Journal of Science-FAS-SEUSL (2025) 06(02) 48-58
ISSN:2738-2184

Graph - Theoretical Analysis of Supramolecular Fuchsine Acid via Revan Topological Indices

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Abstract
Chemical graph theory provides a mathematical framework for modeling molecular structures by representing atoms as vertices and chemical bonds as edges. In Quantitative Structure–Property Relationship (QSPR) and Quantitative Structure–Activity Relationship (QSAR) analyses, degree-based topological indices serve as numerical descriptors that correlate structural features with physicochemical properties. Such indices play a vital role in drug discovery, and molecular modeling. In this work, we investigate the supramolecular sheet structure of fuchsine ($C_{20}H_{19}N_3HCl$), an important magenta dye widely used in microbiological and histological applications. The supramolecular architecture is constructed by arranging fuchsine molecules in an $m \times n$ array, denoted by $F[m,n]$. The associated chemical graph is simple, connected, and finite, comprising $38mn + m + n$ vertices and $42mn$ edges, formulated using Revan degrees of terminal vertices. We derive closed-form expressions for several Revan degree-based topological indices, including the first and second Revan indices (R_1 and R_2), Atomic Bond Connectivity Revan index ($ABCR$), Geometric–Arithmetic Revan index (GAR), first and second hyper Revan indices (HR_1 and HR_2), first and second modified Revan indices (${}^mR_1$ and ${}^mR_2$), and the Forgotten Revan index (FR). This study provides a comprehensive mathematical characterization of the supramolecular fuchsine sheet and enriches the theoretical foundation of Revan-based molecular descriptors.

Keywords: Chemical graph theory; Revan degree; Topological indices; Supramolecular fuchsine; QSPR/QSAR; Mathematical chemistry.

Introduction
Supramolecular chemistry examines the way of creating higher-order structures through molecular interactions. Molecular self-assembly, the primary concept of Supramolecular chemistry is broadly focused on constructing new chemical structures without external direction[1]. Supramolecular structures utilize reversible and fragile non-covalent intermolecular associations, which is a like the linkage of molecules with atoms. This studies the formation of a non-covalently bonded tiny molecule to an extensive molecule. Supramolecular chemistry is widely applied in drug design, biotic procedures, tissue engineering, and as a detector for specific analyses. For instance, Fuchsine $C_{20}H_{19}N_3HCl$ is a supramolecular dye which enhances the effectiveness of a treatment by helping to produce effective drug carriers with minimum side effects. Additionally, Fuchsine is an active agent utilizes for cloth dyeing, bacteria staining and sometimes as a disinfectant. In recent years, Graph Theory has emerged as a crucial mathematical discipline for studying chemical structures. Topological descriptors are employed

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to analyse hydrogen-suppressed molecular graphs, in which the edges represent the molecular bonds and the atoms are located at the vertices [1].

A topological index is a numerical value that characterizes the arrangement of connections in a network. Topological indices, which are important in Chemical Graph Theory, have a well-established significance in studying the chemical properties of medications. Pharmaceutical researchers utilize a wide range of topological descriptors. A topological index quantitatively characterizes the shape of a molecule and is employed in the development of qualitative structure-property relationships/qualitative structure-activity relationships (QSPRs/QSARs). Various graph indexes based on degrees have been documented in the literature [2] and have been applied in specific contexts [3, 4]. There exist three distinct categories of topological indices, as mentioned in [5]: degree-based, distance-based, and spectral-based indices. Degree-based indices are widely favoured among the several categories of indices. Topological indices are highly valuable in the process of chemical validation, as well as in QSAR/QSPR research and the development of pharmaceutical drugs. Extensive research has been conducted on degree-based indices, which are believed to be linked to various characteristics of the chemical compounds under investigation. This study aims to provide a more in-depth analysis of molecular descriptors based on degrees.

Harold Wiener introduced the notion of topological indices while studying paraffins, which are alkenes with a high boiling point [6]. The Wiener index, which is the earliest topological index, was introduced by him in 1947. He assigned it the designation of path number. As advancements were made in the field of chemical graph theory, the path number was officially designated as the Wiener index. The Wiener index is extensively studied in chemical graph theory due to its distinctive theoretical features and wide range of applications [5, 7].

In his seminal 1975 paper, Milan Randic [8] introduced the first realistic degree-based topological index. Originally, Randic referred to it as the branching index, but it was later renamed as the connectedness index. Currently, it is widely recognized and referred to as the Randic index, which is precisely defined as,

$R_{-\frac{1}{2}}(G) = \frac{1}{\sqrt{d_G(U)d_G(v)}}$ where $d_G(u)$ and $d_G(v)$ represents the degrees of vertices u and v.

In 1972, I. Gutman and N. Trinanjtic studied dependency of the total π-electron energy of a molecular on its structure [9]. The calculation can be determined by summing the squares of the degrees at each vertex. Subsequently, this total was named the first Zagreb index, and subsequent investigations have been conducted on it [10]. The first Zagreb index is defined as,

$$M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))$$

and the second Zagreb index as,

$$M_2(G) = \sum_{uv \in E(G)} (d_G(u) d_G(v))$$

Furthermore, the literature has almost 3000 topological indices. In our study, we focus on Reven degree based topological indices. Let us assume that *G* is a connected graph that is finite, simple, and possesses vertex and edge sets that are represented by the notations $V(G)$ and $E(G)$ respectively. The number of vertices that are next to a vertex u is what determines the degree of that vertex, which is denoted by the expression $d_G(u)$. In the context of the graph *G*, let $\Delta(G)$ represent the degree that is highest among the vertices of *G* while $\delta(G)$ denotes the lowest degree among the vertices of *G*. When considering the graph *G*, the Revan vertex degree of u is defined by the expression $r_G(u) = \Delta(G) + \delta(G) - d_G(u)$. In this particular setting, the symbol uv is used to represent the Revan edge that constitutes the connection between the Revan vertices u and v. In this work, we study on the degree-based Revan topological indices.

Kulli [11] introduced the first and second Revan indices based on the Zagreb indices as follows,
$R_1(G) = \sum_{uv\in E(G)}(r_G(u) + r_G(v))$ and $R_2(G) = \sum_{uv\in E(G)}(d_G(u)d_G(v))$.

In [13], Kulli proposed the first and second hyper Revan indices and defined as,

$$HR_1(G) = \sum_{uv\in E(G)} (r_G(u) + r_G(v))^2 \quad HR_2(G) = \sum_{uv\in E(G)} (r_G(u)r_G(v))^2$$

In 2018, the Atomic Bond Connectivity Revan index and Geometric Arithmetic index of a molecular graph *G* [14] were introduced by Kulli and defined as,

$$ABCR(G) = \sum_{uv\in E(G)} \sqrt{\frac{r_G(u) + r_G(v) - 2}{r_G(u)r_G(v)}}$$

$$GAR(G) = \sum_{uv\in E(G)} \frac{2\sqrt{r_G(u)r_G(v)}}{r_G(u)+r_G(v)}$$

The first and second modified Revan indices of a molecular graph *G* were defined by Kulli in [16] as,

$$^{m}R_1(G) = \sum_{uv\in E(G)} \frac{1}{d_G(u)+d_G(v)}$$

$$^{m}R_2(G) = \sum_{uv\in E(G)} \frac{1}{d_G(u)d_G(v)}$$

In 2018, Kulli [15] proposed the forgotten Revan index (F-Revan index) of a molecular graph *G* and formulated as,

$$FR(G) = \sum_{uv\in E(G)} (r_G(u)^2 + r_G(v)^2)$$

Additional information and examples of how Revan indices can be applied can be found in [19-23].

In 2022, A. Ullah et al. conducted a study on the irregular topological indices of the supramolecular sheet of fuchsine acid [24]. In 2024, Kosar et al. [1] calculated and compared various indices, including the Atomic - bond connectivity index, *GA* index, General Randic index, first and second Zagreb index, first hyper Zagreb index, Harmonic index, and Forgotten index. These calculations were performed on the supramolecular structure of Fuchsine acid. This

work aims to examine the Revan topological indices of the supramolecular sheet of fuchsine acid.

Methodology

Within the scope of this study, we take into consideration a supramolecular fuchsine molecule that has the chemical formula $C_{20}H_{19}N_3HCl$. Subsequently, we construct a sheet structure by connecting $a \times b$ units using the unit cell of this compound. We have considered the atoms as vertices and bonds as the edges of this molecular graph. We take this sheet structure as $F[a,b]$. Then we have $38ab + a + b$ vertices and $42ab$ edges. For computing the topological indices, we need to find the edge partitions of $F[a,b]$. Based on Revan degree of Revan end vertices of each Revan edge of $F[a,b]$, three types of edge partitions of Revan edges can be identified.

$$RE_1 = \{uv \in E(F[a,b]) | r(u) = 1, r(v) = 1\}, \qquad |RE_1| = 24ab$$

$$RE_2 = \{uv \in E(F[a,b]) | r(u) = 1, r(v) = 3\}, \qquad |RE_2| = 14ab + 2a + 2b$$

$$RE_3 = \{uv \in E(F[a,b]) | r(u) = 2, r(v) = 1\}, \qquad |RE_3| = 4ab - 2a - 2b$$

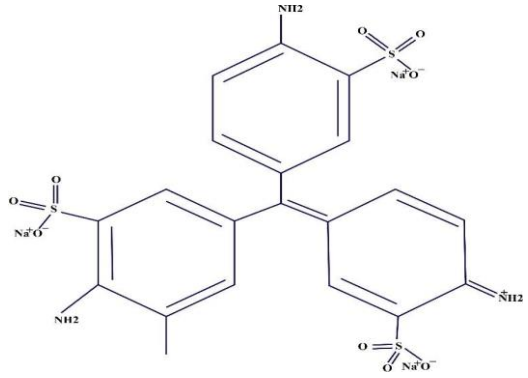

Figure 1: Chemical structure of fuchsine acid

Main Results

Using the edge classification according to the Revan degrees of the end vertices, we now compute the closed-form expressions of the Revan topological indices for the graph $F[a,b]$.

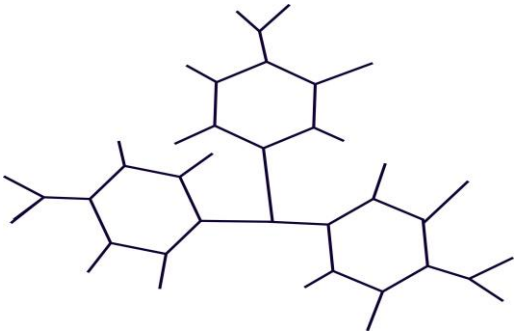

Figure 2: 2D structure of $F[1,1]$

Figure 2 illustrates the 2D structure of $F[1,1]$, which serves as the base unit for the general graph $F[a,b]$. This structure is used to identify the different types of vertices and to determine their corresponding Revan degrees. From this graphical representation, the edges are partitioned according to the Revan degrees of their end vertices. This edge classification enables the computation of the atomic bond connectivity Revan index by systematically counting the number of edges in each partition. The coefficients appearing in the final formula are obtained from this edge partitioning process.

Theorem 1.

The first and second Revan indices of $F[a,b], a,b \geq 1$ *are given by,*

$$R_1(F[a,b]) = 116ab + 2a + 2b$$
$$R_2(F[a,b]) = 74ab + 2a + 2b$$

Proof. The first Revan index is computed as follows.

$$\begin{aligned}
&R_1(F[a,b]) \\
&= \sum_{uv \in E(G)} (r_G(u) + r_G(v)) \\
&= \sum_{uv \in E_1(G)} (r_G(u) + r_G(v)) + \sum_{uv \in E_2(G)} (r_G(u) + r_G(v)) + \sum_{uv \in E_3(G)} (r_G(u) + r_G(v)) \\
&= (24ab)(1+1) + (14ab + 2(a+b))(1+3) + (b(2a-2) + 2a(b-1))(2+1) \\
&= 116ab + 2a + 2b
\end{aligned}$$

The second Revan index of $F[a,b]$ is computed as below.

$$\begin{aligned}
R_2(F[a,b]) &= \sum_{uv \in E(G)} (r_G(u) r_G(v)) \\
&= \sum_{uv \in E_1(G)} (r_G(u) r_G(v)) + \sum_{uv \in E_2(G)} (r_G(u) r_G(v)) + \sum_{uv \in E_3(G)} (r_G(u) r_G(v)) \\
&= (24ab)(1) + (14ab + 2a + 2b)(3) + (b(2a-2) + 2a(b-1))(2) \\
&= 74ab + 2a + 2b
\end{aligned}$$

This is end of the proof.

Theorem 2.

Let $a, b \geq 1$. *The atomic bond connectivity Revan index of* $F[a,b]$ *is given by,*

$$ABCR(F[a,b]) = (14ab + 2a + 2b)\sqrt{\frac{2}{3}} + (14ab - 2a - 2b)\sqrt{\frac{1}{2}}.$$

Proof. By the help of the edge partitions of Revan degree of Revan end vertices of each Revan edge, the atomic bond connectivity Revan index of $F[a,b]$ can be obtained as follows,

$$ABCR(F[a,b]) = \sum_{uv\in E(G)}\sqrt{\frac{r_G(u)+r_G(v)-2}{r_G(u)r_G(v)}}$$

$$= \sum_{uv\in E_1(G)}\sqrt{\frac{r_G(u)+r_G(v)-2}{r_G(u)r_G(v)}} + \sum_{uv\in E_2(G)}\sqrt{\frac{r_G(u)+r_G(v)-2}{r_G(u)r_G(v)}} + \sum_{uv\in E_3(G)}\sqrt{\frac{r_G(u)+r_G(v)-2}{r_G(u)r_G(v)}}$$

$$= (24ab)\sqrt{\frac{1+1-2}{1\times1}} + \big(14ab+2(a+b)\big)\sqrt{\frac{1+3-2}{1\times3}} + \big(b(2a-2)+2a(b-1)\big)\sqrt{\frac{2+1-2}{2\times1}}$$

$$= (14ab+2a+2b)\sqrt{\frac{2}{3}} + (14ab-2a-2b)\sqrt{\frac{1}{2}}$$

We complete the proof.

The Geometric-arithmetic Revan index of $F[a,b]$ is calculated in the next theorem.

Theorem 3.

Let a, b ≥ 1. The geometric-arithmetic Revan index of $F[a,b]$ is given by,

$$GAR(G) = 24ab + (14ab+2a+2b)\frac{\sqrt{3}}{2} + (4ab-2a-2b)\frac{2\sqrt{2}}{3}.$$

Proof. The geometric- arithmetic index of $F[a,b]$can be computed as follows,

$$GAR(F[a,b]) = \sum_{uv\in E(G)}\frac{2\sqrt{r_G(u)r_G(v)}}{r_G(u)+r_G(v)}$$

$$= \sum_{uv\in E_1(G)}\frac{2\sqrt{r_G(u)r_G(v)}}{r_G(u)+r_G(v)} + \sum_{uv\in E_2(G)}\frac{2\sqrt{r_G(u)r_G(v)}}{r_G(u)+r_G(v)} + \sum_{uv\in E_3(G)}\frac{2\sqrt{r_G(u)r_G(v)}}{r_G(u)+r_G(v)}$$

$$= (24ab)\frac{2\sqrt{1}}{1+1} + (14ab+2a+2b)\left(\frac{2\sqrt{1\times3}}{1+3}\right) + 2b(a-1)\frac{2\sqrt{2\times1}}{2+1}$$

$$= 24ab + (14ab+2a+2b)\frac{\sqrt{3}}{2} + (14ab-2a-2b)\frac{2\sqrt{2}}{3}$$

We complete the proof.

Theorem 4.

Let a, b ≥ 1. The first and second hyper Revan indices are given by,

$$HR_1(G) = 356ab + 14a + 14b \text{ and } HR_2(G) = 166ab + 10a + 10b.$$

Proof. Using the edge partitions of Reven degree of end Revan vertices of Revan edges of $F[a,b]$, the first hyper Revan index is can be obtained as follows,

$$HR_1(F[a,b]) = \sum_{uv\in E(G)}(r_G(u)+r_G(v))^2$$

$= \sum_{uv\in E_1(G)}\left(r_G(u)+r_G(v)\right)^2 + \sum_{uv\in E_2(G)}\left(r_G(u)+r_G(v)\right)^2 + \sum_{uv\in E_3(G)}(r_G(u)+r_G(v))^2$

$= \sum_{uv\in E_1(G)}(1)^2 + \sum_{uv\in E_2(G)}(3)^2 + \sum_{uv\in 3(G)}(2)^2$

$= (24ab)(1) + (14ab+2a+2b)(9) + (b(2a-2)+2a(b-1))(4)$

$= 166ab + 10a + 10b.$

Therefore, we complete the proof.

Theorem 5.

Let $a, b \geq 1$. The first and second modified Revan indices are given by,

$${}^{m}R_1(F[a,b]) = RHM_1 = \frac{101ab-a-b}{6}, \text{ and}$$

$${}^{m}R_2(F[a,b]) = RHM_2 = \frac{84ab-4a-4b}{3}.$$

Proof.

$${}^{m}R_1(F[a,b]) = \sum_{uv\in E(G)}\left(\frac{1}{r_G(u)+r_G(v)}\right)$$

$$= \sum_{uv\in E_1(G)}\left(\frac{1}{r_G(u)+r_G(v)}\right) + \sum_{uv\in E_2(G)}\left(\frac{1}{r_G(u)+r_G(v)}\right) + \sum_{uv\in E_3(G)}\left(\frac{1}{r_G(u)+r_G(v)}\right)$$

$$= (24ab)\times\frac{1}{1+1} + (14ab+2a+2b)\times\frac{1}{1+3} + \left(b(2a-2)+2a(b-1)\right)\times\frac{2}{2+1}$$

$$= \frac{101ab-a-b}{6}.$$

$${}^{m}R_2(F[a,b]) = \sum_{uv\in E(G)}\left(\frac{1}{r_G(u)r_G(v)}\right)$$

$$= \sum_{uv\in E_1(G)}\left(\frac{1}{r_G(u)r_G(v)}\right) + \sum_{uv\in E_2(G)}\left(\frac{1}{r_G(u)r_G(v)}\right) + \sum_{uv\in E_3(G)}\left(\frac{1}{r_G(u)r_G(v)}\right)$$

$$= (24ab)\times\frac{1}{1} + (14ab+2a+2b)\times\frac{1}{3} + \left(b(2a-2)+2a(b-1)\right)\times\frac{1}{4}$$

$$= \frac{92ab-a-b}{3}.$$

Theorem 6.

Let $a, b \geq 1$. *The F - Revan index of* $F[a,b]$ *is given by,*

$$FR(F[a,b]) = 208ab + 10a + 10b.$$

Proof.

$$FR(F[a,b]) = \sum_{uv\in E(G)}(r_G(u)^2 + r_G(v)^2)$$

$$= \sum_{uv\in E_1(G)}(r_G(u)^2 + r_G(v)^2) + \sum_{uv\in E_2(G)}(r_G(u)^2 + r_G(v)^2) + \sum_{uv\in E_3(G)}(r_G(u)^2 + r_G(v)^2)$$

$$= (24ab)(1+1) + \big(14ab + 2(a+b)\big)(1+9) + (b(2a-2) + 2a(b-1))(4+1)$$

$$= 208ab + 10a + 10b.$$

Table 1: Comparison of RL indices

G	R_1	R_2	$ABCR$	GAR	HR_1	HR_2	${}^mR_1$	${}^mR_2$	FR
F[1,1]	120	78	22	40	384	186	17	30	228
F[2,2]	472	304	86	159	1480	704	67	121	872
F[3,3]	1056	678	193	358	3288	1554	151	274	1932
F[4,4]	1872	1200	343	637	5808	2736	268	488	3408
F[5,5]	2920	1870	535	996	9040	4250	419	763	5300
F[6,6]	4200	2688	771	1434	12984	6096	604	1100	7608
F[7,7]	5712	3654	1048	1953	17640	8274	823	1498	10332
F[8,8]	7456	4768	1369	2551	23008	10784	1075	1957	13472
F[9,9]	9432	6030	1732	3229	29088	13626	1361	2478	17028
F[10,10]	11640	7440	2137	3986	35880	16800	1680	3060	21000

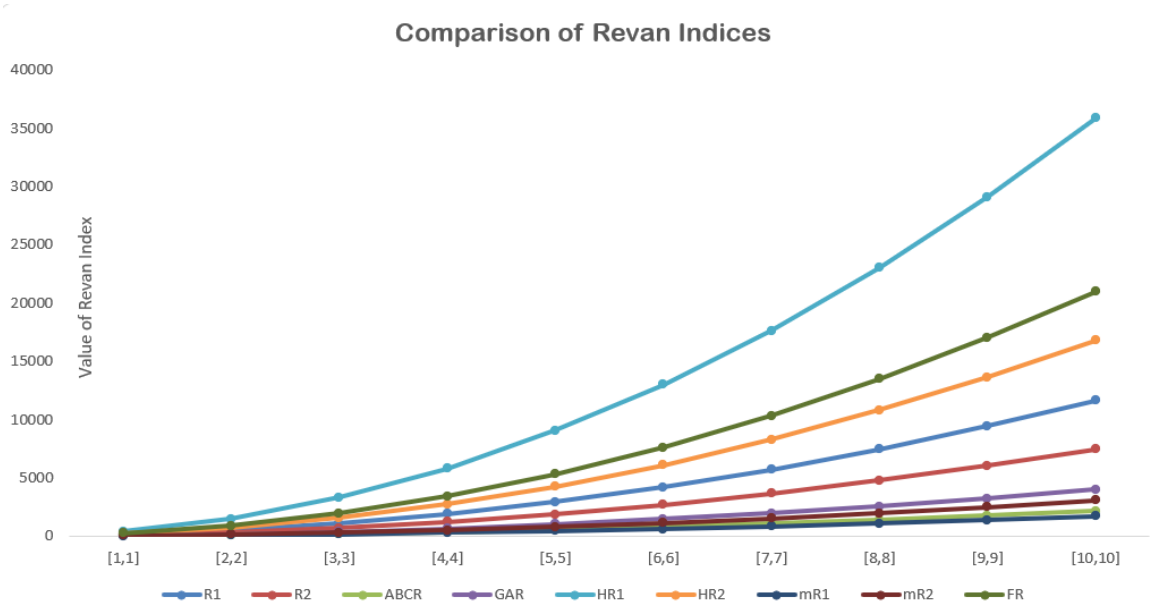

Figure 3: Comparison of Revan indices

Discussion

Table 1 presents a quantitative comparison of the chosen Revan indices for the supramolecular fuchsine acid. Additionally, Figure 3 illustrates a graphical comparison of the Revan indices values provided in Table 1. Furthermore, Figure 3 demonstrates that as the value of $a = b$ increases, the values of Revan topological indices also increase, as seen in Table 1.

Topological indicators are essential for predicting the physicochemical and biological characteristics of chemical compounds from a pharmaceutical and medical perspective. The calculated Revan indices may aid in comprehending molecular stability, reactivity, and structure–activity connections since fuchsine acid and its derivatives are often employed in biological stains and may have antibacterial and diagnostic uses. Without carrying out costly lab tests, these indices may be used in QSAR and QSPR modeling to assess characteristics including bioactivity, toxicity, solubility, and drug–receptor interactions.

Conclusion

This study presents the calculation of the Revan topological indices of the supramolecular graph of Fuchsine acid, which has practical applications in the field of computational chemistry. Furthermore, we have computed various Revan indices, including the first and second Revan indices (R_1 and R_2),the Atomic Bond Connectivity Revan index ($ABCR$), the Geometric-Arithmetic Revan index(GAR), the first and second hyper Revan indices (HR_1 and HR_2), the first and second modified Revan indices ($^mR_1$ and $^mR_2$), and the forgotten Revan index (FR). The numerical comparison of the above mentioned Revan indices is presented in Table 1, while the graphical comparison is provided in Figure 3. The calculated results can be used to determine the eccentricity and spectral based topological indices of supramolecular structures. In future study, we aim to examine the correlation between these Revan index values and the physio-chemical

properties of fuchsine acid. As well as to investigate the importance of these Revan indices compared to other topological indices.

Data availability

All data generated or analysed during this study are included in this manuscript.

Acknowledgements

The authors sincerely thank A. M. F. S. Sino for their dedicated assistance in the typesetting and formatting of this manuscript. Her support greatly contributed to the clarity and professional presentation of this work.

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