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REVIEW ARTICLE

EDGE VERSION MOLECULAR DESCRIPTORS OF POLYCYCLIC AROMATIC HYDROCARBONS

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ABSTRACT

Chemical Graph Theory an important branch of Graph Theory has become a very popu- lar research field among the researchers, due to its wide range of applications in Mathematical Chemistry, Theoretical Chemistry and Pharmaceutical Chemistry. The molecular descriptors are the numerical invariants of a molecular graph used for predicting their Physico-chemical properties and biological activity. In this article, we find closed formulas of edge version of molecular descriptors such as Atom-Bond Connectivity Index, Fourth Atom-Bond Connec- tivity Index, Geometric Arithmetic Index, Fifth Geometric Arithmetic Index, Zagreb Index, Generalized Multiplicative Zagreb Index and F-index of Polycyclic Aromatic Hydrocarbons molecular graph.

KEYWORDS

Molecular Descriptors, Degree based invariants, Line Graph, Polycyclic Aromatic Hydrocarbons

1. INTRODUCTION

Chemical Graph Theory devotes graph theoretic ideas to encrypt the structure of a molecule. A chemical graph refers to a mathematical object that acknowledges the structure of various interconnections of a molecule. A chemical graph is essentially a statement about vertices (nodes) and edges (links) and their relations. A primal concept in chemical graph theory, and in molecular connectivity, is the idea of valence (degree) of a node encrypting atom, i.e., its connectivity degree. For a molecular graph M, with the node set V (M) and link set E(M), a Molecular Descriptor (Topological Index) is a numerical quantity that can be extracted from M. The order of a graph is |V (M)|, represents cardinality of vertex (node) set denoted by m. The size of a graph is |E(M)|, represents cardinality of edge (link) set denoted by n. The valency (degree) of a node u is the number of edges incident to u denoted by $d_M(u)$ or du or deg(u). su= Σ v∈Nu du , where Nu = {v ∈ V (M) : vu ∈ E(M)}. The Line graph L(M) of a graph is the

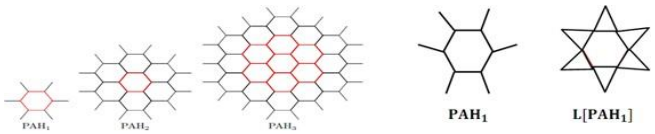

Figure 1: First three members of PAH family and Line graph of its first member

Simple graph is that the links in M are replaced by nodes in L(M) and two nodes in L(M) are connected whenever the corresponding links in M are adjacent. The interest of study of topological indices is mainly associated with its applications in QSAR/QSPR. The applications of line graphs in chemistry was originated from structural chemistry. The first edge version molecular descriptors was introduced in 1981 the advanced theory of molecular branching and complexity. For several molecular descriptors based on line graph of a molecular graph, more about its applications and edge version of other molecular structures and nanotubes [1-12].

The edge version of General Randi´c index was introduced and defined as [13]:

$$ {}_eR_\alpha(M) = \sum_{uv \in E(L(M))} (d_{L(M)}(u).d_{L(M)}(v))^\alpha \qquad (1.1) $$

for α ∈ R and where $d_{L(M)}(u)$ is the valency of the node e and $d_{L(M)}(v)$ is the valency of the node v of line graph M.

In Gutman and Trinajistic defined the edge version of Zagreb index as [2]:

$$ {}_eM_1(M) = \sum_{uv \in E(L(M))} (d_{L(M)}(u) + d_{L(M)}(v))^\alpha \qquad (1.2) $$

where $d_{L(M)}(u)$ is the valency of the node u and $d_{L(M)}(v)$ is the valency of the node v of line graph M.
Similarly,

$$ {}_eM_2(M) = \sum_{uv \in E(L(M))} (d_{L(M)}(u) d_{L(M)}(v))^\alpha \qquad (1.3) $$

Kulli generalized the first and second multiplicative Zagreb indices of a Graph M as [14]:

$$ {}_eM_1^{\alpha}(M) = \prod_{uv \in E(L(M))} (d_{L(M)}(u) + d_{L(M)}(v))^{\alpha} \quad (1.4) $$

where $d_{L(M)}(u)$ is the valency of the node u and $d_{L(M)}(v)$ is the valency of the node v of line graph M.

Similarly,

$$ {}_eM_2^{\alpha}(M) = \prod_{uv \in E(L(M))} (d_{L(M)}(u) d_{L(M)}(v))^{\alpha} \quad (1.5) $$

Recently, Furtula and Gutman defined" forgotten topological index" or" F-index" and its edge version is [15]:

$$ {}_eF(L(M)) = \sum_{x \in V(L(M))} (d_{L(M)}(x))^3 = \sum_{xy \in E(L(M))} [(d_{L(M)}(x))^2 + (d_{L(M)}(y))^2] \quad (1.6) $$

Estrada et al reported the Atom Bond Connectivity index and its edge version is defined [13]:

$$ {}_eABC(M) = \sum_{uv \in E(L((M))} \sqrt{\frac{d_{L(M)}(u) + d_{L(M)}(v) - 2}{d_{L(M)}(u) d_{L(M)}(v)}} \quad (1.7) $$

where $d_{L(M)}(u)$ is the valency of the node e and $d_{L(M)}(v)$ is the valency of the node v of line graph M. The fourth edge version of Atom Bond Connectivity index is defined as

$$ {}_eABC_4(M) = \sum_{uv \in E(L((M))} \sqrt{\frac{s_{L(M)}(u) + s_{L(M)}(v) - 2}{s_{L(M)}(u) s_{L(M)}(v) - 2}} \quad (1.8) $$

where $s_{L(M)}(u)$ is the sum of valency of the nodes adjacent with u and $s_{L(M)}(v)$ is the valency of the nodes adjacent with v of line graph of M.

The difference of geometric and arithmetic mean is defined as the Geometric Arithmetic index introduced by Vukiˆcevi´c and Furtula and its edge version is given [16]:

$$ {}_eGA(M) = \sum_{uv \in E(L(M))} \frac{2\sqrt{d_{L(M)}(u) d_{L(M)}(v)}}{d_{L(M)}(u) + d_{L(M)}(v)} \quad (1.9) $$

And its fifth version is defined as

$$ {}_eGA_5(M) = \sum_{uv \in E(L(M))} \frac{2\sqrt{s_{L(M)}(u) s_{L(M)}(v)}}{s_{L(M)}(u) + s_{L(M)}(v)} \quad (1.10) $$

where $d_{L(M)}(u)$ is the valency of the node ed$_{L(M)}(v)$ is the valency of the node v of line graph M and $s_{L(M)}(u)$ is the sum of valency of the nodes adjacent with u $s_{L(M)}(v)$) is the valency of the nodes adjacent with v of line graph of M .

In a study, they had reported generalized certain degree based and generalized multiplicative indices of Polycyclic Aromatic Hydrocarbons (PAH_n). [14]. In this article, we compute the edge version topological invariants of Polycyclic Aromatic Hydrocarbons (PAH_n).

2. EDGE VERSION MOLECULAR DESCRIPTORS OF POLYCYCLIC AROMATIC HYDROCARBONS (PAHn)

Unless stated otherwise, let M be the molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n) and G be the line graph of the molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n) n > 2. There are $6n^2$ + 6n nodes and $9n^2$ + 3n links in M and also there are $9n^2$ + 3n nodes and 18n2 links in G. Out of $9n^2$ + 3n nodes in G, $9n^2$ – 3n nodes are of degree two and 6n nodes of degree four. Let us consider the edge partition of G based on degree, the first edge partition has 12n links with $d_{L(M)}(u) = 2$ and $d_{L(M)}(v) = 4$ and the second edge partition has $18n^2 – 12n$ links with $d_{L(M)}(u) = d_{L(M)}(v) = 4$. We now compute the edge version of Randi´c, Zagreb, Atom Bond Connectivity with its fourth version and Geometric Arithmetic index with its fifth version of G.

Theorem 2.1 For any n ∈ N, the edge version of GeneralRandi´c index of Polycyclic Aromatic Hydrocarbons is

$$ {}_eR_{\alpha}(G) = 3n[2^{3\alpha+2} + 2^{4\alpha+1}(3n-2)] $$

Proof:

Let G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n). By the definition of edge version of General Randi´c index (1.1) of any graph, we have

$$ \begin{aligned} {}_eR_{\alpha}(G) &= \sum_{uv \in E(L(M))} (d_{L(M)}(u).d_{L(M)}(v))^{\alpha} \\ &= \sum_{(2,4) \in E(L(M))} (2 \times 4)^{\alpha} + \sum_{(4,4) \in E(L(M))} (4 \times 4)^{\alpha} \\ &= 12n(2 \times 4)^{\alpha} + (18n^2 - 12n)(4 \times 4)^{\alpha} \end{aligned} $$

After simplification, we get

$$ {}_eR_{\alpha}(G) = 3n[2^{3\alpha+2} + 2^{4\alpha+1}(3n-2)] $$

Theorem 2.2 For any n ∈ N, the edge version of First Zagreb index of Polycyclic Aromatic Hydrocarbons is

$$ {}_eM_1(G) = n[144n - 24]. $$

Proof:

Let G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n). By the definition of edge version of first Zagreb index (1.2) of any graph, we have

$$ \begin{aligned} {}_eM_1(G) &= \sum_{uv \in E(L(M))} (d_{L(M)}(u) + d_{L(M)}(v)) \\ &= \sum_{(2,4) \in E(L(M))} (2+4) + \sum_{(4,4) \in E(L(M))} (4+4) \\ &= 12n(2+4) + (18n^2 - 12n)(4+4) \\ &= n[144n - 24] \qquad \square \end{aligned} $$

Theorem 2.3 For any n ∈ N, the edge version of Second Zagreb index of Polycyclic Aromatic Hydrocarbons is

Proof:

Let G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n). By the definition of edge version of Second Zagreb index (1.3) of any graph, we have

$$ \begin{aligned} {}_eM_2(G) &= \sum_{uv \in E(L(M))} (d_{L(M)}(u) d_{L(M)}(v)) \\ &= \sum_{(2,4) \in E(L(M))} (2 \times 4) + \sum_{(4,4) \in E(L(M))} (4 \times 4) \\ &= 12n(2 \times 4) + (18n^2 - 12n)(4 \times 4) \\ &= n[288n - 96]. \qquad \square \end{aligned} $$

Theorem 2.4 For any n ∈ N, the edge version of First Multiplicative Zagreb index of Polycyclic Aromatic Hydrocarbons is

$$_eM_1^{\alpha}(G) = 2^{54\alpha n^2-24\alpha n} \times 3^{12\alpha n}$$

Proof:
Let G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n). By the definition of edge version of First Multiplicative Zagreb index (1.4) of any graph, we have

$$\begin{aligned} _eM_1^{\alpha}(G) &= \prod_{uv\in E(L(M))} (d_{L(M)}(u) + d_{L(M)}(v))^{\alpha} \\ &= \prod_{(2,4)\in E(L(M))} (2+4)^{\alpha} + \prod_{(4,4)\in E(L(M))} (4+4)^{\alpha} \\ &= (2+4)^{12n\alpha} \times (4+4)^{(18n^2-12n)\alpha} \\ &= 2^{54\alpha n^2-24\alpha n} \times 3^{12\alpha n} \end{aligned}$$

Theorem 2.5 For any n ∈ N, the edge version of Second Multiplicative Zagreb index of Polycyclic Aromatic Hydrocarbons is

$$_eM_2^{\alpha}(G) = 2^{72\alpha n^2-12\alpha n}.$$

Proof:
Let G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n).
By the definition of edge version of Second Multiplicative Zagreb index (1.5) of any graph, we have

$$\begin{aligned} _eM_2^{\alpha}(G) &= \prod_{uv\in E(L(M))} (d_{L(M)}(u) \times d_{L(M)}(v))^{\alpha} \\ &= \prod_{(2,4)\in E(L(M))} (2\times 4)^{\alpha} + \prod_{(4,4)\in E(L(M))} (4\times 4)^{\alpha} \\ &= (2\times 4)^{12n\alpha} \times (4\times 4)^{(18n^2-12n)\alpha} \\ &= 2^{72\alpha n^2-12\alpha n}. \end{aligned}$$

Theorem 2.6 For any n ∈ N, the edge version of F − index of Polycyclic Aromatic Hydrocarbons is

Proof:
Let G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n). By the definition of edge version of F − index (1.6) of any graph, we have

$$\begin{aligned} _eF(G) &= \sum_{uv\in E(L(M))} [(d_{L(M)}(u))^2 + (d_{L(M)}(v))^2] \\ &= \sum_{(2,4)\in E(L(M))} (2^2+4^2) + \sum_{(4,4)\in E(L(M))} (4^4+4^4) \\ &= 12n(20) + (18n^2-12n)(32) \\ &= n[576n-144]. \qquad \square \end{aligned}$$

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Theorem 2.7 For any n ∈ N, the edge version of Atom Bond connectivity index of Polycyclic Aromatic Hydrocarbons is

$$_eABC(G) = \frac{1}{2}\left[9\sqrt{6}n^2 - 12\sqrt{2}n - 6\sqrt{6}n\right]$$

Proof:
Let G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n).
By the definition of edge version of Atom Bond connectivity index (1.7) of any graph, we have

$$\begin{aligned} _eABC(G) &= \sum_{uv\in E(L(M))} \sqrt{\frac{d_{L(M)}(u)+d_{L(M)}(v)-2}{d_{L(M)}(u)d_{L(M)}(v)}} \\ &= \sum_{(2,4)\in E(L(M))} \sqrt{\frac{2+4-2}{2\times 4}} + \sum_{(4,4)\in E(L(M))} \sqrt{\frac{4+4-2}{4\times 4}} \\ &= 12n\sqrt{\frac{2+4-2}{2\times 4}} + (18n^2-12n)\sqrt{\frac{4+4-2}{4\times 4}} \\ &= 6\sqrt{2}n + \frac{(n(9n-6))}{2}\sqrt{6} \\ &= \frac{1}{2}\left[9\sqrt{6}n^2 - 12\sqrt{2}n - 6\sqrt{6}n\right] \qquad \square \end{aligned}$$

Theorem 2.8 For any n ∈ N, the edge version of Atom Bond connectivity index of Polycyclic Aromatic Hydrocarbons is

$$_eGA(G) = 18n^2 + 2n(3\sqrt{2}-6)$$

Proof:
Let G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n). By the definition of edge version of Geometric Arithmetic index (1.9) of any graph, we have

$$\begin{aligned} _eGA(G) &= \sum_{uv\in E(L(M))} \frac{2\sqrt{d_{L(M)}(u)d_{L(M)}(v)}}{d_{L(M)}(u)+d_{L(M)}(v)} \\ &= \sum_{uv\in(2,4)} \frac{2\sqrt{2\times 4}}{2+4} + \sum_{uv\in(4,4)} \frac{2\sqrt{4\times 4}}{4\times 4} \\ &= (12n)\frac{2\sqrt{2\times 4}}{2+4} + (18n^2-12n)\frac{2\sqrt{4\times 4}}{4\times 4} \\ &= 18n^2 + 2n(3\sqrt{2}-6) \qquad \square \end{aligned}$$

Table 1: The edge partition of G, for n > 1.

(s(u),s(v)) ∀uv ∈ E(G)	Number of edges
(8, 12)	12
(8, 14)	12n − 12
(12, 14)	12
(14, 14)	12n − 18
(14, 16)	12n − 12
(16, 16)	18n^2−36n+18

Theorem 2.9 For n > 1, let G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons [PAHn]. Then

$$\begin{aligned} _eABC_4(G) &= 3[\sqrt{3} + n\sqrt{2} - \sqrt{2}] + \frac{9n^2-18n+9}{8}\sqrt{30} \\ &\quad + \frac{3}{7}[4\sqrt{7} + (n-1)\sqrt{35} + (2n-3)\sqrt{6}] \end{aligned}$$

Proof:
Let G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n).
By the definition of edge version of Fourth Atom Bond Connectivity index

(1.8) of any graph, we have

$$
\begin{aligned}
{}_eABC_4(G) &= \sum_{uv\in E(L(M))}\sqrt{\frac{s_{L(M)}(u)+s_{L(M)}(v)-2}{s_{L(M)}(u)s_{L(M)}(v)-2}} \\
&= \sum_{uv\in(8,12)}\sqrt{\frac{8+12-2}{8\times 12}}+\sum_{uv\in(12,14)}\sqrt{\frac{12+14-2}{12\times 14}}+\sum_{uv\in(16,14)}\sqrt{\frac{16+14-2}{16\times 14}} \\
&+ \sum_{uv\in(8,14)}\sqrt{\frac{8+14-2}{8\times 14}}+\sum_{uv\in(14,14)}\sqrt{\frac{14+14-2}{14\times 14}}++\sum_{uv\in(16,16)}\sqrt{\frac{16+16-2}{16\times 16}} \\
&= 12\sqrt{\frac{8+12-2}{8\times 12}}+12\sqrt{\frac{12+14-2}{12\times 14}}+(12n-12)\sqrt{\frac{16+14-2}{16\times 14}} \\
&+ (12n-12)\sqrt{\frac{8+14-2}{8\times 14}}+(12n-18)\sqrt{\frac{14+14-2}{14\times 14}} \\
&+ (18n^2-36n+18)\sqrt{\frac{16+16-2}{16\times 16}}
\end{aligned}
$$

After Simplification, we get

$$
\begin{aligned}
{}_eABC_4(G) &= 3[\sqrt{3}+n\sqrt{2}-\sqrt{2}]+\frac{9n^2-18n+9}{8}\sqrt{30} \\
&+\frac{3}{7}[4\sqrt{7}+(n-1)\sqrt{35}+(2n-3)\sqrt{6}]
\end{aligned}
$$

Corollary 2.10 If G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons [PAH_1], then

$$
{}_eABC_4(G) = 7.412
$$

Theorem 2.11 For n > 1, let G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n). Then

$$
{}_eGA_5(G) = 18n^2-24n+\frac{4}{5}\left[(4n-4)\sqrt{14}+\sqrt{6}\right]+\frac{24}{13}\sqrt{42}+\frac{4(12n-12)}{11}\sqrt{7}.
$$

Proof:
Let G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons (PAH_n). By the definition of edge version of Fifth Geometric Arithmetic index (1.10) of any graph, we have

$$
\begin{aligned}
{}_eGA_5(G) &= \sum_{uv\in E(L(M))}\frac{2\sqrt{s_{L(M)}(u)s_{L(M)}(v)}}{s_{L(M)}(u)+s_{L(M)}(v)} \\
&= \sum_{(8,12)\in E(L(M))}\frac{2\sqrt{8\times 12}}{8+12}+\sum_{(12,14)\in E(L(M))}\frac{2\sqrt{12\times 14}}{12+14}+\sum_{(14,16)\in E(L(M))}\frac{2\sqrt{14\times 16}}{14+16} \\
&+ \sum_{(8,14)\in E(L(M))}\frac{2\sqrt{8\times 14}}{8+14}+\sum_{(14,14)\in E(L(M))}\frac{2\sqrt{14\times 14}}{14+14}+\sum_{(16,16)\in E(L(M))}\frac{2\sqrt{16\times 16}}{16+16} \\
&= (12)\frac{2\sqrt{9\times 9}}{9+9}+(12)\frac{2\sqrt{9\times 10}}{9+10}+(12n-12)\frac{2\sqrt{10\times 10}}{10+10} \\
&+ (12n-12)\frac{2\sqrt{10\times 17}}{10+17}+(12n-18)\frac{2\sqrt{17\times 17}}{17+17}+(18n^2-36n+18)\frac{2\sqrt{17\times 24}}{17+24} \\
&= 18n^2-24n+\frac{4}{5}\left[(4n-4)\sqrt{14}+\sqrt{6}\right]+\frac{24}{13}\sqrt{42}+\frac{4(12n-12)}{11}\sqrt{7}. \qquad \square
\end{aligned}
$$

Corollary 2.12 If G be the line graph of molecular graph of Polycyclic Aromatic Hydrocarbons [PAH_1], then

$$
{}_eGA_5(G) = 17.7576.
$$

3. CONCLUSION

In this article, we reported closed formulas of edge version of molecular descriptors such as Atom-Bond Connectivity Index, Fourth Atom-Bond Connectivity Index, Geometric Arithmetic Index, Fifth Geometric Arithmetic Index, Zagreb Index, Generalized Multiplicative Zagreb Index and F-index of Polycyclic Aromatic Hydrocarbons molecular graph.

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CONFLICT OF INTEREST

The authors declare that they have no conflict of interest.

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