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Computation Zagreb, Randic, and general sum-connectivity polynomials on symmetrical chemical dendrimer

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Abstract

In this paper, the aim is to redefine some polynomials in a new form on the basis that polyphenylene dendrimer has two growth stages. The third Zagreb polynomial, general sum-connectivity polynomial, and general Randic polynomial are redefined and computed.

Keywords: Graph theory chemical graph , chemical polynomial, Zagreb polynomials, dendrimers.

1.Introduction

Mathematical chemistry is a specialised field within the science of chemistry that employs mathematical theories and concepts to analyse and understand chemical structures. A chemical graph is one branch of mathematical chemistry that connects graph theory and chemical structures. The chemical graph was spark born in the eighteenth century by ideas ideas Isaac Newton, and consider that the first model for representation of atom kinds with specific circles was by John Dalton in (1805). [1][2].The term (molecular structure) appeared in 1861 by Alexander Butlerov and this term refers to every chemical substance have a fixed structure in molecular bases [3].This term development by some scientists like Alexander William Williamson, Johann Wolfgang Döbereiner and Archibald Scott Coupe [4] .in chemical graph the simple graph (without loops and multiple edges) is important because it introduce an accurate description of the molecular graph [5].

Polyphenyl compounds are a class of chemical compounds characterized by the presence of multiple phenyl/benzene rings. These compounds can be synthesized or occur naturally. The separation and characterisation of these compounds can present difficulties due to their inherent unpredictability and the potential for impurities to arise during their synthesis[6]

Dandrimer 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 .[7-12].

Mathematicians have conducted extensive research on numerous chemical substances throughout the course of the last two centuries made a substantial contribution to the advancement of this particular field(for more detiles see [13-18]).

2.*Basic Concepts* : In the recent decades the chemical graph has witnessed great interest for several reasons, the most important of which is that the graph represents an accurate and simplified description of the bonding of chemical atoms, and the chemical graph provides important predictions about the nature of chemical reactions.

In the seventh of decade of the last century the first and second Zagreb indices introduced by Gutman [19],[20]

$$A_1(G) = \sum_{vu \in E(G)} (dv + du)$$

$$A_2(G) = \sum_{vu \in E(G)} (dv .du)$$

In 2011 A. Astaneh-Asl and GH. H. Fath Tabar [21] introduced the three formulas for Zagreb index and its polynomials

$$A_3(G) = \sum_{vu \in E(G)} \left| d_u - d_v \right|$$

and the first, second and third Zagreb polynomials are respectively ,

$$Z_1(G,x) = \sum_{vu \in E(G)} x^{dv+du}$$

$$Z_2(G,x) = \sum_{vu \in E(G)} x^{du.dv}$$

$$Z_3(G,x) = \sum_{vu \in E(G)} x^{|dv-du|}$$

In 2016 [22] Ranjini et al., introduced redefine for first, second and third Zagreb indices as

$$Re\, ZG_1(G) = \sum_{vu \in E(G)} \frac{d_u + d_v}{d_v d_u}$$

$$Re\, ZG_2(G) = \sum_{vu \in E(G)} \frac{d_u d_v}{d_u + d_v}$$

$$Re\, ZG_3(G) = \sum_{vu \in E(G)} (d_u d_v)(d_u + d_v)$$

In 2019 the neighborhood version of the various indices introduced by Sourav Mondal et al.,[23] are defined as

$$NM_1(G) = \sum_{vu \in E(G)} (S_v + S_u)$$

$$NM_2(G) = \sum_{vu \in E(G)} (S_v \times S_u)$$

Recently , in 2021Shanmukha M. C. et al. [24] introduced general sum-connectivity index follow is obtained as :

$$\chi_\alpha(G,x) = \sum_{vu \in E(G)} x^{[dv+du]^\alpha} \text{ , when } \alpha \neq 0 .$$

Also Abdul Jalil M. Khalaf et al.[22] , in 2021 introduce define for the general neighborhood sum-connectivity polynomial and the general Randic respectfully ,

$$R_{\alpha}(G,x) = \sum_{vu \in E(G)} x^{[dv \times du]^{\alpha}}$$

3.*Basic definitions:*

Connected graph : G(V,E) is called connected graph if every pair in G are connected For a graph G(V,E) the vertices and edges denoted V(G) and E(G) respectively [25] ,graph used in this paper is connected graph.

Degree of a vertex: let V(G) is a vertex in graph G the degree of a vertex is the number of edges incident with *v* and is denoted by deg_G or dv [26] .

Neighbors: In a graph G = (V, E), a vertex u is considered a neighbour of vertex v, or equivalently neighbouring to v, if there exists an edge {u, v} ∈ E. In the context of a directed graph, a vertex u is considered an in-neighbor of a vertex v if there exists an edge (u, v) in the set of edges E. Additionally, it is common to refer to two edges or as neighbours if they possess a common vertex.[27].

1.***First Result :***

In Figure 1. at stage i=0, the core of the polyphenylene dendrimer consists of three types of edges with degrees (2,2), (2,3), and (3,4). At stages i ≥ 1, there are four types of edges with degrees (2,2), (2,3), (3,3), and (3,4). The results can be obtained from Table 1 using the forms provided in Table1.

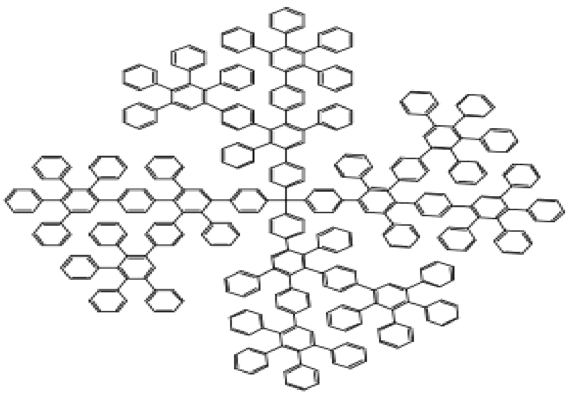

Fig 1. Polyphenylene dendrimer has two growth stages $D_4[i]$

stage / degree	i=0	i=1	i=2
d(2,2)	16	72	184
d(2,3)	8	56	152
d(3,3)	0	36	108
d(3,4)	4	4	4

Table 1 : stages of growth with degree of edge

$d_v, d_u \in E(G)$	No. of edges
d(2,2)	$(56(2^i)-40)$
d(2,3)	$(48(2^i)-40)$
d(3,3)	$(36(2^i)-36)$,
d(3,4)	4

Table 2: forms to calculate number of edges in every degree

Theorem1: Let $D[i]$ polyphenylene dendrimer have i stages of of growth when $i \geq 0$ and let deg(u) and deg(v) are the vertex degrees of u and v, respectively, then redefine the third Zagreb polynomial

$$\operatorname{Re} Z_3(G,x) = \sum_{uv\in E(G)} (56(2^i)-40)x^{(16)} + \sum_{uv\in E(G)} (48(2^i)-40)x^{(30)}$$
$$+ \sum_{uv\in E(G)} (36(2^i)-36)\,x^{(54)} + (4)x^{(84)}$$

Proof: By using the third Zagreb polynomial

$$\operatorname{Re} Z_3(G,x) = \sum_{vu\in E(G)} x^{(dv\times du)(dv+du)}$$

$$= \sum_{vu\in E(G)} (2+2)(2\times 2) + \sum_{vu\in E(G)} (2+3)(2\times 3) + \sum_{vu\in E(G)} (3+3)(3\times 3) + \sum_{vu\in E(G)} (3+4)(3\times 4)$$

$$= \sum_{uv\in E(G)} (56(2^i)-40)x^{(16)} + \sum_{uv\in E(G)} (48(2^i)-40)x^{(30)} + \sum_{uv\in E(G)} (36(2^i)-36)\,x^{(54)} + (4)x^{(84)}$$

Theorem 2: Let $D[i]$ polyphenylene dendrimer have i stages of growth when $i \geq 0$ and let deg(u) and deg(v) are the vertex degrees of u and v, respectively, then redefine the general sum-connectivity polynomial

$$\chi_\alpha(G,x) = \sum_{uv\in E(G)} (56(2^i)-40)x^{(4)^\alpha} + \sum_{uv\in E(G)} (48(2^i)-40)x^{(5)^\alpha}$$
$$+ \sum_{uv\in E(G)} (36(2^i)-36)\,x^{(6)^\alpha} + \sum_{uv\in E(G)} (4)x^{(7)^\alpha}$$

Proof: by using the definition general sum-connectivity polynomial when α it is positive integer number $\alpha \neq 0$

$$\chi_\alpha(G,x) = \sum_{vu\in E(G)} x^{[dv+du]^\alpha}$$

$$= \sum_{vu\in E(G)} x^{(2+2)^{\alpha}} + \sum_{vu\in E(G)} x^{(2+3)^{\alpha}} + \sum_{vu\in E(G)} x^{(3+3)^{\alpha}} + \sum_{vu\in E(G)} x^{(3+4)^{\alpha}}$$

$$= \sum_{uv\in E(G)} (56(2^i)-40)x^{(4)^{\alpha}} + \sum_{uv\in E(G)} (48(2^i)-40)x^{(5)^{\alpha}}$$
$$+ \sum_{uv\in E(G)} (36(2^i)-36)\,x^{(6)^{\alpha}} + \sum_{uv\in E(G)} (4)x^{(7)^{\alpha}}$$

Collorary 1: let $D[i]$ polyphenylene dendrimer with i stages of growth $i=\{0,1,2,\ldots\}$ and let d_v and d_u are degree of edges when $\alpha=1$ then general sum-connectivity polynomial is given by

$$\chi(G,x) = \sum_{uv\in E(G)} (56(2^i)-40)x^{(4)} + \sum_{uv\in E(G)} (48(2^i)-40)x^{(5)}$$
$$+ \sum_{uv\in E(G)} (36(2^i)-36)\,x^{(6)} + \sum_{uv\in E(G)} (4)x^{(7)}$$

Theorem 3: Let $D[i]$ polyphenylene dendrimer have i stages of growth when $i \geq 0$ and let deg(u) and deg(v) are the vertex degrees of u and v, respectively, and α is positive integer, then redefine general Randic polynomial

$$R_{\alpha}(G,x) = \sum_{uv\in E(G)} (56(2^i)-40)x^{(4)^{\alpha}} + \sum_{uv\in E(G)} (36(2^i)-36)\,x^{(6)^{\alpha}}$$
$$+ \sum_{uv\in E(G)} (48(2^i)-40)x^{(9)^{\alpha}} + \sum_{uv\in E(G)} (4)x^{(12)^{\alpha}}$$

Proof: by using the definition general Randic polynomial polynomial when α it is positive integer number $\alpha \neq 0$

$$R_{\alpha}(G,x) = \sum_{vu\in E(G)} x^{[dv \times du]^{\alpha}}$$

$$= \sum_{vu\in E(G)} x^{(2\times 2)^{\alpha}} + \sum_{vu\in E(G)} x^{(2\times 3)^{\alpha}} + \sum_{vu\in E(G)} x^{(3\times 3)^{\alpha}} + \sum_{vu\in E(G)} x^{(3\times 4)^{\alpha}}$$

$$= \sum_{uv\in E(G)} (56(2^i)-40)x^{(4)^{\alpha}} + \sum_{uv\in E(G)} (36(2^i)-36)\,x^{(6)^{\alpha}}$$
$$+ \sum_{uv\in E(G)} (48(2^i)-40)x^{(9)^{\alpha}} + \sum_{uv\in E(G)} (4)x^{(12)^{\alpha}}$$

Collarary2:let $D[i]$ polyphenylene dendrimer with i stages of growth when $i=\{0,1,2,\ldots\}$ and let d_v and d_u are degree of edges when $\alpha=1$ then general Randic polynomial is given by

$$R(G,x) = \sum_{uv\in E(G)} (56(2^i)-40)x^{(4)} + \sum_{uv\in E(G)} (36(2^i)-36)\,x^{(6)}$$
$$+ \sum_{uv\in E(G)} (48(2^i)-40)x^{(9)} + \sum_{uv\in E(G)} (4)x^{(12)}$$

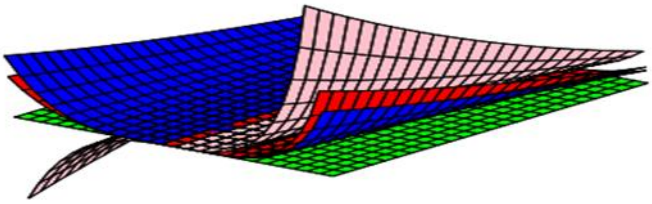

Fig 4. Comparison between 3rd Zagreb (green), sum conn(blue), Randic (red),and harmonic(pink) polynomials.

2. **Second Result**:

In this part, we will present a new formulation for redefining the general Zagreb polynomial, general sum-connectivity polynomials, and the Randic polynomial . New formula for redefine will depends on polyphenylene dendrimer has three growth stages (see Fig 2-3).

In (Fig. 2-3) the stage i= 0 (the core of polyphenlyene dendrimer) there are three types of edges with degree (2,2), (2,3) and (3,3) when $i \geq 0$ by using foems in table6.

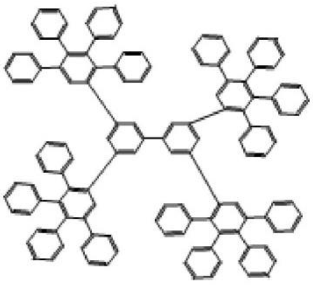

Fig 2. polyphenylene dendrimer has two growth stages $D_2\,[1]$

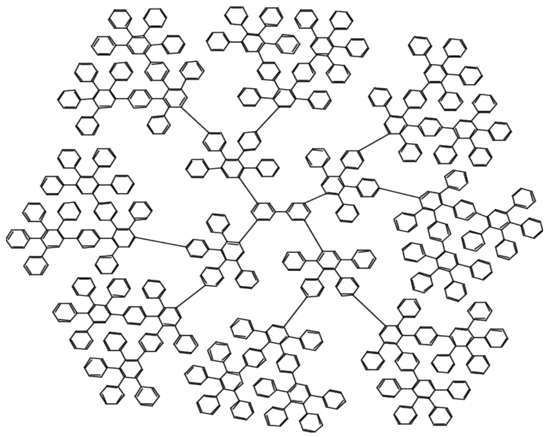

Figure 3. polyphenylene dendrimer has two growth stages $D_2\,[3]$

stage / degree	i=0	i=1	i=2
d(2,2)	8	64	176
d(2,3)	4	52	141
d(3,3)	1	37	109

Table 3 : stages of growth with degree of edge

$d_v, d_u \in E(G)$	No. of edges
d(2,2)	$(56(2^i)-48)$
d(2,3)	$(48(2^i)-44)$
d(3,3)	$(36(2^i)-35)$

Table 4: forms to calculate number of edges in every degree.

Theorem 1 : polyphenylene dendrimer have i stages of of growth when $i \geq 0$ and let deg(u) and deg(v) are the vertex degrees of u and v, respectively, then redefine third Zagreb polynomial

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$$\operatorname{Re} Z_3(G,x) = \sum_{vu\in E(G)} (56(2^i)-48)x^{(16)} + \sum_{vu\in E(G)} (48(2^i)-44)x^{(30)} + \sum_{vu\in E(G)} (36(2^i)-35)\, x^{(54)}$$

Proof : By using definition third Zagreb polynomial

$$\operatorname{Re} Z_3(G,x) = \sum_{vu\in E(G)} x^{(dv\times du)(dv+du)}$$

$$= \sum_{vu\in E(G)} (2+2)(2\times 2) + \sum_{vu\in E(G)} (2+3)(2\times 3) + \sum_{vu\in E(G)} (3+3)(3\times 3)$$

$$= \sum_{vu\in E(G)} (56(2^i)-48)x^{(16)} + \sum_{vu\in E(G)} (48(2^i)-44)x^{(30)} + \sum_{vu\in E(G)} (36(2^i)-35)\, x^{(54)}$$

Theorem 2 : let $D[i]$ polyphenylene dendrimer have i stages of of growth when $i \geq 0$ and let deg(u) and deg(v) are the vertex degrees of u and v, respectively, when α is integer positive number $\alpha \neq 0$,then redefine general sum-connectivity polynomial

$$\chi_\alpha(G,x) = \sum_{vu\in E(G)} (56(2^i)-48)x^{(4)^\alpha} + \sum_{vu\in E(G)} (36(2^i)-35)\, x^{(5)^\alpha} + \sum_{vu\in E(G)} (48(2^i)-44)x^{(6)^\alpha}$$

Proof : by using definition general sum-connectivity polynomial $\chi_\alpha(G,x) = \sum_{vu\in E(G)} x^{[dv+du]^\alpha}$

$$= \sum_{uv\in E(G)} (2+2)^\alpha + \sum_{uv\in E(G)} (2+3)^\alpha + \sum_{uv\in E(G)} (3+3)^\alpha$$

$$= \sum_{vu\in E(G)} (56(2^i)-48)x^{(4)^\alpha} + \sum_{vu\in E(G)} (36(2^i)-35)\, x^{(5)^\alpha} + \sum_{vu\in E(G)} (48(2^i)-44)x^{(6)^\alpha}$$

Theorem 3: let $D[i]$ polyphenylene dendrimer have i stages of of growth when $i \geq 0$ and let deg(u) and deg(v) are the vertex degrees of u and v, respectively, when α is positive integer number and $\alpha \neq 0$, then redefine general Randic polynomial

$$R_\alpha(G,x) = (56(2^i)-48)x^{(4)^\alpha} + (36(2^i)-35)\, x^{(6)^\alpha} + (48(2^i)-44)x^{(9)^\alpha}$$

Proof : by using general Randic polynomial

$$R_\alpha(G,x) = \sum_{vu\in E(G)} x^{[dv\times du]^\alpha}$$

$$= \sum_{vu\in E(G)} (2\times 2)^\alpha + \sum_{vu\in E(G)} (2\times 3)^\alpha + \sum_{vu\in E(G)} (3\times 3)^\alpha$$

$$= \sum_{vu\in E(G)} (56(2^n)-48)x^{(4)^\alpha} + \sum_{vu\in E(G)} (48(2^n)-44)\, x^{(6)^\alpha} + \sum_{vu\in E(G)} (36(2^n)-35)x^{(9)^\alpha} .$$

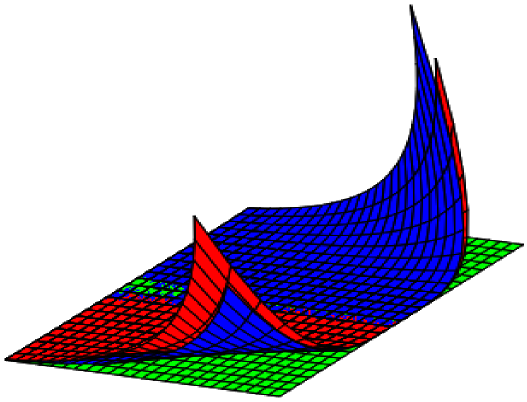

Fig 5. Comparison between 3rd Zagreb (green), sum conn(blue), and Randic (red) plolynomials .

5.*Conclution:*

In this paper the The third Zagreb polynomial, general sum-connectivity polynomial, and general Randic polynomial are redefined and computed depends on the **two of** mathematical structures of some families of denrimers **.** In the future, the scope of research can be used with two positive integers on the same chemical structure or with another structure.

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