DEGREE-BASED TOPOLOGICAL DESCRIPTORS OF SOMEDERIVED GRAPHS BY USING A NOVEL POLYNOMIAL

Nanjundaswamy M[1], Puttaswamy[2], Ammar Alsinai[3<*], Murat Cancan[4]

Article History: Received: 14.03.2023 **Revised:** 25.04.2023 **Accepted:** 09.06.2023

Abstract

Derived graphs are the graphs obtained by some kind of operation on a given and usually smaller graph. By studying the relations between a graph and its derived graph, one can obtain information on one depending on the information on the other. In this paper, we calculate the first and second Zagreb indices of two of the derived graphs, namely double and strong double graphs of circumcoronene series of benzenoid (H_m) by using a novel polynomial called vertex degree polynomial.

Keywords: Derived graphs, vertex degree polynomial, double and strong double graphs of circumcoronene series of benzenoid.

2010 Math. Subject Classification: 05C12, 05C90, 05C76.

[1,2]Department of Mathematics,PES College of Engineering, Mandya, University of Mysore, India
[3,*]Department of Mathematics, University of Mysore, Manasagangotri, Mysore, India.
Email: [3]aliiammar1985@gmail.com
[4]Faculty of Education, Van Yuzuncu Yıl University, Zeve Campus, Tuşba, 65080, Van, Turkey
***Corresponding author Ammar Alsinai:** aliiammar1985@gmail.com.

DOI: 10.31838/ecb/2023.12.s3.466

1. INTRODUCTION

Several topological graph indices have been defined and studied by many mathematicians and chemists. They are defined as topological graph invariants measuring several physical, chemical, pharmacological, pharmaceutical, biological, etc. properties of graphs which are modelling real life situations. They can be grouped into three classes according to the way they are defined: by vertex degrees, by matrices or by distances. In this paper, we consider degree based topological indices of two derived graphs. Let $G = (V, E)$ be a simple graph with $|V(G)| = n$ vertices and $|E(G)| = m$ edges where $V(G) = \{f_1, f_2, ...f_n\}$ and $E(G) = \{f_i f_j | f_i, f_j \in V(G)\}$. That is, we do not allow loops or multiple edges within the set of edges. For any vertex $f \in V(G)$, we denote the degree of v by $d_G(f)$ or d_f. If f_i and f_j are adjacent vertices of G, and if the edge e connects them, this situation will be denoted by $e = f_i f_j$. Adjacency and incidency play a very important role in the spectral graph theory, the sub-area of graph theory dealing with linear algebraic study of graphs. The smallest and biggest vertex degrees in a graph will be denotedby δ and Δ, respectively.

Two of the most important topological graph indices are called the first an second Zagreb indicesdenoted by $M_1(G)$ and $M_2(G)$, respectively:

$$M_1(G) = \sum_{f \in V(G)} d^2(f).$$

$$M_2(G) = \sum_{fg \in E(G)} d(f)d(g).$$

They were first defined in 1972 by Gutman and Trinajstic, [24] and are often referred to due to their uses in Chemistry for QSAR and QSPR studies.
For more new topological indices see [12, 25]. Many papers [1-16] are written on this simple graph invariant. In 2023 [11], Hanan Ahmed et al. introduced new graph polynomial known as vertex degree polynomial defined as:

$$VD(G, x) = \sum_{fg \in E(G)} d(f)x^{d(g)}.$$

Using this new polynomial one can calculate the first and second Zagreb indices. For more com- prehensive and detailed study on vertex degree polynomial of graphs, we mention the following articles [14, 15] for readers.
The authors obtained that the derivative of $VD(G, x)$ at x = 1 is two times the second Zagreb index $M_2(G)$ and the sum of coefficients of the vertex degree polynomial is equal to first Zagreb index $M_1(G)$. This result opens a new gateway to the study of the first and second Zagreb indices and their implications.

Theorem 1.1. *[11] Let G be a graph with vertex degree polynomial $VD(G, x)$. Then*

$$D_x(VD(G, x))|_{x=1} = 2M_2(G),$$
$$(VD(G, x))|_{x=1} = M_1(G).$$

Definition 1.2. *The well-known family of the benzenoid molecular graph is the circumcoronene series of benzenoids (H_m), where $m \geq 1$. This family of graphs is constructed exclusively from benzene C_6 on the circumference. Certain main members of the circumcoronene series of benzenoids are benzene H_1, coronene H_2, circumcoronene H_3, and circumcircumcoronene H_4. Generally, the circumcoronene series of benzenoid (H_m) is shown in Figure 1.*

Definition 1.3. *In order to make a double graph $D(H_m)$ of a graph G, take two copies of the graph G and join the nodes in each copy with their neighbors in the other copy. For example, the graph (H_1) and its double graph $D(H_1)$ are shown in Figure 2. In double graph of the circumcoronene series of benzenoid, there are $12m^2$ vertices and $4(9m^2 - 3m)$ edges, respectively. In $D(H_m)$, we* *have* $12m$ *vertices of degree 4 and* $12(m^2 - m)$ *vertices of degree 6.*

Definition 1.4. *Consider the two copies of graph G, and by joining the closed neighborhoods of one graph's vertex to the vertex in an adjacent graph, one can obtain the strong double graph* $SD(G)$ *of graph G. For example, strong double graph of graph* H_1 *is shown in Figure 3.*

This study is laid out as follows. We will examine some degree-based topological indices known first and second Zagreb indices of double and strong double graphs of circumcoronene series of benzenoid (H_m) by new polynomial named vertex degree polynomial.

2. Main Results

Now we will determine the vertex degree polynomial of double and strong double graphs of circumcoronene series of benzenoid (H_m) and using this new polynomial we calculate the exact values of first $M1(G)$ and second $M_2(G)$ Zagreb indices.

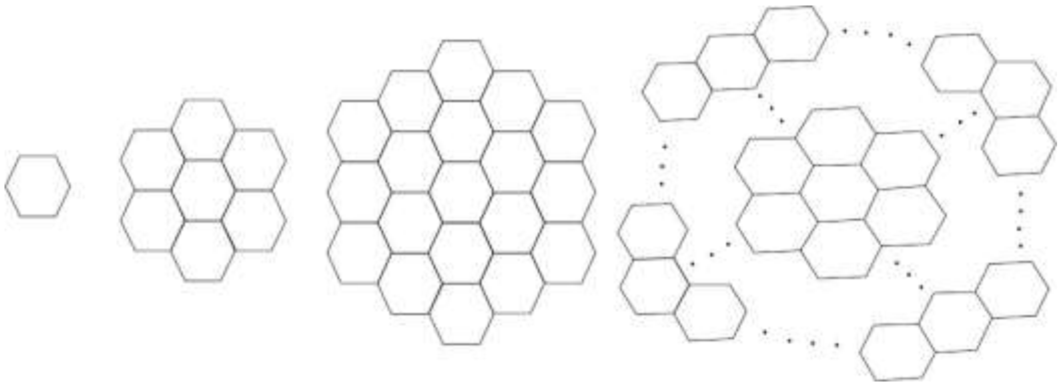

Figure 1: Circumcoronene series of benzenoid (H_1, H_2, H_3 and H_m).

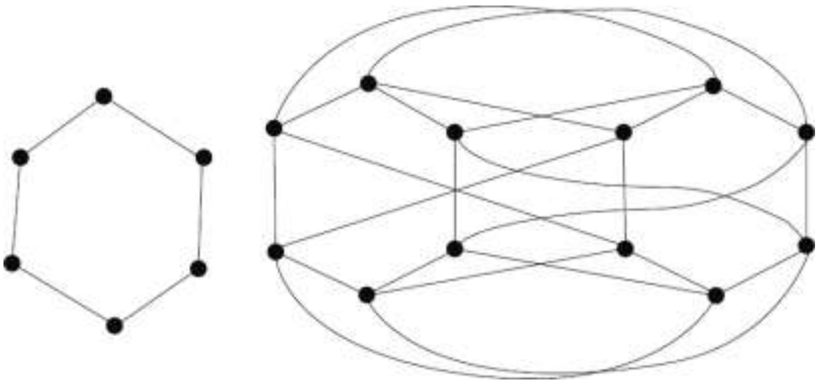

Figure 2: Circumcoronene series of benzenoid (H_1) and its double graph ($D(H_1)$).

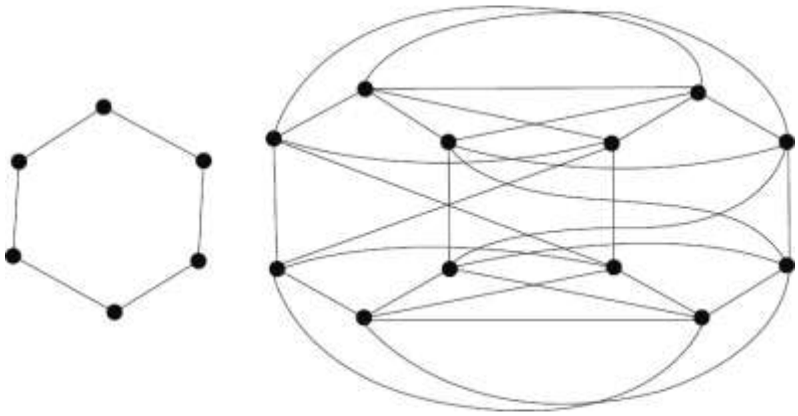

Figure 3: Circumcoronene series of benzenoid (H_1) and its strong double graph ($SD(H_1)$).

Theorem 2.1. *Let* $D(H_m)$ *be the double graph of circumcoronene series of benzenoid graph* (H_m)*;*

then, the vertex degree polynomial of $D(H_m)$ *is*

$$VD(D(H_m),x) = [12(36m^2 - 60m + 24) + 192(m-1)]x^6 + [288(m-1) + 192]x^4.$$

Proof. In the double graph of circumcoronene series of benzenoid, there are $12m^2$ vertices and $4(9m^2 - 3m)$ edges, respectively. There are $12m$ vertices in $D(H_m)$ of degree 4 and $12(m^2 - m)$ of degree 6.
We separate the edges of $D(H_m)$ into:

$$E_1 = \{uv : uv \in E(D(H_m)) \;\; and \;\; du = 4, d_v = 4\}$$

$$E_2 = \{uv : uv \in E(D(H_m)) \;\; and \;\; du = 4, d_v = 6\}$$

$$E_3 = \{uv : uv \in E(D(H_m)) \;\; and \;\; du = 6, d_v = 6\}$$

and $|E_1| = 24$, $|E_2| = 48(m-1)$, $|E_3| = 36m^2 - 60m + 24$. Hence

$$\begin{aligned}
VD(D(H_m),x) &= \sum_{fg\in E(D(H_m))} d(f)x^{d(g)} \\
&= \sum_{fg\in E_1} d(f)x^{d(g)} + \sum_{fg\in E_2} d(f)x^{d(g)} + \sum_{fg\in E_3} d(f)x^{d(g)} \\
&= \sum_{fg\in E_1} (4x^4 + 4x^4) + \sum_{fg\in E_2} (4x^6 + 6x^4) + \sum_{fg\in E_3} (6x^6 + 6x^6) \\
&= 8x^4|E_1| + (4x^6 + 6x^4)|E_2| + 12x^6|E_3| \\
&= 8x^4(24) + (4x^6 + 6x^4)(48(m-1)) + 12x^6(36m^2 - 60m + 24) \\
&= [12(36m^2 - 60m + 24) + 192(m-1)]x^6 + [288(m-1) + 192]x^4.
\end{aligned}$$

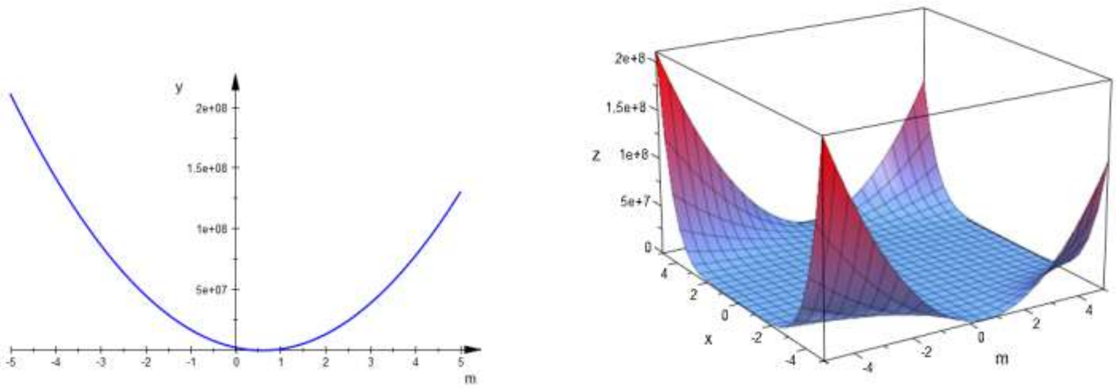

Figure 4: Graphical representation of 2D and 3D of vertex degree polynomial of $D(H_m)$.

Theorem 2.2. *Let* $D(H_m)$ *be the double graph of circumcoronene series of benzenoid graph* (H_m)*; then,*

$$M_1(D(H_m)) = 432m^2 - 240.$$
$$M_2(D(H_m)) = 1296m^2 - 1008m + 96.$$

Proof. Let $D(H_m)$ be the double graph of circumcoronene series of benzenoid graph (H_m); we have

$$VD(D(H_m),x) = [12(36m^2 - 60m + 24) + 192(m-1)]x^6 + [288(m-1) + 192]x^4.$$

Hence, using Theorem 1.1, we get

$$\begin{aligned}
M_1(D(H_m)) &= VD(D(H_m),x)|_{x=1} \\
&= [12(36m^2 - 60m + 24) + 192(m-1)]x^6 + [288(m-1) + 192]x^4|_{x=1}
\end{aligned}$$

$$= [12(36m^2 - 60m + 24) + 192(m-1)] + [288(m-1) + 192]$$
$$= 432m^2 - 720m + 288 + 192m - 192 + 288m - 288 + 192$$
$$= 432m^2 - 240m.$$

And,

$$2M_2(D(H_m)) = D_x(VD(D(H_m), x))|_{x=1}$$
$$= D_x([12(36m^2 - 60m + 24) + 192(m-1)]x^6 + [288(m-1) + 192]x^4)|_{x=1}$$
$$= [72(36m^2 - 60m + 24) + 1152(m-1)]x^5 + [1152(m-1) + 768]x^3|_{x=1}$$
$$= [72(36m^2 - 60m + 24) + 1152(m-1)] + [1152(m-1) + 768]$$
$$= 2592m^2 - 4320m + 1728 + 1152m - 1152 + 1152m - 1152 + 768$$
$$= 2592m^2 - 2016m + 192.$$

Hence,

$$M_2(D(H_m)) = 1296m^2 - 1008m + 96.$$

Theorem 2.3. *Let $SD(H_m)$ be the strong double graph of circumcoronene series of the benzenoidgraph (Hm); then*

$$VD(SD(H_m), x) = \Big(10(6m + 24) + 336(m-1)\Big)x^5 + \Big(240(m-1) + 14(42m^2 - 66m + 24\Big)x^7.$$

Proof. In the strong double graph of circumcoronene series of benzenoid, there are $12m^2$ verticesand $6(7m^2 - 2m)$ edges, respectively. There are $12m$ vertices in $SD(H_m)$ of degree 5 and $12m(m^2 - 1)$ of degree 7. We separate the edges of $SD(H_m)$ into:

$$E_3 = \{uv : uv \in E(SD(H_m)) \ and \ du = 7, d_v = 7\}$$

and $|E_1| = 6m + 24$, $|E_2| = 48(m-1)$, $|E_3| = 42m^2 - 66m + 24$. Hence

$$\begin{aligned} VD(SD(H_m), x) &= \sum_{fg \in E(SD(H_m))} d(f)x^{d(g)} \\ &= \sum_{fg \in E_1} d(f)x^{d(g)} + \sum_{fg \in E_2} d(f)x^{d(g)} + \sum_{fg \in E_3} d(f)x^{d(g)} \\ &= \sum_{fg \in E_1} (5x^5 + 5x^5) + \sum_{fg \in E_2} (5x^7 + 7x^5) + \sum_{fg \in E_3} (7x^7 + 7x^7) \\ &= 10x^5|E_1| + (5x^7 + 7x^5)|E_2| + 14x^7|E_3| \\ &= 10(6m + 24)x^5 + 48(m-1)(5x^7 + 7x^5) + 14(42m^2 - 66m + 24)x^7 \\ &= \Big(10(6m + 24) + 336(m-1)\Big)x^5 + \Big(240(m-1) + 14(42m^2 - 66m + 24\Big)x^7. \end{aligned}$$

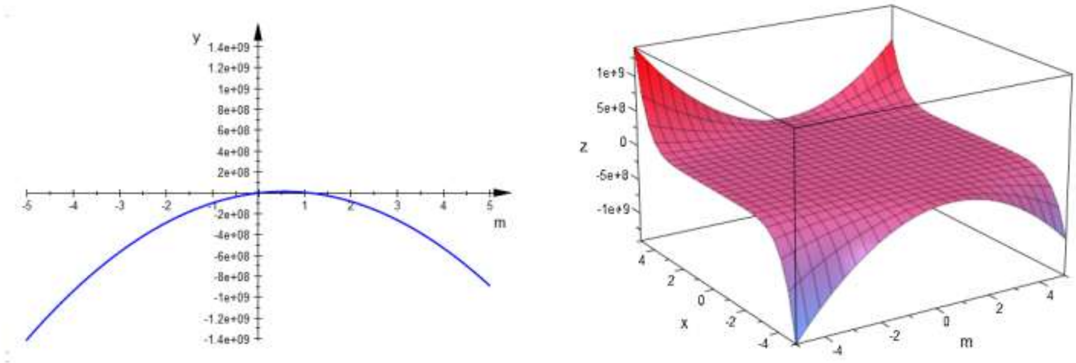

Figure 5: Graphical representation of 2D and 3D of vertex degree polynomial of $SD(H_m)$.

Theorem 2.4. *Let $SD(H_m)$ be the strong double graph of circumcoronene series of the benzenoidgraph (Hm); then*

$$M_1(SD(H_m)) = 336m^2 - 288m.$$
$$M_2(SD(H_m)) = 1176m^2 - 140m + 96.$$

Proof. Let $SD(H_m)$ be the strong double graph of circumcoronene series of the benzenoid graph(Hm), we have

$$VD(SD(H_m),x) = \Big(10(6m+24)+336(m-1)\Big)x^5 + \Big(240(m-1)+14(42m^2-66m+24\Big)x^7.$$

Hence, using Theorem 1.1, we get

$$\begin{aligned}
M_1(SD(H_m)) &= (VD(SD(H_m),x))|_{x=1}\\
&= \Big(10(6m+24)+336(m-1)\Big)x^5 + \Big(240(m-1)+14(42m^2-66m+24\Big)x^7|_{x=1}\\
&= \Big(10(6m+24)+336(m-1)\Big) + \Big(240(m-1)+14(42m^2-66m+24\Big)\\
&= 60m+240+336m-336+240m-240+336m^2-924m+336\\
&= 336m^2-288m.
\end{aligned}$$

And,

$$\begin{aligned}
2M_2(SD(H_m)) &= D_x((VD(SD(H_m),x)))|_{x=1}\\
&= D_x\Big(\Big(10(6m+24)+336(m-1)\Big)x^5 + \Big(240(m-1)+14(42m^2-66m+24\Big)x^7\Big)|_{x=1}\\
&= (50(6m+24)+1680(m-1))x^4 + (1680(m-1)+98(42m^2-66m+24))x^6|_{x=1}\\
&= (50(6m+24)+1680(m-1)) + (1680(m-1)+98(42m^2-66m+24))\\
&= 300m+1200+1680m-1680+1680m-1680+2352m^2-6468m+2352\\
&= 2352m^2-2808m+192
\end{aligned}$$

Hence,

$$M_2(SD(H_m)) = 1176m^2 - 140m + 96.$$

3. REFERENCES

1. A. Alsinai A, A. Alwardi, M. R. Fraahani, N.D. Soner. On the ψk-polynomial of the graph, Eurasian Chemical Communications., 3(4) (2021) 219-226.
2. D. A. Xavier, S. Akhila, A. Alsinai, K. Julietraja, H. Ahmed, A. A. Raja, and E. S. Varghese, Distance-Based Structure Characterization of PAMAM-Related Dendrimers Nanoparticle. Journal of Nanomaterials, (2022). https://doi.org/10.1155/2022/2911196
3. H. Ahmed, A. Alsinai, A. Khan, and H.A. Othman, The Eccentric Zagreb Indices for the Subdivision of Some Graphs and Their Applications, Appl. Math., 16(3), 2022, 467-472. doi:10.18576/amis/160308.
4. A. Alsinai, A. Saleh, H. Ahmed, L.N. Mishra, and N.D. Soner, On fourth leap Zagreb index of graphs, Discrete Mathematics, Algorithms and Applications., 2022. https://doi.org/10.1142/S179383092250077X
5. F. Afzal, A. Alsinai, S. Hussain, D. Afzal, F. Chaudhry, and M.Cancan, On topological aspects of silicate network using M-polynomial. Journal of Discrete Mathematical Sciences and Cryptography, 24(7), (2021), 2109-2119. https://doi.org/10.1080/09720529.2021.1977486

6. A. Alsinai, A. Alwardi, and N. D. Soner, Topological Properties of Graphene Using ψk− polynomial, Proceedings of the Jangjeon Mathematical Society., 24 (2021), 375–388.

7. A. Alsinai, H. Ahmed, A. Alwardi, and N.D.Soner HDR Degree Bassed Indices and MhrPolynomial for the Treatment of COVID-19, Biointerface Research in Applied Chemistry., 12(6) (2021), 7214 – 7225
8. K. Julietraja, A. Alsinai, and A. Alameri, Theoretical Analysis of Superphenalene Using Different] Kinds of VDB Indices. Journal of Chemistry, (2022). https://doi.org/10.1155/2022/5683644

9. S. Hussain, A. Alsinai, D. Afzal, A. Maqbool, F. Afzal, and M. Cancan, Investigation of Closed Formula and Topological Properties of Remdesivir (C27H35N6O8P), Chem. Methodol., 2021, 5(6) 485-497 https://doi.org/10.22034/chemm.2021.138611.

10. M. S. Rosary, A. Alsinai, M. K. Siddiqui, and H. Ahmed, A Perspective Approach to Study the Valency-Based Irregular Indices for Benzenoid Planar Octahedron Structures. Journal of Chemistry, (2023). https://doi.org/10.1155/2023/5512724.

11. H. Ahmed, Anwar Alwardi, Ruby Salestina M., N.D. Soner, *Forgotten domina- tion, hyper domination and modified forgotten domination indices of graphs*, Jour-nal of Discrete Mathematical Sciences and Cryptography, 24(2), 353-368,2021, DOI : 10.1080/09720529.2021.1885805.
12. H. Ahmed, A. Alwardi, R.M Salestina , *Domination topological indices and their polynomials of a firefly graph*, Journal of Discrete Mathematical Sciences and Cryptography 24(2):325- 341, 2021, https://doi.org/10.1080/09720529.2021.1882155
13. H. Ahmed, M.R. Farahani, A. Alwardi, R.M Salestina, *Domination topological properties of some chemical structures using φ_P -polynomial approach*, Eurasian Chemical Communi- cations, 2021, 3(4), 210-218, 2021, DOI: 10.22034/ecc.2021.271992.1133.
14. H. Ahmed, A. Alwardi, R.M. Salestina, *Domination, γ−Domination Topological Indices and φ_P −Polynomial of Some Chemical Structures Applied for the Treatment of COVID-*
15. *19 Patients*, Biointerface research in applide chemistry, 5, 2021, 13290 - 13302. DOI: 10.33263/BRIAC115.1329013302
16. H. Ahmed, R. Rangarajan, A. Alameri, R.M Salestina, *Computation Domination and γ−Domination Topological Indices of Hexane Isomers via φ_P −Polynomial with QSPR Analysis*, Biointerface Research in Applied Chemistry 13(2):182 2022, DOI: 10.33263/BRIAC132.182.
17. H. Ahmed, A. Alwardi, S. Wazzan, *Domination topological properties of polyhydroxybutyrate and polycaprolactone with QSPR analysis*, Nanosystems Physics Chemistry Mathematics 12(6):664-671, 2022, DOI: 10.17586/2220-8054-2021-12-6-664-671
18. A. Alameri, A. Alsharafi, H. Ahmed, *The second hyper-zagreb indices and coindices of disjunction and symmetric difference of graphs*, I. J. of Advanced Chemistry Research,1(1)37-41. 2019.
19. H. Ali, H. M. A. Siddiqui, and M. K. Shafiq, *On degree-based topological descriptors of oxide and silicate molecular structures,* Magnet Research Report, vol. 4, pp. 135–142, 2016.
20. S. Javaraju, H. Ahmed, A. Alsinai, & N. D. Soner, Domination topological properties of carbidopa-levodopa used for treatment Parkinson's disease by using φp-polynomial. *Eurasian Chemical Communications*, *3*(9), (2021), 614-621. https://doi.org/10.22034/ecc.2021.274069.1138
21. .A. Ayache, A. Alameri, M. Alsharafi, H. Ahmed, *The Second Hyper-Zagreb Coindex of Chemical Graphs and Some Applications*, Journal of Chemistry 2021(2):8 pages, DOI: 10.1155/2021/3687533

22. I. Gutman, N. Trinajstic, *Graph theory and molecular orbitals. Total Π-electron energy of alternant hydrocarbons*. Chem. Phys. Lett. 1972, 17, 535–538.
23. A.M. Hanan Ahmed, A. Alwardi, R.M. Salestina, *On Domination Topological Indices of Graphs*, Int. J. Anal. Appl., 19 (1) (2021), 47-64. DOI: 10.28924/2291-8639-19-2021-47.
24. A. Modabish, M. N. Husin, A. Alameri, H. Ahmed, M. Alaeiyan, M. R. Farahani,
25. M. Cancan, *Enumeration of spanning trees in a chain of diphenylene graphs*, Jour- nal of Discrete Mathematical Sciences and Cryptography 25(1):241-251 2022, DOI: 10.1080/09720529.2022.2038931.
26. P. Manuel and I. Rajasingh, *Topological properties of silicate networks*, in Proceedings of the 2009 5th IEEE GCC Conference and Exhibition, pp. 1–5, IEEE, Kuwait City, Kuwait, 2009 March.
27. P. S. Ranjini, V. Lokesha, A. Usha, *Relation between phenylene and hexagonal squeeze using harmonic index*, Int. J. of Graph Theory, 1, 116-21. 2013.