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13. Some Popular Topological Indices of Linear Benzenoid Graphs

By

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A graph is defined as G = (V,E) where V is a nonempty set whose elements are called vertices and E is a set whose elements known as edges such that each edge is associated with an unordered pair of vertices.

The vertex set of a graph G is denoted by V(G) and edge set of G is denoted by E(G). The cardinality of the set V(G) is called order of the graph and the cardinality of E(G) is called size of the graph. The number of edges in a shortest path connected the vertices u and v is called the distance between u and v and it is denoted by d (u,v). The degree of a vertex is the number of edges incident to that vertex and it is denoted by $d_G(v)$. Two vertices u and v in a graph are said to adjacent if there is an edge between u and v otherwise they are not adjacent.

In chemical graphs, atoms are represented by vertices, and bonding is represented by edges in molecular structure. A topological index is a numerical parameter that predicts the characteristics of that chemical graph. Mathematical models, based on polynomial representations of chemical compounds, can be used to predict their properties. Mathematical chemistry is rich in tools such as polynomials and functions which can forecast the properties of compounds.

A hexagonal system is a connected plane graph without cut-vertices, in which all inner faces are hexagons, such that two hexagons are either disjoint or have exactly one common edge, and no three hexagons have share a common edge. Here we consider a linear hexagonal system (Benzenoids) in which two adjacent hexagons have exactly one edge in common.

In mathematical chemistry, topological indices have become a very valuable tool for predicting properties of a compound from its molecular structure. It is possible to correlate the physical, chemical or biological properties of a compound to its molecular structure through numerical values called topological indices, which are derived from the Molecular graph of the compound. Topological indices can be easily used for chemical modeling with the help of software packages. Graph theory has growing applications in different Science and Engineering fields. Topological Index was introduced by Wiener in 1947, called Wiener index, which correlates the topology of alkanes with its boiling points. Here we have derived some of the popular topological indices for linear Benzenoids.

A topological index is a **real** number related to the graph of a chemical compound.

To analyse physio-chemical properties of chemical compounds, topological indices are useful. A topological index of a graph G is a numeric quantity related to structure of G. Some popular topological indices are Wiener index (W) and Wiener polarity index (W_p) introduced by Harold Wiener, first Zagrab (M_1), second Zagrab index (M_2) and Szeged indices (SZ) defined by Ivan Gutman et.al, PI index (PI) studied by Padmakar-Ivan and Reverse Wiener index (RW) determined by A.T. Balaban et.al.

Note that the Weiner index is a distance-based graph invariant defined as the sum of distance between all unordered pairs of vertices of a simple graph G:

$$W(G) = \sum_{\{u,v\}} d(u,v)$$

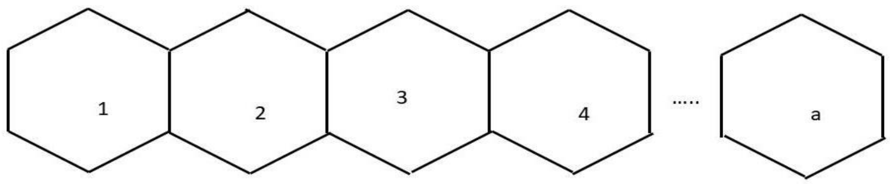
Let K_n and P_n be complete and the simple path with n vertices, respectively. Then

$$W(K_n) = C(n,\ 2) \quad \text{and} \quad W(P_n) = C(n+1,\ 3)$$

The generalized formulae of Wiener index, Szeged index, edge-Szeged index and PI index by cut method other indices Winer polarity index, first Zagrab index, second Zagrab index,Narumi-Katamia index, GA index by defintion, Reverese Wiener index using Wiener index formula for linear cata-condensed linear Benzenoids graphs are more interested and can be calculated with cut method.

Let B_a is a chemical graph of cata-condensed linear Benzenoid with 'a' number of benzenoids. The graph B_a is of order $4a+2$ and size $5a+1$.

The graph with ‘a’ linear cata-condensed Benzenoids is



Theorem 1: The Wiener index of B_a, $W(B_a)=\frac{1}{3}(16a^3+36a^2+26a+3)$.

Theorem 2: The edge Szeged of B_a, $Sz_e(B_a)=\frac{2}{3}(31a^3-9a^2+14a)$.

Theorem 3: The Szeged of B_a, $Sz(B_a)=\frac{1}{3}(44a^3+72a^2+43a+3)$

Theorem 4: The first Zagreb index of B_a, $M_1(B_a)=26a-2$.

Theorem 5: The second Zagreb index of B_a, $M_2(B_a)=33a-9$.

Theorem 6: Padmakar-Ivan index of B_a, $PI(B_a)=24a^2$.

Theorem 7: GA index of B_a, $GA(B_a)=a+5+\frac{8(a-1)\sqrt{6}}{5}$ for $a\geq 2$.

Theorem 8: Narumi –Katamaya index of B_a, $NK(B_a)=2^{2a+4}3^{2a-2}$..

Theorem 9: Wiener – polarity index of B_a, $W_p(B_a)=9a-6$.

- **N. Karunakar**