https://doi.org/10.33472/AFJBS.6.Si3.2024.2288-2300

African Journal of Biological Sciences

Journal homepage: http://www.afjbs.com

Research Paper Open Access

On some Neighborhood Degree – based Topological Indices of Benzopoly perinaphthalene using Direct and NM – Polynomial in Heinz-Quarter Mean Labeling

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Article Info

Volume 6, Issue Si3, June 2024

Received: 18 April 2024

Accepted: 26 May 2024

Published: 20 June 2024

doi: 10.33472/AFJBS.6.Si3.2024.2288-2300

ABSTRACT:

A topological index is a numeric quantity associated with a graph which characterize the topology of graph and is invariant under graph automorphism. In chemical graph theory, various physical properties, chemical reactivity, and biological activities of a molecule are strongly connected to its graphical structure. The M- Polynomial gives degree based topological indices. In this work, some neighborhood degree based topological indices of benzopoly perinaphthalene monoradical series are investigated through NM – Polynomial and direct method. Also compute Heinz-quarter mean labeling of benzopoly perinaphthalene monoradical series structure.

Keywords: Topological index, M – Polynomial, NM – Polynomial, Heinz-Quarter Mean Labeling Benzopoly perinaphthalene monoradical series.

1. Introduction

In chemical graph theory, a molecular graph is a simple graph in which atoms and chemical bonds are represented by vertices and edges respect. A topological index is a function from the collection of graphs to the set of real numbers that describe the topology of the graph and are used in QSPR / QSAR analysis. They play an important role in the study of QSPR/QSAR. In theoretical chemistry, molecular structure descriptors are used for modelling physico-chemical, pharmacological, toxicological, biological and other properties of chemical compounds.

We have two important types of topological Indices.

The first type is degree based topological Indices and the second type is distance – based topological indices. Some more polynomials in the area of chemical graph theory are the clar covering polynomial , PI polynomial , Schultz Polynomial , theta polynomial , Tutte Polynomial etc. The Hosoya Polynomial plays the key role in the distance – based topological indices. In degree based topological Indices [1] the M – Polynomial has a significant role to compute the Indices. It was introduced by Deutsch and Klavzar in 2015 [2].

The M – Polynomial of G is defined as

$$M(G; x, y) = \sum_{\delta \le i \le j \le \Delta} mij(G) x^i y^j$$

Where, $\delta = min\{d_v; v \in V(G)\}$

$\Delta = max\{d_v; v \in V(G)\}$

and $mij(G)$ is the number of edges $uv \in E(G)$, such that $\{d_v, d_u\} = \{i, j\}$. Neighborhood degree – based indices [3– 10] were studied by several authors. To compute these indices very easier, we introduce a polynomial named as Neighborhood M – Polynomial , whose role for neighborhood degree – based indices is parallel to the role of M – Polynomial for degree – based Indices.

The neighborhood M – Polynomial of a graph G is defined as

$$NM(G; x, y) = \sum_{i \le j} mi, j\, x^i y^j$$

Where mi, j is the total number of edges $uv \in E(G)$.

In this paper, we investigate some neighborhood degree based topological indices of Benzoperinaphthalene monoradical series using NM – Polynomial and direct method.

Now we describe some Neighborhood degree – based topological indices.

1. Modal et al., introduced the neighborhood forgotten topological Index in 2019 [11].

$$F_N^*(G) = \sum_{xy \in E(G)} \left(\delta x^2 + \delta y^2\right)$$

2. Verma and Mondal defined the neighborhood harmonic index in 2019 [12].

$$NH(G) = \sum_{xy \in E(G)} \frac{2}{\delta x + \delta y}$$

3. Mondal et al. introduced the neighborhood second zagrab index in 2019 [11].

$$M_2^*(G) = \sum_{xy\in E(G)} \delta x\, \delta y$$

4. Verma and Mondal defined the neighborhood inverse sum index in 2019 [12].

$$M_2^*(G) = \sum_{xy\in E(G)} \delta x\, \delta y$$

5. Verma and Mondal defined the neighborhood general Randic index in 2019 [12].

$$N\mathrm{R}_\alpha(G) = \sum_{xy\in E(G)} (\delta x\, \delta y)^\alpha$$

6. Hosamani proposed the sankruti index in 2020 [13].

$$S(G) = \sum_{xy\in E(G)} \left(\frac{\delta x\, \delta y}{\delta x + \delta y - 2}\right)^3$$

7. Verma and Mondal defined the neighborhood second modified Zagreb index in 2019 [12].

$$M_2^{nm}(G) = \sum_{xy\in E(G)} \frac{1}{\delta x\, \delta y}$$

8. Ghorbani and Hosseinzadeh defined the third version of the Zagreb index in 2013 [14].

$$M_1'(G) = \sum_{xy\in E(G)} (\delta x + \delta y)$$

9. Ghorbani and Hosseinzadeh present in 2010 the 4th atom bond connectivity index as [15].

$$ABC_4(G) = \sum_{xy\in E(G)} \sqrt{\frac{\delta x + \delta y - 2}{\delta x\, .\, \delta y}}$$

Heinz-Quarter Mean Labeling:

A graph G with p vertices and q edges is a Heinz Quarter mean graph if there is an injective function f from the vertices of G to {1,2,3,……….q+1} such that when each edge uv is labeled with

f(e= uv)= $\left\lceil \frac{\sqrt[4]{f(u)f(v)}\left(\sqrt{f(u)}+\sqrt{f(v)}\right)}{2} \right\rceil$ or f(e=uv) = $\left\lfloor \frac{\sqrt[4]{f(u)f(v)}\left(\sqrt{f(u)}+\sqrt{f(v)}\right)}{2} \right\rfloor$

Then the resulting edge labels are distinct.

Benzopolyperinapthalene graph

Figure -1 represents a homologous series of closely peri-condensed monoradical benzenoids consecutively builtup two rings at a time by the C_6H_2 aufbau unit. Molecular graph series of figure-1 is benzopyrene($C_{19}H_{11}$). The monoradical series of benzopolyperinaphthalene be C_{3n+4} (since number of carbon atoms in this series is $3n + 4$, $n \geq 5$for odd n). We develop the edges of the form$E(5,5)$,$E(5,7)$,$E(5,4)$,$E(7,6)$,$E(7,9)$,$E(9,9)$ are shown in the following Table 1.

Graphs	**Edge of the form $E(d_u, d_v)$**	**Sum of edges**
C_{19}	E (5, 5), E (5, 7), E (5, 4), E (7, 6), E (7, 9), E (9, 9)	2, 8, 4, 2, 5, 2
C_{25}	E (5, 5), E (5, 7), E (5, 4), E (7, 6), E (7, 9), E (9, 9)	2, 8, 4, 6, 7, 4
C_{31}	E (5, 5), E (5, 7), E (5, 4), E (7, 6), E (7, 9), E (9, 9)	2, 8, 4, 10, 9, 6

The relations of some neighborhood degree – based topological indices with the NM – Polynomial are shown in table 2.

Topological index	**f (x, y)**	**Derivation from NM (G)**
M_1'	$x + y$	$D_x + D_y(NM(G))\|_{x=y=1}$
M_2^*	Xy	$D_x\,D_y(NM(G))\|_{x=y=1}$
F_N^*	$x^2 + y^2$	$D_x^{\,2} + D_y^{\,2}(NM(G))\|_{x=y=1}$
M_2^{nm}	$\frac{1}{xy}$	$S_x\,S_y(NM(G))\|_{x=y=1}$
NR_α	$(xy)^\alpha$	$D_x^{\,\alpha} D_y^{\,\varepsilon}(NM(G))\|_{x=y=1}$
ND_3	$xy\,(x + y)$	$D_x + D_y\,(D_x\,D_y)(NM(G))\|_{x=y=1}$
ND_5	$\frac{x^2 + y^2}{xy}$	$D_x\,S_y + S_x\,D_y(NM(G))\|_{x=y=1}$
NH	$\frac{2}{x+y}$	$2S_x\,J\,(NM(G))\|_{x=y=1}$
NI	$\frac{xy}{x+y}$	$S_x\,J\,D_x\,D_y(NM(G))\|_{x=y=1}$
S	$\frac{xy}{(x+y-2)^3}$	$S_x^{\,3}\,Q_{-2}\,J\,D_x^{\,3}\,D_y^{\,3}(NM(G))\|_{x=y=1}$

Where,

$$D_x(f(x,y)) = x\frac{\partial(f(x,y))}{\partial x},\ D_y(f(x,y)) = y\frac{\partial(f(x,y))}{\partial y},\ S_x(f(x,y)) = \int_0^x \frac{f(t,y)}{t}\,dt$$

$$Sy(f(x,y)) = \int_0^y \frac{f(x,t)}{t}\,dt,\ J(f(x,y)) = f(x,x),\ Q_\alpha(f(x,y)) = x^\alpha f(x,y)$$

2. Main Results

Theorem: 2.1

Benzopolyperinapthalene monoradical series structure is Heinz-Quarter mean labeling.

Proof:

Let G be a Benzopolyperinapthalene monoradical series structure C_{3n+4} , n≥ 5

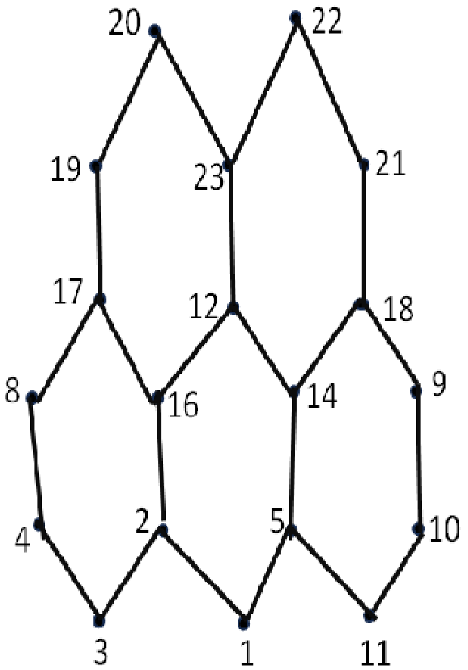

Figure-1 Benzopyrene $C_{3(5)+4} = C_{19}$ (five rings)

Let G = C_{3n+4} , if n =5

Let its vertex set V(G) =$\{u_i , i = 1,2 \dots \dots \dots 19\}$ and edge set E(G) =$\{e_{i,} \ i = 1,2, \dots \dots .23\}$

Define a function f:V(G)→ $\{1,2,3, \dots \dots q + 1\}$ by

$f(u_i)$ = i, 1≤ $i \leq 5$, $f(u_i) = i + 2$, i=6,7,8,9,10 ,

$f(u_i) = i + 3 \,, i = 11,$ $f(u_i) = i + 4, i = 12,13,14,15,16,17,18,19$

We get distinct edge labels as,

$f(u_1u_2) = 1, f(u_2u_3) = 3, f(u_1u_5) = 2, f(u_3u_4) = 4, f(u_4u_6) = 5,$

$f(u_2u_{12}) = 6, f(u_5u_9) = 7, f(u_5u_{11}) = 8, f(u_7u_8) = 9, f(u_8u_9) = 10$

$f(u_6u_{13}) = 11, f(u_7u_{14}) = 12, f(u_{10}u_{11}) = 13, f(u_{10}u_{12}) = 14,$

$\mathrm{f}(u_{11}u_{14}) = 15, f(u_{12}u_{19}) = 16, f(u_{12}u_{13}) = 17, f(u_{13}u_{15}) = 18, f(u_{17}u_{14}) = 19$

$f(u_{15}u_{16}) = 20, f(u_{17}u_{18}) = 21, f(u_{16}u_{19}) = 22, f(u_{18}u_{19}) = 23$

Hence G is a Heinz-Quarter Mean Labeling.

Topological indices of Benzopolyperinapthalene monoradical series

In this section, we compute some neighborhood degree based topological indices by direct formulae.

Theorem: 2.2

Let *G* be a Benzopolyperinaphthalene monoradical series for *n* ≥ 5 where the structure graph satisfies Heinz-Quarter mean labeling then,

i) $F_N^*(G)$ = 462 n – 310

ii) NH (G) = 1.058 + 0.544 n

iii) M_2^* = 228 n – 169

iv) NI = 14.9 n – 2.124

v) NR_α (G) = $2(25)^\alpha + 8(35)^\alpha + 4(20)^\alpha - 8(42)^\alpha + 3(81)^\alpha + n\,[2.(42)^\alpha + (63)^\alpha + (81)^\alpha]$

vi) $S(G)$ = 332.19816 n – 670.672204

vii) $M_2^{nm}(G) = \frac{3984}{14175} + \frac{301}{3969}n$

viii) $M_1'(G)$ = 60 n – 6

ix) $ABC_4(G) = \left(\frac{4\sqrt{2}}{5} + 8\sqrt{\frac{2}{7}} + 2\sqrt{\frac{7}{5}} - 8\sqrt{\frac{11}{42}} - \frac{12}{9}\right) + n\left(2\sqrt{\frac{11}{42}} + \sqrt{\frac{2}{9}} + \frac{4}{9}\right)$

Proof:

Let G be a Benzopolyperinaphthalene monoradical series structure

Then

i) Neighborhood forgotten topological index

$$F_N^*(G) = \sum_{xy\in E(G)} \left(\delta x^2 + \delta y^2\right)$$

$$= (5^2 + 5^2)(2) + (5^2+7^2)(8) + (5^2 + 4^2)(4) + (7^2 + 6^2)(2n - 8) + (7^2 + 9^2)(n) + (9^2 + 9^2)(n - 3)$$

$$F_N^*(G) = 462\,n - 310$$

ii) Neighborhood harmonic index

$$NH(G) = \sum_{xy\in E(G)} \frac{2}{\delta x + \delta y}$$

$$= \frac{2}{5+5}(2) + \frac{2}{5+7}(8) + \frac{2}{5+4}(4) + \frac{2}{7+6}(2n-8) + \frac{2}{7+9}(n) + \frac{2}{9+9}(n-3)$$

$$= \frac{2}{10}(2) + \frac{2}{12}(8) + \frac{2}{9}(4) + \frac{2}{13}(2n-8) + \frac{2}{16}(n) + \frac{2}{18}(n-3)$$

$$NH(G) = 1.058 + 0.544\,n$$

iii) Neighborhood 2nd Zagreb index

$$M_2^* = \sum_{xy\in E(G)} \delta x\,\delta y$$

$= (5 \times 5)(2) + (5 \times 7)(8) + (5 \times 4)(4) + (7 \times 6)(2n - 8) + (7 \times 9)\, n + (9 \times 9)(n - 3)$

$= -169 + 228\, n$

$M_2^* = 228\, n - 169$

iv) Neighborhood inverse sum index

$$NI = \sum_{xy \in E(G)} \frac{\delta x\, \delta y}{\delta x + \delta y}$$

$$= \frac{5\times5}{5+5}(2) + \frac{5\times7}{5+7}(8) + \frac{5\times4}{5+4}(4) + \frac{7\times6}{7+6}(2n-8) + \frac{7\times9}{7+9}(n) + \frac{9\times9}{9+9}(n-3)$$

$NI = 14.9\, n - 2.124$

v) Neighborhood randix index

$$NR_\alpha(G) = \sum_{xy \in E(G)} (\delta x\, \delta y)^\alpha$$

$= (5\times5)^\alpha\ (2) + (5\times7)^\alpha\ (8) + (5\times4)^\alpha\ (4) - (7\times6)^\alpha\ (2n - 8) + (7\times9)^\alpha\ (n) + (9\times9)^\alpha\ (n - 3)$

$= 2(25)^\alpha + 8(35)^\alpha + 4(20)^\alpha - (2n - 8)\ (7\times6)^\alpha + (7\times9)^\alpha\ (n) + (9\times9)^\alpha\ (n - 3)$

$NR_\alpha(G) = 2(25)^\alpha + 8(35)^\alpha + 4(20)^\alpha - 8(42)^\alpha + 3(81)^\alpha + n\,[2.(42)^\alpha + (63)^\alpha + (81)^\alpha]$

vi) Sanskruti index

$$S(G) = \sum_{xy \in E(G)} \left(\frac{\delta x\, \delta y}{\delta x + \delta y - 2} \right)^3$$

$$= 2\left(\frac{5\times5}{5+5-2}\right)^3 + 8\left(\frac{5\times7}{5+7-2}\right)^3 + 4\left(\frac{5\times4}{5+4-2}\right)^3 + \left(\frac{7\times6}{7+6-2}\right)^3 (2n-8) + \left(\frac{7\times9}{7+9-2}\right)^3 (n) + \left(\frac{9\times9}{9+9-2}\right)^3 (n-3)$$

$$= 2\left(\frac{25}{8}\right)^3 + 8\left(\frac{35}{33}\right)^3 + 4\left(\frac{20}{7}\right)^3 + \left(\frac{42}{11}\right)^3 (2n-8) + \left(\frac{63}{14}\right)^3 (n) + \left(\frac{81}{16}\right)^3 (n-3)$$

$S(G) = 332.19816\, n - 670.672204$

vii) The neighborhood second modified zagreb index

$$M_2^{nm}(G) = \sum_{xy\in E(G)} \frac{1}{\delta x\, \delta y}$$

$$= \frac{1}{5\times5}(2)+\frac{1}{5\times7}(8)+\frac{1}{5\times4}(4)+\frac{1}{7\times6}(2n-8)+\frac{1}{7\times9}(n)+\frac{1}{9\times9}(n-3)$$

$$= \frac{1}{25}(2)+\frac{1}{35}(8)+\frac{1}{20}(4)+\frac{2n}{42}-\frac{8}{42}+\frac{n}{63}+\frac{n}{81}-\frac{3}{81}$$

$$= \frac{3984}{14175}+\frac{301}{3969}n$$

viii) Third version of zagreb index

$$M_1'(G) = \sum_{xy\in E(G)} (\delta x + \delta y)$$

= (5 + 5) 2 + (5 + 7) (8) + (5 + 4) (4) + (7 + 6) (2n – 8) + (7 + 9) n + (9 + 9)

$$M_1'(G) = 60\,n - 6$$

ix) Fourth Atom – Bond connectivity index

$$ABC_4(G) = \sum_{xy\in E(G)} \sqrt{\frac{\delta x + \delta y \text{ - } 2}{\delta x\,.\delta y}}$$

$$= \sqrt{\frac{5+5-2}{5\times5}}(2)+\sqrt{\frac{5+7-2}{5\times7}}(8)+\sqrt{\frac{5+4-2}{5\times4}}(4)++\sqrt{\frac{7+6-2}{7\times6}}(2n-8)+ \sqrt{\frac{7+9-2}{7\times9}}(n)+\sqrt{\frac{9+9-2}{9\times9}}(n-3)$$

$$= \left(\frac{4\sqrt{2}}{5}+8\sqrt{\frac{2}{7}}+2\sqrt{\frac{7}{5}}-8\sqrt{\frac{11}{42}}-\frac{12}{9}\right)+\left(2n\sqrt{\frac{11}{42}}+\sqrt{\frac{2}{9}}n+\frac{4}{9}n\right)$$

3. NM – Polynomial of Benzopolyperinaphthalene Monoradical Series

Theorem 3.1

Let G be a Monoradical series of benzopolyperinaphthalene C_{3n+4}, $n \geq 5$ then the NM – Polynomial of G is

NM (G) = $2x^5y^5 + 8x^5y^7 + 4x^5y^4 + (2n-8)x^7y^6 + nx^7y^9 + (n-3)x^9y^9$

Proof

The graph G has C_{3n+4}, $n \geq 5$ vertices and $4n + 3$ edges.

$|E(5, 5)| = |\{uv \in E(G), \delta u = 5, \delta v = 5\}| = 2 = m(5, 5)$
$|E(5, 7)| = |\{uv \in E(G), \delta u = 5, \delta v = 7\}| = 8 = m(5, 7)$

$|E(5, 4)| = |\{uv \in E(G), \delta u = 5, \delta v = 4\}| = 4 = m(5, 4)$

$|E(7, 6)| = |\{uv \in E(G), \delta u = 7, \delta v = 6\}| = 2n - 8 = m(7, 6)$

$|E(7, 9)| = |\{uv \in E(G), \delta u = 7, \delta v = 9\}| = n = m(7, 9)$

$|E(9, 9)| = |\{uv \in E(G), \delta u = 9, \delta v = 9\}| = (n - 3) = m(9, 9)$

From the definition, the NM – Polynomial of G is obtained below.

$$NM(G) = \sum_{i \leq j} mi, j\, x^i y^j$$

$$= m(5, 5)\, x^5y^5 + m(5, 7)\, x^5y^7 + m(5, 4)\, x^5y^4 + m(7, 6)\, x^7y^6 + m(7, 9)\, x^7y^9 + m(9, 9)\, x^9y^9$$

$$= 2\, x^5y^5 + 8\, x^5y^7 + 4\, x^5y^4 + (2n - 8)\, x^7y^6 + n\, x^7y^9 + (n - 3)\, x^9y^9$$

This completes the proof.

Topological Indices of C_{3n+4}, $n \geq 5$ via NM – polynomial.

In this section, we compute some topological indices via NM – polynomial.

Theorem: 3.2

Let G be a C_{3n+4}, ($n \geq 5$) and NM $[G: x, y] = 2\, x^5y^5 + 8\, x^5y^7 + 4\, x^5y^4 + (2n - 8)\, x^7y^6 + n\, x^7y^9 + (n - 3)\, x^9y^9$ then,

i) $F_N^*(G) = 462\, n - 310$
ii) $NH(G) = 1.058 + 0.544\, n$
iii) $M_2^*(G) = 228\, n - 169$
iv) $NI(G) = 96.438 + 7.450\, n$
v) $NR_\alpha(G) = 50^\alpha + 280^\alpha + 80^\alpha - (42)^\alpha (2n - 8) + n (63)^\alpha + (81)^\alpha (n - 3)$
vi) $S(G) = 332.197\, n - 333.463$
vii) $M_2^{nm}(G) = 0.076\, n + 0.282$
viii) $M_1'(G) = 60\, n - 6$
ix) $ABC_4(G) = \left(\frac{4\sqrt{2}}{5} + 8\sqrt{\frac{2}{7}} + 2\sqrt{\frac{7}{5}} - 8\sqrt{\frac{11}{42}} - \frac{12}{9}\right) + n\left(2\sqrt{\frac{11}{42}} + \sqrt{\frac{2}{9}} + \frac{4}{9}\right)$

Proof

NM (G) = $2\,x^5y^5 + 8\,x^5y^7 + 4\,x^5y^4 + (2n-8)\,x^7y^6 + n\,x^7y^9 + (n-3)\,x^9y^9$

i) $(Dx^2 + Dy^2)\,f(x, y) = 2(50)\,x^5y^5 + 8(74)\,x^5y^7 + 4(41)\,x^5y^4 + (2n-8)\,(85)\,x^7y^6 + n(130)\,x^7y^9 + (n-3)\,(162)\,x^9y^9$

$= 100\,x^5y^5 + 592\,x^5y^7 + 164\,x^5y^4 + 85(2n-8)\,x^7y^6 + 130\,n\,x^7y^9 + 162\,(n-3)\,x^9y^9$

$= 462\,n - 310$

ii) $2(S_x\,J)\,f(x, y) = \frac{2\times 2\,x^{10}}{10} + \frac{2\times 8\,x^{12}}{12} + \frac{2\times 4\,x^{9}}{9} + \frac{2(2n-8)x^{13}}{13} + \frac{2\,nx^{16}}{16} + \frac{2(n-3)x^{18}}{18}$

$2(S_x\,J)$ NM $(G)_{x=y=1}$

$$= \frac{4}{10} + \frac{16}{12} + \frac{8}{9} + \frac{2(2n-8)}{13} + \frac{2nx^{16}}{16} + \frac{2\,(n-3)x^{18}}{18}$$

$NH\,(G) = 1.058 + 0.544\,n$

iii) Neighborhood inverse sum index

$(Dx\,Dy)\,f(x, y) = 50\,x^5y^5 + 8(35)\,x^5y^7 + 4(20)\,x^5y^4 + (2n-8)\,42\,x^7y^6 + 63\,n\,x^7y^9 + 81\,(n-3)\,x^9y^9$

$(Dx\,Dy)$ NM $(G)_{x=y=1}$

$= 50 + 280 + 80 + 42\,(2n-8) + 63\,n + 81\,(n-3)$

$M_2^* = 228\,n - 169$

iv) $(S_x\,J\,Dx\,Dy)\,f(x, y) = \frac{50\times 2\,x^{10}}{10\times 2} + \frac{280\,x^{12}}{12}\times\frac{8}{2} + \frac{80\,x^{9}}{9}\times\frac{4}{2} + \frac{42(2n-8)x^{13}}{13\times 2} + \frac{63\,nx^{16}}{16\times 2} + \frac{81(n-3)x^{18}}{18\times 2}$

$$= 5x^{10} + \frac{280\,x^{12}}{3} + \frac{160\,x^{9}}{9} + \frac{21(2n-8)x^{13}}{13} + \frac{63nx^{16}}{32} + \frac{9(n-3)x^{18}}{4}$$

$NI = Sx\,J\,Dx\,Dy$ NM $(G)_{x=y=1}$

$$= 5 + \frac{280}{3} + \frac{160}{9} + \frac{21(2n-8)}{13} + \frac{63n}{32} + \frac{9(n-3)}{4}$$

$NI = 96.438 + 7.450\,n$

v) Randic index

$(Dx\ Dy)\, f(x, y) = 50^{\alpha} x^5y^5 + 280^{\alpha} x^5y^7 + 80^{\alpha} x^5y^4 + 42^{\alpha} (2n - 8) x^7y^6 + 63^{\alpha} n\, x^7y^9 + 81^{\alpha} (n-3)\, x^9y^9$

$NR_{\alpha}(G) = (Dx^{\alpha}\ Dy^{\alpha})\ NM\ (G)_{x=y=1}$

$= 50^{\alpha} + 280^{\alpha} + 80^{\alpha} - 42^{\alpha} (2n - 8) + n\, 63^{\alpha} + 81^{\alpha} (n - 3)$

vi) Sanskruti index

$Sx^3Qx_{(-2)}\ J\ Dx^3Dy^3\ NM\ [G: x, y]_{x=y=1}$

$Dx^3Dy^3 = 31250\ x^5y^5 + 346750\ x^5y^7 + 32000\ x^5y^4 + 74088\ (2n - 8)\ x^7y^6 + 250047\ n\ x^7y^9 + 531441\ (n-3)\ x^9y^9$

$J\ Dx^3Dy^3\ NM\ [G; x, y] = 31250\ x^{10} + 346750\ x^{12} + 32000\ x^9 + 74088\ (2n - 8)\ x^{13} + 250047\ n\ x^{16} + 531441\ (n-3)\ x^{18}$

$Qx_{(-2)}\ J\ Dx^3Dy^3 = 31250\ x^8 + 346750\ x^{10} + 32000\ x^7 + 74088\ (2n - 8)\ x^{11} + 250047\ n\ x^{14} + 531441\ (n-3)\ x^{16}$

$$Sx^3Qx_{(-2)}\ J\ Dx^3Dy^3 = \frac{31250}{512}x^8 + \frac{346750}{1000}x^{10} + \frac{32000}{343}x^7 + \frac{74088}{1331}(2n - 8)x^{11} + \frac{250047}{2744}nx^{14} + \frac{531441}{4096}(n - 3)x^{16}$$

$[Sx^3Qx_{(-2)}\ J\ Dx^3Dy^3]_{x=1} \Rightarrow 61.035 + 346.750 + 93.294 + 55.663\ (2n - 8) + 91.125\ n + 129.746\ (n - 3)$

$S(G) = 332.197\ n - 333.463$

vii) The neighborhood second modified zagreb index

$$M_2^{nm}(G) = \sum_{xy \in E(G)} \frac{1}{\delta u\ \delta v}$$

$(Sx\ Sy)\ (NM(G))_{x=y=1}$

$$Sx\ Sy = \frac{2x^5y^5}{25} + \frac{8x^5y^7}{35} + \frac{4x^5y^4}{20} + \frac{(2n-8)x^7y^6}{42} + \frac{n\,x^7y^9}{63} + \frac{(n-3)x^9y^9}{81}$$

$(Sx\ Sy)\ (NM;\ G)_{x=y=1}$

$$= \frac{2}{25} + \frac{8}{35} + \frac{4}{20} + \frac{2n - 8}{42} + \frac{n}{63} + \frac{n - 3}{81}$$

$M_2^{nm}(G) = 0.076\ n + 0.282$

viii) $(D_x D_y)(NM(G))_{x=y=1}$

$$D_x D_y = 10(2x^5y^5) + 12(8x^5y^7) + 9(4x^5y^4) + 13(2n-8)x^7y^6 + 63(n x^7y^9) + 18((n-3)x^9y^9)$$

$(D_x D_y)(NM(G))_{x=y=1}$

$$\Rightarrow 20 + 96 + 36 + 13(2n-8) + 16n + 18(n-3)$$

$$M_1'(G) = 60n - 6$$

ix) $D_x^{1/2} Q_{x(-2)} J S_x^{1/2} S_y^{1/2} (NM(G))_{x=y=1}$

$$S_y^{1/2} = \frac{2x^5y^5}{\sqrt{5}} + \frac{8x^5y^7}{\sqrt{7}} + \frac{4x^5y^4}{2} + \frac{(2n-8)x^7y^6}{\sqrt{6}} + \frac{n x^7y^9}{\sqrt{9}} + \frac{(n-3)x^9y^9}{\sqrt{9}}$$

$$S_x^{1/2} S_y^{1/2} = \frac{2x^5y^5}{\sqrt{5}\sqrt{5}} + \frac{8x^5y^7}{\sqrt{7}\sqrt{5}} + \frac{4x^5y^4}{2\sqrt{5}} + \frac{(2n-8)x^7y^6}{\sqrt{6}\sqrt{7}} + \frac{n x^7y^9}{\sqrt{9}\sqrt{7}} + \frac{(n-3)x^9y^9}{\sqrt{9}\sqrt{9}}$$

$$J S_x^{1/2} S_y^{1/2} = \frac{2}{5}x^{10} + \frac{8}{\sqrt{35}}x^{12} + \frac{2}{\sqrt{5}}x^9 + \frac{(2n-8)x^{13}}{\sqrt{42}} + \frac{n x^{16}}{\sqrt{63}} + \frac{(n-3)x^{18}}{9}$$

$$Q_{x(-2)} J S_x^{1/2} S_y^{1/2} = \frac{2}{5}x^8 + \frac{8}{\sqrt{35}}x^{10} + \frac{2}{\sqrt{5}}x^7 + \frac{(2n-8)}{\sqrt{42}}x^{11} + \frac{n}{\sqrt{63}}x^{14} + \frac{(n-3)}{9}x^{16}$$

$$D_x^{1/2} Q_{x(-2)} J S_x^{1/2} S_y^{1/2} = \frac{2}{5}\sqrt{8}x^8 + \frac{8}{\sqrt{35}}\sqrt{10}x^{10} + \frac{2}{\sqrt{5}}\sqrt{7}x^7 + \frac{(2n-8)}{\sqrt{42}}\sqrt{11}\,x^{11} + \frac{n}{\sqrt{63}}\sqrt{14}\,x^{14} + \frac{(n-3)}{9}\sqrt{16}x^{16}$$

$$= \frac{4\sqrt{2}}{5} + 8\sqrt{\frac{2}{7}} + 2\sqrt{\frac{7}{5}} + 2n\sqrt{\frac{11}{42}} - 8\sqrt{\frac{11}{42}} + n\sqrt{\frac{2}{9}} + \frac{4n}{9} - \frac{12}{9}$$

4. Conclusion

In this article, we consider the monoradical series of benzopolyperinaphthalene structure. We derived the edge partitions of the molecular graph with respect to the neighborhood degree of the vertex, then computed the different molecular descriptors based on the neighborhood degree sum of nodes via NM-Polynomial. All types of neighborhood degree sum based indices are considered in the paper. Considered topological indices are useful molecular descriptors in the area of chemical graph theory to establish structure-property/structure activity relationship. Thus the results give different properties and activities of the considered structures through mathematical formulations. This Heinz quarter mean labeling is used in circuit design, communication network, coding theory and astronomy.

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