Quantity Structure Activity Relations (QSAR).

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