Advances in Nonlinear Variational Inequalities
ISSN: 1092-910X
Vol 28 No. 7s (2025)

Harmonic and Zagreb Polynomials and Their Applications on Chemical Nano-Structures

Munira W. Mahan[1], Khulood G. Kassid[2] , Mohammed W. Mihan[3], and Mamoon F. Khalf[4]
[1]Department of Material, College of Engineering , University of Basra : munira.mahan@uobasrah.edu.iq
[2,3]Ministry of Education, Basra Education Directorate , Iraq : mmihan62@yahoo.com
[4]College of Education , Samarra University

Article History:
Received: 15-12-2024
Revised:23-1-2025
Accepted:3-2-2025

Abstract: The graph G consists of an ordered pair (V, E), where V represents a nonempty set of elements called vertices for graph G, and E is a family of unordered pairs that may be free of vertices in graph G and is called edges for graph G. G called a simple graph if has not loops and without parallel edges, all graphs that used in this paper are simple graph. The degree of a vertex is number of edges E(G) at that vertex V(G) or V(u) where d_v and d_u are denoted for degree of vertex [1] [2].

Keywords: graph, unordered, consists, loops

Introduction:

Mathematical chemistry that depends on chemical graph is one of the most important field of this science, which converts chemical compounds into mathematical formulas that are easy to deal with based on graph theory by correspond bonds to edges and atoms to vertices in mathematically [3][4].

In **2015** Mohammad A. Iranmansh and Mahboubeh Saheli used the harmonic polynomial as [5][6]

$$H(G) = \sum_{vu \in E(G)} x^{(d_v + d_u - 1)}$$

In **2016** A.R. Bindusree et.al. [7] added a new define to formula of Zagreb polynomials namely fourth and fifth Zagreb polynomials as

$$Z_4(G,x) = \sum_{uv \in E(x)} x^{d_u(d_v + d_u)}$$

$$Z_5(G,x) = \sum_{uv \in E(x)} x^{d_v(d_v + d_u)}$$

Important Concepts:

Nanostar, also known as a nanostructure, is a phrase used to describe an entity that exists at a scale that is midway between microscopic and atomic structures. This phenomenon arises due to a physical measurement that is less than 100 nanometers.[8]

Dendrimer: It is an synthesized molecule or artificially manufactured built up from branched units called monomers .Dendrimers are a new kind of polymeric materials and it is characterized by a combination of a compact molecular structure and a high number of functional groups.[9]

Polyphenyl compounds are organic compounds that consist of numerous phenyl/benzene rings and can be obtained either by synthetic or natural means. The isolation and characterization of these compounds can pose challenges due to their inherent unpredictability and the likelihood of contaminants arising from their synthesis . Consequently, the qualities that have been documented are typically ascertained in substantial quantities or represent a combination of several formations. The aforementioned compounds have demonstrated utility within the field of Material Science, encompassing applications such as organic light emitting diodes, catalysts, transmitters, and other biological uses. Moreover, these compounds have been employed in molecular representations of graphene and discotic liquid crystals owing to their enhanced solubilities, elevated thermal stability, and reduced melting temperatures.[10][11][12][13][14]

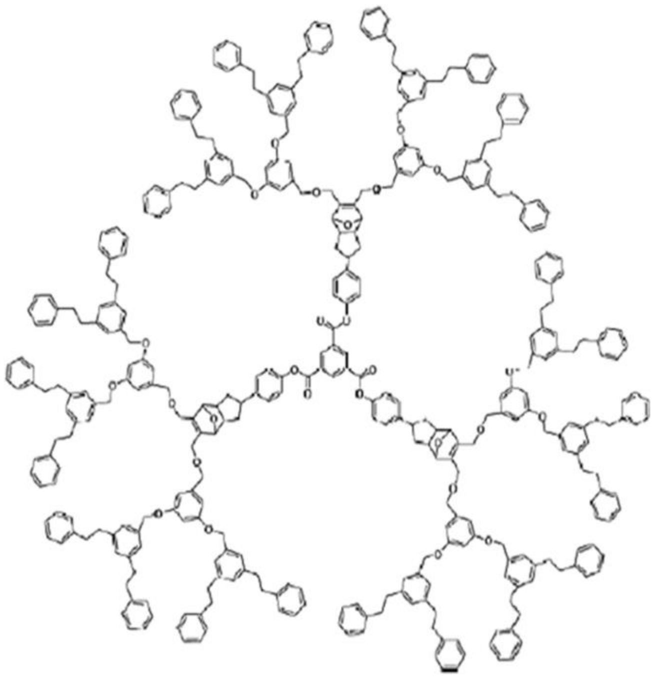

Fig 1 : The polymer dendrimer

The polymer dendrimer in (Fig 1), is nanostar represented as $NS[i]$, where(i) is the number stages of growth, as illustrated. The molecular graph of $NS[i]$ has four types of degrees of the end vertices (2,2), (2,3), (3,3), and (3,4) in symmetrical arrangement with two analogous branches. Hence, by doing a direct calculation, we obtain

$$E_1(NS[i]) = e_{22} = \{ e \in E : d_v = 2, d_u = 2 \}$$

$$E_2(NS[i]) = e_{23} = \{ e \in E : d_v = 2, d_u = 3 \}$$

$$E_3(NS[i]) = e_{33} = \{e \in E : d_v = 3, d_u = 3\}$$

$$E_4(NS[i]) = e_{13} = \{e \in E : d_v = 1, d_u = 3\}$$

In (Fig. 1), we note that there are two similarity branches with four types of end edges, as we explain in (Table 1).

Table 1: the value of degree in $NS[i]$ where $d(v,u)$ = (2,2), (2,3), (3,3), and (1,3) with stage of growth i={1,2,3…}

stage / degree	i=1	i=2	i=3
d(2,2)	18	30	54
d(2,3)	90	186	390
d(3,3)	24	24	24
d(1,3)	15	27	51

Table2 : forms to calculate number of edges in every degree

$d_v, d_u \in E(G)$	No. of edges
d(2,2)	$6 \times (2^i + 1)$
d(2,3)	$6 \times (2^{i+3} - 1)$
d(3,3)	24
d(1,3)	$3 \times (2^{i+1} + 1)$

Results:

Theorem 1: Let $NS[i]$ be the nanostar structures when i={1,2,3…} the fourth Zagreb polynomial is given by

$$Z_4(NS[i],x) = \sum_{NS[i]} 6(2^i + 1)x^8 + \sum_{NS[i]} 6(2^{i+3} - 1)x^{10} + \sum_{NS[i]} 3(2^{i+1} + 1)x^4$$
$$+24x^{18}$$

Proof: by using the fourth Zagreb polynomial definition

$$Z_4(NS[i],x) = \sum_{vu \in E(NS[i])} x^{d_v(d_v+d_u)}$$

$$= \sum_{vu \in E(NS[i])} x^{2(2+2)} + \sum_{vu \in E(NS[i])} x^{2(2+3)}$$
$$+ \sum_{vu \in E(NS[i])} x^{3(3+3)} + \sum_{vu \in E(NS[i])} x^{(1+3)}$$

$$= |E_1(NS[i]|x^8 + |E_2(NS[i]|x^{10} + |E_4(NS[i]|x^{18}$$
$$+ |E_4(NS[i]|x^4$$

$$Z_4(NS[i],x) = \sum_{NS[i]} 6(2^i + 1)x^8 + \sum_{NS[i]} 6(2^{i+3} - 1)x^{10} + \sum_{NS[i]} 3(2^{i+1} + 1)x^4$$
$$+24x^{18}$$

Collorary 1: Let $NS[i]$ nanostar structure polyphenylene dendrimer have stages of growth when $i = 1$ the fourth Zagreb polynomial is

$$Z_4(NS[1],x) = 18x^8 + 90x^{10} + 24x^{18} + 15x^4$$

Theorem 2: Let $NS[i]$ be the nanostar structures when i={1,2,3,…} and the fifth Zagreb polynomial is

Proof : by using the definition of the fifth Zagreb polynomial

$$Z_5(NS[i],x) = \sum_{uv \in E(NS[i])} x^{d_u(d_v+d_u)}$$

$$= \sum_{vu \in E(NS[i])} x^{2(2+2)} + \sum_{vu \in E(NS[i])} x^{3(2+3)}$$
$$+ \sum_{vu \in E(NS[i])} x^{3(3+3)} + \sum_{vu \in E(NS[i])} x^{(1+3)}$$

$$=\left|E_1(NS[i]\right|x^8+\left|E_2(NS[i]\right|x^{15}+\left|E_3(NS[i]\right|x^{18}$$
$$+\left|E_4(NS[i]\right|x^{12}$$

$$Z_5(NS[i],x)=\sum_{vu\in E(NS[i])}6(2^i+1)x^8+\sum_{vu\in E(NS[i])}(4\times 2^i-2)x^{12}+\sum_{vu\in E(NS[i])}6(2^{i+3}-1)x^{15}$$
$$+\sum_{vu\in E(NS[i])}3(2^{i+1}+1)x^{12}+24x^{18}$$

Collorary 2: Let $NS[i]$ nanostar structure polyphenylene dendrimer have stages of growth when $i=1$ the fifth Zagreb polynomial is

$$Z_5(NS[1],x)=18x^8+4x^{12}+90x^{15}+24x^{18}+15x^{12}$$

Theorem 3: Let $NS[i]$ be the nanostar structure when i={0,1,2,3,…} and the harmonic polynomial is

$$H(NS[i],x)=\sum_{vu\in E(NS[i])}6(2^i+1)x^3+\sum_{vu\in E(NS[i])}6(2^{i+3}-1)x^4+\sum_{vu\in E(NS[i])}3(2^{i+1}+1)x^3$$
$$+(24)x^5$$

Proof : by using the definition of the harmonic polynomial

$$H(NS[i],x)=\sum_{vu\in E(NS[i])}x^{d_v+d_u-1}$$

$$=\sum_{vu\in E(NS[i])}x^{(2+2)-1}+\sum_{vu\in E(NS[i])}x^{(2+3)-1}$$
$$+\sum_{vu\in E(NS[i])}x^{(3+3)-1}+\sum_{vu\in E(NS[i])}x^{(1+3)-1}$$

$$=\left|E_1(NS[i]\right|x^3+\left|E_2(NS[i]\right|x^4+\left|E_3(NS[i]\right|x^5$$
$$+\left|E_4(NS[i]\right|x^3$$

$$H(NS[i],x)=\sum_{vu\in E(NS[i])}6(2^i+1)x^3+\sum_{vu\in E(NS[i])}6(2^{i+3}-1)x^4+\sum_{vu\in E(NS[i])}3(2^{i+1}+1)x^3$$
$$+(24)x^5$$

$$H(NS[i],x) = 9x^3 + (6\times 2^i + 3\times 2^{i+1})x^3 + 6(2^{i+3} - 1)x^4 + (24)x^5$$

Collorary 3: Let $NS[i]$ nanostar structure polyphenylene dendrimer have stages of growth when $i = 1$ the Harmonic polynomial is

$$H(NS[1],x) = 33x^3 + 90x^4 + 24x^5$$

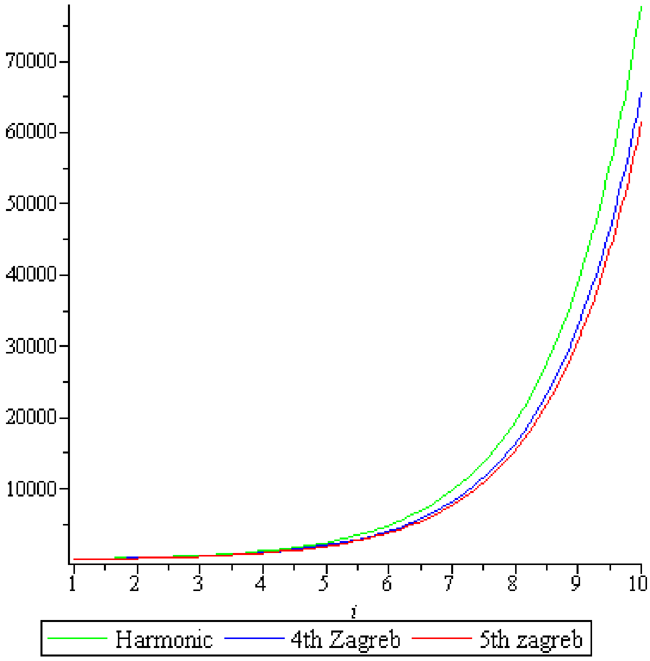

Fig .2: compare between polynomials

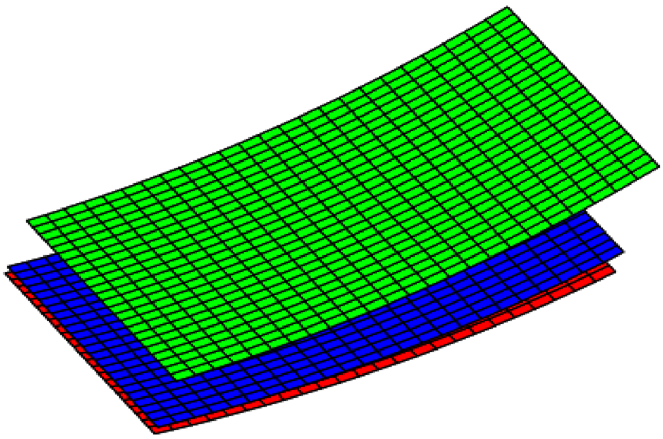

Fig .3: compare (3D) between polynomials

References :

[1] Mamoon Fattah Khalf, Habib Azanchiler, Nbeel E. Arif , Sara Eslamian. Vol 27 No.1 (2024).Advances in Nonliner Vaitional Inequalities

[2] Norman Biggs, E. Keith Lloyd, and Robin J. Wilson. (1998). *Graph Theory, 1736-1936.* New Yourk, United state of Amarica: Oxford University press.

[3] Prakash, N.(2018, Jan. 28). *Origins and Development of Graph Theory prior to 20th Century.*

[4] Carlson, s. C. (2023). Grath Theory. *Britannica*.

[5] Mohammed A. Iranmanesh and Mahboubeh Saheli. (2015). On the harmonic index and harmonic polynomial of Caterpillars with diameter four. *Iranian Journal of Mathematical Chemistry*, 41-49.

[6]Balaban, A. (1995). Chemical Graphs: Looking Back and Glimpsing Ahead. *J. Chem. Inf. Comput. Sci.*

[7] Young Chel Kwun,, Manzoor Ahmad Zahid, Waqas Nazeer,Ashaq Ali, Maqbool Ahmad, and Shin Min Kang. (2018). On the Zagreb polynomials of benzenoid systems. *DE GRUYTER, 16*, 734–740.

[8] Tony Augustine and Santiago Roy. (2022). Topological Study on Triazine-Based Covalent-Organic Frameworks. *symmetry*.

[9]C. Lima, M. R. (2011). Structural and Thermodynamic Characterization of Polyphenylbenzenes. *J. of Phy. Chem.*, 11876-11888.

[10] M. Unroe, B. R. (1987). One Pot Sythesis of p-Polyphenyls via the Intermolecular Cyclization of 3-Dimethyl-aminohex-5-en-1-ynes. *Synthesis*.

[11] Narwal, L. (2017). Role of Mathematics in chemistry and its future. *International Research Journal of Mangment Science and Technology, 8*(3).

[12] Mohammed W. Mihan, Habib Azanchiler, Nabeel E.Arif and Sara Eslameian. "Computation Zagreb, Randic, and general sum-connectivity polynomials on symmetrical chemical dendrimer." *Communications on Applied Nonlinear Analysis* 31 (2024): 551-559.

[13] Mohammed W. Mihan, Habib Azanchiler, Nabeel E.Arif and Sara Eslameian. "On Graph Polynomials and Their Applications of Nanostar." *Communications on Applied Nonlinear Analysis* 31 (2024): 583-594.

[14] Zainab Aziz Touma, Asaad Y. Ayied, and Ghaidda Ali Makki. "Genetic Polymorphisms Of The DNMT3b Gene In Local And Imported Calves." *Journal of Pharmaceutical Negative Results* 13.8 (2022): 1739-1745.