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Characterizations of Physico-Chemical Properties for Non-kekulean benzenoid hydrocarbon Using M-polynomial

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Abstract

In the last few decades, nanomaterials have found widespread application in a variety of industries, including electronics, building, food processing, pharmaceuticals, cosmetics, and aviation. These nanoparticles could enhance medical therapy, diagnostics, and preventive methods. These days, drug delivery and cellular imaging are two applications of benzonoid systems in biotechnology and medicine. Non-kekulean benzoid hydrocarbons offer a great way to evaluate the structural characteristics of their series due to their regular structures. This work involves the computation of several degree-based topological indices that are helpful in figuring out how reactive the associated molecules are. In particular, we found these calculations to be helpful in examining the thermodynamic parameter entropy, which could be important for successfully reworking the structure of non-kekulean benzoid hydrocarbons.

Keywords: Non-kekulean Benzoid hydrocarbons, topological indices, M-polynomial.

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1|Introduction

Graph theory is the branch of mathematics deal with the study of graph, which are mathematical structures used to model pairwise relations between objects. The study of graph theory officially began in 1735 [1]. Graph theory is frequently used to investigate networks, models, and circuits. Schedules and routes might be as diverse as vast collection and linen delivery. The fields of computing, biology, chemistry, physics, electrical, civil engineering, communication science, operations research, architecture, genetics, sociology, psychology, anthropology, linguistics, and economics have all found major applications for this theory. It is known as "mathematical chemistry" since it is mostly employed in applied chemistry. Vertex and edges are the basic building blocks of graph theory. Vertex V is simply defined as a figure's node and edge E is the connection between two vertices. In graph theory, the terms "QSAR" and "QSPR" refer to a compound's structure or formula [2, 3]. Since Corwin's initial work, quantitatives structure-activity and structure-property relationships (QSAR/QSPR) have been established and applied, as is currently known.

The melting and boiling points in homologous series predicted by Mills is probably the first QSPR to come to mind. The ability of QSAR or QSPR to predict the endpoint values of compounds that were not used to build correlations i.e., chemicals that were not utilized in the learning process, is what gives these techniques their predictive strength. The two primary methods for assessing predictability are internal cross validation and external validation using a set of test compounds. For scientific and legal reasons, only QSARs and QSPRs that have undergone external validation can now be deemed valid. To determine a compound's structure, we used the TIs [4, 5, 6, 7].

A topological index (or molecular structure descriptor) is a numerical number connected to chemical composition for correlating chemical structure with various physical attributes, chemical reactivity, or biological activity, according to the IUPAC definition. While examining the boiling points of alkanes, Wiener developed the concept of the topological index. Numerous such “structure descriptors" have been proposed thus far and continue to be so often without any consideration of whether they correspond with any of the "various physical properties, chemical reactivity, or biological activity. The molecular graph based structure descriptors are particularly abundant [8, 9, 10]. Development of concepts for the subject of graph theory called molecular topology (MT). Many physico-chemical and biological parameters can be accurately and quickly estimated using (MT), which has been shown to be a reliable method. (MT) principles, which include converting a chemical molecule into a molecular network with atoms as nodes and connections as links, are used to measure topological index [11, 12]. Assume that the molecular graph $G = (V, E)$ has $E(G)$ as the line set (G) and $V(G)$ as the node set. The nodes and edges in a graph G are denoted by the symbols $|V(G)|$ and $|E(G)|$, respectively. $d(u)$, which is the degree of node $u(V)$, represents the number of nodes that are adjacent to it. The line between the vertex pairs u and v is designated as $e = uv$, where $e \in E(G)$ [13, 14].

For instance, there are three types of topological indices; degree-based, distance-based, and counting-based. Theoretical chemistry and biochemistry are two fields where degree-based topological indices are extremely helpful [15]. A key factor in examining the physico chemical characteristics of compound structures is topological index. Topological indices come in five different varieties: degree, distance, eigenvalues, matching, and mixing. For measurement, numerous graph polynomials have been created information on the molecular graph's structure [17].

Visual polynomial discovered applications for molecules in chemistrys Unsaturated compound orbitals and significant concepts where to get the structural descriptors that are utilised to create structural attributes model. Different topological indices exist, but we utilised polynomial. A graph's algebraic counterparts are called graph polynomials. Generally speaking this is invariant, at least for graph isomorphisms. Algebraic graph polynomials in abundance have already been introduced, some of which are significant; Polynomials such as Hosoya polynomials, Tutte polynomials, M-Polynomials, Schultz polynomials, modified Schultz polynomials, and matching polynomials. This polynomial is recognised as being the most typical polynomial connected to decisions. Therefore, the computation of the distance-based topological index is a single polynomial computation [18].

- Mathematical chemistry is helpful to study the quantitative models for helping comprehend the world of chemistry by understanding the elements that make up molecules.
- In this study, the application of chemical graph theory is used to determine the chemical structure and chemical properties of Non-kekulean benzenoid hydrocarbon using M-polynomial

- Mathematical chemistry is helpful for the study of chemical structure and chemical properties of molecules.
- Mathematical chemistry is helpful for taking measurements performing dimensional analysis determining temperature and density.

2.2|Literature Review

There're many different polynomials including Hosoya polynomial, forgotten polynomial and Zagreb polynomial but they give only 1 or 2 topological indices [19, 20, 21]. The M-polynomial is latest polynomial and can give more than ten degree based molecular descriptors[22, 23]. In this section, we will study about M-polynomial existing in literature.

Topological indices. In this section we will study about the topological indices that we used in this work.
The M-polynomial of a graph G is formulated as [24] for further study see [25, 26]

$$M(G;y,z)=\sum_{\delta\leq i\leq j\leq\triangle} m_{ij}y^iz^j \tag{1}$$

Here $\delta = min\{d(s)/s \in V(G)\}$, $\triangle = max\{d(s)/s \in V(G)\}$ and $m_{ij}(G)$ is the edge $rs \in E(G)$ s.t. $\{d(r),d(s)\}=\{i,j\}$.
The topological index introduced by Wiener in 1947 [27] was first and named path numbers, now called as the Wiener index [28]. Later in 1975, Milan Randić found Randić indexas

$$R_{-\frac{1}{2}}(G)=\sum_{rs\in E(G)}\frac{1}{\sqrt{d_rd_s}} \tag{2}$$

General Randić index introduced in [29] and in [30]. The general Randić and inverse Randić indices are formulated as

$$R_\alpha(G)=\sum_{rs\in E(G)}(d_rd_s)^\alpha RR_\alpha(G)=\sum_{rs\in E(G)}\frac{1}{(d_rd_s)^\alpha} \tag{3}$$

The first and second Zagreb indices were introduced by Gutman and Trinajstić [31] and defined as

$$M_1(G)=\sum_{rs\in E(G)}(d_r+d_s)M_2(G)=\sum_{rs\in E(G)}(d_rd_s) \tag{4}$$

Gutman and Furtula [32] developed forgotten topological index and described as:

$$F(G)=\sum_{rs\in E(G)}[d(r)^2+d(s)^2] \tag{5}$$

The second modified Zagreb index defined as

$$mM_2(G)=\sum_{rs\in E(G)}\frac{1}{d_rd_s} \tag{6}$$

Ranjini, lokesha and Usha [33] redefined third Zagreb index which was described as:

$$ReZG_3(G)=\sum_{rs\in E(G)}d_r\cdot d_s(d_r+d_s) \tag{7}$$

The symmetric division deg index introduced [34] used for surface determination of polychlorobiphenyls [35] and formulated as

$$SDD(G)=\sum_{rs\in E(G)}\left(\frac{min(d_r,d_s)}{max(d_r,d_s)}+\frac{max(d_r,d_s)}{min(d_r,d_s)}\right) \tag{8}$$

The other version of the Randić index is the Hormonic index [36] and formulated as

$$H(G)=\sum_{rs\in E(G)}\frac{2}{d_r+d_s} \tag{9}$$

Inverse sum index is

$$I(G) = \sum_{rs \in E(G)} \frac{d_r d_s}{d_r + d_s} \tag{10}$$

The augmented Zagreb index is formulated as [38]

$$A(G) = \sum_{rs \in E(G)} \left(\frac{d_r d_s}{d_r + d_s - 2} \right)^3 \tag{11}$$

Estrada et al. [39] introduced Atom-bond connectivity index. Vukičević [40] proposed Geometric Arithmetic index.

$$GA(G) = \sum_{rs \in E(G)} \frac{2\sqrt{d_r d_s}}{(d_r + d_s)}$$

The first and second K-Banhatti indices were introduced by Kulli in [41] as

$$B_1(G) = \sum_{ue} d_u + d_e$$

$$B_2(G) = \sum_{ue} d_u \times d_e$$

where ue means that the vertex u and edge e are incidents in G
The modified first and second K-Banhatti indices are defined as [42]

$$mB_1(G) = \sum_{ue} \frac{1}{d_u + d_e}$$

$$mB_2(G) = \sum_{ue} \frac{1}{d_u \times d_e}$$

The first and second hyper K-Banhatti indices are defined by Kulli in [43] as

$$HB_1(G) = \sum_{ue} [d_u + d_e]^2$$

$$HB_2(G) = \sum_{ue} [d_u \times d_e]^2$$

The harmonic K-Banhatti index is calculated as [44]

$$H_b(G) = \sum_{ue} \frac{2}{d_u + d_e}$$

Methods and proofs

Derivation of some topolgical indices from M.Polynomial where

$$D_a M(a,b) = a \frac{\partial}{\partial a} M(a,b),$$

$$D_b M(a,b) = b \frac{\partial}{\partial b} M(a,b),$$

$$S_a M(a,b) = \int \frac{M(a,b)}{a} da,$$

$$S_b M(a,b) = \int \frac{M(a,b)}{b} db,$$

$$JM(a,b) = f(a,a),$$

$$Q_{-2}M(a,b) = a^{-2}M(a,b),$$

$$L_aM(a,b) = f(a^2,b),$$

$$L_bM(a,b) = f(a,b^2),$$

$$D_a^{1/2}M(a,b) = \sqrt{a\frac{\partial M(a,b)}{\partial a}}\sqrt{M(a,b)},$$

$$D_b^{1/2}M(a,b) = \sqrt{b\frac{\partial M(a,b)}{\partial b}}\sqrt{M(a,b)},$$

$$S_a^{1/2}M(a,b) = \sqrt{\int \frac{M(a,b)}{a}da}\sqrt{M(a,b)},$$

$$S_b^{1/2}M(a,b) = \sqrt{\int \frac{M(a,b)}{b}db}\sqrt{M(a,b)},$$

The Table 1 is constructed using the Figure 1 for $G_n; n \geq 1$.

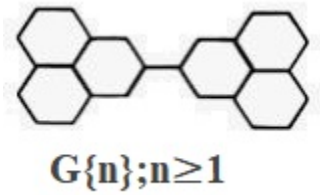

FIGURE 1. Non-kekulean benzenoid hydrocarbon

Table 1: Non-kekulean benzenoid hydrocarbon using Figure 1				
	Types of edges	$(2,2)$	$(2,3)$	$(3,3)$
	Count of edges	8	$12+4n$	$13n-6$

Derivation of M-Polynomial. Using Table 1, we can compute the M-Polynomial of non-kekulean benzenoid hydrocarbon, simple and undirected graph $G_n; n \geq 1$ as follows:

$$MP(NKB;\xi,\eta) = \sum_{i\leqslant j} mp_{ij}(NKB)\xi^i\eta^j$$

$$\begin{aligned} &= \sum_{2\leqslant 2} mp_{22}(NKB)\xi^2\eta^2 + \sum_{2\leqslant 3} mp_{23}(NKB)\xi^2\eta^3 + \sum_{3\leqslant 3} mp_{33}(NKB)\xi^3\eta^3 \\ &= |E_{(2,2)}|\xi^2\eta^2 + |E_{(2,3)}|\xi^2\eta^3 + |E_{(3,3)}|\xi^3\eta^3 \\ &= (8)\xi^2\eta^2 + (12+4n)\xi^2\eta^3 + (13n-6)\xi^3\eta^3 \end{aligned}$$

Consider the non-kekulean benzenoid hydrocarbon $G_n; n \geq 1$ structure.

1.: First Zagreb Index

$$\begin{aligned} M_1(NKB) &= (D_\xi + D_\eta)\left(MP(NKB;\xi,\eta)\right)|_{\xi=\eta=1} \\ &= 89n + 56 \end{aligned}$$

2.: Second Zagreb Index

$$\begin{aligned} M_2(NKB) &= (D_\xi D_\eta)\left(MP(NKB;\xi,\eta)\right)|_{\xi=\eta=1} \\ &= 141n + 50 \end{aligned}$$

3.: First K- Banhatti Index

$$\begin{aligned} B_1(NKB) &= (D_\xi + D_\eta + 2D_\xi Q_{-2}J)\left(MP(NKB;\xi,\eta)\right)|_{\xi=1} \\ &= 226n + 112 \end{aligned}$$

4.: Modified first K- Banhatti Index

$$\begin{aligned} mB_1(NKB) &= S_\xi Q_{-2}J\left(MP(NKB;\xi,\eta)\right)|_{\xi=1} \\ &= 5.93n + 6.8 \end{aligned}$$

5.: Symmetric Index

$$\begin{aligned} SSD(NKB) &= (D_\xi S_\eta + S_\xi D_\eta)\left(MP(NKB;\xi,\eta)\right)|_{\xi=\eta=1} \\ &= 30.6n + 30 \end{aligned}$$

6.: Harmonic Index

$$\begin{aligned} H\left(NKB\right) &= 2S_\xi J\left(MP(NKB;\xi,\eta)\right)|_{\xi=1} \\ &= \frac{89n + 102}{15} \end{aligned}$$

7.: Inverse Index

$$\begin{aligned} I\left(NKB\right) &= S_\xi J D_\xi D_\eta\left(MP(NKB;\xi,\eta)\right)|_{\xi=1} \\ &= 24.3n + 13.4 \end{aligned}$$

8.: Atom- bond connectivity Index

$$\begin{aligned} ABC\left(NKB\right) &= D_\xi^{1/2} Q_{-2} J S_\xi^{1/2} S_\eta^{1/2}\left(M(NKB;\xi,\eta)\right)|_{\xi=1} \\ &= 11.49n + 10.14 \end{aligned}$$

9.: Geometric - Arithmetic Index

$$\begin{aligned} GA\left(NKB\right) &= 2S_\xi J D_\xi^{1/2} D_\eta^{1/2}\left(MP(NKB;\xi,\eta)\right)|_{\xi=1} \\ &= 16.91n + 13.75 \end{aligned}$$

10.: K-Harmoni Banhatti index

$$H_b\left(NKB\right) = 2S_\xi Q_{-2} J(L_\xi + L_\eta)(MP\left(NKB;\xi,\eta\right))|_{\xi=1} \qquad = 11.86n + 13.6$$

11.: Randic index

$$\begin{aligned} R_\alpha\left(NKB\right) &= D_\xi^\alpha D_\eta^\alpha\left(MP(NKB;\xi,\eta)\right) \\ &= \left\{ \begin{array}{c} n(2^{\alpha+2}\times 3^\alpha + 3^{2\alpha}\times 13) + 2^{2\alpha+3} \\ +2^{\alpha+2}\times 3^{\alpha+1} - 3^{2\alpha+1}\times 2 \end{array} \right\} \end{aligned}$$

Proof: Let

$$MP(NKB;\xi,\eta) = (8)\xi^2\eta^2 + (12+4n)\xi^2\eta^3 + (13n-6)\xi^3\eta^3$$

Now, we apply the formulas and compute the following required results.

1.: $D_\xi\left(MP(NKB;\xi,\eta)\right) = 2(8)\xi,\eta\mu^2\nu\xi,\eta^2 + 2(12+4n)\xi^2\eta^3 + 3(13n-6)\xi^3\eta^3;$

2.: $D_\eta\left(MP(NKB;\xi,\eta)\right) = 2(8)\xi^2\eta^2 + 3(12+4n)\xi^2\eta^3 + 3(13n-6)\xi^3\eta^3;$

3.: $D_\xi D_\eta\left(MP(NKB;\xi,\eta)\right) = 4(8)\xi^2\eta^2 + 6(12+4n)\xi^2\eta^3 + 9(13n-6)\xi^3\eta^3;$

4.: $S_\xi D_\eta\left(MP(NKB;\xi,\eta)\right) = \frac{2}{2}(8)\xi^2\eta^2 + \frac{3}{2}(12+4n)\xi,\eta^3 + \frac{3}{3}(13n-6)\xi^3,\eta^3;$

5.: $S_\eta\left(MP(NKB;\xi,\eta)\right) = \frac{1}{2}(8)\xi^2\eta^2 + \frac{1}{3}(12+4n)\xi^2\eta^3 + \frac{1}{3}(13n-6)\xi^3\eta^3;$

6.: $D_\xi S_\eta\left(MP(NKB;\xi,\eta)\right) = \frac{2}{2}(8)\xi^2\eta^2 + \frac{2}{3}(12+4n)\xi^2\eta^3 + \frac{3}{3}(13n-6)\xi^3\eta^3;$

7.: $J\left(MP(NKB;\xi,\eta)\right) = (8)\xi^4 + (12+4n)\xi^5 + (13n-6)\xi^6;$

8.: $S_\xi J\left(MP(NKB;\xi,\eta)\right) = \frac{1}{4}(8)\xi^4 + \frac{1}{5}(12+4n)\xi^5 + \frac{1}{6}(13n-6)\xi^6;$

9.: $S_\xi J D_\xi D_\eta\left(MP(NKB;\xi,\eta)\right) = \frac{1}{4}4(8)\xi^4 + \frac{1}{5}6(12+4n)\xi^5 + \frac{1}{6}9(13n-6)\xi^6;$

10.: $D_\xi^\alpha D_\eta^\alpha\left(MP(NKB;\xi,\eta)\right) = 2^{2\alpha}(8)\xi^2\eta^2 + 2^\alpha.3^\alpha(12+4n)\xi^2\eta^3 + 3^{2\alpha}(13n-6)\xi^3\eta^3;$

11.: $S_\eta^{1/2}\left(MP(NKB;\xi,\eta)\right) = \frac{1}{\sqrt{2}}(8)\xi^2\eta^2 + \frac{1}{\sqrt{3}}(12+4n)\xi^2\eta^3 + \frac{1}{\sqrt{3}}(13n-6)\xi^3\eta^3;$

12.: $S_\xi^{1/2}S_\eta^{1/2}\left(MP(NKB;\xi,\eta)\right) = \frac{1}{\sqrt{2}\sqrt{2}}(8)\xi^2\eta^2 + \frac{1}{\sqrt{6}}(12+4n)\xi^2\eta^3 + \frac{1}{\sqrt{9}}(13n-6)\xi^3\eta^3;$

13.: $JS_\xi^{1/2}S_\eta^{1/2}\left(MP(NKB;\xi,\eta)\right) = \frac{1}{\sqrt{2}\sqrt{2}}(8)\xi^4 + \frac{1}{\sqrt{6}}(12+4n)\xi^5 + \frac{1}{\sqrt{9}}(13n-6)\xi^6;$

14.: $Q_{-2}JS_\xi^{1/2}S_\eta^{1/2}\left(MP(NKB;\xi,\eta)\right) = \frac{1}{\sqrt{2}\sqrt{2}}(8)\xi^2 + \frac{1}{\sqrt{6}}(12+4n)\xi^3 + \frac{1}{\sqrt{9}}(13n-6)\xi^4;$

20: $D_\xi^{1/2}Q_{-2}JS_\xi^{1/2}S_\eta^{1/2}\left(MP(NKB;\xi,\eta)\right) = 4\sqrt{2}\xi^2 + \frac{\sqrt{3}}{\sqrt{6}}(12+4n)\xi^3 + \frac{\sqrt{4}}{\sqrt{9}}(13n-6)\xi^4;$

21.: $D_\eta^{1/2}\left(MP(NKB;\xi,\eta)\right) = \sqrt{2}(8)\xi^2\eta^2 + \sqrt{3}(12+4n)\xi^2\eta^3 + \sqrt{3}(13n-6)\xi^3\eta^3;$

22.: $D_\xi^{1/2}D_\eta^{1/2}\left(MP(NKB;\xi,\eta)\right) = 2(8)\xi^2\eta^2 + \sqrt{6}(12+4n)\xi^2\eta^3 + 3(13n-6)\xi^3\eta^3;$

23.: $JD_\xi^{1/2}D_\eta^{1/2}\left(MP(NKB;\xi,\eta)\right) = 2(8)\xi^4 + \sqrt{6}(12+4n)\xi^5 + 3(13n-6)\xi^6;$

24.: $S_\xi JD_\xi^{1/2}D_\eta^{1/2}\left(MP(NKB;\xi,\eta)\right) = 4\xi^4 + \frac{\sqrt{6}}{5}(12+4n)\xi^5 + \frac{3}{6}(13n-6)\xi^6;$

25.: $Q_{-2}J\left(MP(NKB;\xi,\eta)\right) = (8)\xi^2 + (12+4n)\xi^3 + (13n-6)\xi^4;$

26.: $D_\xi Q_{-2}J\left(M(NKB;\xi,\eta)\right) = 2(8)\xi^2 + 3(12+4n)\xi^3 + 4(13n-6)\xi^4;$

27.: $L_\xi\left(MP(NKB;\xi,\eta)\right) = (8)\xi^4\eta^2 + (12+4n)\xi^4\eta^3 + (13n-6)\xi^5\eta^3;$

28.: $L_\eta(MP(NKB;\xi,\eta)) = (8)\xi^2\eta^4 + (12+4n)\xi^2\eta^5 + (13n-6)\xi^3\eta^5;$

29: $\left(L_\xi + L_\eta\right)\left(MP(NKB;\xi,\eta)\right) = \begin{pmatrix} (8)\xi^4\eta^2 + (12+4n)\xi^4\eta^3 + (13n-6)\xi^5\eta^3 + \\ (8)\xi^2\eta^4 + (12+4n)\xi^2\eta^5 + (13n-6)\xi^3\eta^5 \end{pmatrix};$

30.: $J(L_\xi + L_\eta)\left(MP(NKB;\xi,\eta)\right) = \begin{pmatrix} (8)\xi^6 + (12+4n)\xi^7 + (13n-6)\xi^8 + \\ (8)\xi^6 + (12+4n)\xi^7 + (13n-6)\xi^8 \end{pmatrix};$

31.: $Q_{-2}J(L_\xi + L_\eta)\left(MP(NKBV;\xi,\eta)\right) = \begin{pmatrix} (8)\xi^4 + (12+4n)\xi^5 + (13n-6)\xi^6 + (8)\xi^4 \\ +(12+4n)\xi^5 + (13n-6)\xi^6 \end{pmatrix};$

32.: $S_\xi Q_{-2}J(L_\xi + L_\eta)\left(MP(NKB;\xi,\eta)\right) = \begin{pmatrix} 2\xi^4 + \frac{1}{5}(12+4n)\xi^5 + \frac{1}{6}(13n-6)\xi^6 + 2\xi^4 + \\ \frac{1}{5}(12+4n)\xi^5 + \frac{1}{6}(13n-6)\xi^6 \end{pmatrix}.$

Now we apply the above results on the topological indices.

1.: First Zagreb Index

For $G_n; n \geq 1$, First Zagreb index is as follows:

$$M_1(NKB) = (D_\xi + D_\eta)\left(MP(NKB;\xi,\eta)\right)|_{\xi=\eta=1}$$

$$\begin{aligned}
&= \left\{ \begin{array}{c} 2(8)\xi^2\eta^2 + 2(12+4n)\xi^2\eta^3 + 3(13n-6)\xi^3\eta^3 \\ +2(8)\xi^2\eta^2 + 3(12+4n)\xi^2\eta^3 + 3(13n-6)\xi^3\eta^3 \end{array} \right\} \\
&= \left\{ \begin{array}{c} 2(8) + 2(12+4n) + 3(13n-6) + 2(8) \\ +3(12+4n) + 3(13n-6) \end{array} \right\} \\
&= \left\{ \begin{array}{c} 16 + 24 + 8n + 39n - 18 + 16 \\ +36 + 12n + 39n - 18 \end{array} \right\} \\
&= 89n + 56
\end{aligned}$$

2.: Second Zagreb Index

For $G_n; n \geq 1$, Second Zagreb index is as follows:

$$M_2(NKB) = (D_\xi D_\eta)\left(MP(NKB;\xi,\eta)\right)|_{\xi=\eta=1}$$

$$\begin{aligned}
&= 4(8)\xi^2\eta^2 + 6(12+4n)\xi^2\eta^3 + 9(13n-6)\xi^3\eta^3 \\
&= 4(8) + 6(12+4n) + 9(13n-6) \\
x &= 32 + 72 + 12n + 117n - 54 \\
&= 141n + 50
\end{aligned}$$

3.: First K- Banhatti Index

For $G_n; n \geq 1$, First K- Banhatti index is as follows:

$$B_1(NKB) = (D_\xi + D_\eta + 2D_\xi Q_{-2}J)\left(MP(NKB;\eta,\xi)\right)|_{\xi=1}$$

$$\begin{aligned}
&= \left(\begin{array}{c} 2(8)\xi^2\eta^2 + 2(12+4n)\xi^2\eta^3 + 3(13n-6)\xi^3\eta^3 \\ +2(8)\xi^2\eta^2 + 3(12+4n)\xi^2\eta^3 + 3(13n-6)\xi^3\eta^3 \\ +2\left(2(8)\xi^2 + 3(12+4n)\xi^3 + 4(13n-6)\xi^4\right) \end{array} \right) \\
&= \left(\begin{array}{c} 2(8) + 2(12+4n) + 3(13n-6) + 2(8) + 3(12+4n) \\ +3(13n-6) + 2\left(2(8) + 3(12+4n) + 4(13n-6)\right) \end{array} \right) \\
&= \left(\begin{array}{c} = 16 + 24 + 8n + 39n - 18 + 16 + 36 + 12n \\ +39n - 18 + 32 + 72 + 24n + 104n - 48 \end{array} \right) \\
&= 226n + 112
\end{aligned}$$

4.: Modified first K- Banhatti Index

For $G_n; n \geq 1$, Modified first K- Banhatti index is as follows:

$$mB_1(NKB) = S_\xi Q_{-2}J\left(MP(NKB;\xi,\eta)\right)|_{\xi=1}$$

$$\begin{aligned}
&= \left\{ \begin{array}{c} 2\xi^4 + \frac{1}{5}(12+4n)\xi^5 + \frac{1}{6}(13n-6)\xi^6 + 2\xi^4 \\ +\frac{1}{5}(12+4n)\xi^5 + \frac{1}{6}(13n-6)\xi^6 \end{array} \right\} \\
&= \left\{ \begin{array}{c} 2 + \frac{1}{5}(12+4n) + \frac{1}{6}(13n-6) + 2 \\ +\frac{1}{5}(12+4n) + \frac{1}{6}(13n-6) \end{array} \right\} \\
&= \left\{ \begin{array}{c} 2 + \frac{1}{5}12 + \frac{1}{5}4n + \frac{1}{6}13n - 1 + 2 \\ +\frac{1}{5}12 + \frac{1}{5}4n + \frac{1}{6}13n - 1 \end{array} \right\} \\
&= 5.93n + 6.8
\end{aligned}$$

5.: Symmetric Index

For $G_n; n \geq 1$, Symmetric index is as follows:

$$SSD(NKB) = (D_\xi S_\eta + S_\xi D_\eta)\left(MP(NKB;\xi,\eta)\right)|_{\xi=\eta=1}$$

$$\begin{aligned}
&= \left\{ \begin{array}{c} \frac{2}{2}(8)\xi^2\eta^2 + \frac{2}{3}(12+4n)\xi^2\eta^3 + \frac{3}{3}(13n-6)\xi^3\eta^3 \\ +\frac{2}{2}(8)\xi^2\eta^2 + \frac{3}{2}(12+4n)\xi^2\eta^3 + \frac{3}{3}(13n-6)\xi^3\eta^3 \end{array} \right\} \\
&= \left\{ \begin{array}{c} 8 + \frac{2}{3}(12+4n) + (13n-6) + 8 \\ +\frac{3}{2}(12+4n) + (13n-6) \end{array} \right\} \\
&= \left\{ \begin{array}{c} 8 + \frac{2}{3}(12) + \frac{2}{3}(4n) + 13n - 6 + 8 \\ +\frac{3}{2}(12) + \frac{3}{2}(4n) + 13n - 6 \end{array} \right\} \\
&= 30.6n + 30
\end{aligned}$$

6.: Harmonic Index

For $G_n; n \geq 1$, Harmonic index is as follows:

$$\begin{aligned}
H(NKB) &= 2S_\xi J\left(MP(NKB;a,\eta)\right)|_{a=1} \\
&= 2\left(\frac{1}{4}(8)\xi^4 + \frac{1}{5}(12+4n)\xi^5 + \frac{1}{6}(13n-6)\xi^6\right) \\
&= 4 + \frac{2}{5}(12) + \frac{2}{5}4n + \frac{1}{3}(13n) - 2 \\
&= \frac{89n+102}{15}
\end{aligned}$$

7.: Inverse Index

For $G_n; n \geq 1$, Inverse index is as follows:

$$\begin{aligned}
I(NKB) &= S_\xi J D_\xi D_\eta\left(MP(NKB;\xi,\eta)\right)|_{\xi=1} \\
&= \frac{1}{4}4(8)\xi^4 + \frac{1}{5}6(12+4n)\xi^5 + \frac{1}{6}9(13n-6)\xi^6 \\
&= (8) + \frac{6}{5}(12) + \frac{6}{5}(4n) + \frac{3}{2}(13n) - 9 \\
&= 24.3n + 13.4
\end{aligned}$$

8.: Atom- bond connectivity Index

For $G_n; n \geq 1$, Atom- bond connectivity index is as follows:

$$\begin{aligned}
ABC(NKB) &= D_\xi^{1/2} Q_{-2} J S_\xi^{1/2} S_\eta^{1/2}\left(MP(NKB;\xi,\eta)\right)|_{\xi=1} \\
&= 4\sqrt{2}\xi^2 + \frac{\sqrt{3}}{\sqrt{6}}(12+4n)\xi^3 + \frac{\sqrt{4}}{\sqrt{9}}(13n-6)\xi^4 \\
&= 4\sqrt{2} + \frac{\sqrt{3}}{\sqrt{6}}(12) + \frac{\sqrt{3}}{\sqrt{6}}(4n) + \frac{2}{3}(13n) - \frac{2}{3}(6) \\
&= 4\sqrt{2} + \frac{\sqrt{3}}{\sqrt{6}}(12) + \frac{\sqrt{3}}{\sqrt{6}}(4n) + \frac{2}{3}(13n) - 4 \\
&= 11.49n + 10.14
\end{aligned}$$

9.: Geometric - Arithmetic Index

For $G_n; n \geq 1$, Geometric - Arithmetic index is as follows:

$$\begin{aligned}
GA(NKB) &= 2S_\xi J D_\xi^{1/2} D_\eta^{1/2}\left(MP(NKB;\xi,\eta)\right)|_{\xi=1} \\
&= 2\left(4\xi^4 + \frac{\sqrt{6}}{5}(12+4n)\xi^5 + \frac{3}{6}(13n-6)\xi^6\right) \\
&= 8 + \frac{\sqrt{6}}{5}(24) + \frac{\sqrt{6}}{5}(8n) + (13n) - (6) \\
&= 16.91n + 13.75
\end{aligned}$$

10.: K-Harmonic Banhatti Index

For $G_n; n \geq 1$, K-Harmonic Banhatti index is as follows:

$$H_b(NKB) = 2S_\xi Q_{-2} J(L_\xi + L_\eta)(MP(NKB;\xi,\eta))|_{\xi=1}$$

$$\begin{aligned} &= \left\{ 2 \left(\begin{array}{c} 2\xi^4 + \frac{1}{5}(12+4n)\xi^5 + \frac{1}{6}(13n-6)\xi^6 + 2\xi^4 \\ +\frac{1}{5}(12+4n)\xi^5 + \frac{1}{6}(13n-6)\xi^6 \end{array} \right) \right\} \\ &= \left\{ \begin{array}{c} 4 + \frac{24}{5} + \frac{8}{5}n + \frac{1}{3}(13n) - 2 + 4 \\ +\frac{24}{5} + \frac{8}{5}n + \frac{1}{3}(13n) - 2 \end{array} \right\} \\ &= 11.86n + 13.6 \end{aligned}$$

11.: Randic Index

For $G_n; n \geq 1$, Randic index is as follows:

$$R_\alpha(NKB) = D_\xi^\alpha D_\eta^\alpha (MP(NKB;\xi,\eta))$$

$$\begin{aligned} &= \left\{ \begin{array}{c} 2^{2\alpha}(8)\xi^2\eta^2 + 2^\alpha \times 3^\alpha (12+4n)\xi^2\eta^3 \\ +3^{2\alpha}(13n-6)\xi^3\eta^3 \end{array} \right\} \\ &= \left\{ \begin{array}{c} 2^{2\alpha} \times 2^3 + 2^\alpha \times 3^\alpha \times 2^2 \times 3 + 2^2 n \\ +3^{2\alpha}(13n) - 3^{2\alpha} \times 2 \times 3 \end{array} \right\} \\ &= \left\{ \begin{array}{c} 2^{2\alpha+3} + 2^{\alpha+2} \times 3^{\alpha+1} + 2^{\alpha+2}. \times 3^\alpha n \\ +3^{2\alpha}(13n) - 3^{2\alpha+1} \times 2 \end{array} \right\} \\ &= \left\{ \begin{array}{c} n(2^{\alpha+2} \times 3^\alpha + 3^{2\alpha} \times 13) + 2^{2\alpha+3} \\ +2^{\alpha+2} \times 3^{\alpha+1} - 3^{2\alpha+1} \times 2 \end{array} \right\} \end{aligned}$$

Here are some cases for Randic Index with different values of α. Special Cases:

Case 1::

For $\alpha = 1$

$$\begin{aligned} R_\alpha(NKB) &= \left\{ \begin{array}{c} n(2^{\alpha+2} \times 3^\alpha + 3^{2\alpha} \times 13) + 2^{2\alpha+3} \\ +2^{\alpha+2} \times 3^{\alpha+1} - 3^{2\alpha+1} \times 2 \end{array} \right\} \\ R_1(NKB) &= \left\{ \begin{array}{c} n(2^{1+2} \times 3^1 + 3^2 \times 13) + 2^{2+3} \\ +2^{1+2} \times 3^{1+1} - 3^{2+1} \times 2 \end{array} \right\} \\ &= \left\{ \begin{array}{c} n\left(2^3 \times 3 + 3^2 \times 13\right) + 2^5 \\ +2^3 \times 3^2 - 3^3 \times 2 \end{array} \right\} \\ &= n(24 + 117) + 32 + 72 - 54 \\ &= 141n + 50 \end{aligned}$$

Case 2::

For $\alpha = -1$

$$\begin{aligned} R_\alpha(NKB) &= \left\{ \begin{array}{c} n(2^{\alpha+2} \times 3^\alpha + 3^{2\alpha} \times 13) + 2^{2\alpha+3} \\ +2^{\alpha+2} \times 3^{\alpha+1} - 3^{2\alpha+1} \times 2 \end{array} \right\} \\ R_{-1}(NKB) &= \left\{ \begin{array}{c} n(2^{-1+2} \times 3^{-1} + 3^{-2} \times 13) + 2^{-2+3} \\ +2^{-1+2} \times 3^{-1+1} - 3^{-2+1} \times 2 \end{array} \right\} \\ &= \left\{ \begin{array}{c} n(2^1 \times 3^{-1} + 3^{-2} \times 13) \\ +2^1 + 2^1 \times 3^0 - 3^{-1} \times 2 \end{array} \right\} \\ &= 2.111n + 3.333 \end{aligned}$$

Case 3::

For $\alpha = 1/2$

$$\begin{aligned} R_{\alpha}(NKB) &= \left\{ \begin{array}{c} n(2^{\alpha+2} \times 3^{\alpha} + 3^{2\alpha} \times 13) \\ +2^{2\alpha+3} + 2^{\alpha+2} \times 3^{\alpha+1} - 3^{2\alpha+1} \times 2 \end{array} \right\} \\ R_{1/2}(NKB) &= \left\{ \begin{array}{c} n(2^{1/2+2} \times 3^{1/2} + 3^{2/2} \times 13) + 2^{2/2+3} \\ +2^{1/2+2} \times 3^{1/2+1} - 3^{2/2+1} \times 2 \end{array} \right\} \\ R_{1/2}(NKB) &= n(9.797 + 39) + 27.393 \\ &= 48.797n + 27.393 \end{aligned}$$

Case 4::

For $\alpha = -1/2$

$$\begin{aligned} R_{\alpha}(NKB) &= \left\{ \begin{array}{c} n(2^{\alpha+2} \times 3^{\alpha} + 3^{2\alpha} \times 13) + 2^{2\alpha+3} \\ +2^{\alpha+2} \times 3^{\alpha+1} - 3^{2\alpha+1} \times 2 \end{array} \right\} \\ R_{-1/2}(NKB) &= \left\{ \begin{array}{c} n(2^{-1/2+2} \times 3^{-1/2} + 3^{-2/2} \times 13) + 2^{-2/2+3} \\ +2^{-1/2+2} \times 3^{-1/2+1} - 3^{-2/2+1} \times 2 \end{array} \right\} \\ &= n(1.632 + 4.333) + 6.898 \\ &= 5.965n + 6.898 \end{aligned}$$

5|Conclusion

We examined a number of significant compounds, such as the benzeniod network for Non-kekulean benzoid hydrocarbons, in order to assess their valency-based features. The findings are helpful in predicting many different molecular characteristics of chemical compounds, including pi, boiling temperature, electron energy, medicinal configuration, and a host of other ideas. We first generalize the graph and find the valency Table 1 using the Figure 1 for $G_n; n \geq 1$. After that we developed the formula for M-Polynomial of non-kekulean benzenoid hydrocarbon. With the help of the Table 1 and the formula for M-Polynomial, we calculate the first & second Zagreb index, first & modified first K- Banhatti index, symmetric index, harmonic index, inverse index, atom- bond connectivity index, geometric - arithmetic index, k-harmoni banhatti index, and randic index. Together with thermodynamic entropy, chemical structure, energy, and computer sciences, the entropies can play a critical role in bridging gaps in knowledge and establishing the foundation for future interdisciplinary study. We intend to extend this approach to a range of chemical configurations, which will alter the direction of future research in this area. We may also compute further results for these symmetric chemical compounds by using the valency-based technique.
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Author Contribution

Dr Muhammad Kamran and Dr Saba Mehmood supervised and all other authors contribute equally. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest

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