

Retraction

Retracted: Computation of M-Polynomial and Topological Indices of Phenol Formaldehyde

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This article has been retracted by Hindawi, as publisher, following an investigation undertaken by the publisher [1]. This investigation has uncovered evidence of systematic manipulation of the publication and peer-review process. We cannot, therefore, vouch for the reliability or integrity of this article.

Please note that this notice is intended solely to alert readers that the peer-review process of this article has been compromised.

Wiley and Hindawi regret that the usual quality checks did not identify these issues before publication and have since put additional measures in place to safeguard research integrity.

We wish to credit our Research Integrity and Research Publishing teams and anonymous and named external researchers and research integrity experts for contributing to this investigation.

The corresponding author, as the representative of all authors, has been given the opportunity to register their agreement or disagreement to this retraction. We have kept a record of any response received.

References

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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 Klav-žar [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

$$M(G; a, b) = \sum_{\delta \le i \le j \le \Delta} m_{ij} a^i b^j, \tag{1}$$

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 $\{d(u), d(v)\} = \{i, j\}$, and $d(u), d(v)(1 \le \delta \le d(u))$, and $d(v) \le \Delta \le |V(G)| - 1)$ 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]

$$R_{\alpha}(G) = \sum_{uv \in E(G)} (d(u)d(v))^{\alpha}.$$
 (3)

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

$$\begin{split} M_1(G) &= \sum_{uv \in E(G)} \, (d(u) + d(v)), \\ M_2(G) &= \sum_{uv \in E(G)} \, (d(u)d(v)). \end{split} \tag{4}$$

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

$$B_1(G) = \sum_{ue} \left[d(u) + \tilde{\Re}(e) \right], \tag{5}$$

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

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

$$mB_1(G) = \sum_{ue} \frac{1}{d(u) + \tilde{\mathfrak{R}}(e)}.$$
 (6)

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

$$H_b(G) = \sum_{ue} \frac{2}{d(u) + \Re(e)}.$$
(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 Vukičevic' 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 structureproperty 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.

$$\begin{split} D_a f(a,b) &= x \frac{\partial f(a,b)}{\partial a}, D_y f(a,b) = b \frac{\partial f(a,b)}{\partial b}, \\ S_a f(a,b) &= \int \frac{f(a,b)}{a} da, S_b f(a,b) = \int \frac{f(a,b)}{b} db, \\ Jf(a,b) &= f(a,a), Q_a f(a,b) = a^a f(a,b), \\ L_a f(a,b) &= f(a^2,b), L_b f(a,b) = f(a,b^2), \\ D_a^{1/2} f(a,b) &= \sqrt{a \frac{\partial f(a,b)}{\partial a}} \cdot \sqrt{f(a,b)}, D_b^{1/2} f(a,b) = \sqrt{b \frac{\partial f(a,b)}{\partial b}} \cdot \sqrt{f(a,b)}, \\ S_a^{1/2} f(a,b) &= \sqrt{\int \frac{f(a,b)}{a} da} \cdot \sqrt{f(a,b)}, S_b^{1/2} f(a,b) = \sqrt{\int \frac{f(a,b)}{b} db} \cdot \sqrt{f(a,b)}, \end{split}$$

$$\end{split}$$

where f(a, b) is a function of M-polynomial which is computed for given graph.

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	$(D_a D_b)(M(G; a, b)) _a = b = 1$
First K-Banhatti index	$(D_a + D_b + 2D_aQ_{-2}J)(M(G; a, b)) _{a=1}$
Modified first K-Banhatti index	$S_a Q 2J(L_a + L_b)(M(G; a, b)) _{a=1}$
Randić index	$(D^{lpha}_a \ D^{lpha}_b)(M(G;a,b)) \mid_{a=b=1}$
Symmetric index	$(D_a S_b + S_a D_b)(M(G; a, b)) a=b=1$
Harmonic index	$2S_a J(M(G;a,b)) _{a=1}$
Inverse sum index	$S_a J D_a D_b (M(G; a, b)) \mid_{a=1}$
K harmonic Banhatti index	$2S_aQ 2J(L_a + L_b)(M(G; a, b)) _{a=1}$
Atom-bond connectivity index	$D_a^{1/2}Q 2JS_a^{1/2}S_b^{1/2} \left. \left(M(G;a,b) ight) ight _{a=1}$
Geometric-arithmetic index	$2S_a J D_a^{1/2} D_b^{1/2} (M(G; a, b)) _{a=1}$

TABLE 1: Derivation of some topological indices from M-polynomial.

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:

$$\begin{split} M(PF;a,b) &= \sum_{i \leq j} m_{ij}(G) a^i b^j \\ &= \sum_{1 \leq 3} m_{13}(G) a b^3 + \sum_{2 \leq 2} m_{22}(G) a^2 b^2 \\ &+ \sum_{2 \leq 3} m_{23}(G) a^2 b^3 + \sum_{3 \leq 3} m_{33}(G) a^3 b^3 \\ &= \left| E_{\{1,3\}} \right| a b^3 + \left| E_{\{2,2\}} \right| a^2 b^2 + \left| E_{\{2,3\}} \right| a^2 b^3 + \left| E_{\{3,3\}} \right| a^3 b^3 \\ &= (p+1) a b^3 + (2p+1) a^2 b^2 + (4p-2) a^2 b^3 + (2p-1) a^3 b^3. \end{split}$$

$$\end{split}$$

$$(14)$$

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

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

TABLE 2: Degree-based edge partition.

Types of edges	(1, 3)	(2, 2)	(2, 3)	(3, 3)
Frequency	p + 1	2p + 1	4 <i>p</i> – 2	2p - 1

- (ii) Second Zagreb index: $M_2(PF) = (D_a D_b)(M(PF; a, b))|_{a=b=1} = 53p 14$
- (iii) First K-Banhatti index: $B_1(PF) = (D_a + D_b + 2D_a Q_{-2}J)(M(PF; a, b))|_{a=1} = 96p 20$
- (iv) Modified first K-Banhatti index: $mB_1(PF) = S_aQ_{-2}$ $J(L_a + L_b)(M(PF; a, b))|_{a=1} = 3.57p - 0.01$
- $\begin{array}{l} (\nu) \ Randić \quad index: \quad R_{\alpha}(PF) = (D_{a}^{\alpha}D_{b}^{\alpha})(M(PF;a,b))| \\ \\ a=b=1 = 3^{\alpha}(p+1) + 2^{2\alpha}(2p+1) + 2^{\alpha} \cdot 3^{\alpha}(4p-2) + 3^{2\alpha} \\ (2p-1) \end{array}$
- (vi) Symmetric index: $SDD(PF) = (D_aS_b + S_aD_b)(M(P + F; a, b))|_{a=b=1} = 20p 1$
- (vii) Harmonic index: $H(PF) = 2S_a J(M(PF; a, b))|_{a=1}$ = 3.77n - 0.13
- (viii) Inverse sum index: $I(PF) = S_a JD_a D_b(M(PF; a, b))|_{a=1} = 10.55p 3.15$
- (ix) Atom-bond connectivity index: $ABC(PF) = D_a^{1/2}Q_{-2}$ $JS_a^{1/2}S_b^{1/2}(M(PF; a, b))|_{a=1} = 6.4p - 0.57$
- (x) Geometric-arithmetic index: $GA(PF) = 2S_a J D_a^{1/2}$ $D_b^{1/2} (M(PF; a, b))|_{a=1} = 8.78p - 1.09$
- (xi) K harmonic Banhatti index: $H_b(PF) = 2S_aQ_{-2}J(L_a + L_b)(M(PF; a, b))|_{a=1} = 7.14p 0.03$

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



FIGURE 1: Phenol formaldehyde polymer (PF) chain structure.

$$\begin{split} D_a(M(PF;a,b)) &= (p+1)ab^3 + 2(2p+1)a^2b^2 \\ &+ 2(4p-2)a^2b^3 + 3(2p-1)a^3b^3, \end{split}$$

$$\begin{split} D_b(M(PF;a,b)) &= 3(p+1)ab^3 + 2(2p+1)a^2b^2 \\ &+ 3(4p-2)a^2b^3 + 3(2p-1)a^3b^3, \end{split}$$

$$\begin{split} D_a D_b (M(PF;a,b)) &= 3(p+1)ab^3 + 4(2p+1)a^2b^2 \\ &+ 6(4p-2)a^2b^3 + 9(2p-1)a^3b^3, \end{split}$$

$$\begin{split} S_a D_b(M(PF;a,b)) &= 3(p+1)ab^3 + (2p+1)a^2b^2 \\ &+ \frac{3(4p-2)}{2}a^2b^3 + (2p-1)a^3b^3 \end{split}$$

$$\begin{split} S_b(M(PF;a,b)) &= \frac{(p+1)}{3}ab^3 + \frac{(2p+1)}{2}a^2b^2 \\ &+ \frac{(4p-2)}{3}a^2b^3 + \frac{(2p-1)}{3}a^3b^3, \end{split}$$

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

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

$$\begin{split} S_a J(M(PF;a,b)) &= \frac{(3p+2)}{4} a^4 + \frac{(4p-2)}{5} a^5 + \frac{(2p-1)}{6} a^6, \\ S_a J D_a D_b(M(PF;a,b)) &= \frac{(11p+7)}{4} a^4 + \frac{(24p-12)}{5} a^5 \\ &+ \frac{(18p-9)}{6} a^6, \end{split}$$

$$\begin{split} D^{\alpha}_{a}D^{\alpha}_{b}(M(PF\,;\,a,\,b)) &= 3^{\alpha}(p+1)ab^{3}+2^{2\alpha}(2p+1)a^{2}b^{2} \\ &+ 2^{\alpha}3^{\alpha}(4p-2)a^{2}b^{3}+3^{2\alpha}(2p-1)a^{3}b^{3}, \end{split}$$

$$\begin{split} S_b^{1/2}(M(PF;a,b)) &= \frac{(p+1)}{\sqrt{3}}ab^3 + \frac{(2p+1)}{\sqrt{2}}a^2b^2 \\ &+ \frac{(4p-2)}{\sqrt{3}}a^2b^3 + \frac{(2p-1)}{\sqrt{3}}a^3b^3 \end{split}$$

$$S_a^{1/2}S_b^{1/2}(M(PF;a,b)) = \frac{(p+1)}{\sqrt{3}}ab^3 + \frac{(2p+1)}{2}a^2b^2 + \frac{(4p-2)}{\sqrt{6}}a^2b^3 + \frac{(2p-1)}{3}a^3b^3,$$

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

$$\begin{aligned} Q_{-2}JS_a^{1/2}S_b^{1/2}(M(PF;a,b)) &= (1.58p+1.08)a^2 \\ &+ \frac{(4p-2)}{\sqrt{6}}a^3 + \frac{(2p-1)}{3}a^4, \end{aligned}$$

$$\begin{split} D_a^{1/2} Q_{-2} J S_a^{1/2} S_b^{1/2} (M(G;a,b)) &= \sqrt{2} (1.58p + 1.08) a^2 \\ &+ \sqrt{\frac{3}{6}} (4p-2) a^3 + \frac{2(2p-1)}{3} a^4 , \end{split}$$

$$\begin{split} D_b^{1/2}(M(PF;a,b)) &= \sqrt{3}(p+1)ab^3 + \sqrt{2}(2p+1)a^2b^2 \\ &+ \sqrt{3}(4p-2)a^2b^3 + \sqrt{3}(2p-1)a^3b^3, \end{split}$$

$$\begin{split} D_a^{1/2} D_b^{1/2} (M(PF;a,b)) &= \sqrt{3}(p+1)ab^3 + 2(2p+1)a^2b^2 \\ &+ \sqrt{6}(4p-2)a^2b^3 + 3(2p-1)a^3b^3, \end{split}$$

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

$$\begin{split} S_a J D_a^{1/2} D_b^{1/2} \big(M(PF; a, b) \big) &= \frac{\sqrt{3}(p+1)}{4} a^4 + \frac{(2p+1)}{2} a^4 \\ &+ \frac{\sqrt{6}(4p-2)}{5} a^5 + \frac{(2p-1)}{2} a^6, \end{split}$$

$$Q_{-2}J(M(PF; a, b)) = (3n+2)a^2 + (4p-2)a^3 + (2p-1)a^4,$$

$$D_a Q_{-2} J(M(PF; a, b)) = 2(3n+2)a^2 + 3(4p-2)a^3 + 4(2p-1)a^4,$$

$$\begin{split} L_a(M(PF;a,b)) &= (p+1)a^2b^3 + (2p+1)a^4b^2 \\ &+ (4p-2)a^4b^3 + (2p-1)a^6b^3, \\ L_b(M(PF;a,b)) &= (p+1)ab^6 + (2p+1)a^2b^4 \\ &+ (4p-2)a^2b^6 + (2p-1)a^3b^6, \end{split}$$

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).

р	$M_1 \ (PF)$	$M_2(PF)$	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

$$\begin{split} (L_a+L_b)(M(PF\,;a,b)) &= (p+1)a^2b^3 + (2p+1)a^4b^2 \\ &\quad + (4p-2)a^4b^3 + (2p-1)a^6b^3 \\ &\quad + (p+1)ab^6 + (2p+1)a^2b^4, \\ &\quad + (4p-2)a^2b^6 + (2p-1)a^3b^6, \end{split}$$

$$\begin{split} J(L_a+L_b)(M(PF;a,b)) &= (p+1)a^5 + (4p+2)a^6 + (5p-1)a^7 \\ &+ (4p-2)a^8 + (4p-2)a^9, \end{split}$$

$$\begin{split} Q_{-2}J(L_a+L_b)(M(PF\,;a,b)) &= (p+1)a^3 + (4p+2)a^4 \\ &+ (5p-1)a^5 + (4p-2)a^6 + (4p-2)a^7, \end{split}$$

$$S_{a}Q_{-2}J(L_{a} + L_{b})(M(PF; a, b)) = \frac{(p+1)}{3}a^{3} + \frac{(4p+2)}{4}a^{4} + \frac{(5p-1)}{5}a^{5} + \frac{(4p-2)}{6}a^{6} + \frac{(4p-2)}{7}a^{7}.$$
(15)

- (i) First Zagreb index: $M_1(PF) = (D_a + D_b)(M(PF; a, b))|_{a=b=1} = 44p 8$
- (ii) Second Zagreb index: $M_2(PF) = (D_a D_b)(M(PF; a, b))|_{a=b=1} = 53p 14$
- (iii) First K-Banhatti index: $B_1(PF)=(D_a+D_b+2D_a$
 $Q_{-2}J)(M(PF\,;a,b))|_{a=1}=96p-20$
- (iv) Modified first K-Banhatti index: $mB_1(PF) = S_aQ_{-2}$ $J(L_a + L_b)(M(PF; a, b))|_{a=1} = 3.57p - 0.01$
- (v) Randić index: $R_{\alpha}(PF) = (D_{a}^{\alpha}D_{b}^{\alpha})(M(PF; a, b))|_{a=b=1} = 3^{\alpha}(p+1) + 2^{2\alpha}(2p+1) + 2^{\alpha} \cdot 3^{\alpha}(4p-2) + 3^{2\alpha}(2p-1)$
- (vi) Symmetric index: $SDD(PF) = (D_aS_b + S_aD_b)(M(P F; a, b))|_{a=b=1} = 20p 1$

- (vii) Harmonic index: $H(PF) = 2S_a J(M(PF; a, b))|_{a=1}$ = 3.77*n* - 0.13
- (viii) Inverse sum index: $I(PF)=S_aJD_aD_b(M(PF; a, b))$ $|_{a=1} = 10.55p - 3.15$
- (ix) Atom-bond connectivity index: $ABC(PF) = D_a^{1/2} Q_{-2}JS_a^{1/2}S_b^{1/2}(M(PF; a, b))|_{a=1} = 6.4p 0.57$
- (x) Geometric-arithmetic index: $GA(PF) = 2S_a J D_a^{1/2} D_b^{1/2} (M(PF; a, b))|_{a=1} = 8.78p 1.09$
- (xi) K harmonic Banhatti index: $H_b(PF) = 2S_aQ_{-2}J(L_a + L_b)(M(PF; a, b))|_{a=1} = 7.14p 0.03$

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 CH_2 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:

р	$R_1(PF)$	$R_{1/2}(PF)$	$R_{-1/2}(PF)$	$R_{-1}(PF)$
1	39	17.36	3.81	1.58
2	92	38.89	7.69	3.3
3	145	60.42	11.57	5.02
4	198	81.95	15.45	6.74
5	251	103.48	19.33	8.46
6	304	125.01	23.21	10.18
7	357	146.54	27.09	11.9
8	410	168.07	30.97	13.62
9	463	189.6	34.85	15.34
10	516	211.13	38.73	17.06

TABLE 4: Numerical behaviour of $R_1(PF)$, $R_{1/2}(PF)$, $R_{-1/2}(PF)$, and $R_{-1}(PF)$.



FIGURE 2: Graphical comparison of topological indices.

(a) Comparison of M1(PF), M2(PF), SDD(PF), H(PF), and I(PF)

(b) Comparison of B1(PF), mB1(PF), Hb(PF), ABC(PF), and GA(PF)





Proposition 4. Consider the cross-linked phenol formaldehyde (PF) structure.

- (i) First Zagreb index: $M_1(PF) = (D_a + D_b)(M(PF; a, b))|_{a=b=1} = 309n$
- (ii) Second Zagreb index: $M_2(PF) = (D_a D_b)(M(PF; a, b))|_{a=b=1} = 373n$

FIGURE 3: Comparison of $R_{\alpha}(PF)$ for $\alpha = 1, 1/2, -1/2$, and -1.

- (iii) First K-Banhatti index: $B_1(PF) = (D_a + D_b + 2D_a Q_{-2}J)(M(PF; a, b))|_{a=1} = 679n$
- (iv) Modified first K-Banhatti index: $mB_1(PF) = S_aQ_{-2}$ $J(L_a + L_b)(M(PF; a, b))|_{a=1} = 24.19n$



FIGURE 4: Cross-linked phenol formaldehyde (PF) structure.

TABLE 5: Degree-based edge partition for n > 1.

Types of edges	(1, 2)	(1,3)	(2, 3)	(3, 3)
Frequency	2 <i>n</i>	9 <i>n</i>	39 <i>n</i>	12 <i>n</i>

- (v) Randić index: $R_{\alpha}(PF) = (D_a^{\alpha}D_b^{\alpha})(M(PF; a, b))|$ $_{a=b=1} = 2^{\alpha}(2n) + 3^{\alpha}(9n) + 2^{\alpha} \cdot 3^{\alpha}(39n) + 3^{2\alpha}(12n)$
- (vi) Symmetric index: $SDD(PF) = (D_aS_b + S_aD_b) (M(P F; a, b))|_{a=b=1} = 143.5n$
- (vii) Harmonic index: $H(PF) = 2S_a J(M(PF; a, b))|_{a=1}$ = 25.43n
- (viii) Inverse sum index: $I(PF) = S_a J D_a D_b(M(PF; a, b))$ $|_{a=1} = 72.88n$
- (ix) Atom-bond connectivity index: $ABC(PF) = D_a^{1/2} Q_{-2}JS_a^{1/2}S_b^{1/2}(M(PF; a, b))|_{a=1} = 44.34n$
- (x) Geometric-arithmetic index: $GA(PF) = 2S_a J D_a^{1/2}$ $D_b^{1/2}(M(PF; a, b))|_{a=1} = 53.52n$
- (xi) K harmonic Banhatti index: $H_b(PF) = 2S_aQ_{-2}J(L_a + L_b)(M(PF; a, b))|_{a=1} = 48.39n$

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

$$\begin{split} D_a(M(PF;a,b)) &= 2nab^2 + 9nab^3 + 78na^2b^3 + 36na^3b^3, \\ D_b(M(PF;a,b)) &= 4nab^2 + 27nab^3 + 117na^2b^3 + 36na^3b^3, \\ D_aD_b(M(PF;a,b)) &= 4nab^2 + 27nab^3 + 234na^2b^3 + 108na^3b^3, \\ S_aD_b(M(PF;a,b)) &= 4nab^2 + 27nab^3 + \frac{117n}{2}a^2b^3 + 12na^3b^3, \\ S_b(M(PF;a,b)) &= nab^2 + 3nab^3 + 13na^2b^3 + 4na^3b^3, \\ D_aS_b(M(PF;a,b)) &= nab^2 + 3nab^3 + 26na^2b^3 + 12na^3b^3, \end{split}$$

$$J(M(PF; a, b)) = 2na^3 + 9na^4 + 39na^5 + 12na^6,$$

$$\begin{split} S_a J(M(PF;a,b)) &= \frac{2n}{3}a^3 + \frac{9n}{4}a^4 + \frac{39n}{5}a^5 + 2na^6, \\ JD_a D_b(M(PF;a,b)) &= 4na^3 + 27na^4 + 234na^5 + 108na^6, \\ S_a JD_a D_b(M(PF;a,b)) &= \frac{4n}{3}a^3 + \frac{27n}{4}a^4 + \frac{234n}{5}a^5 + 18na^6, \\ D_a^{\alpha} D_b^{\alpha}(M(PF;a,b)) &= 2^{\alpha} \cdot 2nab^2 + 3^{\alpha} \cdot 9nab^3 \\ &+ 2^{\alpha} \cdot 3^{\alpha} \cdot 39na^2b^3 + 3^{2\alpha} \cdot 12na^3b^3, \end{split}$$

$$\begin{split} S_b^{1/2}(M(PF;a,b)) &= \frac{2n}{\sqrt{2}}ab^2 + \frac{9n}{\sqrt{3}}ab^3 + \frac{39n}{\sqrt{3}}a^2b^3 + \frac{12n}{\sqrt{3}}a^3b^3, \\ S_a^{1/2}S_b^{1/2}(M(PF;a,b)) &= \frac{2n}{\sqrt{2}}ab^2 + \frac{9n}{\sqrt{3}}ab^3 + \frac{39n}{\sqrt{6}}a^2b^3 + \frac{12n}{3}a^3b^3, \\ JS_a^{1/2}S_b^{1/2}(M(PF;a,b)) &= \frac{2n}{\sqrt{2}}a^3 + \frac{9n}{\sqrt{3}}a^4 + \frac{39n}{\sqrt{6}}a^5 + 4na^6, \\ Q_{-2}JS_a^{1/2}S_b^{1/2}(M(PF;a,b)) &= \frac{2n}{\sqrt{2}}a + \frac{9n}{\sqrt{3}}a^2 + \frac{39n}{\sqrt{6}}a^3 + 4na^4, \\ D_a^{1/2}Q_{-2}JS_a^{1/2}S_b^{1/2}(M(PF;a,b)) &= \frac{2n}{\sqrt{2}}a + \frac{9n\sqrt{2}}{\sqrt{2}}a^2 + \frac{9n\sqrt{2}}{3}a^2 + \frac{39n\sqrt{3}}{3}a^2 + \frac{39n\sqrt{3}}{3}a^3 + 8na^4, \end{split}$$

$$\begin{split} D_b^{1/2}(M(PF;a,b)) &= \sqrt{2}(2n)ab^2 + \sqrt{3}(9n)ab^3 \\ &+ \sqrt{3}(39n)a^2b^3 + \sqrt{3}(12n)a^3b^3, \end{split}$$

$$\begin{split} D_a^{1/2} D_b^{1/2} (M(PF;a,b)) &= \sqrt{2} (2n) a b^2 + \sqrt{3} (9n) a b^3 \\ &+ \sqrt{6} (39n) a^2 b^3 + 36n a^3 b^3, \end{split}$$

$$\begin{split} JD_a^{1/2}D_b^{1/2}(M(PF\,;a,b)) &= \sqrt{2}(2n)a^3 + \sqrt{3}(9n)a^4 \\ &+ \sqrt{6}(39n)a^5 + 36na^6, \end{split}$$

$$\begin{split} S_a J D_a^{1/2} D_b^{1/2} (M(PF;a,b)) &= \frac{\sqrt{2}(2n)}{3} a^3 + \frac{\sqrt{3}(9n)}{4} a^4 \\ &+ \frac{\sqrt{6}(39n)}{5} a^5 + 6na^6, \end{split}$$

п	$M_1(PF)$	$M_2(PF)$	SDD(PF)	H(PF)	I(PF)	$B_1(PF)$	$mB_1(PF)$	$H_b(PF)$	ABC(PF)	GA(PF)
1	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	127.15	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 6: 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).

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

п	$R_1(PF)$	$R_{1/2}(PF)$	$R_{-1/2}(PF)$	$R_{-1}(PF)$
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

 $Q_{-2}J(M(PF; a, b)) = 2na + 9na^2 + 39na^3 + 12na^4,$

 $D_a Q_{-2} J(M(PF; a, b)) = 2na + 18na^2 + 117na^3 + 48na^4,$

 $L_a(M(PF; a, b)) = 2na^2b^2 + 9na^2b^3 + 39na^4b^3 + 12na^6b^3,$

 $L_b(M(PF; a, b)) = 2nab^4 + 9nab^6 + 39na^2b^6 + 12na^3b^6$

$$\begin{split} (L_a+L_b)(M(PF;a,b)) &= 2na^2b^2+9na^2b^3+39na^4b^3\\ &+12na^6b^3+2nab^4+9nab^6\\ &+39na^2b^6+12na^3b^6, \end{split}$$

 $J(L_a + L_b)(M(PF; a, b)) = 2na^4 + 11na^5 + 48na^7 + 39na^8 + 24na^9,$

 $\begin{aligned} Q_{-2}J(L_a+L_b)(M(PF;a,b)) &= 2na^2+11na^3 \\ &+ 48na^5+39na^6+24na^7, \end{aligned}$

$$S_a Q_{-2} J(L_a + L_b) (M(PF; a, b)) = na^2 + \frac{11n}{3}a^3 + \frac{48n}{5}a^5 + \frac{39n}{6}a^6 + \frac{24n}{7}a^7.$$
(17)

- (i) First Zagreb index: $M_1(PF) = (D_a + D_b)(M(PF; a, b))|_{a=b=1} = 309n$
- (ii) Second Zagreb index: $M_2(PF) = (D_a D_b)(M(PF; a, b))|_{a=b=1} = 373n$
- (iii) First K-Banhatti index: $B_1(PF) = (D_a + D_b + 2D_a Q_{-2}J)(M(PF; a, b))|_{a=1} = 679n$
- (iv) Modified first K-Banhatti index: $mB_1(PF) = S_aQ_{-2}$ $J(L_a + L_b)(M(PF; a, b))|_{a=1} = 24.19n$
- (v) Randić index: $R_{\alpha}(PF) = (D_a^{\alpha}D_b^{\alpha})(M(PF; a, b))|$ $_{a=b=1} = 2^{\alpha}(2n) + 3^{\alpha}(9n) + 2^{\alpha} \cdot 3^{\alpha}(39n) + 3^{2\alpha}(12n)$
- (vi) Symmetric index: $SDD(PF) = (D_aS_b + S_aD_b)(M(P F; a, b))|_{a=b=1} = 143.5n$







FIGURE 6: Comparison of $R_{\alpha}(FP)$ for $\alpha = 1, 1/2, -1/2$, and -1.

- (vii) Harmonic index: $H(PF) = 2S_a J(M(PF; a, b))|_{a=1}$ = 25.43*n*
- (viii) Inverse sum index: $I(PF) = S_a J D_a D_b (M(PF; a, b))$ $|_{a=1} = 72.88n$
- (ix) Atom-bond connectivity index: $ABC(PF) = D_a^{1/2} Q_{-2} J S_a^{1/2} S_b^{1/2} (M(PF; a, b))|_{a=1} = 44.34n$
- (x) Geometric-arithmetic index: $GA(PF) = 2S_a J D_a^{1/2}$ $D_b^{1/2} (M(PF; a, b))|_{a=1} = 53.52n$
- (xi) K harmonic Banhatti index: $H_b(PF) = 2S_aQ_{-2}J(L_a + L_b)(M(PF; a, b))|_{a=1} = 48.39n$

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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References

- I. Poljansek and M. Krajnc, "Characterization of phenolformaldehyde prepolymer resins by in line FT-IR spectroscopy," *Acta Chimica Slovenica*, vol. 52, no. 3, p. 238, 2005.
- [2] I. Gutman, "Degree-based topological indices," Croatica Chemica Acta, vol. 86, no. 4, pp. 351–361, 2013.
- [3] I. Gutman, E. Milovanovic, and I. Milovanovic, "Beyond the Zagreb indices," *Graphs and Combinatorics*, vol. 17, no. 1, pp. 74–85, 2020.
- [4] S. Noureen, A. Ali, and A. A. Bhatti, "On the extremal Zagreb indices of n-vertex chemical trees with fixed number of segments or branching vertices," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 84, pp. 513– 534, 2020.
- [5] E. Deutsch and S. Klavžar, "M-polynomial and degree-based topological indices," *Iranian Journal of Mathematical Chemistry*, vol. 6, no. 2, pp. 93–102, 2015.
- [6] D. Afzal, F. Afzal, M. R. Farahani, and S. Ali, "On computation of recently defined degree-based topological indices of some families of convex polytopes via M-polynomial," *Complexity*, vol. 2021, Article ID 5881476, 11 pages, 2021.

- [7] M. Ahmad, M. Saeed, M. Javaid, and E. Bonyah, "Molecular descriptor analysis of certain isomeric natural polymers," *Journal of Chemistry*, vol. 2021, Article ID 9283246, 26 pages, 2021.
- [8] Y. M. Chu, M. Imran, A. Q. Baig, S. Akhter, and M. K. Siddiqui, "On M-polynomial-based topological descriptors of chemical crystal structures and their applications," *The European Physical Journal Plus*, vol. 135, no. 11, pp. 1–19, 2020.
- [9] R. H. Khan, A. Q. Baig, R. Kiran, I. Haider, M. Rizwan, and A. Elahi, "M-Polynomials and Degree-Based Topological Indices of Dexamethasone, Chloroquine and Hydroxychloroquine; using in COVID-19," *International Journal of Scientific Engineering and Science*, vol. 4, no. 7, pp. 47–52, 2020.
- [10] M. Munir, W. Nazeer, S. Rafique, and S. M. Kang, "M-polynomial and degree-based topological indices of polyhex nanotubes," *Symmetry*, vol. 8, no. 12, p. 149, 2016.
- [11] M. Munir, W. Nazeer, S. Rafique, and S. M. Kang, "M-polynomial and related topological indices of nanostar dendrimers," *Symmetry*, vol. 8, no. 9, p. 97, 2016.
- [12] M. Hu, H. Ali, M. A. Binyamin, B. Ali, J. B. Liu, and C. Fan, "On distance-based topological descriptors of chemical interconnection networks," *Journal of Mathematics*, vol. 2021, Article ID 5520619, 10 pages, 2021.
- [13] N. Salamat, M. Kamran, S. Ali, M. Alam, and R. H. Khan, "Several characterizations on degree-based topological indices for star of david network," *Journal of Mathematics*, vol. 2021, Article ID 9178444, 11 pages, 2021.
- [14] H. Wiener, "Structural determination of paraffin boiling points," *Journal of the American Chemical Society*, vol. 69, no. 1, pp. 17–20, 1947.
- [15] M. Randic, "Characterization of molecular branching," *Journal of the American Chemical Society*, vol. 97, no. 23, pp. 6609–6615, 1975.
- [16] A. Aslam, S. Ahmad, M. A. Binyamin, and W. Gao, "Calculating topological indices of certain OTIS interconnection networks," *Open Chemistry*, vol. 17, no. 1, pp. 220–228, 2019.
- [17] M. Azeem, A. Aslam, Z. Iqbal, M. A. Binyamin, and W. Gao, "Topological aspects of 2D structures of trans-Pd(NH2)S lattice and a metal-organic superlattice," *Arabian Journal of Chemistry*, vol. 14, no. 3, article 102963, 2021.
- [18] X. Zhao, H. Ali, B. Ali, M. A. Binyamin, J. B. Liu, and A. Raza, "Statistics and calculation of entropy of dominating David derived networks," *Complexity*, vol. 2021, Article ID 9952481, 15 pages, 2021.
- [19] B. Bollobás and P. Erdös, "Graphs of extremal weights," Ars Combinatoria, vol. 50, pp. 225–233, 1998.
- [20] I. Gutman and K. C. Das, "The first Zagreb index 30 years after," MATCH Communications in Mathematical and in Computer Chemistry, vol. 50, no. 1, pp. 83–92, 2004.
- [21] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, no. 4, pp. 535–538, 1972.
- [22] I. Gutman, N. Trinajstic, and C. F. Wilcox, "Graph theory and molecular orbitals. XII. Acyclic polyenes," Journal of Chemical Physics, vol. 62, no. 9, pp. 3399–3405, 1975.
- [23] V. R. Kulli, "On K Banhatti indices of graphs," *Journal of Computer and Mathematical Sciences*, vol. 7, no. 4, pp. 213–218, 2016.
- [24] V. R. Kulli, "Hyper Zagreb-K-Banhatti indices of graphs," *International Journal of Mathematics Trends and Technology*, vol. 66, no. 8, pp. 123–130, 2020.

- [25] V. R. Kulli, "New K Banhatti topological indices," *International Journal of Fuzzy Mathematical Archive*, vol. 12, no. 1, pp. 29–37, 2017.
- [26] V. R. Kulli, "Harmonic Zagreb-K-Banhatti Index of a Graph," *International Journal of Mathematics Trends and Technology*, vol. 66, no. 10, pp. 123–132, 2020.
- [27] C. K. Gupta, V. Lokesha, S. B. Shwetha, and P. S. Ranjini, "On the symmetric division deg index of graph," *Southeast Asian Bulletin of Mathematics*, vol. 40, no. 1, pp. 41–51, 2016.
- [28] V. Lokesha and T. Deepika, "Symmetric division deg index of tricyclic and tetracyclic graphs," *International Journal of Scientific and Engineering Research*, vol. 7, pp. 53–55, 2016.
- [29] L. Zhong, "The harmonic index for graphs," Applied Mathematics Letters, vol. 25, no. 3, pp. 561–566, 2012.
- [30] E. Estrada, L. Torres, L. Rodriguez, and I. Gutman, "An atombond connectivity index: modelling the enthalpy of formation of alkanes," *Indian Journal of Chemistry*, vol. 37A, pp. 849– 855, 1998.
- [31] D. Vukicevic and B. Furtula, "Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges," *Journal of Mathematical Chemistry*, vol. 46, no. 4, pp. 1369–1376, 2009.