Research Article

Computation of Revan Topological Indices for Phenol-Formaldehyde Resin

Muhammad Kamran, Nadeem Salamat, Riaz Hussain Khan, Muhammad Abaid Ullah, Muhammad Shazib Hameed, and M. K. Pandit

1 Department of Mathematics, Khwaja Fareed University of Engineering & Information Technology, Rahim Yar Khan, Punjab 64200, Pakistan
2 Department of Life Sciences, Khwaja Fareed University of Engineering & Information Technology, Rahim Yar Khan, Punjab 64200, Pakistan
3 Department of Mathematics, Jahangirnagar University, Savar, Dhaka, Bangladesh

Correspondence should be addressed to M. K. Pandit; mkpandit@juniv.edu

Received 25 January 2022; Revised 1 April 2022; Accepted 5 April 2022; Published 27 April 2022

1. Introduction

Phenol-formaldehyde (PF) resin is a synthetic polymer created when phenol and formaldehyde combine. It is employed for a variety of purposes in many industries due to its molding ability. Phenolic resins are utilized in circuit boards such as PCBs and numerous electronic devices such as buttons, knobs, cameras, and vacuum cleaners. It is true. Laminate, fabric, and paper are all examples of where it is employed. Based on industrial practice, there are two types of production processes. In an alkaline solution, excess formaldehyde reacts with phenol. In the second approach, an excessive amount of phenol reacts with [1]. Formaldehyde is an acidic solution. It was initially used in the early twentieth century.

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 properties of compounds. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. They described the structure of molecules numerically and displayed that it is 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]. Atoms are represented by vertices in chemical networks, and bonding is represented by vertices in chemical graph theory [3, 4]. A topological index is the numerical parameter that predicts the characteristics of that chemical graph.

In this article, \( G \) be a connected simple chemical structure, with \( V(G) \) vertices set and \( E(G) \) edges set. The degree of any vertex \( u \) is denoted by \( \delta(u) \). The edge between vertices \( u \) and \( v \) is denoted by \( uv \). In the present work, we have calculated degree-based Revan topological indices. Let \( \delta(G) \) be the minimum degree and \( \Delta(G) \) be the maximum degree in \( G \). The Revan degree of vertex \( u \) is \( \delta_u = \delta(G) + \delta(G) - \delta(u) \).

The topological index was evolved by Wiener, in 1945, while researching the alkane’s boiling point [5, 6]. 1st degree-based topological index was represented by Milan Randić,
Revan 1st and 2nd topological indices were introduced by Kulli in [8]; for study, see [9].

\[ R_1(G) = \sum_{uv \in \Gamma(G)} (\mathcal{A}_u + \mathcal{A}_v), \]

\[ R_2(G) = \sum_{uv \in \Gamma(G)} (\mathcal{A}_u \cdot \mathcal{A}_v). \]

(1)

The 1st and 2nd hyper Revan indices were introduced by Kulli in [10] as follows:

\[ HR_1(G) = \sum_{uv \in \Gamma(G)} (\mathcal{A}_u + \mathcal{A}_v)^2, \]

\[ HR_2(G) = \sum_{uv \in \Gamma(G)} (\mathcal{A}_u \cdot \mathcal{A}_v)^2. \]

(2)

The 1st and 2nd modified Revan indices were introduced by Kulli in [11] as follows:

\[ mR_1(G) = \sum_{uv \in \Gamma(G)} \frac{1}{(\mathcal{A}_u + \mathcal{A}_v)}, \]

\[ mR_2(G) = \sum_{uv \in \Gamma(G)} \frac{1}{(\mathcal{A}_u \cdot \mathcal{A}_v)}. \]

(3)

The sum connectivity Revan index was defined by Kulli in [12].

\[ SR(G) = \sum_{uv \in \Gamma(G)} \frac{1}{(\mathcal{A}_u + \mathcal{A}_v)}. \]

(4)

The product connectivity Revan index was defined by Kulli in [13].

\[ PR(G) = \sum_{uv \in \Gamma(G)} \frac{1}{(\mathcal{A}_u \cdot \mathcal{A}_v)}. \]

(5)

The F-Revan was introduced as [14].

\[ FR(G) = \sum_{uv \in \Gamma(G)} \left( \mathcal{A}_u^2 + \mathcal{A}_v^2 \right). \]

(6)

The symmetric division Revan index is defined as follows: the method of [15] is used for surface determination of polychlorobiphenyls [16] and formulated as follows:

\[ SDD(G) = \sum_{uv \in \Gamma(G)} \left( \frac{\mathcal{A}_u}{\mathcal{A}_v} + \frac{\mathcal{A}_v}{\mathcal{A}_u} \right). \]

(7)

The harmonic Revan index is defined as: [15].

\[ H(G) = \sum_{uv \in \Gamma(G)} \frac{2}{\mathcal{A}_u + \mathcal{A}_v}. \]

(8)

Inverse sum Revan index is: [15].

\[ I(G) = \sum_{uv \in \Gamma(G)} \frac{\mathcal{A}_u \cdot \mathcal{A}_v}{\mathcal{A}_u + \mathcal{A}_v}. \]

(9)

2. Formation of the Phenol-Formaldehyde Resin Polymer Chain

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

3. Formation of the Crosslinked Phenol-Formaldehyde Resin 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.

3.1. Results

Theorem 1. The first Revan index of the phenol-formaldehyde resin polymer chain is follows:

\[ R_1(G) = 28h, \]

\[ R_1(G) = \sum_{uv \in \Gamma(G)} (\mathcal{A}_u + \mathcal{A}_v), \]

\[ = (3 + 1)(h + 1) + (2 + 2)(2h + 1) + (2 + 1)(4h + 1) (2h - 1) \]

\[ = 4(h + 1) + 4(2h + 1) + 3(4h - 2) + 2(2h - 1) \]

\[ = 28h. \]

(10)

and the crosslinked phenol-formaldehyde resin PF's structure is as follows:

\[ R_1(G) = 187n. \]

(11)

Results are obtained using Figure 1 and Table 1.

Proof. Let
Theorem 3. The hyper first Revan index of the phenol-formaldehyde resin polymer chain is as follows:

$$HR_1 (G) = \sum_{uv \in \Gamma (G)} (|\mathfrak{S}_u| + |\mathfrak{S}_v|)^2,$$

$$= (3 + 1)^2 (h + 1) + (2 + 2)^2 (2h + 1) + (2 + 1)^2 (4h - 2) + (1 + 1)^2 (2h - 1)$$

$$= 16(h + 1) + 16(2h + 1) + 9(4h - 2) + 4(2h - 1)$$

$$= 92h + 10.$$
Using the same formula for Figure 2 and Table 2, we get the result of the crosslinked phenol-formaldehyde (PF) resin structure as follows:

\[ HR_1(G) = 593n. \]  

(21)

\[ HR_2(G) = \sum_{uv \in \Gamma(G)} (\mathcal{I}_u \cdot \mathcal{I}_v)^2, \]

\[ HR_2(G) = \sum_{1,3 \in \Gamma(G)} (\mathcal{I}_u \cdot \mathcal{I}_v)^2 + \sum_{2,2 \in \Gamma(G)} (\mathcal{I}_u \cdot \mathcal{I}_v)^2 + \sum_{2,3 \in \Gamma(G)} (\mathcal{I}_u \cdot \mathcal{I}_v)^2 + \sum_{3,3 \in \Gamma(G)} (\mathcal{I}_u \cdot \mathcal{I}_v)^2 \]

(24)

\[ = (3 \cdot 1)^2 (h + 1) + (2 \cdot 2)^2 (2h + 1) + (2 \cdot 1)^2 (4h - 2) + (1 \cdot 1)^2 (2h - 1) \]

\[ = 9(h + 1) + 16(2h + 1) + 4(4h - 2) + (2h - 1) \]

\[ = 59h + 16. \]

Using the same formula for Figure 2 and Table 2, we get the result of the crosslinked phenol-formaldehyde (PF) resin structure as follows:

\[ HR_2(G) = 321n. \]  

(25)

\[ mR_1(G) = \frac{37}{12} h - \frac{2}{3}, \]  

(26)

and the crosslinked phenol-formaldehyde (PF) resin structure is given below:

\[ HR_2(G) = 321n. \]  

(23)

The result is obtained using Figure 1 and Table 1.

**Theorem 4.** The second hyper Revan index of the phenol-formaldehyde resin polymer chain is as follows:

\[ HR_2(G) = 59h + 16, \]  

(22)

**Proof.** Let

Using the same formula for Figure 2 and Table 2, we get the result of the crosslinked phenol-formaldehyde (PF) resin structure as follows:

\[ HR_2(G) = 321n. \]  

(25)

\[ mR_1(G) = \frac{433}{20} n. \]  

(27)

The result is obtained using Figure 1 and Table 1.
Proof. Let

\[ mR_1(G) = \sum_{uv \in \Gamma(G)} \frac{1}{3_u + 3_v}, \]

\[ mR_1(G) = \sum_{1,3 \in \Gamma(G)} \frac{1}{3_u} + \sum_{2,3 \in \Gamma(G)} \frac{1}{3_u + 3_v} + \sum_{3,3 \in \Gamma(G)} \frac{1}{3_u + 3_v}, \]

\[ = \frac{(h + 1)}{(3 + 1)} + \frac{(2h + 1)}{(2 + 2)} + \frac{(4h - 2)}{(2 + 1)} + \frac{(2h - 1)}{(1 + 1)} \]

\[ = \frac{(h + 1)}{4} + \frac{(2h + 1)}{4} + \frac{(4h - 2)}{3} + \frac{(2h - 1)}{2} \]

\[ = \frac{37h - 2}{12}, \]

Using the same formula for Figure 2 and Table 2, we get the result of crosslinked phenol-formaldehyde (PF) resin structure as follows:

\[ mR_1(G) = \frac{433}{20} n. \]

(29)

□

Theorem 6. The modified second Revan index of the phenol-formaldehyde resin polymer chain is as follows:

\[ mR_2(G) = \sum_{uv \in \Gamma(G)} \frac{1}{3_u \cdot 3_v}, \]

\[ mR_2(G) = \sum_{1,3 \in \Gamma(G)} \frac{1}{3_u \cdot 3_v} + \sum_{2,3 \in \Gamma(G)} \frac{1}{3_u + 3_v} + \sum_{3,3 \in \Gamma(G)} \frac{1}{3_u + 3_v} \]

\[ = \frac{(h + 1)}{(3 + 1)} + \frac{(2h + 1)}{(2 + 2)} + \frac{(4h - 2)}{(2 + 1)} + \frac{(2h - 1)}{(1 + 1)} \]

\[ = \frac{(h + 1)}{3} + \frac{(2h + 1)}{4} + \frac{(4h - 2)}{2} + (2h - 1) \]

\[ = \frac{29h - 17}{12}, \]

(30)

and the crosslinked phenol-formaldehyde (PF) resin structure is as below:

\[ mR_2(G) = \frac{209}{6} n, \]

(31)

The result is obtained using Figure 1 and Table 1.

Proof. Let

\[ mR_2(G) = \frac{209}{6} n. \]

(32)

□

Theorem 7. The sum Revan index of the phenol-formaldehyde (PF) resin polymer chain is given below:

\[ SR(G) = 5.22h - 0.86, \]

(33)

and the crosslinked phenol-formaldehyde (PF) resin structure is as follows:

\[ SR(G) = 5.22h - 0.86, \]

□
Theorem 8. The product Reivan index of the phenol-formaldehyde resin polymer chain is given:

\[
SR(G) = 36.39n. \tag{35}
\]

Proof. Let

\[
SR(G) = \sum_{u,v \in V(G)} \frac{1}{\sqrt{(3_u + 3_v)}}
\]

\[
SR(G) = \sum_{1,3 \in \Gamma(G)} \frac{1}{\sqrt{(3_u + 3_v)}} + \sum_{2,2 \in \Gamma(G)} \frac{1}{\sqrt{(3_u + 3_v)}} + \sum_{2,3 \in \Gamma(G)} \frac{1}{\sqrt{(3_u + 3_v)}} + \sum_{3,3 \in \Gamma(G)} \frac{1}{\sqrt{(3_u + 3_v)}}
\]

\[
= \frac{(h + 1)}{\sqrt{3}} + \frac{(2h + 1)}{\sqrt{4}} + \frac{(4h - 2)}{\sqrt{2}} + \frac{(2h - 1)}{\sqrt{2}}
\]

\[
= 5.22h - 0.86.
\]

Using the same formula for Figure 2 and Table 2, we get the result of the crosslinked phenol-formaldehyde (PF) resin structure as below:

\[
SR(G) = 36.39n. \tag{37}
\]

The result is obtained using Figure 1 and Table 1.

\[\begin{align*}
\text{PR}(G) &= 6.41h - 1.34, \tag{38} \\
\text{and the crosslinked phenol-formaldehyde (PF) resin structure is given below:} & \\
\text{PR}(G) &= 45.59n. \tag{39}
\end{align*}\]

The result is obtained using Figure 1 and Table 1.

Proof. Let

\[
PR(G) = \sum_{u,v \in V(G)} \frac{1}{\sqrt{(3_u + 3_v)}}
\]

\[
PR(G) = \sum_{1,3 \in \Gamma(G)} \frac{1}{\sqrt{(3_u + 3_v)}} + \sum_{2,2 \in \Gamma(G)} \frac{1}{\sqrt{(3_u + 3_v)}} + \sum_{2,3 \in \Gamma(G)} \frac{1}{\sqrt{(3_u + 3_v)}} + \sum_{3,3 \in \Gamma(G)} \frac{1}{\sqrt{(3_u + 3_v)}}
\]

\[
= \frac{(h + 1)}{\sqrt{(3 \cdot 1)} + \frac{(2h + 1)}{\sqrt{(2 \cdot 2)}} + \frac{(4h - 2)}{\sqrt{(2 \cdot 1)}} + \frac{(2h - 1)}{\sqrt{(1 \cdot 1)}}}
\]

\[
= \frac{(h + 1)}{\sqrt{3}} + \frac{(2h + 1)}{\sqrt{4}} + \frac{(4h - 2)}{\sqrt{2}} + \frac{(2h - 1)}{\sqrt{2}}
\]

\[
= 6.41h - 1.34.
\]

Using the same formula for Figure 2 and Table 2, we get the result of the crosslinked phenol-formaldehyde (PF) resin structure as below:

\[
PR(G) = 45.59n. \tag{41}
\]

Theorem 9. The F-Reivan index of the phenol-formaldehyde resin polymer chain is shown below:

\[
FR(G) = 50h + 6. \tag{42}
\]

and the crosslinked phenol-formaldehyde (PF) resin structure is as follows:
The result is obtained using Figure 1 and Table 1.

**Proof.** Let

\[ \text{FR}(G) = 335n. \]  \hspace{1cm} (43)

Using the same formula for Figure 2 and Table 2, we get the result of the crosslinked phenol-formaldehyde (PF) resin structure as below:

\[ \text{FR}(G) = 335n. \]  \hspace{1cm} (45)

**Theorem 10.** The harmonic Revan index of the phenol-formaldehyde resin polymer chain is as follows:

\[ \text{HR}(G) = \frac{37 \cdot h - 4}{3}. \]  \hspace{1cm} (46)

**Proof.** Let

\[ \text{HR}(G) = \sum_{u \in \Gamma(G)} \left( \frac{2}{3u} + \frac{2}{3v} \right) \]

\[ = \left( \frac{2}{3} \right) \left( h + 1 \right) + \left( \frac{2}{3} \right) \left( 2h + 1 \right) + \left( \frac{2}{3} \right) \left( 4h - 2 \right) + \left( \frac{2}{3} \right) \left( 2h - 1 \right) \]

\[ = 10(h + 1) + 8(2h + 1) + 5(4h - 2) + 2(2h - 1) \]

\[ = 50h + 6. \]

Using the same formula for Figure 2 and Table 2, we get the result of the crosslinked phenol-formaldehyde (PF) resin structure as given below:

\[ \text{FR}(G) = 335n. \]  \hspace{1cm} (49)

and the crosslinked phenol-formaldehyde (PF) resin structure is below:

\[ \text{HR}(G) = \frac{433}{10} \cdot n. \]  \hspace{1cm} (47)

**Theorem 11.** The sum division Revan index of phenol-formaldehyde resin polymer chain is as follows:

\[ \text{SDR}(G) = \frac{64}{3} \cdot h - \frac{5}{3}. \]  \hspace{1cm} (50)

and the crosslinked phenol-formaldehyde (PF) resin structure is given below:

\[ \text{SDR}(G) = \frac{935}{6} \cdot n. \]  \hspace{1cm} (51)
The result of the crosslinked phenol-formaldehyde (PF) resin structure as below:

**Theorem 12.** The inverse Reivan index of the phenol-formaldehyde resin polymer chain is given below:

\[
\text{IR}(G) = \sum_{uv \in \Gamma(G)} \frac{3u \cdot 3v}{(3u + 3v)}
\]

Using the same formula for Figure 2 and Table 2, we get the result of the crosslinked phenol-formaldehyde (PF) resin structure as below:

\[
\text{SDR}(G) = \frac{935}{6} n
\]

Using the same formula for Figure 2 and Table 2, we get the result of the crosslinked phenol-formaldehyde (PF) resin structure is given below:

\[
\text{IR}(G) = \frac{77}{12} h - \frac{1}{12}
\]

**Proof.** Let

\[
\text{SDR}(G) = \sum_{uv \in \Gamma(G)} \left[ \frac{3u + 3v}{3u} \right],
\]

\[
\text{SDR}(G) = \sum_{1,3 \in \Gamma(G)} \left[ \frac{3u + 3v}{3u} \right] + \sum_{2,2 \in \Gamma(G)} \left[ \frac{3u + 3v}{3u} \right] + \sum_{2,3 \in \Gamma(G)} \left[ \frac{3u + 3v}{3u} \right] + \sum_{3,3 \in \Gamma(G)} \left[ \frac{3u + 3v}{3u} \right]
\]

\[
= \frac{3}{1} + \frac{1}{3} (h + 1) + \frac{2}{2} \left( 2h + 1 \right) + \frac{1}{1} \left( 4h - 2 \right) + \frac{1}{1} \left( 2h - 1 \right)
\]

\[
= \frac{10}{3} (h + 1) + 2(2h + 1) + \frac{5}{2} (4h - 2) + 2(2h - 1)
\]

\[
= \frac{64}{3} n - \frac{5}{3}
\]
Using the same formula for Figure 2 and Table 2, we get the result of the crosslinked phenol-formaldehyde (PF) resin structure as below:

\[ \text{IR} \left( \frac{G}{\text{equiv}} \right) = \frac{823}{20} n. \]  

4. Numerical and Graphical Representation

The numerical and graphical representation of the results for the phenol-formaldehyde resin polymer chain is exhibited in Figures 3 and 4. Table 1 depicts the mathematical equations as topological indices. Furthermore, these indices are being

Comparison

<table>
<thead>
<tr>
<th>Figure 4: Comparison of $mR_1$ (PF), $mR_2$ (PF), SR (PF), PR (PF), $H(R)$, and IR (PF).</th>
</tr>
</thead>
<tbody>
<tr>
<td>( mR_1(G) )</td>
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<tr>
<td>( mR_2(G) )</td>
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<tr>
<td>( SR(G) )</td>
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<tr>
<td>( PR(G) )</td>
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<tr>
<td>( HR(G) )</td>
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<td>( IR(G) )</td>
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</tbody>
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Comparison

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<tr>
<th>Figure 5: Comparison of ( R_1 ) (PF), ( R_2 ) (PF), ( HR_1 ) (PF), ( HR_2 ) (PF), FR (G), and SDR (PF).</th>
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<tbody>
<tr>
<td>( R_1(G) )</td>
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<tr>
<td>( R_2(G) )</td>
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<tr>
<td>( HR_1(G) )</td>
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<tr>
<td>( HR_2(G) )</td>
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<tr>
<td>( FR(G) )</td>
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<td>( SDR(G) )</td>
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Comparison

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<tr>
<th>Figure 6: Comparison of $mR_1$ (PF), $mR_2$ (PF), SR (PF), PR (PF), $H(R)$, and IR (PF).</th>
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<tbody>
<tr>
<td>( mR_1(G) )</td>
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<tr>
<td>( mR_2(G) )</td>
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<tr>
<td>( SR(G) )</td>
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<td>( PR(G) )</td>
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<td>( HR(G) )</td>
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<td>( IR(G) )</td>
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</tbody>
</table>
illustrated graphically in Figures 3 and 4. 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 Table 1.

The numerical and graphical representation of above computed results for crosslinked phenol-formaldehyde (PF) resin structure is depicted in Figures 5 and 6. Table 2 depicts 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 Table 2.

5. Conclusion

In this research article, the Revan vertex degree of phenol-formaldehyde resin was found and subjected to calculate degree-dependent Revan topological indices. These topological indices will be helpful to improve the for the synthetic production and quality of PCBs and numerous electronic devices on commercial bases.

Data Availability

The data used to support the findings of this study are available and can be provided over e-mail, querying directly the authors at kamrankfueit@gmail.com and mkpandit@juniv.edu.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors’ Contributions

Nadeem Salamat (NS) and Muhammad Kamran (MK) extracted and analyzed the data and drafted the figures. Riaz Hussan Khan (RHK), Muhammad Shazaib Hameed (MSH), and M. K. Pandit (MKP) conceptualized and drafted the graphs. Muhammad Kamran, Riaz Hussan Khan, and M. K. Pandit drafted the manuscript. Muhammad Kamran and Muhammad Abaid Ullah (MA) reviewed this article and corrected the English. Nadeem Salamat and Muhammad Kamran contributed equally to this work and are to be considered as co-first authors.

References