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Degree Based Topological Indices of Chemical Graphs

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Abstract

In chemical graph theory and in mathematical chemistry, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory. A chemical graph is a labeled graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Its vertices are labeled with the kinds of the corresponding atoms and edges are labeled with the types of bonds. A hydrogen-depleted molecular graph or hydrogen-suppressed molecular graph is the molecular graph with hydrogen vertices deleted. There are various topological indices such as distance based topological indices and degree based topological indices etc. In this paper I computed the edge version of ABC index, ABC_4 index, Randic connectivity index, sum connectivity index, GA index and GA_5 index of molecular graphs such as benzopolyperinaphthalene monoradical series. The results are analyzed and the general formulas are derived for the above mentioned graphs.
Key words: Topological indices, benzopolyperinaphthalene monoradical series.

1.Introduction And Preliminary Results

A molecular graph is a straightforward graph communication to the carbon atom skeleton of a organic molecule. In the molecular graph, the vertices articulate to the carbon molecules and the edges speak to the carbon-carbon bonds. A single nimber, in graph anal tical termes, représentions a chemical structure, is named as topological descriptor. A topological descriptor Wren corresponds with a molécule propreté, it Can bé détermine as molécule index or topological index. Good interaction with the structure was establish between the molecular propretés for: the rmodynamic properties (for illustration: boiling points, heat of combustion, enthalpy of formation, etc.) and several boiling properties. Therefore, a topological index restore a chemical structure into a particular number, valuable in QSPR/QSAR studies. In this paper all molecular graphs are designed to be connected, finite, loopless and deprived of parallel edges. Let G be a graph with n vertices and m edges. The degree of a vertex is the number of vertices adjacent to u and is symbolized as d(u) or d_u. By these terminologies, specific

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topological indices are well-defined in the consecutive way. The oldest degree based topological index is Randic index symbolise as $\chi(G)$ and bestowed by Randic [12].

Definition1. The Randic index for a molecular graph G is defined as $\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$.

There is a correlation among Randic index and certain physiochemical properties of alkanes: surface area, boiling points, energy level, etc. An alteration of Randic connectivity index is the sum-connectivity index. It was granted by Zhou and Trinajstic [16]. They formulated upper and lower bounds of this index for trees in terms of other graph invariants.

Definition 2. For a molecular graph G, the sum connectivity index is defined as $S(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}$.

Estrada *et al.* in [3] suggested a degree based topological index of graphs, which is named to be atom-bond connectivity index. It can be used as mechanism to model the thermodynamic properties of organic compounds.

Definition 3. The ABC index for a molecular graph G, is defined as

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

Geometric-artithmetic index is identified with a variation of physiochemical properties. It can be used as avaiable tool for QSPR/QSAR research. Vukicevic and Furtula in [15] introduced the geometric-arithmetic □GA□ index.

Definition 4. Let G be a molecular graph, then geometric-arithmetic index is defined as

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

Ghorbani and Hosseinzadeh in [7] confessed the fourth atom-bond connectivity index(ABC_4).

Definition 5. Let G be a molecular graph, then ABC_4 index is defined as

$$ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}.$$

where S_u is the summation of degrees of all the neighbors of vertex v in G.

Recently Graovac *et al*. in [9] suggested fifth GA index (GA_5). As an elemental topological index, the fifth geometric index is used to analysis the chemical properties of chemical compounds, nanomaterial and drugs.

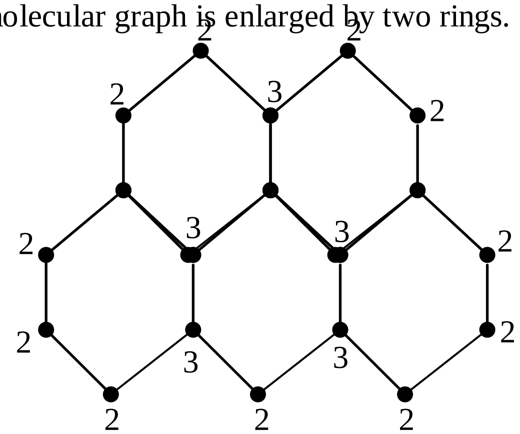
Definition 6. Let F be molecular graph, then GA_5 index is defined as

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}.$$

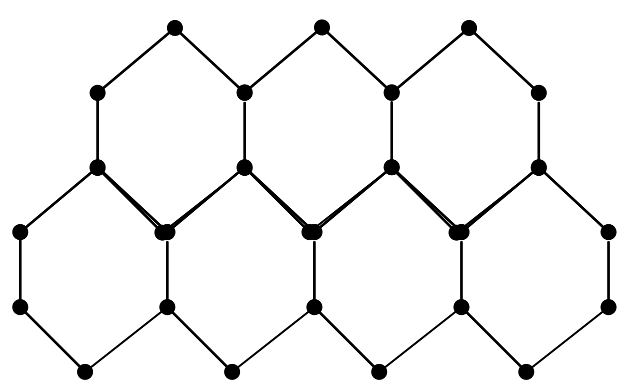
Das and Trinajstic in [2] combined the ABC and GA indices for molecular graphs and chemical trees also related their two indices for general graphs. More recent Gan *et al*. in [8] introduced some sharp lower and upper bounds on ABC. Chen and Li in [1] gave sharp lower bound for sum-connectivity index having n- vertex unicyclic graphs by k pendant vertices. Farhani in [4] explored various topological indices in polyhex nanotubes: Randic connectivity index, sum connectivity index, geometric-arithmetic index, atom-bond connectivity index, first and second Zagreb indices and Zagreb polynomials. In this paper, Randic, ABC, sum connectivity, ABC_4, GA connectivity and GA_5 indices of monoradical series of benzopolyperinaphthalene were computed.

2. RESULTS AND DISCUSSIONS

Figure. 1 presents a homologous series of closely peri-condensed monoradical benzenoids[10] consecutively built up two rings at a time by the C_6H_2 aufbau unit. The first and second molecular graphs of this series conformed to phenalenyl ($C_{13}H_9$), benzo[cd]pyrene ($C_{19}H_{11}$). Also Figure.1 presents the analytical expression for the SC (structural count) vs. a membership index number. This analytical expression is of degree 4 in n as each successive molecular graph is enlarged by two rings.



$C_{3(5)+4} = C_{19}$ (five rings)



$C_{3(7)+4} = C_{25}$ (seven rings)

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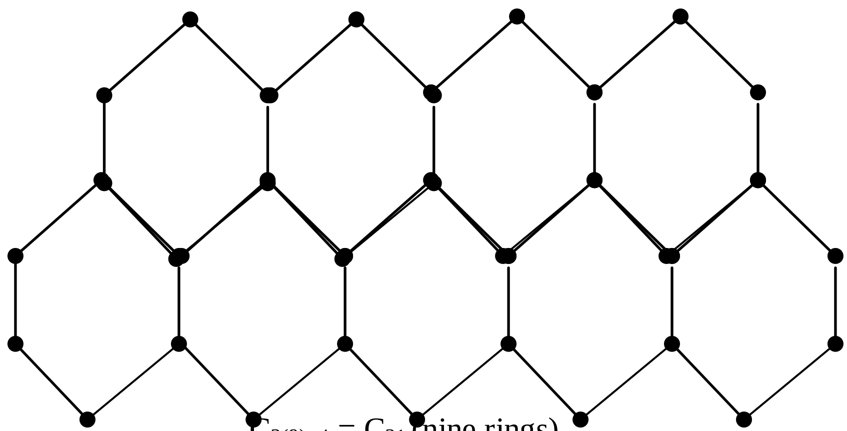

$C_{3(9)+4} = C_{31}$ (nine rings)

Figure 1. Benzopolyperinaphthalene monoradical series

2.1 Randic connectivity index of benzopolyperinaphthalene monoradical series

Consider the monoradical series of benzopolyperinaphthalene be C_{3n+4} (since number of carbon atoms in this series is 3n + 4, n ≥ 5 for odd n). The edges of G = C_{3n+4} can be subdivide into edges of form $E(d_u, d_v)$, where uv is an edge. We progress the edges of the form E(2,2), E(2,3) and E(3,3).

We know that $\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$.

$$\chi(C_{3n+4}) = |E(2,2)| \sum_{uv\in E(2,2)(G)} \frac{1}{\sqrt{d_u d_v}} + |E(2,3)| \sum_{uv\in E(2,3)(G)} \frac{1}{\sqrt{d_u d_v}} + |E(3,3)| \sum_{uv\in E(3,3)(G)} \frac{1}{\sqrt{d_u d_v}}$$

From table 1 and figure 1, $\chi(C_{3n+4}) = 3 + \frac{2n}{\sqrt{6}} + \frac{2n-3}{3}$.

This is true for all odd n, n ≥ 5.

Table 1: Edge partition formed by sum of adjacent vertices of each line.

Graphs	Edge of the form $E(d_u, d_v)$	Sum of edges (successively)
$C_{3(5)+4} = C_{19}$	E(2,2), E(2,3), E(3,3)	6, 10, 7
$C_{3(7)+4} = C_{25}$	E(2,2), E(2,3), E(3,3)	6, 14,11

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$C_{3(9)+4} = C_{31}$	E(2,2), E(2,3), E(3,3)	6, 18,15

2.2 Sum connectivity index of benzopolyperinaphthalene monoradical series

We know that $S(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}$.

$$S(C_{3n+4}) = |E(2,2)| \sum_{uv\in E(2,2)(G)} \frac{1}{\sqrt{d_u + d_v}} + |E(2,3)| \sum_{uv\in E(2,2)(G)} \frac{1}{\sqrt{d_u + d_v}}$$

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

$$= \frac{6}{\sqrt{4}} + \frac{2n}{\sqrt{5}} + \frac{2n-3}{\sqrt{6}} \text{ (from table 1 and figure 1)}$$

$$S(C_{3n+4}) = 3 + \frac{2n}{\sqrt{5}} + \frac{2n-3}{\sqrt{6}}.$$

2.3 ABC index of benzopolyperinaphthalene monoradical series

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

$$ABC(C_{3n+4}) = |E(2,2)| \sum_{uv\in E(2,2)(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} + |E(2,3)| \sum_{uv\in E(2,3)(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

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

$$= \frac{6}{\sqrt{2}} + \frac{2n}{\sqrt{2}} + \frac{2n}{3} \text{ (from table 1 and figure 1)}$$

$$ABC(C_{3n+4}) = \frac{2n+6}{\sqrt{2}} + \frac{2n}{3}.$$

2.4 GA index of benzopolyperinaphthalene monoradical series

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We know that GA(G) = $\sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$.

$$GA(C_{3n+4}) = |E(2,2)| \sum_{uv\in E(2,2)(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} + |E(2,3)| \sum_{uv\in E(2,2)(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

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

$$= 6\left[\frac{2\sqrt{4}}{4}\right] + \frac{4n\sqrt{6}}{5} + (2n-3)\left[\frac{2\sqrt{9}}{6}\right] \text{ (from table 1 and figure 1)}$$

$$GA(C_{3n+4}) = 6 + \frac{4n\sqrt{6}}{5} + (2n-3).$$

2.5 ABC_4 index of benzopolyperinaphthalene monoradical series

The edges of G can be divide into edges of form E(d_u, d_v), where uv is an edge. We develop the edges of the form E(5,5), E(5,7), E(5,4), E(7,6), E(7,9), E(9,9) that are shown in table 2.

Table 2: Edge partition formed by sum of degrees of neighbors of the head-to-head vertices of every edge.

Graphs	Edge of the form E(d_u, d_v)	Sum of edges (successively)
$C_{3(5)+4} = C_{19}$	E(5,5), E(5,7), E(5,4), E(7,6), E(7,9), E(9,9)	2, 8, 4, 2, 5, 2
$C_{3(7)+4} = C_{25}$	E(5,5), E(5,7), E(5,4), E(7,6), E(7,9), E(9,9)	2, 8, 4, 6, 7, 4
$C_{3(9)+4} = C_{31}$	E(5,5), E(5,7), E(5,4), E(7,6), E(7,9), E(9,9)	2, 8, 4, 10, 9, 6

We know that $ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}$ where S_u is the summation of degrees of all the neighbors of vertex v in G.

$$ABC_4(C_{3n+4}) = |E(5,5)| \sum_{uv\in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} + |E(5,7)| \sum_{uv\in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}$$

$$+ |E(5,4)| \sum_{uv\in E(G)} \sqrt{\frac{S_u+S_v-2}{S_uS_v}} + |E(7,6)| \sum_{uv\in E(G)} \sqrt{\frac{S_u+S_v-2}{S_uS_v}} + |E(7,9)| \sum_{uv\in E(G)} \sqrt{\frac{S_u+S_v-2}{S_uS_v}}$$

$$+ |E(9,9)| \sum_{uv\in E(G)} \sqrt{\frac{S_u+S_v-2}{S_uS_v}}$$

From table 2 and figure 1,

$$ABC_4(C_{3n+4}) = 2\sqrt{\frac{8}{25}} + 8\sqrt{\frac{10}{35}} + 4\sqrt{\frac{7}{20}} + (2n-8)\sqrt{\frac{11}{42}} + n\sqrt{\frac{14}{63}} + (n-3)\sqrt{\frac{16}{81}}.$$

2.6 GA_5 index of benzopolyperinaphthalene monoradical series

We know that $GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{S_u+S_v}$.

$$GA_5(C_{3n+4}) = |E(5,5)| \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{S_u+S_v} + |E(5,7)| \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{S_u+S_v}$$

$$+ |E(5,4)| \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{S_u+S_v} + |E(7,6)| \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{S_u+S_v} + |E(7,9)| \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{S_u+S_v}$$

$$+ |E(9,9)| \sum_{uv\in E(G)} \frac{2\sqrt{S_uS_v}}{S_u+S_v}$$

From table 2 and figure 1,

$$GA_5(C_{3n+4}) = 2\left[\frac{2\sqrt{5.5}}{5+5}\right] + 8\left[\frac{2\sqrt{5.7}}{5+7}\right] + 4\left[\frac{2\sqrt{5.4}}{5+4}\right] + (2n-8)\left[\frac{2\sqrt{6.7}}{6+7}\right] + n\left[\frac{2\sqrt{9.7}}{9+7}\right] + (n-3)\left[\frac{2\sqrt{9.9}}{9+9}\right]$$

$$= 2\left[\frac{2\sqrt{25}}{10}\right] + 8\left[\frac{2\sqrt{35}}{12}\right] + 4\left[\frac{2\sqrt{20}}{9}\right] + (2n-8)\left[\frac{2\sqrt{42}}{13}\right] + n\left[\frac{2\sqrt{63}}{16}\right] + (n-3)\left[\frac{2\sqrt{81}}{18}\right]$$

$$GA_5(G) = 2 + \frac{4\sqrt{35}}{3} + \frac{8\sqrt{20}}{9} + (4n-16)\frac{\sqrt{42}}{13} + n\frac{\sqrt{63}}{8} + (n-3).$$

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