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13. Some Popular Topological Indices of Linear Benzenoid Graphs

By

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In graph theory a graph 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 number of vertices and the number of edges in a graph are called order and size of the graph respectively. The distance between any pair of vertices is the number of edges between them in the shortest path between them.

In chemical graphs, vertices represent atoms, and edges represent the bonding between vertices in a molecular structure. Topological indices are employed in mathematical chemistry to predict properties of chemical compounds by analyzing their molecular graph. These indices represent different structural features and are instrumental in estimating properties like boiling point, melting points, solubility and toxicity.

A hexagonal system is a connected planar graph without cut-vertices, in which all inner faces are hexagons, such that any two hexagons are either disjoint or have exactly one edge in common, and no three hexagons have share a common edge.

The concept of **topological indices** plays a critical role in mathematical chemistry, where they are used to predict various properties of chemical compounds based on their molecular structure. These indices are derived using graph theory, and they serve as a bridge between a molecule's topology (structure) and its chemical properties.

One of the **first topological indices**, introduced by **Wiener** in 1947, is known as the **Wiener index**. This index correlates the molecular topology of alkanes with properties like boiling points. The Wiener index is calculated as the sum of the shortest path distances between all pairs of vertices (atoms) in the molecule's graph representation.

In more recent times, the application of graph theory has grown in the fields of chemistry, biology, and materials science. As a result, various topological indices have been developed to describe and predict the properties of chemical compounds. Among these indices, there are several that are particularly useful for describing **linear benzenoids** — a class of compounds consisting of fused benzene rings in a linear arrangement. These compounds are important due to their relevance in materials science and organic chemistry.

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:

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

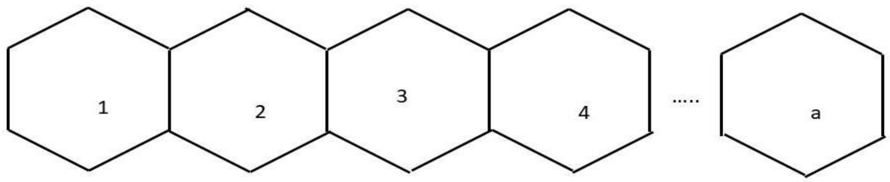
Let K_n and P_n be complete and the simple path graphs with n vertices, respectively. Then

their Weiner indices are C(n,2) and C(n+1,3) respectively.

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, $W(B_a)=\frac{1}{3}\left(16a^3+36a^2+26a+3\right)$.

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

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

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**