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Eccentricity Of Topological Indices In Chemical Graph

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Abstract:Topological index is an invariant of molecular graphs which correlates the structure with different physical and chemical invariant of the compound like boiling point, chemical reactivity, stability, Kovat's constant etc. Eccentricity-based topological indices, like eccentric connectivity index, connective eccentric index, first Zagreb eccentricity index, and second Zagreb eccentricity index graphs.

Keywords: Eccentric degree, topological index, chemical graph.

1 Introduction

Let $G(V, E)$ be a simple and disconnected graph with n vertices and m edges. Let $u \in V$ then be the eccentricity of a vertex where u is a maximum distance of u from other vertices of graph G. Which is denoted by $e(u)$, That is denoted by $e(u) = max\ \{d(u, v); v \in V\ \}$, where $d(u, v)$ is a distance between u and v. The de- gree of vertex u, is number of vertices which are attached to u by the edges. The eccentric connectivity index is introduced by Sharm, Goswami, and madan [**?**].

I. B. Furtula, A. Graovac, D. Vuki cevi c [4], introduced the Atom-bond connectivity index of tree in 2009 as follows: $ABC^{P_3}(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_{P_3}(u) + d_{P_3}(v) - 2}{d_{P_3}(u)d_{P_3}(v)}}$

In 2022, A. Ali, B. Furtula,I. Rečzepović[1] defined the Atom-bond sum connectivity index of a graph G as follows:

$$ABS^{P_3}(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_{P_3}(u) + d_{P_3}(v) - 2}{d_{P_3}(u) + d_{P_3}(v)}}$$

B. Furtula, A. Graovac, D. Vuki cevi c, Augmented Zagreb index[5], and it is defined in 2010:

$$AGI^{P_3}(G) = \sum_{uv\in E(G)} \left(\frac{d_{P_3}(u)d_{P_3}(v)}{d_{P_3}(u) + d_{P_3}(v) - 2}\right)^3$$

V.R.Kulli [15], defined the Sum augmented and multiplicative sum augmented indices in 2023 as follows:

$$SAI^{P_3}(G) = \sum_{uv\in E(G)} \left(\frac{d_{P_3}(u) + d_{P_3}(v)}{d_{P_3}(u) + d_{P_3}(v) - 2}\right)^3$$

Yan Yuan, Bo Zhou, N.Trinajstic,[19] introduced the Geometric-arithmetic index defined in 2010.

$$AGI^{P_3}(G) = \sum_{uv\in E(G)} \frac{d_{P_3}(u) + d_{P_3}(v)}{2\sqrt{d_{P_3}(u)d_{P_3}(v)}}$$

Shegehall V.S,and Kanabur R. [17] introduced the Arithmetic-geometric index defined in 2015.

$$AGI^{P_3}(G) = \sum \frac{d_{P_3}(u) + d_{P_3}(v)}{2\sqrt{d_{P_3}(u)d_{P_3}(v)}}$$

I. Gutman and N. Trinajstić in [8] introduced the First Zagreb index and Second Zagreb index in 1972 as follows:

$$M_1^{P_3}(G) = \sum_{uv \in E(G)} (d_{P_3}(u) + d_{P_3}(v)), \quad M_2^{P_3}(G) = \sum_{uv \in E(G)} d_{P_3}(u) d_{P_3}(v)$$

In 2012, M. Ghorbani and N. Azimi [9] defined the first and second Multiple Zagreb indices of a graph G as follows:

$$PM_1^{P_3}(G) = \prod_{uv \in E(G)} (d_{P_3}(u) + d_{P_3}(v)), \quad PM_2^{P_3}(G) = \prod_{uv \in E(G)} d_{P_3}(u) d_{P_3}(v)$$

In 2009, The Augmented Zagreb index was introduced by Fartula et al.[4] and it is defined as follows:

$$AZI^{P_3}(G) = \sum_{uv \in E(G)} \left(\frac{d_{P_3}(u) d_{P_3}(v)}{d_{P_3}(u) + d_{P_3}(v) - 2} \right)^3$$

The Harmonic index was introduced by Zhong[20], and defined as follows:

$$HI^{P_3}(G) = \sum_{uv \in E(G)} \frac{2}{d_{P_3}(u) + d_{P_3}(v)}$$

G. H. Shirdel et al.[18] introduced the hyper Zagreb index and defined it as follows:

$$HM^{P_3}(G) = \sum_{uv\in E(G)} [d_{P_3}(u) + d_{P_3}(v)]^2$$

Inspired by work on the P_3-degree of the graphs [3] and Fenofibrate graphs, we find the followings:

2 Main results for fenofibrate

In this section, we calculate the $P_3(G)$-degree based- topological indices Atom-bond connectivity index, Atom-bond Sum connectivity index, Augmented Zagreb index, Sum Augmented Zagreb index, Geometric-arithmetic index, Arithmetic-geometric index of Fenofibrate.

In fenofibrate the chemical formal is $C_{20}H_{21}O_4Cl$ as a graph G. We partition the edges of graph G into edges of the type $E_{(d_{P_3}(u),d_{P_3}(v))}$ where uv is an edge. In graph G we get edges of the type.

The graph G of fenofibrate has

$d_{P_3}(u), d_{P_3}(v) : uv \in E(G)$	Number of edges
(2,4)	2
(2,5)	1
(2,7)	2
(3,9)	2
(4,4)	4
(4,5)	3
(4,6)	2
(4,7)	4
(5,7)	1
(6,6)	1
(6,9)	1
(7,7)	2
(7,9)	1

Theorem 2.1. *The P_3-Atom bond connectivity index of fenofibrate is 15.4128661804.*

***Proof*:** $$ABC^{P_3}(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_{P_3}(u) + d_{P_3}(v) - 2}{d_{P_3}(u)d_{P_3}(v)}}$$

$$ABC^{P_3}(G) = 2\sqrt{\frac{2+4-2}{2\times 4}} + 1\sqrt{\frac{2+5-2}{2\times 5}} + 2\sqrt{\frac{2+7-2}{2\times 7}} + 2\sqrt{\frac{2+9-2}{2\times 9}} + 4\sqrt{\frac{4+4-2}{4\times 4}} +$$

$$3\sqrt{\frac{4+5-2}{4\times5}}+2\sqrt{\frac{4+6-2}{4\times6}}+4\sqrt{\frac{4+7-2}{4\times7}}+1\sqrt{\frac{5+7-2}{5\times7}}+1\sqrt{\frac{6+6-2}{6\times6}}+1\sqrt{\frac{6+9-2}{6\times9}}+2\sqrt{\frac{7+7-2}{7\times7}}+1\sqrt{\frac{7+9-2}{7\times9}}$$

$$= 15.4128661804$$

Theorem 2.2. *The P_3-Atom bond sum connectivity index of fenofibrate is 19.5101765314*

***Proof*:** $ABS^{P_3}(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_{P_3}(u)+d_{P_3}(v)-2}{d_{P_3}(u)+d_{P_3}(v)}}$

$$ABS^{P_3}(G) = 2\sqrt{\frac{2+4-2}{2+4}} + 1\sqrt{\frac{2+5-2}{2+5}} + 2\sqrt{\frac{2+7-2}{2+7}} + 2\sqrt{\frac{3+9-2}{3+9}} + 4\sqrt{\frac{4+4-2}{4+4}} + 3\sqrt{\frac{4+5-2}{4+5}} + 2\sqrt{\frac{4+6-2}{4+6}} + 4\sqrt{\frac{4+7-2}{4+7}} + 1\sqrt{\frac{5+7-2}{5+7}} + 1\sqrt{\frac{6+6-2}{6+6}} + 1\sqrt{\frac{6+9-2}{6+9}} + 2\sqrt{\frac{7+7-2}{7+7}} + 1\sqrt{\frac{7+9-2}{7+9}}$$

$= 19.5101765314$

Theorem 2.3. *The P_3-Augmented Zagreb index of fenofibrate is 803.4583483625.*

Proof: $AGI^{P_3}(G) = \sum_{uv\in E(G)} \left(\frac{d_{P_3}(u)d_{P_3}(v)}{d_{P_3}(u) + d_{P_3}(v) - 2}\right)^3$

$$AGI^{P_3}(G) = 2\left(\frac{2\times4}{2+4-2}\right)^3 + 1\left(\frac{2\times5}{2+5-2}\right)^3 + 2\left(\frac{2\times7}{2+7-2}\right)^3 + 2\left(\frac{3\times9}{3+9-2}\right)^3 + 4\left(\frac{4\times4}{4+4-2}\right)^3 + 3\left(\frac{4\times5}{4+5-2}\right)^3 + 2\left(\frac{4\times6}{4+6-2}\right)^3 + 4\left(\frac{4\times7}{4+7-2}\right)^3 + 1\left(\frac{5\times7}{5+7-2}\right)^3 + 1\left(\frac{6\times6}{6+6-2}\right)^3 + 1\left(\frac{6\times9}{6+9-2}\right)^3 + 2\left(\frac{7\times7}{7+7-2}\right)^3 + 1\left(\frac{7\times9}{7+9-2}\right)^3$$

$= 803.4583483625$

Theorem 2.4. *The P_3-Sum Augmented Zagreb index of fenofibrate is 53.5461920958.*

Proof: $SAI^{P_3}(G) = \sum_{uv\in E(G)} \left(\frac{d_{P_3}(u) + d_{P_3}(v)}{d_{P_3}(u) + d_{P_3}(v) - 2}\right)^3$

$$AGI^{P_3}(G) = 2\left(\frac{2+4}{2+4-2}\right)^3 + 1\left(\frac{2+5}{2+5-2}\right)^3 + 2\left(\frac{2+7}{2+7-2}\right)^3 + 2\left(\frac{3+9}{3+9-2}\right)^3 + 4\left(\frac{4+4}{4+4-2}\right)^3 + 3\left(\frac{4+5}{4+5-2}\right)^3 + 2\left(\frac{4+6}{4+6-2}\right)^3 + 4\left(\frac{4+7}{4+7-2}\right)^3 + 1\left(\frac{5+7}{5+7-2}\right)^3 + 1\left(\frac{6+6}{6+6-2}\right)^3 + 1\left(\frac{6+9}{6+9-2}\right)^3 + 2\left(\frac{7+7}{7+7-2}\right)^3 + 1\left(\frac{7+9}{7+9-2}\right)^3$$

$= 53.5461920958$

Theorem 2.5. *The P_3-Geometric-arithmetic index of fenofibrate is 23.9454695786.*

Proof: $GAI^{P_3}(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_{P_3}(u)d_{P_3}(v)}}{d_{P_3}(u) + d_{P_3}(v)}$

$$GAI^{P_3}(G) = 2\left[\frac{2\sqrt{2\times4}}{2+4}\right] + 1\left[\frac{2\sqrt{2\times5}}{2+5}\right] + 2\left[\frac{2\sqrt{2\times7}}{2+7}\right] + 2\left[\frac{2\sqrt{3\times9}}{3+9}\right] + 4\left[\frac{2\sqrt{4\times4}}{4+4}\right] + 3\left[\frac{2\sqrt{4\times5}}{4+5}\right] + 2\left[\frac{2\sqrt{4\times6}}{4+6}\right] + 4\left[\frac{2\sqrt{4\times7}}{4+7}\right] + 1\left[\frac{2\sqrt{5\times7}}{5+7}\right] + 1\left[\frac{2\sqrt{6\times6}}{6+6}\right] + 1\left[\frac{2\sqrt{6\times9}}{6+9}\right] + 2\left[\frac{2\sqrt{7\times7}}{7+7}\right] + 1\left[\frac{2\sqrt{7\times9}}{7+9}\right]$$

$= 53.5461920958$

Theorem 2.6. *The P_3-Arithmetic Geometric index of fenofibrate is 712.3678963134*

Proof: $AGI^{P_3}(G) = \sum_{uv\in E(G)} \frac{d_{P_3}(u) + d_{P_3}(v)}{2\sqrt{d_{P_3}(u)d_{P_3}(v)}}$

$$AGI^{P_3}(G) = 2\left[2^{\frac{2+4}{2\times 4}}\right] + 1\left[2^{\frac{2+5}{2\times 5}}\right] + 2\left[2^{\frac{2+7}{2\times 7}}\right] + 2\left[2^{\frac{3+9}{3\times 9}}\right] + 4\left[2^{\frac{4+4}{4\times 4}}\right] + 3\left[2^{\frac{4+5}{4\times 5}}\right] +$$

$$2\left[2^{\frac{4+6}{4\times 6}}\right] + 4\left[2^{\frac{4+7}{4\times 7}}\right] + 1\left[2^{\frac{5+7}{5\times 7}}\right] + 1\left[2^{\frac{6+6}{6\times 6}}\right] + 1\left[2^{\frac{6+9}{6\times 9}}\right] + 2\left[2^{\frac{7+7}{7\times 7}}\right] + 1\left[2^{\frac{7+9}{7\times 9}}\right]$$

$$= 712.3678963134$$

Theorem 2.7. *The P_3-First Zagreb index of fenofibrate is 263*

$$M_1^{P_3}(G) = \sum_{uv\in E(G)} [d_{P_3}(u) + d_{P_3}(v)] \text{ For } P_3\text{-degree,}$$

***Proof*:** $M_1^{P_3}(G) = \sum_{uv\in E(G)} [d_{P_3}(u) + d_{P_3}(v)]$

$M_1^{P_3}(G) = 2(2+4) + 1(2+5) + 2(2+7) + 2(3+7) + 4(4+4) + 3(4+5) + 2(4+6) +$

$4(4+7) + 1(5+7) + 1(6+6) + 1(6+9) + 2(7+7) + 1(7+9).$

$= 263$

Theorem 2.8. *The P_3-Second Zagreb index of fenofibrate is 686.*

$$M_2^{P_3}(G) = \sum_{uv\in E(G)} [d_{P_3}(u) d_{P_3}(v)] \text{ For } P_3\text{-degree,}$$

***Proof*:** $M_2^{P_3}(G) = \sum_{uv\in E(G)} [d_{P_3}(u) d_{P_3}(v)],$

$M_2^{P_3}(G) = 2(2\times 4) + 1(2\times 5) + 2(2\times 7) + 2(3\times 7) + 4(4\times 4) + 3(4\times 5) + 2(4\times$

$6) + 4(4\times 7) + 1(5\times 7) + 1(6\times 6) + 1(6\times 9) + 2(7\times 7) + 1(7\times 9)$

$= 686$

Theorem 2.9. *The P_3-First Multiple Zagreb index of Fenofibrate is* $2.66987675 \times 10^{16}$.

***Proof*:** $PM_1^{P_3}(G) = \prod_{uv\in E(G)} [d_{P_3}(u) + d_{P_3}(v)]$ *For P_3-degree,*

$PM_1^{P_3}(G) = 2(2+4) \times 1(2+5) \times 2(2+7) \times 2(3+9) \times 4(4+4) \times 3(4+5) \times 2(4+$

$6) \times 4(4+7) \times 1(5+7) \times 1(6+6) \times 1(6+9) \times 2(7+7) \times 1(7+9)$

$= 2.66987675 \times 10^{16}$

Theorem 2.10. *The P_3-Second Multiple Zagreb index of fenofibrate is* $4.44008593\times$

10^{19}.

Proof : $PM^{P_3}(G) = \prod_{uv\in E(G)} [d_{P_3}(u)d_{P_3}(v)]$ *For* P_3-*degree,*

$PM^{P_3}(G) = 2(2\times 4)\times 1(2\times 5)\times 2(2\times 7)\times 2(3\times 9)\times 4(4\times 4)\times 3(4\times 5)\times 2(4\times 6)\times 4(4\times 7)\times 1(5\times 7)\times 1(6\times 6)\times 1(6\times 9)\times 2(7\times 7)\times 1(7\times 9)$

$= 4.44008593 \times 10^{19}$

Theorem 2.11. *The* P_3-*harmonic index of fenofibrate is 6.8014790765.*

Proof : $HI^{P_3}(G) = \sum_{uv\in E(G)} \frac{2}{d_{P_3}(u) + d_{P_3}(v)}$ *For* P_3-*degree*

$HI^{P_3}(G) = \sum_{uv\in E(G)} \frac{2}{d_{P_3}(u) + d_{P_3}(v)}$

$HI^{P_3}(G) = 2(\frac{2}{2+4}) + 1(\frac{2}{2+5}) + 2(\frac{2}{2+7}) + 2(\frac{2}{3+9}) + 4(\frac{2}{4+4}) + 3(\frac{2}{4+5}) + 2(\frac{2}{4+6}) + 4(\frac{2}{4+7}) + 1(\frac{2}{5+7}) + 1(\frac{2}{6+6}) + 1(\frac{2}{6+9}) + 2(\frac{2}{7+7}) + 1(\frac{2}{7+9})$

$= 6.8014790765$

Theorem 2.12. *The P_3-Hyper index of fenofibrate is 3227.*

Proof : $HM^{P_3}(G) = \sum_{uv\in E(G)} [d_{P_3}(u) + d_{P_3}(v)]^2$ *For P_3-degree*

$HM^{P_3}(G) = 2(2+4)^2 + 1(2+5)^2 + 2(2+7)^2 + 2(3+9)^2 + 4(4+4)^2 + 3(4+5)^2 +$

$2(4+6)^2 + 4(4+7)^2 + 1(5+7)^2 + 1(6+6)^2 + 1(6+9)^2 + 2(7+7)^2 + 1(7+9)^2$

$= 3227$

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