ISSN: 1672 - 6553

JOURNAL OF DYNAMICS AND CONTROL

VOLUME 9 ISSUE 10: P69-87

STUDY ON SOME TOPOLOGICAL INDICES OF PHTHALOCYANINES

[1]Padmapriya P., [2]Aswathi M. P.

[1]Department of Mathematics, Vidyavardhaka College of Engineering, Mysuru - 570 002 India
[2]Department of Mathematics, PG Studies and Research Center, St. Philomena's College (Autonomous), Mysuru - 570 015, India

JOURNAL OF DYNAMICS AND CONTROL
https://doi.org/10.71058/jodac.v9i10008

STUDY ON SOME TOPOLOGICAL INDICES OF PHTHALOCYANINES

[1]**Padmapriya P.,** [2]**Aswathi M. P.**

[1]*Department of Mathematics, Vidyavardhaka College of Engineering, Mysuru - 570 002 India.*
[2]*Department of Mathematics, PG Studies and Research Center, St. Philomena's College (Autonomous), Mysuru - 570 015, India*
[1] *padmapriyap7@gmail.com,* [2]*aswathimancheri586@gmail.com*

Abstract: *Chemical graph theory is the application of discrete mathematics to chemistry applied to model, physical and biological properties of chemical compounds. In this paper we establish Atom-Bond Connectivity Index ABC(G), Geometric Arithmetic Index GA(G), First and Second Zagreb Indices M1(G) and M2(G), Randic Index R(G), Sum Connectivity Index SCI(G), Harmonic Index H(G), Augmented Zagreb Index AZI(G), Forgotten Index F(G), Inverse Sum Indeg Index ISI(G), Hyper-Zagreb Index HM(G) for Phthalocyanine Tetrasulfonic Acid, Phthalocyanine Octacarboxylic Acid, Anthraquinone Cyanines, Phthalocyanine Porphyrin and zinc bis(1,4-didecylbenzo) bis(3,4-pyridoporphyrazine).*

Keywords: *Degree, Topological indices, Molecular graph.*

1 Introduction

Graph theory is a branch of mathematics concerned with networks of points connected by lines. The subject of graph theory has its beginnings in recreational math problems but it has grown into a significant area of mathematical reasearch, with applications in Chemistry, Operational research, Social sciences, and Computer science. Also, many branches of mathematics, such as group theory, matrix theory, probability, and topology have close connections with graph theory. Euler's formula relating the number of edges, vertices, and faces of a convex polyhedron was studied and generalized by Cauchy and ĹHuillier and represents the beginning of the branch of mathematics known as topology.

A topological graph index, also called a molecular descriptor, is a mathematical formula that can be applied to any graph, which is model of some molecular structure. Graph in this index is used to analyze mathematical values and further investigate some physicochemical properties of a molecule.

Molecular descriptors play a significant role in mathematical chemistry, especially in quantitative structure-property relationship (QSPR), and quantitative structure-activity relationship (QSAR) investigations. An example of a molecular descriptor is a topological descriptor. Nowadays, there are numerous topological indices, some applied in chemistry. They can be classified by the structural properties of the graphs used for their calculation. There is a rapidly increasing interest in this topic, therefore topological graph indices are researched worldwide. In this paper we discuss about some degree based topological indices of phthalocyanines.

Several graph invariants found applications and are currently used in chemistry, pharmacology, environmental sciences, etc.[6, 15, 16]. One of these is the so-called atombond connectivity index (ABC). The ABC index was introduced by E. Estrada et al. in 1998 and it is defined as [4].

 https://doi.org/10.71058/jodac.v9i10008

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

It was shown that ABC can be used for modeling thermodynamic properties of organic chemical compounds [2]. However, this paper did not receive much attention. In 2008, Estrada published another paper, applying ABC as tool for explaining the stability of branched alkanes [5]. This work attracted the attention of mathematically oriented scholars, resulting in a remarkable number of researches on the mathematical properties of the ABC index.

The Geometric-arithmetic index was introduced by D. Vukicevic et. al. in 2009[17] and it is defined as

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

For physicochemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and acentric factor, it is noted in that the predictive power of GA index is somewhat better than predictive power of the Randic connectivity index[18].

The Zagreb indices M_1 and M_2 were first introduced by Gutman and Trinajstić in 1972[9], and they are defined as

$$M_1(G) = \sum_{uv\in E(G)} [d_u + d_v].$$

$$M_2(G) = \sum_{uv\in E(G)} [d_u \times d_v].$$

The quantities of the Zagreb indices were found to occur within certain approximate expressions for the total p-electron energy[3].

The so-called sum-connectivity index is a recent invention by B. Zhou and N. Trinajstić[19]. They noticed that in the definition of Randics branching index, there is no a priori reason for using the product $d_u d_v$ of vertex degrees, and this term may be replaced by the sum $d_u + d_v$.

$$SCI(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

The sum connectivity index is also a variant of the well known Randic index[1] which was proposed for measuring the extent of branching of certain chemical compounds. The Randic index of a graph G is defined as

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

The sum connectivity index and Randic index correlate well among themselves and the predictive abilities of these topological indices are practically same in most of the cases.

https://doi.org/10.71058/jodac.v9i10008

In the 1980's, Siemion Fajtlowicz created a computer program for automatic generation of conjectures in graph theory[12]. Then he examined the possible relations between countless graph invariants, among which there was a vertex-degree-based quantity known as

$$H(G) = \sum_{uv \in E(G)} \frac{1}{d_u + d_v}.$$

With a single exception H(G) did not attract anybodys attention, especially not of chemists. Only in 2012, Zhang re-introduced this quantity, and called it harmonic index.

Motivated by the success of the ABC index, Furtula et. al. put forward its modified version, that they somewhat inadequately named augmented Zagreb index[6]. It is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3.$$

Preliminary studies, indicate that AZI has an even better correlation potential than ABC, and the same will be confirmed also in the later sections of the present article. Until now, only a few properties of the augmented Zagreb index have been established.

Furtula and Gutman[7] are introduced a new topological index namely, forgotten index and it is clearly stated that the forgotten index is a special case of the earlier much studied general first Zagreb index .

$$F(G) = \sum_{uv \in E(G)} [(d_u)^2 + (d_v)^2].$$

They also established a few basic properties of it. In 2014 unexpected chemical application of the Forgotten index was discovered and it is proved that the forgotten topological index can significantly enhance the physicochemical applicability of the first Zagreb index[10].

The inverse sum indeg index ISI(G)[11] of a simple graph G is defined as

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

Sedlar et. al.[13] studied the properties of the inverse sum indeg index, the descriptor that was selected as a significant predictor of total surface area of octane isomers and for which the extremal graphs obtained with the help of Math.

In 2013, Shirdel et. al.[14] introduced a new degree-based topological index named hyper-Zagreb index as

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2$$

In this paper we compute the Atom-Bond Connectivity Index, Geometric Arith- metic Index,

https://doi.org/10.71058/jodac.v9i10008

First and Second Zagreb Indices, Randic Index, Sum Connectivity Index, Harmonic Index, Augmented Zagreb Index, Forgotten Index, Inverse Sum Indeg Index, Hyper-Zagreb Index of Phthalocyanine Tetrasulfonic Acid, Phthalocyanine Octacarboxylic Acid, Anthraquinone Cyanines, Phthalocyanine Porphyrin and zinc bis(1,4-didecylbenzo)bis(3,4-pyridoporphyrazine).

2 Phthalocyanine Tetrasulfonic Acid

In this section we focus on the Phthalocyanine Tetrasulfonic Acid. Let G be the molecular graph of Phthalocyanine tetrasulfonic acid, See Figure 2.1. The order and size of Phthalocyanine tetrasulfonic acid are 61 and 70 respectively. The edge partition of G with respect to the degrees of the end-vertices of edges given in the Table 2.1.

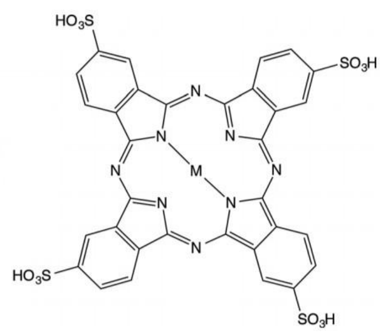

Figure 2.1: Molecular graph of Phthalocyanine Tetrasulfonic Acid

$(d_u, d_v) : u, v \in E(G)$	(1, 4)	(2, 4)	(1, 2)	(2, 3)	(2, 2)	(3, 3)	(4, 4)
Number of edges	8	4	4	30	4	16	4

Table 2.1: Partition of the edge set of Phthalocyanine tetrasulfonic acid based on the degree of end vertices of each edge.

Theorem 2.1. *Let G be the molecular graph of phthalocyanine tetrasulfonic acid then the Atom bond connectivity index is $ABC(G) = 49.858$.*

Proof. By using the Table 2.1 in the definition of the Atom bond connectivity index, we get

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

$$= 8\sqrt{\frac{1+4-2}{1\times 4}} + 4\sqrt{\frac{2+4-2}{2\times 4}} + 4\sqrt{\frac{1+2-2}{1\times 2}} + 30\sqrt{\frac{2+3-2}{2\times 3}}$$

$$+4\sqrt{\frac{2+2-2}{2\times 2}} + 16\sqrt{\frac{3+3-2}{3\times 3}} + 4\sqrt{\frac{4+4-2}{4\times 4}}$$

$$= 49.858.$$

https://doi.org/10.71058/jodac.v9i10008

□

Theorem 2.2. *The Geometric arithmetic index of G is* $GA(G) = 67.262$.
Proof. By using the Table 2.1 in the definition of the Geometric arithmetic index, we get

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

$$= 8\left[\frac{2\sqrt{1\times 4}}{1+4}\right] + 4\left[\frac{2\sqrt{2\times 4}}{2+4}\right] + 4\left[\frac{2\sqrt{1\times 2}}{1+2}\right] + 30\left[\frac{2\sqrt{2\times 3}}{2+3}\right] + 4\left[\frac{2\sqrt{2\times 2}}{2+2}\right]$$

$$+16\left[\frac{2\sqrt{3\times 3}}{3+3}\right] + 4\left[\frac{2\sqrt{4\times 3}}{4+3}\right]$$

$$= 67.262$$

□

Theorem 2.3. *The First and Second Zagreb indices of G are* $M_1(G) = 366$ *and* $M_2(G) = 460$ *respectively.*

Proof. By using the Table 2.1 in definitions of the first and second Zagreb indices, we get

$$M_1(G) = \sum_{uv\in E(G)} [d_u + d_v]$$

$$= 8[1+4] + 4[2+4] + 4[1+2] + 30[2+3] + 4[2+2] + 16[3+3] +4[4+3]$$

$$=366.$$

$$M_2(G) = \sum_{uv\in E(G)} [d_u \times d_v]$$

$$= 8[1\times 4] + 4[2\times 4] + 4[1\times 2] + 30[2\times 3] + 4[2\times 2] + 16[3\times 3] +4[4\times 3]$$

$$=460.$$

□

Theorem 2.4. *The Randic indices of G is* $R(G) = 28.96$.

Proof. By using the Table 2.1 in the definition of Randic index, we get

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

$$= 8\left[\frac{1}{\sqrt{1\times 4}}\right] + 4\left[\frac{1}{\sqrt{2\times 4}}\right] + 4\left[\frac{1}{\sqrt{1\times 2}}\right] + 30\left[\frac{1}{\sqrt{2\times 3}}\right] + 4\left[\frac{1}{\sqrt{2\times 2}}\right] + 16\left[\frac{1}{\sqrt{3\times 3}}\right]$$

$$+4\left[\frac{1}{\sqrt{4\times 3}}\right]$$

$$= 28.96$$

□

Theorem 2.5. *The Sum connectivity index of G is* $SCI(G) = 30.962$.
Proof. By using the Table 2.1 in the definition of Sum connectivity index, we get

$$SCI(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}$$

 https://doi.org/10.71058/jodac.v9i10008

$$= 8\left[\frac{1}{\sqrt{1+4}}\right] + 4\left[\frac{1}{\sqrt{2+4}}\right] + 4\left[\frac{1}{\sqrt{1+2}}\right] + 30\left[\frac{1}{\sqrt{2+3}}\right] + 4\left[\frac{1}{\sqrt{2+2}}\right]$$
$$+16\left[\frac{1}{\sqrt{3+3}}\right] + 4\left[\frac{1}{\sqrt{4+3}}\right]$$
$$= 30.962.$$

□

Theorem 2.6. *The Harmonic index of G is $H(G) = 27.664$.*

Proof. By using the Table 2.1 in the definition of Harmonic index, we get

$$H(G) = \sum_{uv\in E(G)} \frac{1}{d_u + d_v}$$
$$= 8\left[\frac{1}{1+4}\right] + 4\left[\frac{1}{2+4}\right] + 4\left[\frac{1}{1+2}\right] + 30\left[\frac{1}{2+3}\right] + 4\left[\frac{1}{2+2}\right] + 16\left[\frac{1}{3+3}\right]$$
$$+4\left[\frac{1}{4+3}\right]$$
$$= 27.664.$$

□

Theorem 2.7. *The Augmented Zagreb index of G is $AZI(G) = 592.496$.*

Proof. By using the Table 2.1 in the definition of Augmented Zagreb index, we get

$$AZI(G) = \sum_{uv\in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$$
$$= 8\left[\frac{1\times 4}{1+4-2}\right]^3 + 4\left[\frac{2\times 4}{2+4-2}\right]^3 + 4\left[\frac{1\times 2}{1+2-2}\right]^3 + 30\left[\frac{2\times 3}{2+3-2}\right]^3$$
$$+4\left[\frac{2\times 2}{2+2-2}\right]^3 + 16\left[\frac{3\times 3}{3+3-2}\right]^3 + 4\left[\frac{4\times 3}{4+3-2}\right]^3$$
$$= 592.496$$

□

Theorem 2.8. *The Forgotten index of G is $F(G) = 1046$.*

Proof. By using the Table 2.1 in the definition of Forgotten index, we get

$$F(G) = \sum_{uv\in E(G)} [(d_u)^2 + (d_v)^2]$$
$$=8[(1)^2 + (4)^2] + 4[(2)^2 + (4)^2] + 4[(1)^2 + (2)^2] + 30[(2)^2 + (3)^2]$$
$$+ 4[(2)^2 + (2)^2] + 16[(3)^2 + (3)^2] + 4[(4)^2 + (3)^2]$$
$$=1046.$$

□

Theorem 2.9. *The Inverse sum indeg index of G is $ISI(G) = 85.252$.*

Proof. By using the Table 2.1 in the definition of Inverse sum indeg, we get index

$$ISI(G) = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u + d_v}$$
$$= 8\left[\frac{1\times 4}{1+4}\right] + 4\left[\frac{2\times 4}{2+4}\right] + 4\left[\frac{1\times 2}{1+2}\right] + 30\left[\frac{2\times 3}{2+3}\right] + 4\left[\frac{2\times 2}{2+2}\right]$$
$$+16\left[\frac{3\times 3}{3+3}\right] + 4\left[\frac{4\times 3}{4+3}\right]$$

https://doi.org/10.71058/jodac.v9i10008

= 85.252.

□

Theorem 2.10. *The Hyper-Zagreb index of G is* $HM(G) = 1966$*.*

Proof. By using the Table 2.1 in the definition of Hyper-Zagreb index, we get

$$HM(G) = \sum_{uv\in E(G)} (d_u + d_v)^2$$

$$=8[(1+4)^2] + 4[(2+4)^2] + 4[(1+2)^2] + 30[(2+3)^2] + 4[(2+2)^2] + 16[(3+3)^2] + 4[(4+3)^2]$$

$$=1966.$$

□

3 Phthalocyanine Octacarboxylic Acid

In this section,we focus on Phthalocyanine Octacarboxylic Acid. Consider the molecular graph of Phthalocyanine Octacarboxylic acid as H. The order and size of Phthalocyanine Octacarboxylic acid are 73 and 82 respectively. See Figure 3.1. The edge partition of H with respect to the degrees of the end-vertices of edges is given in the Table 3.1.

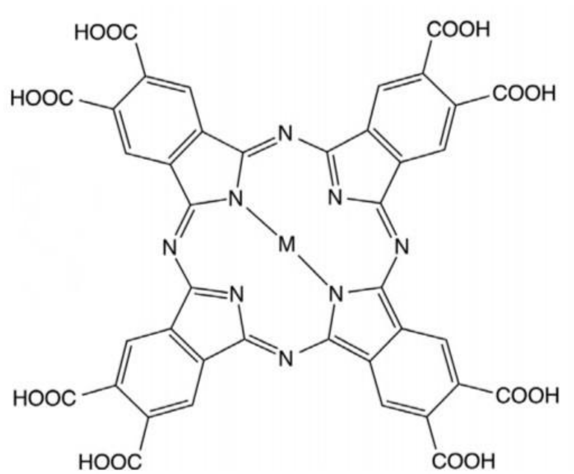

Figure 3.1: Molecular graph of Phthalocyanine Octacarboxylic Acid

$(d_u, d_v) : u, v \in E(G)$	(1, 3)	(2, 3)	(1, 2)	(3, 3)
Number of edges	8	38	8	28

Table 3.1: Partition of the edge set of Phthalocyanine Octacarboxylic acid based on the degree of end vertices of each edge.

Theorem 3.1. *The Atom bond connectivity index of H is* $ABC(H) = 57.698$*.*

Proof. By using the Table 3.1 in the definition of the Atom bond connectivity index, we get

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

https://doi.org/10.71058/jodac.v9i10008

$$= 8\sqrt{\frac{1+3-2}{1\times 3}} + 38\sqrt{\frac{2+3-2}{2\times 3}} + 8\sqrt{\frac{1+2-2}{1\times 2}} + 28\sqrt{\frac{3+3-2}{3\times 3}}$$

$$= 57.698.$$

□

Theorem 3.2. *The Geometric arithmetic index of G is GA*(H) = 79.866*.*

Proof. By using the Table 3.1 in the definition of the Geometric arithmetic index, we get

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

$$= 8\left[\frac{2\sqrt{1\times 3}}{1+3}\right] + 38\left[\frac{2\sqrt{2\times 3}}{2+3}\right] + 8\left[\frac{2\sqrt{2\times 1}}{2+1}\right] + 28\left[\frac{2\sqrt{3\times 3}}{3+3}\right]$$

$$= 79.866.$$

□

Theorem 3.3. *The First and Second Zagreb indices of G are* M_1(H) = 414 *and* M_2(H) = 520 *respectively.*

Proof. By using the Table 3.1 in definitions of the first and second Zagreb indices, we get

$$M_1(H) = \sum_{uv\in E(H)} [d_u + d_v]$$

$$= 8[1+3] + 38[2+3] + 8[2+1] + 28[3+3]$$

$$=414.$$

$$M_2(H) = \sum_{uv\in E(H)} [d_u \times d_v]$$

$$= 8[1\times 3] + 38[2\times 3] + 8[2\times 1] + 28[3\times 3]$$

$$=520.$$

□

Theorem 3.4. *The Randic indices of G is* $R(H) = 35.1$*.*

Proof. By using the Table 3.1 in the definition of Randic index, we get

$$R(H) = \sum_{uv\in E(H)} \frac{1}{\sqrt{d_u d_v}}$$

$$= 8\left[\frac{1}{\sqrt{1\times 3}}\right] + 38\left[\frac{1}{\sqrt{2\times 3}}\right] + 8\left[\frac{1}{\sqrt{2\times 1}}\right] + 28\left[\frac{1}{\sqrt{3\times 3}}\right]$$

$$= 35.1.$$

□

Theorem 3.5. *The Sum connectivity index of G is* $SCI(H) = 37.026$*.*

Proof. By using the Table 3.1 in the definition of Sum connectivity index, we get

$$SCI(H) = \sum_{uv\in E(H)} \frac{1}{\sqrt{d_u + d_v}}$$

$$= 8\left[\frac{1}{\sqrt{1+3}}\right] + 38\left[\frac{1}{\sqrt{2+3}}\right] + 8\left[\frac{1}{\sqrt{2+1}}\right] + 28\left[\frac{1}{\sqrt{3+3}}\right]$$

$$= 37.026.$$

□

Theorem 3.6. *The Harmonic index of G is* $H(H)$

https://doi.org/10.71058/jodac.v9i10008

= 80.528.

Proof. By using the Table 3.1 in the definition of Harmonic index, we get

$$H(H) = \sum_{uv\in E(H)} \frac{1}{d_u + d_v}$$

$$= 8\left[\frac{1}{1+3}\right] + 38\left[\frac{1}{2+3}\right] + 8\left[\frac{1}{2+1}\right] + 28\left[\frac{1}{3+3}\right]$$

= 80.528.

□

Theorem 3.7. *The Augmented Zagreb index of G is AZI(H) = 713.92.*

Proof. By using the Table 3.1 in the definition of Augmented Zagreb index, we get

$$AZI(H) = \sum_{uv\in E(H)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$$

$$= 8\left[\frac{1\times 3}{1+3-2}\right]^3 + 38\left[\frac{2\times 3}{2+3-2}\right]^3 + 8\left[\frac{2\times 1}{2+1-2}\right]^3 + 28\left[\frac{3\times 3}{3+3-2}\right]^3$$

= 713.92

□

Theorem 3.8. *The Forgotten index of G is $F(H)$ = 1118.*

Proof. By using the Table 3.1 in the definition of Forgotten index, we get

$$F(H) = \sum_{uv\in E(H)} [(d_u)^2 + (d_v)^2]$$

$=8[(1)^2 + (3)^2] + 38[(2)^2 + (3)^2] + 8[(2)^2 + (1)^2] + 28[(3)^2 + (3)^2]$

=1118.

□

Theorem 3.9. *The Inverse sum indeg index of G is $ISI(H)$* = 98.928.

Proof. By using the Table 3.1 in the definition of Inverse sum indeg, we get index

$$ISI(H) = \sum_{uv\in E(H)} \frac{d_u d_v}{d_u + d_v}$$

$$= 8\left[\frac{1\times 3}{1+3}\right] + 38\left[\frac{2\times 3}{2+3}\right] + 8\left[\frac{2\times 1}{2+1}\right] + 28\left[\frac{3\times 3}{3+3}\right]$$

= 98.958.

□

Theorem 3.10. *The Hyper-Zagreb index of G is HM* (H) = 2158*.*

Proof. By using the Table 3.1 in the definition of Hyper-Zagreb index, we get

$$HM(H) = \sum_{uv\in E(H)} (d_u + d_v)^2$$

$=8[(1 + 3)^2] + 38[(2 + 3)^2] + 8[(2 + 1)^2] + 28[(3 + 3)^2]$

=2158.

□

4 Anthraquinone cyanines

In this section, we focus on Anthraquinone cyanines. Consider the molecular graph of Anthraquinone cyanine as I. The order and size of Anthraquinone cyanine are 81 and 96 respectively. See Figure 4.1. The edge partition of I with respect to the degrees of the end-vertices of edges given by Table 4.1.

https://doi.org/10.71058/jodac.v9i10008

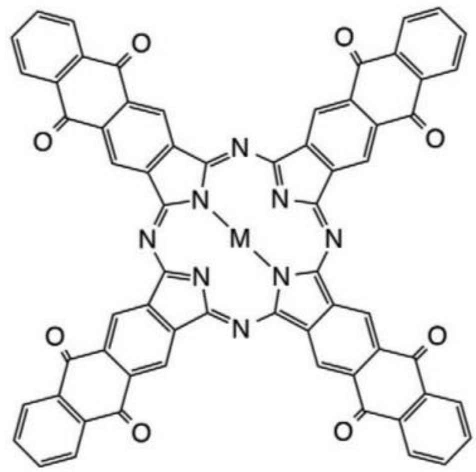

Figure 4.1: Molecular graph of Anthraquinone cyanines

$(d_u, d_Y) : u, v \in E(G)$	(2, 2)	(2, 3)	(3, 1)	(3, 3)
Number of edges	12	36	8	40

Table 4.1: Partition of the edge set of Anthraquinone cyanines based on the degree of end vertices of each edge.

Theorem 4.1. *The Atom bond connectivity index of H is* $ABC(\mathrm{I}) = 67.104$*.*

Proof. By using the Table 4.1 in the definition of the Atom bond connectivity index, we get

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

$$= 12\sqrt{\frac{2+2-2}{2\times 2}} + 36\sqrt{\frac{2+3-2}{2\times 3}} + 8\sqrt{\frac{3+1-2}{3\times 1}} + 40\sqrt{\frac{3+3-2}{3\times 3}}$$

$$= 67.104.$$

□

Theorem 4.2. *The Geometric arithmetic index of G is* $GA(\mathrm{I}) = 94.172$*.*

Proof. By using the Table 4.1 in the definition of the Geometric arithmetic index, we get

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

$$= 12\left[\frac{2\sqrt{2\times 2}}{2+2}\right] + 36\left[\frac{2\sqrt{2\times 3}}{2+3}\right] + 8\left[\frac{2\sqrt{3\times 1}}{3+1}\right] + 40\left[\frac{2\sqrt{3\times 3}}{3+3}\right]$$

$$= 94.172.$$

□

Theorem 4.3. *The First and Second Zagreb indices of G are* $M_1(\mathrm{I}) = 500$ *and* $M_2(\mathrm{I}) = 648$

https://doi.org/10.71058/jodac.v9i10008

respectively.

Proof. By using the Table 4.1 in definitions of the first and second Zagreb indices, we get

$$M_1(I) = \sum_{uv\in E(I)} [d_u + d_v]$$
$$= 12[2+2] + 36[2+3] + 8[3+1] + 40[3+3]$$
$$=500.$$

$$M_2(I) = \sum_{uv\in E(I)} [d_u \times d_v]$$
$$= 12[2\times 2] + 36[2\times 3] + 8[3\times 1] + 40[3\times 3]$$
$$=648.$$

□

Theorem 4.4. *The Randic indices of G is R*(*I*) = 38.624*.*

Proof. By using the Table 4.1 in the definition of Randic index, we get

$$R(I) = \sum_{uv\in E(I)} \frac{1}{\sqrt{d_u d_v}}$$
$$= 12\left[\frac{1}{\sqrt{2\times 2}}\right] + 36\left[\frac{1}{\sqrt{2\times 3}}\right] + 8\left[\frac{1}{\sqrt{3\times 1}}\right] + 40\left[\frac{1}{\sqrt{3\times 3}}\right]$$
$$= 38.624.$$

□

Theorem 4.5. *The Sum connectivity index of G is SCI*(*I*) = 42.412*.*

Proof. By using the Table 4.1 in the definition of Sum connectivity index, we get

$$SCI(I) = \sum_{uv\in E(I)} \frac{1}{\sqrt{d_u + d_v}}$$
$$= 12\left[\frac{1}{\sqrt{2+2}}\right] + 36\left[\frac{1}{\sqrt{2+3}}\right] + 8\left[\frac{1}{\sqrt{3+1}}\right] + 40\left[\frac{1}{\sqrt{3+3}}\right]$$
$$= 42.412.$$

□

Theorem 4.6. *The Harmonic index of G is H*(I) = 37.72.

Proof. By using the Table 4.1 in the definition of Harmonic index, we get

$$H(I) = \sum_{uv\in E(I)} \frac{1}{d_u + d_v}$$
$$= 12\left[\frac{1}{2+2}\right] + 36\left[\frac{1}{2+3}\right] + 8\left[\frac{1}{3+1}\right] + 40\left[\frac{1}{3+3}\right]$$
$$= 37.72.$$

□

Theorem 4.7. *The Augmented Zagreb index of G is AZI*(I) = 866.6*.*

Proof. By using the Table 4.1 in the definition of Augmented Zagreb index, we get

$$AZI(I) = \sum_{uv\in E(I)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$$
$$= 12\left[\frac{2\times 2}{2+2-2}\right]^3 + 36\left[\frac{2\times 3}{2+3-2}\right]^3 + 8\left[\frac{3\times 1}{3+1-2}\right]^3 + 40\left[\frac{3\times 3}{3+3-2}\right]^3$$
$$= 866.6.$$

https://doi.org/10.71058/jodac.v9i10008

□

Theorem 4.8. *The Forgotten index of G is* F(I) = 1364.

Proof. By using the Table 4.1 in the definition of Forgotten index, we get

$$F(I) = \sum_{uv \in E(I)} [(d_u)^2 + (d_v)^2]$$

=12[(2)^2 + (2)^2] + 36[(2)^2 + (3)^2] + 8[(3)^2 + (1)^2] + 40[(3)^2 + (3)^2]

=1364.

□

Theorem 4.9. *The Inverse sum indeg index of G is* $ISI(I)$ = 121.2.

Proof. By using the Table 4.1 in the definition of Inverse sum indeg, we get index

$$ISI(I) = \sum_{uv \in E(I)} \frac{d_u d_v}{d_u + d_v}$$

$$= 12\left[\frac{2 \times 2}{2+2}\right] + 36\left[\frac{2 \times 3}{2+3}\right] + 8\left[\frac{3 \times 1}{3+1}\right] + 40\left[\frac{3 \times 3}{3+3}\right]$$

$$= 121.2.$$

□

Theorem 4.10. *The Hyper-Zagreb index of G is* HM(I) = 2660.

Proof. By using the Table 4.1 in the definition of Hyper-Zagreb index, we get

$$HM(I) = \sum_{uv \in E(I)} (d_u + d_v)^2$$

=12[(2+23)^2] + 36[(2 + 3)^2] + 8[(3 + 1)^2] + 40[(3 + 3)^2]

=2660.

□

5 Phthalocyanine Porphyrin

The porphyrin families of compounds are cyclic tetrapyrolles many of which are intermediates of the heme biosynthetic pathway. The majority of the compounds of interest to the clinical chemist are not in fact porphyrins (with the exception of protoporphyrin) but porphyrinogens in which all four methylene bridges are in the reduced form. Characterization of the type of porphyria depends upon the identification of particular patterns of porphyrins in blood, urine, and feces.

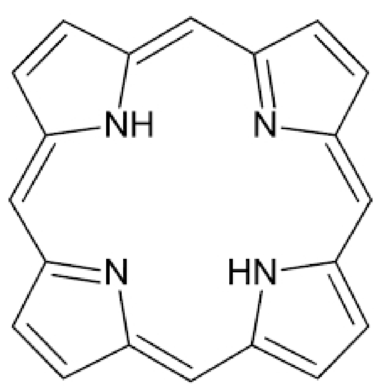

Figure 5.1: Molecular graph of Phthalocyanine Porphyrin (P)

The Molecular graph of Phthalocyanine Porphyrin is denoted by P. The edge partition of P with respect to the degrees of the end-vertices of edges given by Table 5.1.

https://doi.org/10.71058/jodac.v9i10008

$(d_u, d_v) : u, v \in E(G)$	(2, 2)	(2, 3)	(3, 1)	(3, 3)
Number of edges	4	20	2	4

Table 5.1: Partition of the edge set of Phthalocyanine Porphyrin based on the degree of end vertices of each edge.

Theorem 5.1. *The Atom bond connectivity index of P is $ABC(P) = 21.264$.*

Proof. By using the Table 5.1 in the definition of the Atom bond connectivity index, we get

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

$$= 4\sqrt{\frac{2+2-2}{2\times 2}} + 20\sqrt{\frac{2+3-2}{2\times 3}} + 2\sqrt{\frac{3+1-2}{3\times 1}} + 4\sqrt{\frac{3+3-2}{3\times 3}}$$

$$= 21.264.$$

□

Theorem 5.2. *The Geometric arithmetic index of G is $GA(P) = 29.312$.*
Proof. By using the Table 5.1 in the definition of the Geometric arithmetic index, we get

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

$$= 4\left[\frac{2\sqrt{2\times 2}}{2+2}\right] + 20\left[\frac{2\sqrt{2\times 3}}{2+3}\right] + 2\left[\frac{2\sqrt{3\times 1}}{3+1}\right] + 4\left[\frac{2\sqrt{3\times 3}}{3+3}\right]$$

$$= 29.312.$$

□

Theorem 5.3. *The First and Second Zagreb indices of G are $M_1(P) = 148$ and $M_2(P) = 178$ respectively.*

Proof. By using the Table 5.1 in definitions of the first and second Zagreb indices, we get

$$M_1(P) = \sum_{uv \in E(P)} [d_u + d_v]$$
$$= 4[2+2] + 20[2+3] + 2[3+1] + 4[3+3]$$
$$=148.$$

$$M_2(P) = \sum_{uv \in E(P)} [d_u \times d_v]$$
$$= 4[2\times 2] + 20[2\times 3] + 2[3\times 1] + 4[3\times 3]$$
$$=178.$$

□

Theorem 5.4. *The Randic indices of G is $R(P) = 12.646$.*

Proof. By using the Table 5.1 in the definition of Randic index, we get

$$R(P) = \sum_{uv \in E(P)} \frac{1}{\sqrt{d_u d_v}}$$

https://doi.org/10.71058/jodac.v9i10008

$$= 4\left[\frac{1}{\sqrt{2\times 2}}\right] + 20\left[\frac{1}{\sqrt{2\times 3}}\right] + 2\left[\frac{1}{\sqrt{3\times 1}}\right] + 4\left[\frac{1}{\sqrt{3\times 3}}\right]$$
$$= 12.646.$$

□

Theorem 5.5. *The Sum connectivity index of G is* $SCI(P)$ = 13.572.

Proof. By using the Table 5.1 in the definition of Sum connectivity index, we get

$$SCI(P) = \sum_{uv\in E(P)} \frac{1}{\sqrt{d_u + d_v}}$$
$$= 4\left[\frac{1}{\sqrt{2+2}}\right] + 20\left[\frac{1}{\sqrt{2+3}}\right] + 2\left[\frac{1}{\sqrt{3+1}}\right] + 4\left[\frac{1}{\sqrt{3+3}}\right]$$
$$= 13.572.$$

□

Theorem 5.6. *The Harmonic index of G is* H(P) = 12.332.

Proof. By using the Table 5.1 in the definition of Harmonic index, we get

$$H(P) = \sum_{uv\in E(P)} \frac{1}{d_u + d_v}$$
$$= 4\left[\frac{1}{2+2}\right] + 20\left[\frac{1}{2+3}\right] + 2\left[\frac{1}{3+1}\right] + 4\left[\frac{1}{3+3}\right]$$
$$= 12.332.$$

□

Theorem 5.7. *The Augmented Zagreb index of G is* AZI(P) = 244.31.

Proof. By using the Table 5.1 in the definition of Augmented Zagreb index, we get

$$AZI(P) = \sum_{uv\in E(P)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$$
$$= 4\left[\frac{2\times 2}{2+2-2}\right]^3 + 20\left[\frac{2\times 3}{2+3-2}\right]^3 + 2\left[\frac{3\times 1}{3+1-2}\right]^3 + 4\left[\frac{3\times 3}{3+3-2}\right]^3$$
$$= 244.31.$$

□

Theorem 5.8. *The Forgotten index of G is* F(P) = 384.

Proof. By using the Table 5.1 in the definition of Forgotten index, we get

$$F(P) = \sum_{uv\in E(P)} [(d_u)^2 + (d_v)^2]$$
$$=4[(2)^2 + (2)^2] + 20[(2)^2 + (3)^2] + 2[(3)^2 + (1)^2] + 4[(3)^2 + (3)^2]$$
$$=384.$$

□

Theorem 5.9. *The Inverse sum indeg index of G is* ISI(P) = 35.5.

Proof. By using the Table 5.1 in the definition of Inverse sum indeg, we get index

$$ISI(P) = \sum_{uv\in E(P)} \frac{d_u d_v}{d_u + d_v}$$
$$= 4\left[\frac{2\times 2}{2+2}\right] + 20\left[\frac{2\times 3}{2+3}\right] + 2\left[\frac{3\times 1}{3+1}\right] + 4\left[\frac{3\times 3}{3+3}\right]$$
$$= 35.5.$$

□

Theorem 5.10. *The Hyper-Zagreb index of G is*

https://doi.org/10.71058/jodac.v9i10008

$HM(\mathrm{P}) = 740.$

Proof. By using the Table 5.1 in the definition of Hyper-Zagreb index, we get

$$HM(P) = \sum_{uv\in E(P)} (d_u + d_v)^2$$

$$=4[(2+23)^2] + 20[(2 + 3)^2] + 2[(3 + 1)^2] + 4[(3 + 3)^2]$$

$$=740.$$

□

6 Zinc bis(1,4-didecylbenzo)bis(3,4-pyridoporphyrazine)

In this section, we focus on zinc bis(1,4-didecylbenzo) bis(3,4-pyridoporphyrazine). Consider the molecular graph of zinc bis(1,4-didecylbenzo)bis(3,4-pyridoporphyrazine) as **J**. The order and size of zinc bis(1,4-didecylbenzo)bis(3,4-pyridoporphyrazine) is 167 and 178 respectively. See Figure 6.1. The edge partition of **J** with respect to the degrees of the end-vertices of edges is given in Table 6.1.

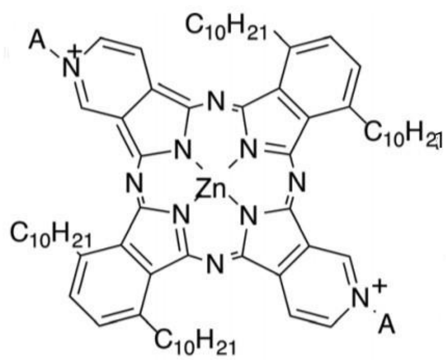

Figure 6.1: Molecular graph of zinc bis(1,4-didecylbenzo)bis(3,4-pyridoporphyrazine)

$(d_u, d_v) : u, v \in E(G)$	(1, 4)	(4, 3)	(3, 2)	(2, 2)	(3, 1)	(3, 3)	(4, 4)
Number of edges	84	8	20	4	2	24	36

Table 6.1: Partition of the edge set of zinc bis(1,4-didecylbenzo) bis(3,4-pyridoporphyrazine) based on the degree of end vertices of each edge.

Theorem 6.1. *Let J be the molecular graph of zinc bis(1,4-didecylbenzo)bis(3,4-pyridoporphyrazine) then the atom bond connectivity index is* $ABC(J) = 134.52$.

Proof. By using the Table 6.1 in the definition of the Atom bond connectivity index, we get

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

https://doi.org/10.71058/jodac.v9i10008

$$= 84\sqrt{\frac{1+4-2}{1\times 4}} + 8\sqrt{\frac{4+3-2}{4\times 3}} + 20\sqrt{\frac{3+2-2}{3\times 2}} + 4\sqrt{\frac{2+2-2}{2\times 2}}$$

$$+2\sqrt{\frac{3+1-2}{3\times 1}} + 24\sqrt{\frac{3+3-2}{3\times 3}} + 36\sqrt{\frac{4+4-2}{4\times 4}}$$

$$= 134.52.$$

□

Theorem 6.2. *The Geometric arithmetic index of G is GA(J) = 160.424.*
Proof. By using the Table 6.1 in the definition of the Geometric arithmetic index, we get

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

$$= 84\left[\frac{2\sqrt{1\times 4}}{1+4}\right] + 8\left[\frac{2\sqrt{4\times 3}}{4+3}\right] + 20\left[\frac{2\sqrt{3\times 2}}{3+2}\right] + 4\left[\frac{2\sqrt{2\times 2}}{2+2}\right] + 2\left[\frac{2\sqrt{3\times 1}}{3+1}\right]$$

$$+24\left[\frac{2\sqrt{3\times 3}}{3+3}\right] + 36\left[\frac{2\sqrt{4\times 4}}{4+4}\right]$$

$$= 160.424$$

□

Theorem 6.3. *The First and Second Zagreb indices of G are* $M_1(J) = 1032$ *and* $M_2(J) = 1366$ *respectively.*

Proof. By using the Table 6.1 in definitions of the first and second Zagreb indices, we get

$$M_1(J) = \sum_{uv\in E(J)} [d_u + d_v]$$

$$= 84[1+4] + 8[4+3] + 20[3+2] + 4[2+2] + 2[3+1] + 24[3+3] +36[4+4]$$

$$=1032.$$

$$M_2(J) = \sum_{uv\in E(J)} [d_u \times d_v]$$

$$= 84[1\times 4] + 8[4\times 3] + 20[3\times 2] + 4[2\times 2] + 2[3\times 1] + 24[3\times 3] +36[4\times 4]$$

$$=1366.$$

□

Theorem 6.4. *The Randic indices of G is R(G) = 72.622.*

Proof. By using the Table 2.1 in the definition of Randic index, we get

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

$$= 84\left[\frac{1}{\sqrt{1\times 4}}\right] + 8\left[\frac{1}{\sqrt{4\times 3}}\right] + 20\left[\frac{1}{\sqrt{3\times 2}}\right] + 4\left[\frac{1}{\sqrt{2\times 2}}\right] + 2\left[\frac{1}{\sqrt{3\times 1}}\right]$$

https://doi.org/10.71058/jodac.v9i10008

$$+24\left[\frac{1}{\sqrt{3\times 3}}\right]+36\left[\frac{1}{\sqrt{4\times 4}}\right]$$
$$= 72.622.$$

□

Theorem 6.5. *The Sum connectivity index of G is SCI(J) = 75.022.*

Proof. By using the Table 6.1 in the definition of Sum connectivity index, we get

$$SCI(J) = \sum_{uv\in E(J)} \frac{1}{\sqrt{d_u + d_v}}$$

$$= 84\left[\frac{1}{\sqrt{1+4}}\right]+8\left[\frac{1}{\sqrt{4+3}}\right]+20\left[\frac{1}{\sqrt{3+2}}\right]+4\left[\frac{1}{\sqrt{2+2}}\right]+2\left[\frac{1}{\sqrt{3+1}}\right]$$

$$+24\left[\frac{1}{\sqrt{3+3}}\right]+36\left[\frac{1}{\sqrt{4+4}}\right]$$
$$= 75.022.$$

□

Theorem 6.6. *The Harmonic index of G is H(J) = 63.88.*

Proof. By using the Table 6.1 in the definition of Harmonic index, we get

$$H(J) = \sum_{uv\in E(J)} \frac{1}{d_u + d_v}$$

$$= 84\left[\frac{1}{1+4}\right]+8\left[\frac{1}{4+3}\right]+20\left[\frac{1}{3+2}\right]+4\left[\frac{1}{2+2}\right]+2\left[\frac{1}{3+1}\right]$$

$$+24\left[\frac{1}{3+3}\right]+36\left[\frac{1}{4+4}\right]$$
$$= 63.88.$$

□

Theorem 6.7. *The Augmented Zagreb index of G is AZI(J) =1464.534.*

Proof. By using the Table 6.1 in the definition of Augmented Zagreb index, we get

$$AZI(J) = \sum_{uv\in E(J)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$$

$$= 84\left[\frac{1\times 4}{1+4-2}\right]^3+8\left[\frac{4\times 3}{4+3-2}\right]^3+20\left[\frac{3\times 2}{3+2-2}\right]^3+4\left[\frac{2\times 2}{2+2-2}\right]^3$$

$$+2\left[\frac{3\times 1}{3+1-2}\right]^3+24\left[\frac{3\times 3}{3+3-2}\right]^3+36\left[\frac{4\times 4}{4+4-2}\right]^3$$

$$= 1464.534.$$

□

Theorem 6.8. *The Forgotten index of G is F(J) = 3524.*

Proof. By using the Table 6.1 in the definition of Forgotten index, we get

$$F(J) = \sum_{uv\in E(J)} [(d_u)^2 + (d_v)^2]$$

$$=84[(1)^2 + (4)^2] + 8[(4)^2 + (3)^2] + 20[(3)^2 + (2)^2] + 4[(2)^2 + (2)^2]$$

https://doi.org/10.71058/jodac.v9i10008

$$+ 2[(3)^2 + (1)^2] + 24[(3)^2 + (3)^2] + 36[(4)^2 + (4)^2]$$
$$=3524.$$

□

Theorem 6.9. *The Inverse sum indeg index of G is ISI(J) =218.412.*

Proof. By using the Table 6.1 in the definition of Inverse sum indeg, we get index

$$ISI(J) = \sum_{uv\in E(J)} \frac{d_u d_v}{d_u + d_v}$$

$$= 84\left[\frac{1\times 4}{1+4}\right] + 8\left[\frac{4\times 3}{4+3}\right] + 20\left[\frac{3\times 2}{3+2}\right] + 4\left[\frac{2\times 2}{2+2}\right] + 2\left[\frac{3\times 1}{3+1}\right]$$

$$+24\left[\frac{3\times 3}{3+3}\right] + 36\left[\frac{4\times 4}{4+4}\right]$$

$$= 218.412.$$

□

Theorem 6.10. *The Hyper-Zagreb index of G is HM(J) = 6256.*

Proof. By using the Table 6.1 in the definition of Hyper-Zagreb index, we get

$$HM(J) = \sum_{uv\in E(J)} (d_u + d_v)^2$$

$$=84[(1 + 4)^2] + 8[(4 + 3)^2] + 20[(3 + 2)^2] + 4[(2 + 2)^2] + 2[(3 + 1)^2]$$
$$+ 24[(3 + 3)^2] + 36[(4 + 4)^2]$$
$$=6256.$$

□

Conclusion

In this paper, we computed the Atom-Bond Connectivity Index, Geometric Arithmetic Index, First and Second Zagreb Indices, Randic Index, Sum Connectivity Index, Harmonic Index, Augmented Zagreb Index, Forgotten Index, Inverse Sum Indeg Index, Hyper-Zagreb Index of Phthalocyanine Tetrasulfonic Acid, Phthalo- cyanine Octacarboxylic Acid, Anthraquinone Cyanines, Phthalocyanine Porphyrin and zinc bis(1,4-didecylbenzo)bis(3,4-pyridoporphyrazine) with the help of graph theory and mathematical derivation. It is interesting to investigate this index for other chemical structures via their molecular graphs.

References

[1] A. Ali, L. Zhong, and I. Gutman, Harmonic index and its Generalization Extremal Results and Bounds, *Match Communications in Mathematical and in Computer Chemistry*, **81**, (2019), 249-311.

[2] K. C. Das, I. Gutman and B. Furtula, On Atom Bond Connectivity Index, *Faculty of Science and Mathematics,* **26**, (2012), 733-738.

[3] K. C. Das, K. xu and J. Nam, Zagreb index of Graph, Springer- Verlag Berlin Heidelberg, **10(3)**, (2015), 567-582.

[4] E. Estrada, L. Torres, L. Rodriguez and I.

https://doi.org/10.71058/jodac.v9i10008

Gutman, An atombond connectivity index: Modelling the enthalpy of formation of alkanes, *Indian J. Chem.,* **37**, (1998), 849-855.

[5] E. Estrada, Atombond connectivity and the energetic of branched alkanes, *Chem. Phys. Lett.* **463**, (2008), 422-425.

[6] B. Furtula, A. Graovac and D. Vukicevic, Augmented Zagreb index, *J. Math. Chem,* **48**, (2010), 370-380.

[7] B. Furtula and I . Gutman, A Forgotten topological index, *J. Math. Chem.* **53**, (2015), 1184-1190.

[8] I. Gutman, Degree Based Topological Indices, *Croatica Chemica Acta,* **86(4)**, (2013), 351-361.

[9] I. Gutman and N. Trinajstić, Graph Theory and molecular orbitals, Total π-electron energy of alternant hydrocarbons, *Chemical Physics letters*, **17**, (1972), 535-538.

[10] A. Khaksari and M. Ghorbani, On the Forgotten Topological Index, *Iranian Journal of Mathematical Chemistry,* **8(3)**, (2017), 327-338.

[11] K. Pattabiraman, Inverse sum indeg index of graphs, *AKCE International Journal of Graphs and Combinatorics,* **15(2)**, (2017), 155-167.

[12] M. Randic, On characterisation of molecular branching, *Journal of the American Chemical society,* **97**, (1975), 6609-6615.

[13] J. Sedlar, D. Stevanoic and A. Vasilyev, On the inverse sum indeg index, *Discrete Applied Mathematics,* **184**, (2015), 202-212.

[14] G.H. Shirdel, H. Rezapour and A.M. Sayadi, The Hyper -Zagreb index of Graph Operations, *Iran. J. Math. Chem.,* **4(2)**, (2013), 213-220.

[15] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, WileyVCH, Weinheim, (2000).

[16] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, WileyVCH, Weinheim, (2009).

[17] D. Vukicevic and B. Furtula, Tological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.*, **46**, (2009), 1369-1376.

[18] Y. Yuan, B. Zhou and N. Trinajsti´c, On geometric-arithmetic index, *Journal of mathematical chemistry,* **47(2)**, (2010), 833-841.

[19] B. Zhou and N.Trinajstić, On a novel connectivity index, *J. Math. Chem.,* **46**, (2009), 1252-1270.