INDIAN JOURNAL OF SCIENCE AND TECHNOLOGY

SYSTEMATIC REVIEW

Johan Zagreb Indices of Some Chemical Network Graphs

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OPEN ACCESS

Received: 23-06-2023

Accepted: 29-07-2023

Published: 26-09-2023

Citation: Monolisa S, Rajam K, Lancy A, Mary U (2023) Johan Zagreb Indices of Some Chemical Network Graphs. Indian Journal of Science and Technology 16(35): 2902-2906. https://doi.org/10.17485/IJST/v16i35.1556-icrms

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Funding: None

Competing Interests: None

Published By Indian Society for Education and Environment (iSee)

ISSN
Print: 0974-6846
Electronic: 0974-5645

Abstract

Nowadays, molecular descriptors are the most significant invariants utilised in molecular modeling, and as a result, they are controlled by statistics, chemo metrics, and chemo informatics. Topological indices (TIs) are receiving more and more attention from chemists and biologists, because of their significance in QSPR (Quantitative Structure Property Relationships) and QSAR (Quantitative Structure Activity Relationships). In this, Johan Zagreb chromatic indices of some chemical network graphs are presented. **Objectives:** The major objective of this article is to investigate the structure of three types of chemical network graphs, Hourglass, Jagged Rectangle, and Rhombic Benzenoid and to identify some Johan Zagreb indices for predicting their physical and chemical properties. **Methods:** Topological indices are usually based on underlying connectivity as characterized by degrees, distance or degree distance**.** Here, the study uses degree counting and edge sub division methods corresponding with Johan coloring of graphs. **Findings:** In this, we established a family of Johan Zagreb Indices, including the First, Second, and Third Johan Zagreb Indices and Hyper First and Second Johan Zagreb Indices, Augmented Johan Zagreb Index, Redefined First, Second, Third Johan Zagreb Indices. **Novelty:** There are many different chromatic indices that have already been used in the literature but Johan Zagreb chromatic indices deliver better results than the ones that have been already exists. Also we determined Python programming, which we used to compute the Zagreb Johan topological indices of graphs.

Keywords: Chromatic Indices; Hourglass Benzenoid; Jagged Rectangle Benzenoid; Rhombic Benzenoid; Johan Zagreb Indices; QSPR/QSAR

1 Introduction

Compounds of chemical molecules tend to be represented as graphs, with nodes and edges denoting the atoms and bonds, respectively. In particular, chemical graph theory is applied in mathematical chemistry to investigate and study the structure of complicated chemical networks and basic chemical structures. Numerical parameter called topological indices is used to describe how a graph is structured. In addition to their many other uses, they have contributed significantly to the development of mathematical chemistry as molecular descriptors [1,2]. The topological structure of

a chemical molecule is represented by an undirected and linked graph G = (V,E). Molecules are the basic building units of compounds, consisting of a variety of components bound together. When the set of vertices (or nodes (V)) symbolizes the atoms of the molecule, the set of edges or link (E) depicts the connections between them [3].

In this, we extend the concept of chromatic Zagreb indices [4–7] into the Johan Zagreb indices for molecular graph structure of some chemical network. In General, graph coloring refers to the assignment of colors, labels or weight to the vertices of graph subject to certain conditions. Let C = $\{c_1, c_2, c_3, \cdots, c_l\}$, l ∈ N sufficiently large is a set of distinct colors, a proper vertex coloring of a graph G is a vertex coloring φ: V(G) → C of G such that no two distinct adjacent vertices have the same color. The minimum number of colors in proper vertex coloring of G is called the chromatic number of G and is denoted as χ(G). Unless mentioned otherwise, we follow the convention that, among the colors in the coloring C = $\{c_1, c_2, c_3, \ldots c_l\}$, l = χ(G), the color c_1 will be assigned to maximum possible number of vertices in G, then color

c_2 will be assigned to maximum possible number of remaining uncolored vertices and proceeding like this, at the final step, the color c_l will be given for the remaining uncolored vertices. This convention is called the rainbow neighbourhood convention [8]. The coloring φ: V(G) → C can be written as $\varphi(v_i) = c_l$, in other words we say that φ(vi)=l. A maximal proper coloring of a graph G is a Johan coloring denoted J - coloring, if and only if every vertex of G belongs to a rainbow neighbourhood of G. The maximum number of colors in a J -coloring is denoted by J(G). To learn more about topological indices and their uses refer [9,10].

Python programmes are simple to understand and can generally run in a matter of seconds. Here, we use a python code to find a family of Zagreb Johan indices for a molecular graph and to generate a number of Zagreb indices for the mentioned molecular networks.

2 Main Results

2.1 Some Family of Johan Zagreb Indices of Rhombic Benzenoid Graph RBr

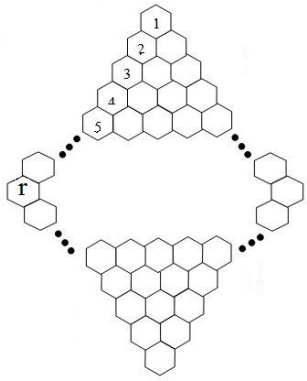

Fig 1. Rhombic Benzenoid graph RB_r

Theorem 2.1. The family of some Johan Zagreb Index of the molecular graph of Rhombic Benzenoid RB_r is

(1) $JZI_1(RB_r)=9r^2+12r-3$.
(2) $JZI_2(RB_r)=6r^2+8r-2$.
(3) $JZI_3(RB_r)=3r^2+4r-1$.
(4) $HJZI_1(RB_r)=27r^2+36r-9$.
(5) $HJZI_2(RB_r)=12r^2+16r-4$.
(6) $AJZI_2(RB_r)=24r^2+32r-8$.
(7) $ReJZI_1(RB_r)=\frac{9}{2}r^2+6n-\frac{3}{2}$.
(8) $ReJZI_2(RB_r)=2n^2+\frac{8}{3}r-\frac{2}{3}$.
(9) $ReJZI_3(RB_r)=18r^2+24r-6$.

Proof. Let us consider the Rhombic Benzenoid graph RB_r. We presume that the vertex setto be $V = (a_1, a_2, a_3 \ldots, a_p; p = 2r(n+2)\}$ and edge set to be E= $\{b_1, b_2, b_3 \ldots, b_q; q = 3r^2 + 4r)\}$, where r denotes the order of the

series. This graph is Johan colourable. The coloring of the graph is as follows,

$$C(a_i) = \begin{cases} c_1 \ if \ i \equiv 1(mod\ 2) \\ c_2 \ if \ i \equiv 0(mod\ 2) \end{cases}$$

In the graph RB_r, we use two colors and the coloring partition given as follows,

Color Class	No of Times Obtain
$(1,2)$	$3r^2+4r-1$

(2.1)

Using the above coloring partition, the first Johan Zagreb Index is,

$$JZI_1(RB_r) = \sum_{i=1}\sum_{j=2}(\varphi(v_i) + \varphi(v_j)]\ \forall\ v_i v_j \in E(RB_r)$$

$=3r^2+4r-1(3)$

$=9r^2+12r-3JZI(RB)=9r+12r-3.$

2.2 Johan Zagreb Index of Hourglass Benzenoid Graph HBr

Theorem 3.1. The family of some Johan Zagreb Index of the molecular Hourglass Benzenoid graph HB_r is,

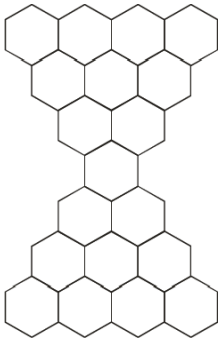

Fig 2. Hourglass Benzenoid graph HB_r

(1) $JZI_1(HB_r)=9r^2+27r-18.$
(2) $JZI_2(HB_r)=6r^2+18r-12.$
(3) $JZI_3(HB_r)=3r^2+9r-6.$
(4) $JZJI_1(HB_r) = 27r^2 + 81r - 54.$
(5) $HJZI_2(HB_r) = 12r^2 + 36r - 24.$
(6) $AJZI_2(HB_r) = 24r^2 + 72r - 48.$
(7) $ReJZI_1(HB_r)=9r^2+ 27r-9.$
(8) $ReJZI_2(HB_r) = 2r^2 + 6r - 4.$
(9) $ReJZI_3(HB_r)=18r^2+54r-36.$HBsetto be $V = \{a_1, a_2, a_3 \ldots, a_p; p = 2(r^2+4r+2)\}$ and edge set to be E= $\{b_1, b_2, b_3 \ldots, b_q; q = 3r^2+9r+6)\}$,wcolourable. The coloring of the graph is as follows,

$$C(a_i) = \begin{cases} c_1 \ if \ i \equiv 1(mod\ 2) \\ c_2 \ if \ i \equiv 0(mod\ 2) \end{cases}$$

In the graph HB_r, we use two colors and the coloring partition given as follows,

Color Class	No of Times Obtain
$(1,2)$	$3r^2+9r-6$

(3.1)

Using the above coloring partition the first Johan Zagreb Index is,

$$JZI_1(HB_r) = \sum_{i=1}\sum_{j=2}(\varphi(v_i) + \varphi(v_j)]\ \forall\ v_i v_j \in E(HB_r)$$

$= 3r^2+9r-6(3)$

$=9r^2+27r-18JZI(HB)=9r+27r-18.$ The proof is Similar for the all other indices.

2.3 Some Johan Zagreb Indices of Jagged Rectangle Benzenoid Graph JBr

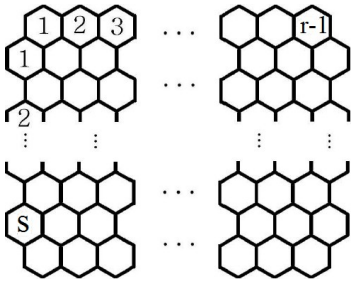

Fig 3. Jagged Rectangle Benzenoid graph $JB_{r,s}$

Theorem 4.1. The family of some Johan Index of the molecular Jagged Rectangle Benzenoid graph JB_r is
(1) $JZI_1(JB_r) = 18rs + 15r + 3s - 12$.
(2) $JZI_2(JB_r) = 12rs+10r+3s-8$.
(3) $JZI_3(JB_r)=6rs+5r+s-4$.
(4) $HJZI_1(JB_r) = 54rs + 45r + 9s - 36$.
(5) $HJZI_2(JB_r) = 24rs + 20r + 4s - 16$.
(6) $AJZI_2(JB_r)=48rs + 40r+ 8s -32$.
(7) $ReJZI_1(JB_r)= \frac{9}{2}rs+\frac{15}{2}r+\frac{3}{2}s-6$.
(8) $ReJZI_2(JB_r)=4rs+\frac{15}{3}r+\frac{2}{3}s-\frac{8}{3}$.
(9) $ReJZI_3(JB_r)=36rs+30r+6s-24$.

Proof: Let us consider the Jagged Rectangle Benzenoid graph JB_r. We presume that the vertex set to be $V = (a_1, a_2, a_3 \ldots, a_p; p = 4rs+4r+2s-2)\}$ and edge set to be E= $(b_1, b_2, b_3 \ldots, b_q; q = 6rs+5r+s-4)\}$, where r denotes the order of the series. This graph is Johan colourable.

$$C(a_i) = \begin{cases} c_1 \ if \ i \equiv 1(mod\ 2) \\ c_2 \ if \ i \equiv 0(mod\ 2) \end{cases}$$

In the graph JB_r, we use two colors and the coloring partition given as follows,

Color Class	No of Times Obtain
$(1,2)$	$6rs+5r+s-4$

(4.1)

Using the above coloring partition, the first Johan Zagreb Index is,

$$JZI_1(JB_r) = \sum_{i=1}\sum_{j=2}(\varphi(v_i) + \varphi(v_j)]\ \forall\ v_i v_j \in E(JB_r)$$

=6rs+5r+s−4(3)
=18rs+15r+3s−12JZI(JB)=18rs+15r+3s−12. The proof is Similar for the all other Indices.

2.4 Python Programming for Family of Zagreb Johan Indices of Jagged Rectangle Benzenoid Graphs

r=int(input("Enter r Value:"))
s=int(input("Enter s Value:"))
$JZI1JR_{r,s}$= 18 *r *s + 15 *r + 3 *s − 12
$JZI2JR_{r,s}$= 12 *r *s + 10 *r + 2 *s − 8
$JZI3JR_{r,s}$= 6 *r *s + 5 *r + s − 4
$HJZ1JR_{r,s}$= 54 *r *s + 45 *r + 9s − 36
$HJZI2JR_{r,s}$=24*r*s+20 *r+4s−16

$AJZIJR_{r,s}$= 48 *r *s + 40*r + 8s – 32
$ReJZI1JR_{r,s}$=9*r*s+= $\frac{15}{2}$ *r+$\frac{3}{2}$s–6$ReJZI2JR$=4*r*s+$\frac{10}{2}$*r+s−$\frac{8}{2}$
$ReJZI3JR$ =36 *r*s+30*r+6*s−24
print("$ZJI1(JR_{r,s})$ =: ",$ZJI1JR_{r,s}$)
print("$ZJI2(JR_{r,s})$=:",$ZJI2JR_{r,s}$)
print("$ZJI3(JR_{r,s})$ =: ",$ZJI3JR_{r,s}$)
print("$HZJI1(JR_{r,s})$=:",$HZJI1JR_{r,s}$)
print("$HZJI2(JR_{r,s})$=:", $HZJI2JR_{r,s}$)
print("$AZJI(JR_{r,s})$=:",$AZJIJR_{r,s}$)
print("$ReZJI1(JR_{r,s})$=:", $ReZJI1JR_{r,s}$)
print("$ReZJI2(JR_{r,s})$=:", $ReZJI2JR_{r,s}$)
print("$ReZJI3(JR_{r,s})$=:",$ReZJI3JR_{r,s}$)

3 Conclusion

This study introduces a number of Johan Zagreb Indices that are relevant to chemical graph theory. Although many various chromatic indices have been employed in the literature, Johan Zagreb chromatic indices outperform those that have already been developed. Additionally, it provides the Python Program to calculate these indices. The physico-chemical characteristics of chemical molecules are predicted using them. The creation of new indices will aid in the discovery of drugs more in future study. Interdisciplinary research is quite valuable in this situation, that this explanation would encourage some readers to research these indices in more depth. So hopefully more research can be done in the fascinating field of graph theoretical indices.

4 Declaration

This work has been presented in "International conference on Recent Strategies in Mathematics and Statistics" 112 (ICRSMS2022), Organized by the Department of Mathematics of Stella Maris College and of IIT Madras during 19 to 21 May, at Chennai, India The Organizer claims the peer review responsibility.

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