Hindawi
Journal of Chemistry
Volume 2022, Article ID 8131276, 8 pages
https://doi.org/10.1155/2022/8131276

Research Article

Network-Based Modeling of the Molecular Topology of Fuchsine Acid Dye with Respect to Some Irregular Molecular Descriptors

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Received 31 October 2022; Revised 1 December 2022; Accepted 9 December 2022; Published 26 December 2022

Academic Editor: J. O. Caceres

Fuchsine acid is one of the supramolecular dyes used in Masson's trichrome stain and has enormous applications in histology. It is also used in Van Gieson's method with picric acid to show red collagen fibers and in Masson's trichrome to show smooth muscle in contrast to collagen. In addition to these, it has several other important applications in electronic fields and photonic devices as an organic semiconductor. Therefore, it is of utmost importance to investigate and predict the complex molecular topology of fuchsine acid, which serves as a foundation for the link with its physicochemical properties. In this article, the supramolecular sheet of fuchsine acid is modeled topologically based on the edge partition, and closed formulae are derived for some of its important irregular molecular descriptors, with the ultimate object of throwing some light on the effectiveness of the computed molecular descriptors for QSAR and QSPR analyses.

1. Introduction

Supramolecular structures have the same relationship with molecules as molecular structures have with atoms. The molecular structure is at the heart of the chemistry of many essential industrial and biological materials, despite the fact that atoms play an important role in chemistry paradigms. The chemistry of the intermolecular link, which connects molecules together into supermolecules rather than the covalent bond, which binds atoms together into molecules, is emphasized in the growing supramolecular systems paradigm. The chemistry of molecular assemblies and the intermolecular connection, the chemistry beyond the molecule, and the chemistry of the noncovalent bond are all examples of supramolecular chemistry. The structure and dynamics of a tiny molecule (known as a guest) that is not covalently bonded to a bigger molecule (termed a host) are studied in supramolecular chemistry. Fuchsine acid is one of the supramolecular dyes used in Masson's trichrome stain and is widely used in histology. It is used in Van Gieson's method with picric acid to show red collagen fibers and in Masson's trichrome to show smooth muscle in contrast to collagen. In addition to these, it has several other important applications in electronic fields and photonic devices as an organic semiconductor.

An important area of applied mathematics called graph theory is used to model numerous real-world issues in fields like science and technology. There are numerous applications of chemical graph theory in the field of chemistry. By adopting a visual representation (a chemical graph) of these chemical compounds, chemical graph theory offers a wealth of knowledge about molecules and atoms. If every vertex in graph G has the same degree, then the graph is regular. It is irregular otherwise. Regular graphs are very important in graph theory because they have many interesting mathematical characteristics. Knowing how far a particular graph deviates from being regular, or how significant its irregularity is, is crucial for solving various applications and issues. Numerous quantitative graph irregularity measurements have been proposed for this purpose. The earliest numerical measure of graph irregularity appears to have been put out by Von Collatz and Sinogowitz [1]. Theoretical chemistry is

concerned with predicting the physical features of chemical structures. In the field of chemical sciences, chemical graph theory plays a significant role. A molecular graph is a molecule-based graph with vertices representing atoms and edges representing bonds or links between them. The degree of a vertex is the number of edges that are connected with it. In chemistry, biology, and common networks, the quantitative topological classification of the irregularity of graphs [2, 3] is becoming increasingly important for evaluating the structure of deterministic and arbitrary networks and systems.

The topology of a molecule as well as the irregularity of the structure plays an important role in determining quantities like enthalpy and entropy. A topological index [4] is a numerical value that represents some important molecular structural information. In quantitative structure-property relation (QSPR) and quantitative structure-activity relation (QSAR) investigations, these indices are frequently employed to represent the physicochemical properties of chemical compounds [5–13]. One can consult references [14–26] for more information on the topological characterization of microstructure and nanostructure and the importance and applicability of the molecular descriptors. Topological indices include eccentric-based, degree-based, and distance-based indices; here, we are concerned about the degree-based topological indices [27–30]. We considered $C_{20}H_{19}N_3HCl$ supramolecular fuchsine and made the sheet by using its unit cell.

Let M be the graph, p and q be the vertices, d_p and d_q represent the degree of the vertex, pq stands for the edge that connects the vertices p and q. The irregular topological indices can be defined as follows:

The Albertson index (AL) [31] is defined as follows:

$$\mathrm{AL}(M) = \sum_{pq\in E} \left|d_p - d_q\right|. \tag{1}$$

The irregularity indices IRL and IRLU [32] are defined as follows:

$$\mathrm{IRL}(M) = \sum_{pq\in E} \left|\ln d_p - \ln d_q\right|, \tag{2}$$

$$(M) = \sum_{pq\in E} \frac{\left\|d_p - d_q\right\|}{\min\left(d_p - d_q\right)}. \tag{3}$$

The total irregularity index (IRRT) [33] is defined as follows:

$$\mathrm{IRRT}(M) = \frac{1}{2} \sum_{pq\in E} \left|d_p - d_q\right|. \tag{4}$$

The $IRF(M)$ irregularity index, which was introduced by Gutman [3] is defined as follows:

$$\mathrm{IRF}(M) = \sum_{pq\in E} \left|d_p - d_q\right|^2. \tag{5}$$

The Randic index [34] is defined as follows:

$$\mathrm{IRA}(M) = \sum_{pq\in E} \left(d_p{}^{-1/2} - d_q{}^{-1/2}\right)^2. \tag{6}$$

Below are the definitions of some more degree-based irregularity topological indices [35].

$$\mathrm{IRDIF}(M) = \sum_{pq\in E} \left|\frac{d_p}{d_q} - \frac{d_q}{d_p}\right|. \tag{7}$$

$$\mathrm{IRLF}(M) = \sum_{pq\in E} \frac{\left|d_p - d_q\right|}{\sqrt{d_p d_q}}, \tag{8}$$

$$LA(M) = 2\sum_{pq\in E} \frac{\left|d_p - d_q\right|}{\left(d_p + d_q\right)}, \tag{9}$$

$$\mathrm{IRDI}(M) = \sum_{pq\in E} \ln\left\{1 + \left|d_p - d_q\right|\right\}, \tag{10}$$

$$\mathrm{IRGA}(M) = \sum_{pq\in E} \ln\frac{d_p + d_q}{2\sqrt{d_p d_q}}, \tag{11}$$

$$\mathrm{IRB}(M) = \sum_{pq\in E} \left(d_p{}^{(1/2)} - d_q{}^{(1/2)}\right)^2. \tag{12}$$

The above irregular topological indices are very important to describe the topology of a molecular structure for QSPR and QSAR analyses. Here, in this paper, motivated by the enormous applications of fuchsine acid in industry and the importance of irregular topological indices (equations (1)–(12)), we intend to model the supramolecular sheet of fuchsine acid topologically based on the edge partition and derive closed formulae for the above-mentioned irregular molecular descriptors with the ultimate object of throwing some light on the effectiveness of the computed molecular descriptors for QSAR/QSPR analysis.

2. Edge Partition-Based Topological Modeling of Fuchsine Acid

The chemical structure of fuchsine acid is shown in Figure 1. The 2D graphical model of the molecular graph of fuchsine acid is shown in Figure 2. In order to define its molecular graph, we define a as the number of columns and b as the number of rows. The general molecular graph is denoted by $C_{20}H_{19}N_3HCl[a,b]$. As a result, the total number of vertices is $38ab + a + b$ and the total number of edges is $42ab$. The edge partition of $C_{20}H_{19}N_3HCl[a,b]$ established on degree of end vertices of each edge is given in Table 1.

3. Main Results

3.1. Computation of Irregular Topological Indices of Fuchsine Acid. In this section, we compute and derive closed formulae for the Albertson index $\mathrm{AL}(M)$, the irregularity indices $\mathrm{IRL}(M)$ and $\mathrm{IRLU}(M)$, the total irregularity index $\mathrm{IRRT}(M)$, the $\mathrm{IRF}(M)$ irregularity index, the $\mathrm{IRA}(M)$

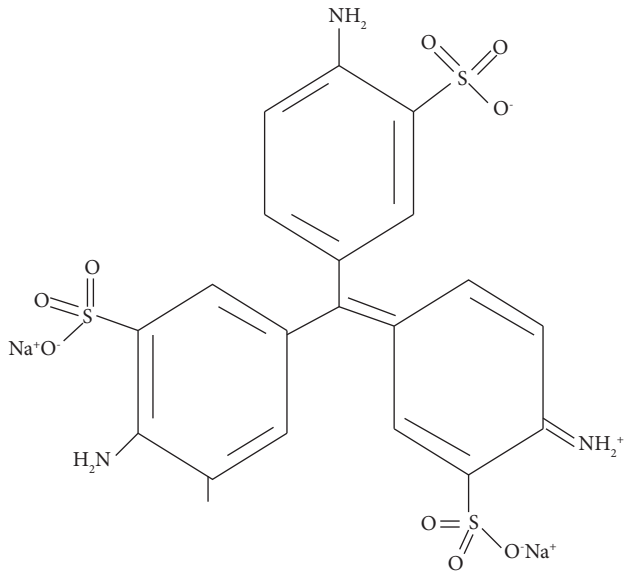

Figure 1: Chemical structure of fuchsine acid.

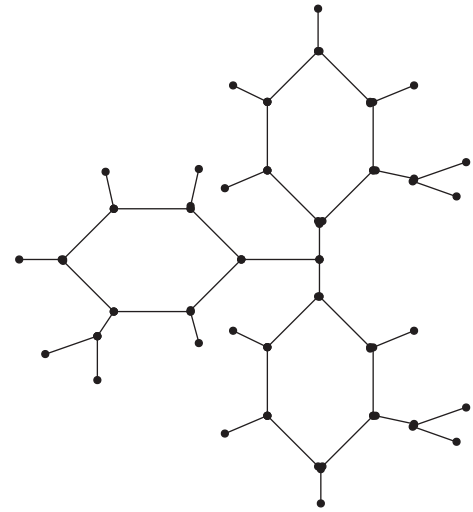

Figure 2: 2D structure of fuchsine $C_{20}H_{19}N_3HCl[1,1]$.

Table 1: The edge partition of $C_{20}H_{19}N_3HCl[a,b]$, established on degree of end vertices of each edge.

(d_p, d_q)	Frequency
(1, 3)	$14ab + 2(a+b)$
(2, 3)	$4ab - 2(a+b)$
(3, 3)	$24ab$

irregularity index, the IRDIF(M) irregularity index, the IRLF(M) irregularity index, the LA(M) irregularity index, the IRDI(M) irregularity index, the IRGA(M) irregularity index, and the IRB(M) irregularity index.

3.1.1. Theorems. Let $M(a,b)$ be the graph of 2D structure of $C_{20}H_{19}N_3HCl[a,b]$ supramoelcular sheet of fuchsine, then the irregularity indices of $M(a,b)$ are as follows:

(1) $\mathrm{AL}(M) = 32ab + 2(a+b)$

(2) $\mathrm{IRL}(M) = 16.992ab + 1.386(a+b)$

(3) $\mathrm{IRLU}(M) = 30ab + 3(a+b)$

(4) $\mathrm{IRRT}(M) = 16ab + a + b$

(5) $\mathrm{IRF}(M) = 60ab + 6(a+b)$

(6) $\mathrm{IRA}(M) = 2.556ab + 0.324(a+b)$

(7) $\mathrm{IRDIF}(M) = 40.67ab + 3.668(a+b)$

(8) $\mathrm{IRLF}(M) = 17.788ab + 1.493(a+b)$

(9) $\mathrm{LA}(M) = 15.6ab + 1.2(a+b)$

(10) $\mathrm{IRDI}(M) = 18.144ab + 0.81(a+b)$

(11) $\mathrm{IRGA}(M) = 2.082ab + 0.246(a+b)$

(12) $\mathrm{IRB}(M) = 7.894ab + 0.868(a+b) < listaend >$

3.1.2. Proofs. Figure 2 will be used to prove all of the above theorems. We can confirm the values from Table 1 for the edges of $M(a,b)$. Consider M be the graph of fuchsine acid. Then by using Table 1 and equations (1)–(12) we compute the following topological indices and derive closed formulae for them.

(1) **AL(M)**

Using Table 1 and (1), we estimate the value of this index as follows:

$$\begin{aligned}\mathrm{AL}(M) &= \sum_{pq\in E}\left|d_p - d_q\right| = [14ab + 2(a+b)]|3-1| + [4ab - 2(a+b)]|3-2| + (24ab)|3-3| \\ &= 28ab + 4(a+b) + 4ab - 2a - 2b + 0 = 32ab + 2a + 2b = 32ab + 2(a+b).\end{aligned} \tag{13}$$

(2) **IRL(M)**

By using Table 1 and (2), we estimate the value of this index as follows:

$$\begin{aligned}\mathrm{IRL}(M) &= \sum_{pq\in E}\left|\ln d_p - \ln d_q\right| = [14ab + 2(a+b)]|\ln 3 - \ln 1| + [4ab - 2(a+b)]|\ln 3 - \ln 2| + (24ab)|\ln 3 - \ln 3| \\ &= [14ab + 2a + 2b](1.098) + [4ab - 2a - 2b](0.405) + 0 \\ &= 15.372ab + 2.196a + 2.196b + 1.62ab - 0.81a - 0.81b = 16.992ab + 1.386(a+b).\end{aligned} \tag{14}$$

(3) **IRLU (M)**

By using Table 1 and (3), we estimate the value of this index as follows:

$$\begin{aligned}\mathrm{IRLU}(M) &= \sum_{pq\in E}\frac{\left\|d_p - d_q\right\|}{\min\left(d_p - d_q\right)} = [12ab + 2(a+b)]\frac{|3-1|}{\min(3,1)} + [4ab - 2(a+b)]\frac{|3-2|}{\min(3,2)} \\ &+ (24ab)\frac{|3-3|}{\min(3,3)} = (14ab + 2a + 2b)(2) + (4ab - 2a - 2b)(0.5) + 0 = 28ab \\ &+ 4a + 4b + 2ab - a - b = 30ab + 3(a+b).\end{aligned} \tag{15}$$

(4) **IRRT (M)**

We compute the value of this index by using Table 1 and (4) as follow:

$$\begin{aligned}\mathrm{IRRT}(M) &= \frac{1}{2}\sum_{pq\in E}\left|d_p - d_q\right| = \frac{1}{2}[14ab + 2(a+b)]|3-1| + \frac{1}{2}[4ab - 2(a+b)]|3-2| + \frac{1}{2}(24ab)|3-3| \\ &= 14ab + 2a + 2b + 2ab - a - b = 16ab + a + b.\end{aligned} \tag{16}$$

(5) **IRF (M)**

We compute the value of this index by using Table 1 and (5) as follow:

$$\begin{aligned}\mathrm{IRF}(M) &= \sum_{pq\in E}\left|d_p - d_q\right|^2, \\ &= [14ab + 2(a+b)](3-1)^2 + [4ab - 2(a+b)](3-2)^2 + (24ab)(3-3)^2, \\ &= (14ab + 2a + 2b)(4) + (4ab - 2a - 2b)(1) + 0ab + 8a + 8b + 4ab - 2a - 2b, \\ &= 60ab + 6(a+b).\end{aligned} \tag{17}$$

(6) **IRA (M)**

By using Table 1 and (6), we estimate the value of this index as follows:

$$\begin{aligned}\mathrm{IRA}(M) &= \sum_{pq\in E}\left(d_p{}^{-1/2} - d_q{}^{-1/2}\right)^2 = [14ab + 2(a+b)]\left[(3)^{-1/2} - (2)^{-1/2}\right]^2 + [4ab - 2(a+b)]\left[(3)^{-1/2} - (2)^{-1/2}\right]^2 \\ &+ (24ab)\left[(3)^{-1/2} - (3)^{-1/2}\right]^2 = (14ab + 2a + 2b)(0.178) + (4ab - 2a - 2b)(0.016) + 0 = 2.492ab \\ &+ 0.356a + 0.356b + 0.064ab - 0.032a - 0.032b = 2.556ab + 0.324(a+b).\end{aligned} \tag{18}$$

(7) **IRDIF (M)**

By using Table 1 and (7), we estimate the value of this index as follows:

$$\begin{aligned}\mathrm{IRDIF}(M) &= \sum_{pq\in E}\left|\frac{d_p}{d_q} - \frac{d_q}{d_p}\right|, \\ &= [14ab + 2(a+b)]\left|\frac{3}{1} - \frac{1}{3}\right| + [4ab - 2(a+b)]\left|\frac{3}{2} - \frac{2}{3}\right| + (24ab)\left|\frac{3}{3} - \frac{3}{3}\right|, \\ &= (14ab + 2a + 2b)(2.667) + (4ab - 2a - 2b)(0.833) + 0, \\ &= 37.338ab + 5.334a + 5.334b + 3.332ab - 1.666a - 1.666b, \\ &= 40.67ab + 3.668(a+b).\end{aligned} \tag{19}$$

(8) **IRLF (M)**

We compute the value of this index by using Table 1 and (8) as follow:

$$\begin{aligned}IRLF(M) &= \sum_{pq\in E}\frac{\left|d_p - d_q\right|}{\sqrt{d_p d_q}}, \\ &\cdot [14ab + 2(a+b)]\frac{|3-1|}{\sqrt{3\times 1}} + [4ab - 2(a+b)]\frac{|3-2|}{\sqrt{3\times 2}} + (24ab)\frac{|3-3|}{\sqrt{3\times 3}}, \\ &= (14ab + 2a + 2b)(1.154) + (4ab - 2a - 2b)(0.408) + 0, \\ &= 16.156ab + 2.309a + 2.309b + 1.632ab - 0.816a - 0.816b, \\ &= 17.788ab + 1.493(a+b).\end{aligned} \tag{20}$$

(9) **LA (M)**

We compute the value of this index by using Table 1 and (9) as follow:

$$LA(M) = 2\sum_{pq\in E}\frac{\left|d_p - d_q\right|}{\left(d_p + d_q\right)} = 2[14ab + 2(a+b)]\frac{|3-1|}{(3+1)} + 2[(4ab - 2(a+b))]\frac{|3-2|}{(3+2)} + (24ab)\frac{|3-3|}{(3+3)}$$
$$= (14ab + 2b + 2b)(1) + 2(4ab - 2a - 2b)(0.2) + 0$$
$$= 14ab + 2a + 2b + 1.6ab - 0.8a - 0.8b = 15.6ab + 1.2(a+b). \tag{21}$$

(10) **IRDI (M)**

By using Table 1 and (10), we estimate the value of this index as follows:

$$IRDI(M) = \sum_{pq\in E}\ln\left\{1 + \left|d_p - d_q\right|\right\} = [14ab + 2(a+b)]\ln\{1 + |3-1|\} + [4ab - 2(a+b)]\ln\{1 + |3-2|\}$$
$$+ (24ab)\ln\{1 + |3-3|\} = (14ab + 2a + 2b)(1.098) + (4ab - 2a - 2b)(0.693) + 0$$
$$= 15.372ab + 2.196a + 2.197b + 2.772ab - 1.386a - 1.386b = 18.144ab + 0.81(a+b). \tag{22}$$

(11) **IRGA (M)**

By using Table 1 and (11), we estimate the value of this index as follows:

$$\mathrm{IRGA}(M) = \sum_{pq\in E}\ln\frac{d_p + d_q}{2\sqrt{d_p d_q}} = [14ab + 2(a+b)]\ln\frac{3+1}{2\sqrt{3\times 1}} + [4ab - 2(a+b)]\ln\frac{3+2}{2\sqrt{3\times 2}} + (24ab)\ln\frac{3+3}{2\sqrt{3\times 3}}$$
$$= (14ab + 2a + 2b)(0.143) + (4ab - 2a - 2b)(0.020) + 0 = 2.002ab + 0.286a + 0.286b$$
$$+ 0.08ab - 0.04a - 0.04b = 2.082ab + 0.246(a+b). \tag{23}$$

(12) **IRB (M)**

By using Table 1 and (12), we estimate the value of this index as follows:

$$\mathrm{IRB}(M) = \sum_{pq\in E}\left(d_p{}^{1/2} - d_q{}^{1/2}\right)^2 = [14ab + 2(a+b)]\left(3^{1/2} - 1^{1/2} + [4ab - 2(a+b)]\left(3^{1/2} - 2^{1/2} + (24ab)\left(3^{1/2} - 3^{1/2}\right)^2\right.\right.$$
$$= (14ab + 2a + 2b)(0.535) + (4ab - 2a - 2b)(0.101) + 0 = 7.49ab + 1.07a + 1.07b + 0.404ab$$
$$- 0.202a - 0.202b = 7.894ab + 0.868(a+b). \tag{24}$$

3.2. Numerical and Graphical Interpretation of the Derived Formulae. Here, the numerical values of the irregularity indices obtained for different values of a and b are present in the form of Table 2 and Figure 3. It is evident from Table 2 as well as Figure 3 that the values of all indices are rising with an increase in the values of a, b. However, some of the irregularity indices grow very slowly as compared to others, as can be seen from Table 2 and Figure 3 that the values of irregularity indices IRGA (M) and IRA (M) are very low as compare to other indices. The derivation of closed formulae and numerical computation of these irregularity indices of fuchsine acid is valuable not only for QSPR/QSAR studies but also for investigation of the physicochemical properties such as enthalpy of vaporization, entropy, boiling and melting points, toxicity, resistance, and so on.

Table 2: Comparison of irregularity indices for $C_{20}H_{19}N_3HCl[a,b]$.

Irregularity indices	$a=1$ $b=1$	$a=2$ $b=2$	$a=3$ $b=3$	$a=4$ $b=4$
(1) $AL(M)=32ab+2(a+b)$	36	136	300	528
(2) $\mathrm{IRL}(M)=16.992ab+1.386(a+b)$	19.764	73.512	161.244	282.96
(3) $\mathrm{IRLU}(M)=30ab+3(a+b)$	36	132	288	504
(4) $\mathrm{IRRT}(M)=16ab+a+b$	18	68	150	264
(5) $\mathrm{IRF}(M)=60ab+6(a+b)$	72	264	576	1008
(6) $\mathrm{IRA}(M)=2.556ab+0.324(a+b)$	3.204	11.520	24.948	43.488
(7) $\mathrm{IRDIF}(M)=40.67ab+3.668(a+b)$	48.006	177.352	388.038	680.064
(8) $\mathrm{IRLF}(M)=17.788ab+1.493(a+b)$	20.774	77.124	169.05	296.552
(9) $LA(M)=15.6ab+1.2(a+b)$	18	67.2	147.6	259.2
(10) $\mathrm{IRDI}(M)=18.144ab+0.81(a+b)$	19.764	75.816	168.152	296.784
(11) $\mathrm{IRGA}(M)=2.082ab+0.246(a+b)$	2.574	9.312	20.214	35.28
(12) $\mathrm{IRB}(M)=7.894ab+0.868(a+b)$	9.63	35.048	76.254	133.248

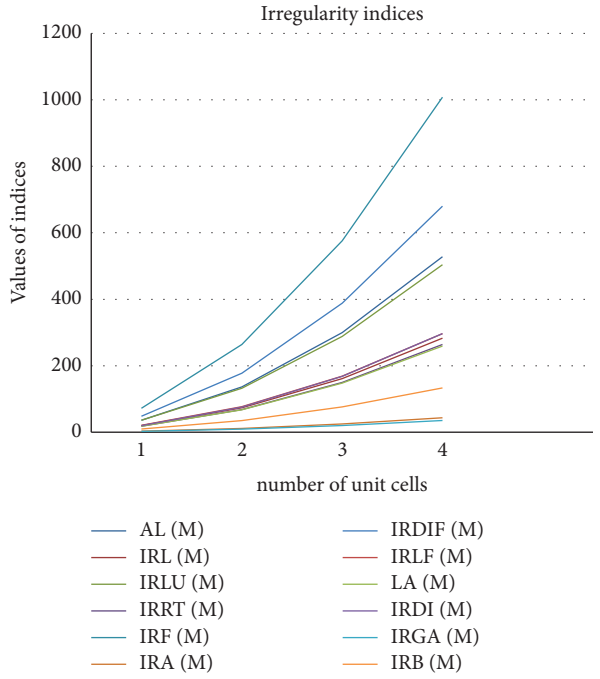

Figure 3: Comparison of irregular topological indices of 2D structure of supramolecular sheet of fuchsine acid $C_{20}H_{19}N_3HCl[a,b]$.

4. Conclusions

In this article, the supramolecular sheet of fuchsine acid is modeled topologically based on the edge partition and derived closed formulae for some of its important irregular molecular descriptors viz. Albertson index $AL(M)$, the total irregularity index $\mathrm{IRRT}(M)$, the $\mathrm{IRF}(M)$ irregularity index, the irregularity indexes $\mathrm{IRL}(M)$ and $\mathrm{IRLU}(M)$, the $\mathrm{IRA}(M)$ irregularity index, the $\mathrm{IRDIF}(M)$ irregularity index, the $LA(M)$ irregularity index, the $\mathrm{IRDI}(M)$ irregularity index, the $\mathrm{IRLF}(M)$ irregularity index, the $\mathrm{IRGA}(M)$ irregularity index, and the $\mathrm{IRB}(M)$ irregularity index. Based on the closed formulae, the numerical values of the irregularity indices are obtained, and a comparative analysis of the topological indices is performed. The derivation of closed formulae and numerical computation of these irregularity indices of fuchsine acid are valuable not only for QSPR/QSAR studies but also for the investigation of the physicochemical properties such as enthalpy of vaporization, entropy, boiling and melting points, toxicity, resistance, and so on.

Data Availability

The data used to support the findings of this study are included within the article.

Additional Points

No code was used to produce the results in this article.

Conflicts of Interest

The authors declare that there are no conflicts of interest.

Authors' Contributions

Asad Ullah, Shams udin and Shahid Zaman equally contributed to this manuscript.

Acknowledgments

The authors Asad Ullah, Anila Hamraz, and Shamsudin gratefully acknowledge the financial support to conduct this study derived from the Higher Education Commission of Pakistan (Grant No. 20-11682/NRPU/R&D/HEC/2020).

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