Research Article

Computation of M-Polynomial and Topological Indices of Phenol Formaldehyde

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Phenol formaldehyde (phenolic resin) has a wide range of moldings. However, it has immense consumption in manufacturing electrical equipment due to its insulating property. Phenolic resin retains properties at the freezing point, and also its age cannot be determined. Due to its insulator property, it has wide use in electrical equipment. In this article, degree-based topological indices of phenol formaldehyde are determined with the help of M-polynomial. We calculate the Zagreb index, Randić index, K-Banhatti indices, modified K-Banhatti indices, atom-bond connectivity index, geometric arithmetic index, symmetric index, inverse sum index, and harmonic index.

1. Introduction

Phenol formaldehyde (PF) is a synthetic polymer that is formed by the reaction of phenol and formaldehyde. Due to its molding power, it is used for many purposes in different industries. An in-circuit board like PCB and many electronic equipment like buttons, knobs, cameras, and vacuum cleaner phenolic resins are used. It is also used in laminate, fabric, and paper. There are two methods of production in industrial practice. In the first method, excess formaldehyde reacts with phenol in an alkaline solution. In the second method, excess phenol reacts with formaldehyde in an acidic solution [1]. It was firstly used in the first decades of 20th century.

In chemical graphs, atoms are represented by vertices, and bonding is represented by edges in molecular structure. A topological index is a numerical parameter that predicts the characteristics of that chemical graph. Mathematical models, based on polynomial representations of chemical compounds, can be used to predict their properties. Mathematical chemistry is rich in tools such as polynomials and functions which can forecast the properties of compounds. Topological indices are numerical parameters of a graph that characterize its topology and are usually graph invariant. They describe the structure of molecules numerically and are used in the development of quantitative structure-activity relationships (QSARs). These numerical values correlate structural facts and chemical reactivity, biological activities, and physical properties [2–4].

In this work, G be connected chemical structure, with V(G) vertices and E(G) edge sets. d(u) is degree of vertex u. The edge among vertices u and v is indicated by uv. Let e = uv be an edge in G, and then u and e are incident as are v and e. Let d(e) indicate the degree of an edge e of G, which is obtained by d(e) = d(u) + d(v) − 2 with e = uv. Presently, topological indices based on degrees are calculated with the help of M-polynomials. In 2015, Deutsch and Klavžar [5] introduced M-polynomial, as for similar role as distance-based Hosoya polynomial. For further study, see [6–12]. The M-polynomial of G is written as

\[ M(G; a, b) = \sum_{\delta \subseteq \Delta} m_\delta a^b, \]  

(1)
where \( \delta(G) = \min \{ d(v) : v \in V(G) \} \) and \( \Delta(G) = \max \{ d(v) : v \in V(G) \} \) are the minimum and maximum degree of \( G \), respectively, and \( m_{ij}(G) \) is the edge \( uv \in E(G) \) such that \( d(u), d(v) \in \{ i, j \} \), and \( d(u), d(v) \in \{ 1 \leq \delta \leq d(u), d(v) \leq \Delta \leq |V(G)| - 1 \} \) are the degrees of vertices \( u, v \in V(G) \); see also [10, 11].

The origin of topological index is from Wiener index, in 1945. This was defined by Wiener as he was examining the boiling point of alkanes [13, 14] (for further study, see [12]). The Randić index, invented by Milan Randić, is the first degree-based topological index [15] (for further research, see [16-18]) and is as

\[
R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}. 
\]

(2)

Generalized Randić index is defined as [19]

\[
R_a(G) = \sum_{uv \in E(G)} (d(u)d(v))^a. 
\]

(3)

The 1st and 2nd Zagreb indices were introduced by Gutman and Trinajstić [20-22] as

\[
M_1(G) = \sum_{uv \in E(G)} (d(u) + d(v)),
M_2(G) = \sum_{uv \in E(G)} (d(u)d(v)). 
\]

(4)

The first K-Banhatti index was introduced by Kulli in [23, 24] as

\[
B_1(G) = \sum_{u \in V} \left[ d(u) + R(e) \right], 
\]

where \( ue \) means that the vertex \( u \) and edge \( e \) are incident in \( G \).

The modified first K-Banhatti index is defined as [25]

\[
mB_1(G) = \sum_{u \in V} \frac{1}{d(u) + R(e)}. 
\]

(6)

The harmonic K-Banhatti index is calculated as [25, 26]

\[
H_b(G) = \sum_{u \in V} \frac{2}{d(u) + R(e)}.
\]

(7)

The symmetric division index is defined [27] and used to determine surface of polychlorobiphenyls [28] and formulated as

\[
SDD(G) = \sum_{uv \in E(G)} \left( \frac{\min\{d(u),d(v)\}}{\max\{d(u),d(v)\}} + \frac{\max\{d(u),d(v)\}}{\min\{d(u),d(v)\}} \right). 
\]

(8)

The Harmonic index is defined as [29]

\[
H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}. 
\]

(9)

Inverse sum index is defined as [29]

\[
I(G) = \sum_{uv \in E(G)} \frac{d(u)d(v)}{d(u) + d(v)}. 
\]

(10)

Atom-bond connectivity (ABC) index introduced by Estrada et al. [30] as

\[
ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}. 
\]

(11)

Geometric-arithmetic (GA) index was introduced by Vukičević et al. [31] as

\[
GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}. 
\]

(12)

Topological indices encode information regarding molecular size, shape, branching, etc. in numerical form, which is used for measuring topological similarity between chemical compounds and in quantitative structure-property relationship (QSPR)/quantitative structure-activity relationship (QSAR) studies. Randić index has been closely correlated with many chemical properties and found to parallel the boiling point and Kovats constants. The first and second Zagreb indices provide quantitative measures of molecular branching. The atom-bond connectivity (ABC) index provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes. For certain physicochemical properties, the predictive power of GA index is somewhat better than predictive power of the Randić connectivity index. We can find topological index with the help of Table 1.

\[
D_{LJ} f(a,b) = x \frac{\partial f(a,b)}{\partial a}, \quad D_{H} f(a,b) = \frac{\partial f(a,b)}{\partial b}, 
\]

\[
S_{LJ} f(a,b) = \int \frac{f(a,b)}{a} da, \quad S_{H} f(a,b) = \int \frac{f(a,b)}{b} db, 
\]

\[
L_{r} f(a,b) = f(a, b), \quad Q_{r} f(a,b) = a^r f(a,b), 
\]

\[
D_{LJ}^2 f(a,b) = \sqrt{\frac{\partial f(a,b)}{\partial a}} \sqrt{f(a,b)}, \quad D_{H}^2 f(a,b) = \sqrt{\frac{\partial f(a,b)}{\partial b}} \sqrt{f(a,b)}, 
\]

\[
S_{LJ}^2 f(a,b) = \int \frac{f(a,b)}{a} da \sqrt{f(a,b)}, \quad S_{H}^2 f(a,b) = \int \frac{f(a,b)}{b} db \sqrt{f(a,b)}, 
\]

(13)

where \( f(a,b) \) is a function of M-polynomial which is computed for given graph.
2. Formation and Result for Phenol Formaldehyde Polymer Chain

In alkaline or acidic solution, when phenol and methanal are heated phenol formaldehyde (PF), polymer chain is formed in condensation reaction. Ortho and para substitute phenol is produced in the first step, then ortho isomer reacts with other same molecule, and polymer chain is produced. A polymer chain is formed when in acidic condition, and methanal and phenol rings in 2 or 4 position react with 0.5:1 ratio.

In Table 2, \( p \) represents number of units.

**Theorem 1.** Consider the phenol formaldehyde polymer chain (PF); then, its M-polynomial is as follows.

**Proof.** From Figure 1, and using Table 2, we can compute the M-polynomial of chemical structure of phenol formaldehyde polymer chain (PF) as follows:

\[
M(PF; a, b) = \sum_{\subgraph} m_{ij}(G) a^i b^j
\]

\[
= \sum_{i=1} m_{13}(G) a^3 b^2 + \sum_{i=2} m_{22}(G) a^2 b^3
+ \sum_{i=3} m_{33}(G) a^1 b^4
\]

\[
= E_{(1,3)} a^3 b^2 + E_{(2,2)} a^2 b^3 + E_{(3,3)} a b^4
= (p+1) a^3 b^2 + (2p+1) a^2 b^3 + (4p-2) a b^4 + (2p-1) a^1 b^4.
\]

\[\text{(14)}\]

**Proposition 2.** Consider the phenol formaldehyde polymer (PF) chain structure.

\[\text{(i) First Zagreb index: } M_1(PF) = (D_a + D_b)(M(PF; a, b))_{a=b=1} = 44p - 8\]

**Proof.** Let \( M(PF; a, b) = (p+1) a^3 b^2 + (2p+1) a^2 b^3 + (4p-2) a b^4 + (2p-1) a^1 b^4. \) Now, we apply the formulas from Table 1, and compute the following required results.

| Topological index | Derivative from \( M(G; a, b) \) |
|-------------------|---------------------------------|
| First Zagreb index | \((D_a + D_b)(M(G; a, b))_{a=b=1}\) |
| Second Zagreb index | \((D_2 D_a)(M(G; a, b))_{a=b=1}\) |
| First K-Banhatti index | \((D_a + D_b + 2D_a Q_{-2})J(M(G; a, b))_{a=b=1}\) |
| Modified first K-Banhatti index | \(S_a Q_a J(L_a + L_b)(M(G; a, b))_{a=b=1}\) |
| Randić index | \((D_a S_a + S_a D_a)(M(G; a, b))_{a=b=1}\) |
| Symmetric index | \(2S_a J(M(G; a, b))_{a=b=1}\) |
| Harmonic index | \(S_a J D_a D_b(M(G; a, b))_{a=b=1}\) |
| Inverse sum index | \(2S_a Q_a J(J(L_a + L_b)(M(G; a, b))_{a=b=1}\) |
| K harmonic Banhatti index | \(2S_a J D_a D_b(M(G; a, b))_{a=b=1}\) |
| Atom-bond connectivity index | \(2S_a J D_a D_b(M(G; a, b))_{a=b=1}\) |
| Geometric-arithmetic index | \(2S_a J D_a D_b(M(G; a, b))_{a=b=1}\) |

**Table 2: Degree-based edge partition.**

| Types of edges | Frequency |
|---------------|-----------|
| (1, 3)        | \(p + 1\) |
| (2, 2)        | \(2p + 1\) |
| (2, 3)        | \(4p - 2\) |
| (3, 3)        | \(2p - 1\) |

\[\text{(ii) Second Zagreb index: } M_2(PF) = (D_a D_b)(M(PF; a, b))_{a=b=1} = 53p - 14\]

\[\text{(iii) First K-Banhatti index: } B_1(PF) = (D_a + D_b + 2D_a Q_{-2})J(M(PF; a, b))_{a=b=1} = 96p - 20\]

\[\text{(iv) Modified first K-Banhatti index: } mB_1(PF) = S_a Q_a J(J(L_a + L_b)(M(PF; a, b))_{a=b=1} = 3.57p - 0.01\]

\[\text{(v) Randić index: } R_a(PF) = (D_a^2 D_b^2)(M(PF; a, b))_{a=b=1} = 3^a(p + 1) + 2^a(2p + 1) + 2^a(4p - 2) + 3^a(2p - 1)\]

\[\text{(vi) Symmetric index: } SDD(PF) = (D_a S_b + S_a D_b)(M(PF; a, b))_{a=b=1} = 20p - 1\]

\[\text{(vii) Harmonic index: } H(PF) = 2S_a J(M(PF; a, b))_{a=b=1} = 3.77n - 0.13\]

\[\text{(viii) Inverse sum index: } I(PF) = S_a J D_a D_b(M(PF; a, b))_{a=b=1} = 10.55p - 3.15\]

\[\text{(ix) Atom-bond connectivity index: } ABC(PF) = D_{a}^{1/2} Q_{-2} J S_a J D_a^{1/2}(M(PF; a, b))_{a=b=1} = 6.4p - 0.57\]

\[\text{(x) Geometric-arithmetic index: } GA(PF) = 2S_a J D_a^{1/2} D_{a}^{1/2}(M(PF; a, b))_{a=b=1} = 8.78p - 1.09\]

\[\text{(xi) K harmonic Banhatti index: } H_b(PF) = 2S_a Q_{-2} J(J(L_a + L_b)(M(PF; a, b))_{a=b=1} = 7.14p - 0.03\]

\[\text{Proof. Let } M(PF; a, b) = (p+1) a^3 b^2 + (2p+1) a^2 b^3 + (4p-2) a b^4 + (2p-1) a^1 b^4. \]
Figure 1: Phenol formaldehyde polymer (PF) chain structure.

\[
D_a(M(PF; a, b)) = (p + 1)ab^3 + 2(2p + 1)a^2b^2
+ 2(4p - 2)a^2b^3 + 3(2p - 1)a^3b^3,
\]

\[
D_b(M(PF; a, b)) = 3(p + 1)ab^3 + 2(2p + 1)a^2b^2
+ 3(4p - 2)a^2b^3 + 3(2p - 1)a^3b^3,
\]

\[
D_aD_b(M(PF; a, b)) = 3(p + 1)ab^3 + 4(2p + 1)a^2b^2
+ 6(4p - 2)a^2b^3 + 9(2p - 1)a^3b^3,
\]

\[
S_aD_b(M(PF; a, b)) = 3(p + 1)ab^3 + (2p + 1)a^2b^2
+ \frac{3(4p - 2)}{2}a^2b^3 + (2p - 1)a^3b^3,
\]

\[
S_b(M(PF; a, b)) = \frac{(p + 1)}{3}ab^3 + \frac{(2p + 1)}{2}a^2b^2
+ \frac{(4p - 2)}{3}a^2b^3 + \frac{(2p - 1)}{3}a^3b^3,
\]

\[
D_aS_b(M(PF; a, b)) = \frac{(p + 1)}{3}ab^3 + \frac{(2p + 1)}{2}a^2b^2
+ \frac{2(4p - 2)}{3}a^2b^3 + (2p - 1)a^3b^3,
\]

\[
J(M(PF; a, b)) = (3p + 2)a^4 + (4p - 2)a^5 + (2p - 1)a^6,
\]

\[
S_aJ(M(PF; a, b)) = \frac{(3p + 2)}{4}a^4 + \frac{(4p - 2)}{5}a^5
+ \frac{(2p - 1)}{6}a^6,
\]

\[
S_bJ_aD_b(M(PF; a, b)) = \frac{(11p + 7)}{4}a^4 + \frac{(24p - 12)}{5}a^5
+ \frac{(18p - 9)}{6}a^6,
\]

\[
D_a^2D_b^2(M(PF; a, b)) = 3^6(p + 1)ab^3 + 2^{2a}(2p + 1)a^2b^2
+ 2^{2a}(4p - 2)a^2b^3 + 3^{2a}(2p - 1)a^3b^3,
\]

\[
S_a^{1/2}S_b^{1/2}(M(PF; a, b)) = \frac{(p + 1)}{\sqrt{3}}ab^3 + \frac{(2p + 1)}{\sqrt{2}}a^2b^2
+ \frac{(4p - 2)}{\sqrt{3}}a^2b^3 + \frac{(2p - 1)}{\sqrt{3}}a^3b^3,
\]

\[
JS_a^{1/2}S_b^{1/2}(M(PF; a, b)) = (1.58p + 1.08)a^4
+ \sqrt{\frac{3}{6}}(4p - 2)a^5 + \frac{2(2p - 1)}{3}a^6,
\]

\[
Q_aJS_a^{1/2}S_b^{1/2}(M(PF; a, b)) = (1.58p + 1.08)a^2
+ \sqrt{\frac{3}{6}}(4p - 2)a^3 + \frac{2(2p - 1)}{3}a^4,
\]

\[
D_a^2Q_aJS_a^{1/2}S_b^{1/2}(M(G; a, b)) = \sqrt{2}(1.58p + 1.08)a^2
+ \sqrt{\frac{3}{6}}(4p - 2)a^3 + \frac{2(2p - 1)}{3}a^4,
\]

\[
D_a^{1/2}D_b^{1/2}(M(PF; a, b)) = \sqrt{3}(p + 1)ab^3 + \sqrt{2}(2p + 1)a^2b^2
+ \sqrt{3}(4p - 2)a^2b^3 + \sqrt{3}(2p - 1)a^3b^3,
\]

\[
D_a^{1/2}D_b^{1/2}(M(PF; a, b)) = \sqrt{3}(p + 1)ab^3 + 2(2p + 1)a^2b^2
+ \sqrt{6}(4p - 2)a^2b^3 + 3(2p - 1)a^3b^3,
\]

\[
JD_a^{1/2}D_b^{1/2}(M(PF; a, b)) = \sqrt{3}(p + 1)a^4 + 2(2p + 1)a^4
+ \sqrt{6}(4p - 2)a^5 + 3(2p - 1)a^6,
\]

\[
JS_aJD_a^{1/2}D_b^{1/2}(M(PF; a, b)) = \frac{\sqrt{3}(p + 1)}{4}a^4 + \frac{(2p + 1)}{2}a^4
+ \frac{\sqrt{6}(4p - 2)}{5}a^5 + \frac{(2p - 1)}{2}a^6,
\]

\[
Q_aJ(M(PF; a, b)) = (3n + 2)a^2 + (4p - 2)a^3 + (2p - 1)a^4,
\]

\[
D_aQ_aJ(M(PF; a, b)) = 2(3n + 2)a^2 + 3(4p - 2)a^3 + 4(2p - 1)a^4,
\]

\[
L_a(M(PF; a, b)) = (p + 1)a^2b^3 + (2p + 1)a^3b^2
+ (4p - 2)a^4b^3 + (2p - 1)a^6b^3,
\]

\[
L_a(M(PF; a, b)) = (p + 1)ab^6 + (2p + 1)a^2b^4
+ (4p - 2)a^2b^5 + (2p - 1)a^3b^6,
\]
Table 3: Numerical comparison of $M_1(PF)$, $M_2(PF)$, SDD(PF), $H(PF)$, $I(PF)$, $B_1(PF)$, $mB_1(PF)$, $H_b(PF)$, ABC(PF), and GA(PF).

| p  | $M_1(PF)$ | $M_2(PF)$ | SDD(PF) | $H(PF)$ | $I(PF)$ | $B_1(PF)$ | $mB_1(PF)$ | $H_b(PF)$ | ABC(PF) | GA(PF) |
|----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 1  | 36    | 39    | 19    | 3.64  | 7.4   | 76    | 3.56  | 7.11  | 5.83  | 7.69  |
| 2  | 80    | 92    | 39    | 7.41  | 17.95 | 172   | 7.13  | 14.25 | 12.23 | 16.47 |
| 3  | 124   | 145   | 59    | 11.18 | 28.5  | 268   | 10.7  | 21.39 | 18.63 | 25.25 |
| 4  | 168   | 198   | 79    | 14.95 | 39.05 | 364   | 14.27 | 28.53 | 25.03 | 34.03 |
| 5  | 212   | 251   | 99    | 18.72 | 49.6  | 460   | 17.84 | 35.67 | 31.43 | 42.81 |
| 6  | 256   | 304   | 119   | 22.49 | 60.15 | 556   | 21.41 | 42.81 | 37.83 | 51.59 |
| 7  | 300   | 357   | 139   | 26.26 | 70.7  | 652   | 24.98 | 49.95 | 44.23 | 60.37 |
| 8  | 344   | 410   | 159   | 30.03 | 81.25 | 748   | 28.55 | 57.09 | 50.63 | 69.15 |
| 9  | 388   | 463   | 179   | 33.8  | 91.8  | 844   | 32.12 | 64.23 | 57.03 | 77.93 |
| 10 | 432   | 516   | 199   | 37.57 | 102.35| 940   | 35.69 | 71.37 | 63.43 | 86.71 |

\[
(L_a + L_b)(M(PF; a, b)) = (p + 1)a^2b^3 + (2p + 1)a^4b^2 \\
+ (4p - 2)a^3b^4 + (2p - 1)a^6b^3 \\
+ (p + 1)a^4b^2 + (2p + 1)a^2b^4. \\
+(4p - 2)a^3b^4 + (2p - 1)a^6b^3,
\]

\[
J(L_a + L_b)(M(PF; a, b)) = (p + 1)a^2 + (4p + 2)a^6 + (5p - 1)a^7 \\
+ (4p - 2)a^8 + (4p - 2)a^9,
\]

\[
Q_2J(L_a + L_b)(M(PF; a, b)) = (p + 1)a^2 + (4p + 2)a^4 \\
+ (5p - 1)a^3 + (4p - 2)a^5 + (4p - 2)a^6.
\]

\[
S_6Q_2J(L_a + L_b)(M(PF; a, b)) = \frac{(p + 1)}{3}a^3 \\
+ \frac{(4p + 2)}{4}a^4 + \frac{(5p - 1)}{5}a^5 \\
+ \frac{(4p - 2)}{6}a^6 + \frac{(4p - 2)}{7}a^7. \\
(15)
\]

3. Numerical and Graphical Representation

“The numerical representation of the above computed results is depicted in Tables 3 and 4, and the graphical representation is dedicated in Figures 2 and 3. We can easily see from Figures 2 and 3 that all indices are in increasing order as the value of n is increasing.”

4. Formation and Result Cross-Linked Phenol Formaldehyde Structure

The polymer chain reacts with formaldehyde to produce branching. Branching is possible when methanal reacts with higher proportion, because it provides a CH₂ and on heating resin is produced.

Theorem 3. Consider the cross-linked phenol formaldehyde (PF) structure; then, its M-polynomial is as follows.

Proof. From Figure 4, and using Table 5, we can compute the M-polynomial of chemical structure of phenol formaldehyde (PF) network as follows:
Proposition 4. Consider the cross-linked phenol formaldehyde (PF) structure.

(i) First Zagreb index: \( M_1(PF) = (\sum_{i,j} m_{ij} G_{ab}^i G_{ab}^j) \left. \right|_{a=b=1} = 309n \)

(ii) Second Zagreb index: \( M_2(PF) = (\sum_{i,j} m_{ij} G_{ab}^i G_{ab}^j) \left. \right|_{a=b=1} = 373n \)

(iii) First K-Banhatti index: \( B_1(PF) = (\sum_{i,j} m_{ij} G_{ab}^i G_{ab}^j) \left. \right|_{a=b=1} = 679n \)

(iv) Modified first K-Banhatti index: \( mB_1(PF) = (\sum_{i,j} m_{ij} G_{ab}^i G_{ab}^j) \left. \right|_{a=b=1} = 24.19n \)

\[ M(PF; a, b) = \sum_{i,j} m_{ij} G_{ab}^i G_{ab}^j = \sum_{i=1}^m m_{1i} G_{ab}^i G_{ab}^j \]

\[ + \sum_{j=1}^m m_{ji} G_{ab}^i G_{ab}^j \]

\[ = |E_{1,1}| a^2 b + |E_{1,3}| a^3 b \]

\[ + |E_{2,1}| a^2 b^2 + |E_{1,3}| a^3 b^2 \]

\[ = 2nab^2 + 9nab^3 + 39na^2 b^3 + 12na^3 b^3. \]

\[ (16) \]

(a) Comparison of \( M_1(PF) \), \( M_2(PF) \), \( SDD(PF) \), \( H(PF) \), and \( I(PF) \)

(b) Comparison of \( B_1(PF) \), \( mB_1(PF) \), \( Hb(PF) \), \( ABC(PF) \), and \( GA(PF) \)

Figure 2: Graphical comparison of topological indices.

Figure 3: Comparison of \( R_\alpha(PF) \) for \( \alpha = 1, 1/2, -1/2, \) and \(-1\).
Table 5: Degree-based edge partition for n > 1.

| Types of edges | (1, 2) | (1, 3) | (2, 3) | (3, 3) |
|----------------|-------|-------|-------|-------|
| Frequency      | 2n    | 9n    | 39n   | 12n   |

(v) Randić index: $R_{\alpha}(PF) = (D_a^\alpha D_b^\alpha)(M(PF; a, b))|_{a=b=1} = 2^n(2n) + 3^n(9n) + 2^n \cdot 3^n(39n) + 3^{2n}(12n)$

(vi) Symmetric index: SDD(PF) = $(D_aS_b + S_aD_b)(M(PF; a, b))|_{a=b=1} = 143.5n$

(vii) Harmonic index: $H(PF) = 2S_aJ(M(PF; a, b))|_{a=1} = 25.43n$

(viii) Inverse sum index: $I(PF) = S_bJD_aD_b(M(PF; a, b))|_{a=1} = 72.88n$

(ix) Atom-bond connectivity index: $ABC(PF) = D_a^{1/2}Q_{-2}S_a^{1/2}S_b^{1/2}(M(PF; a, b))|_{a=1} = 44.34n$

(x) Geometric-arithmetic index: $GA(PF) = 2S_aJ^{1/2}D_b^{1/2}(M(PF; a, b))|_{a=1} = 53.52n$

(xi) K harmonic Banhatti index: $H_b(PF) = 2S_aQ_{-2}J(L_a + L_b)(M(PF; a, b))|_{a=1} = 48.39n$

\[ S_aJ(M(PF; a, b)) = \frac{2n}{3}a^3 + \frac{9n}{4}a^4 + \frac{39n}{5}a^5 + 2na^6, \]
\[ IJD_aD_b(M(PF; a, b)) = 4na^3 + 27na^4 + 234na^5 + 108na^6, \]
\[ S_aJD_aD_b(M(PF; a, b)) = \frac{4n}{3}a^3 + \frac{27n}{4}a^4 + \frac{234n}{5}a^5 + 18na^6, \]
\[ D_a^2D_b^2(M(PF; a, b)) = 2^n \cdot 2 nab^2 + 3^n \cdot 9 nab^3 + 2^n \cdot 3^n \cdot 39 na^2 b^3 + 3^{2n} \cdot 12 na^3 b^3, \]
\[ S_b^{1/2}(M(PF; a, b)) = \frac{2n}{\sqrt{2}}a b^2 + \frac{9n}{\sqrt{3}}a b^3 + \frac{39n}{\sqrt{6}}a^2 b^3 + \frac{12n}{3}a^4 b^3, \]
\[ S_a^{1/2}S_b^{1/2}(M(PF; a, b)) = \frac{2n}{\sqrt{2}}a b^2 + \frac{9n}{\sqrt{3}}a b^3 + \frac{39n}{\sqrt{6}}a^2 b^3 + \frac{12n}{3}a^4 b^3, \]
\[ JS_a^{1/2}S_b^{1/2}(M(PF; a, b)) = \frac{2n}{\sqrt{2}}a + \frac{9n}{\sqrt{3}}a^2 + \frac{39n}{\sqrt{6}}a^3 + 4na^4, \]
\[ Q_{-2}JS_a^{1/2}S_b^{1/2}(M(PF; a, b)) = \frac{2n}{\sqrt{2}}a + \frac{9n}{\sqrt{3}}a^2 + \frac{39n}{\sqrt{6}}a^3 + 4na^4, \]
\[ D_a^{1/2}Q_{-2}JS_a^{1/2}S_b^{1/2}(M(PF; a, b)) = \frac{2n}{\sqrt{2}}a + \frac{9n}{\sqrt{3}}a^2 + \frac{39n}{\sqrt{6}}a^3 + 8na^4, \]
\[ D_b^{1/2}(M(PF; a, b)) = \sqrt{2}(2n)ab^2 + \sqrt{3}(9n)ab^3 + \sqrt{5}(39n)a b^3, \]
\[ D_a^{1/2}D_b^{1/2}(M(PF; a, b)) = \sqrt{2}(2n)ab^2 + \sqrt{3}(9n)ab^3 + \sqrt{6}(39n)a b^3 + 36na^3 b^3, \]
\[ JD_a^{1/2}D_b^{1/2}(M(PF; a, b)) = \sqrt{2}(2n)a^3 + \sqrt{3}(9n)a^4 + \sqrt{6}(39n)a^5 + 36na^6, \]
\[ S_aJD_a^{1/2}D_b^{1/2}(M(PF; a, b)) = \frac{\sqrt{2}(2n)}{3}a^3 + \frac{\sqrt{3}(9n)}{4}a^4 + \frac{\sqrt{6}(39n)}{5}a^5 + 6na^6, \]

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**Proof.** Let $M(PF; a, b) = 2 nab^2 + 9 nab^3 + 39 na^2 b^3 + 12na^3 b^3$. Now, we apply the formulas from Table 1, and compute the following required results.

\[ D_a(M(PF; a, b)) = 2 nab^2 + 9 nab^3 + 78 na^2 b^3 + 36na^3 b^3, \]
\[ D_b(M(PF; a, b)) = 4 nab^2 + 27 nab^3 + 117 na^2 b^3 + 36na^3 b^3, \]
\[ D_aD_b(M(PF; a, b)) = 4 nab^2 + 27 nab^3 + 234 na^2 b^3 + 108na^3 b^3, \]
\[ S_aD_b(M(PF; a, b)) = 4 nab^2 + 27 nab^3 + \frac{117n}{2}a^2 b^3 + 12na^3 b^3, \]
\[ S_b(M(PF; a, b)) = nab^2 + 3 nab^3 + 13 na^2 b^3 + 4na^3 b^3, \]
\[ D_aS_b(M(PF; a, b)) = nab^2 + 3 nab^3 + 26na^2 b^3 + 12na^3 b^3, \]
\[ J(M(PF; a, b)) = 2na^3 + 9na^4 + 39 na^5 + 12na^6, \]
Table 6: Numerical comparison of $M_1(PF)$, $M_2(PF)$, $SDD(PF)$, $H(PF)$, $I(PF)$, $B_1(PF)$, $mB_1(PF)$, $H_1(PF)$, ABC(PF), and GA(PF).

| $n$ | $M_1(PF)$ | $M_2(PF)$ | SDD(PF) | $H(PF)$ | $I(PF)$ | $B_1(PF)$ | $mB_1(PF)$ | $H_1(PF)$ | ABC(PF) | GA(PF) |
|-----|-----------|-----------|---------|---------|---------|-----------|------------|-----------|---------|--------|
| 1   | 309       | 373       | 143.5   | 25.43   | 72.88   | 679       | 24.19      | 48.39     | 44.34   | 53.52  |
| 2   | 618       | 746       | 287     | 50.86   | 145.76  | 1358      | 48.38      | 96.78     | 88.68   | 107.04 |
| 3   | 927       | 1119      | 430.5   | 76.29   | 218.64  | 2037      | 72.57      | 145.17    | 133.02  | 160.56 |
| 4   | 1236      | 1492      | 574     | 101.72  | 291.52  | 2716      | 96.76      | 193.56    | 177.36  | 214.08 |
| 5   | 1545      | 1865      | 717.5   | 127.12  | 364.4   | 3395      | 120.95     | 241.95    | 221.7   | 267.6  |
| 6   | 1854      | 2238      | 861     | 152.58  | 437.28  | 4074      | 145.14     | 290.34    | 266.04  | 321.12 |
| 7   | 2163      | 2611      | 1004.5  | 178.01  | 510.16  | 4753      | 169.33     | 338.73    | 310.38  | 374.64 |
| 8   | 2472      | 2984      | 1148    | 203.44  | 583.04  | 5432      | 193.52     | 387.12    | 354.72  | 428.16 |
| 9   | 2781      | 3357      | 1291.5  | 228.87  | 655.92  | 6111      | 217.71     | 435.51    | 399.06  | 481.68 |
| 10  | 3090      | 3730      | 1435    | 254.3   | 728.8   | 6790      | 241.9      | 483.9     | 443.4   | 535.2  |

Table 7: Numerical behaviour of $R_1(PF)$, $R_{1/2}(PF)$, $R_{-1/2}(PF)$, and $R_{-1}(PF)$.

| $n$ | $R_1(PF)$ | $R_{1/2}(PF)$ | $R_{-1/2}(PF)$ | $R_{-1}(PF)$ |
|-----|-----------|---------------|----------------|-------------|
| 1   | 373       | 149.95        | 26.53          | 11.83       |
| 2   | 746       | 299.9         | 53.06          | 23.66       |
| 3   | 1119      | 449.85        | 79.59          | 35.49       |
| 4   | 1492      | 599.8         | 106.12         | 47.32       |
| 5   | 1865      | 749.75        | 132.65         | 59.15       |
| 6   | 2238      | 899.7         | 159.18         | 70.98       |
| 7   | 2611      | 1049.65       | 185.71         | 82.81       |
| 8   | 2984      | 1199.6        | 212.24         | 94.64       |
| 9   | 3357      | 1349.55       | 238.77         | 106.47      |
| 10  | 3730      | 1499.5        | 265.3          | 118.3       |

\[ Q_2(J(M(PF; a, b)) = 2na + 9na^2 + 39na^3 + 12na^4, \]
\[ D_2Q_2(J(M(PF; a, b)) = 2na^2b^2 + 2na^3b^2 + 39na^3b^3 + 12na^4b^3, \]
\[ L_1(M(PF; a, b)) = 2nab^2 + 9nab^3 + 39nab^3 + 12nab^3b^3, \]
\[ L_2(M(PF; a, b)) = 2nab^4 + 9nab^6 + 39nab^6 + 12nab^6b^6, \]
\[ (L_a + L_b)(M(PF; a, b)) = 2na^2b^2 + 2na^3b^3 + 39na^3b^3 + 12na^4b^3 + 2nab^4 + 9nab^6 + 39nab^6 + 12nab^6, \]
\[ J(L_a + L_b)(M(PF; a, b)) = 2na^4 + 11na^5 + 48na^7 + 39na^8 + 24na^9, \]
\[ Q_2(J(L_a + L_b)(M(PF; a, b)) = 2na^2 + 11na^3 + 48na^5 + 39na^6 + 24na^7, \]
\[ S_nQ_2(J(L_a + L_b)(M(PF; a, b)) = na^2 + \frac{11n}{3}a^3 + \frac{48n}{5}a^5 + \frac{39n}{6}a^4 + \frac{24n}{7}a^3. \]

(i) First Zagreb index: $M_1(PF) = (D_a + D_b)(M(PF; a, b)) \big|_{a=b=1} = 309n^2$
(ii) Second Zagreb index: $M_2(PF) = (D_a + D_b)(M(PF; a, b)) \big|_{a=b=1} = 373n^2$
(iii) First K-Banhatti index: $B_1(PF) = (D_a + D_b + 2D_a Q_2)(M(PF; a, b)) \big|_{a=1} = 679n^2$
(iv) Modified first K-Banhatti index: $mb_1(PF) = S_nQ_2(\big|_{a=1} = 24.19n^2$
(v) Randić index: $R_q(PF) = (D_a^2D_b^2)(M(PF; a, b)) \big|_{a=b=1} = 2a(2n) + 3a(9n) + 2a \cdot 3a(39n) + 3^2a(12n)$
(vi) Symmetric index: $SDD(PF) = (D_aS_aD_b)(M(PF; a, b)) \big|_{a=b=1} = 143.5n^2$
Figure 5: Graphical comparison of topological indices.
(vii) Harmonic index: \( H(PF) = 2S_a J(M(PF; a, b)) \big|_{a=1} = 25.43n \)

(viii) Inverse sum index: \( I(PF) = S_{a/2} D_a D_b(M(PF; a, b)) \big|_{a=1} = 72.88n \)

(ix) Atom-bond connectivity index: \( ABC(PF) = D_{a}^{1/2} Q_{a, b} M^{1/2}(M(PF; a, b)) \big|_{a=1} = 44.34n \)

(x) Geometric-arithmetic index: \( GA(PF) = 2S_{a/2} D_{a}^{1/2} D_{b}^{1/2}(M(PF; a, b)) \big|_{a=1} = 53.52n \)

(xi) K harmonic Banhatti index: \( H_b(PF) = 2S_{a} Q_{a, b} J(L_{a} + L_{b})(M(PF; a, b)) \big|_{a=1} = 48.39n \)

5. Numerical and Graphical Representation

The numerical representation of the above computed results is depicted in Tables 6 and 7, and the graphical representation is dedicated in Figures 5 and 6. Tables 6 and 7 depict the mathematical equations as topological indices. Furthermore, these indices are being illustrated graphically in Figures 5 and 6. It has been observed clearly from the figures that all indices are in an ascending order as the value of \( n \) is increasing gradually. Thus, the increasing trend indicates that the values of topological indices are increasing accordingly in Tables 6 and 7.

6. Conclusion

In this article, the M-polynomial of phenol formaldehyde was found, and then, degree-dependent topological indices were calculated. These topological indices will be helpful for the preparation of electronic devices such as buttons, knobs, cameras, and vacuum cleaners. The numerical values that are found in this manuscript are valuable for betterment synthetic production and quality on a commercial base. For the assessment of the production, quality is easily measured by these numerical values.

Data Availability

No data availability for this research.

Conflicts of Interest

The authors declare no conflicts of interest.

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