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Retraction

Retracted: On the Temperature Indices of Molecular Structures of Some Networks

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This article has been retracted by Hindawi following an investigation undertaken by the publisher [1]. This investigation has uncovered evidence of one or more of the following indicators of systematic manipulation of the publication process:

(1) Discrepancies in scope
(2) Discrepancies in the description of the research reported
(3) Discrepancies between the availability of data and the research described
(4) Inappropriate citations
(5) Incoherent, meaningless and/or irrelevant content included in the article
(6) Manipulated or compromised peer review

The presence of these indicators undermines our confidence in the integrity of the article's content and we cannot, therefore, vouch for its reliability. Please note that this notice is intended solely to alert readers that the content of this article is unreliable. We have not investigated whether authors were aware of or involved in the systematic manipulation of the publication process.

Wiley and Hindawi regrets 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 own 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

[1] A. Jahanbani, R. Khoeilar, and M. Cancan, "On the Temperature Indices of Molecular Structures of Some Networks," *Journal of Mathematics*, vol. 2022, Article ID 4840774, 7 pages, 2022.

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Research Article

On the Temperature Indices of Molecular Structures of Some Networks

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The topological index is a molecular predictor that is commonly supported in the research of QSAR of pharmaceuticals to numerically quantify their molecular features. Theoretical and statistical study of drug-like compounds improves the drug design and finding workflow by rationalizing lead detection, instant decision, and mechanism of action comprehension. Using molecular structure characterization and edge segmentation technique, we computed the general temperature topological indices for OTIS networks.

1. Introduction

Mathematical chemistry may be a theoretic science in which artificial structures square measure by the employment of scientific instruments. The artificial diagram hypothesis maybe a part of this field where chart hypothesis devices square measure applied to scientifically demonstrate concoctions. As the graph has vertices that can be pictured by processor nodes and edges represent links between these nodes/processors [1]. The primary application in chemistry was the boiling purpose of the paraffin [1–3].

Topological indices are numerical values that are attributed to a molecular structure. Today, topological indices have been considered by many researchers because they have applications in various sciences, see [4–8].

Aslam et al. [9], obtained new results for OTIS networks by using some of the topological indices. Zahra et al. [3], discussed the swapped networks by using topological indices. In [10], the authors computed some of the topological indices for OTIS networks. Baig et al. [11] discussed some of the DOX and DSL networks by using the topological indices. In [6], the authors obtained some of the new results for anticancer drugs by using the multiplicative topological indices. In [12], the author discussed carbon nanocones and nanotori by using some of the topological indices. Therefore, in this paper, we obtain new results for OTIS networks by using some topological indices.

For a simple graph $\mathcal{G}$, we denoted the vertex set by $V(\mathcal{G}) = \{x_1, x_2, x_3, \ldots, x_n\}$ and the edge set by $\xi(\mathcal{G})$, $|\xi(\mathcal{G})| = \varepsilon$. The degree of the vertex $x \in V(\mathcal{G})$ is denoted by ζ_x.

For any graphs $\mathcal{G}$ with n vertices, the temperature of a vertex x is defined in [13] as

$$\psi(x) = \frac{\zeta_x}{n - \zeta_x}. \tag{1}$$

Kulli in [14] defined the following topological indices as

The general first temperature index

$$\psi_1^{\omega}(\mathcal{G}) = \sum_{xy \in \xi(\mathcal{G})} (\psi(x) + \psi(y))^{\omega}. \tag{2}$$

The general second temperature index

$$\psi_2^{\omega}(\mathcal{G}) = \sum_{xy \in \xi(\mathcal{G})} (\psi(x) \times \psi(y))^{\omega}. \tag{3}$$

The general temperature index

$$\psi_{\omega}(\mathcal{G}) = \sum_{xy \in \xi(\mathcal{G})} (\psi(x)^{\omega} + \psi(y)^{\omega}), \tag{4}$$

where $\omega \in R$.

2. Results for NP_n Network

In this section, we compute the exact formulas for the OTIS networks NP_n of some general temperature indices, and we also examine the relationships between these topologies with graphical diagrams.

Let P_n be the path of n vertices and NP_n be OTIS (swapped) network with basis network P_n, see Figure 1.

We start by computing the general first temperature index.

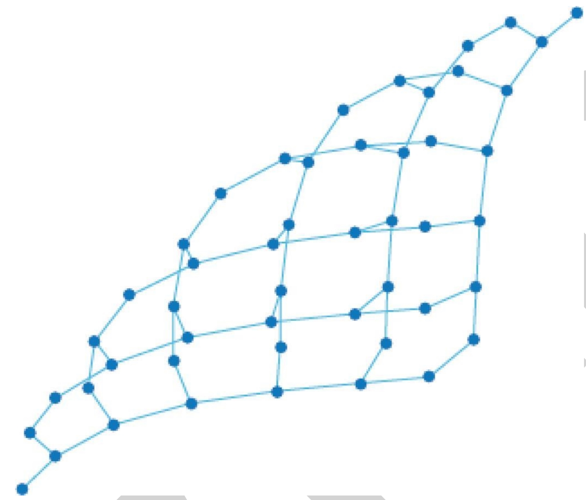

Figure 1: The graph of NP_7.

Theorem 1. *For NP_n network, we have*

$$\psi_1^{\omega}(NP_n) = 2\left(\frac{1}{n^2-1}+\frac{3}{n^2-3}\right)^{\omega} + 3\left(\frac{4}{n^2-2}\right)^{\omega} + (6n-14)\left(\frac{2}{n^2-2}+\frac{3}{n^2-3}\right)^{\omega} + \left(\frac{3(n-2)(n-3)}{2}\right)\left(\frac{6}{n^2-3}\right)^{\omega}. \tag{5}$$

Proof. The OTIS networks NP_n have n^2 vertices and $3(n^2-n)/2$, edges. Hence, there are three partitions, $V_{\{1\}} = \{y \in V(\mathrm{NP}_n) | \zeta_y = 1\}$, $V_{\{2\}} = \{y \in V(\mathrm{NP}_n) | \zeta_y = 2\}$ and $V_{\{3\}} = \{y \in V(\mathrm{NP}_n) | \zeta_y = 3\}$. Hence, we can write that

$$\xi_1 = \{\varepsilon = xy \in \xi(\mathrm{NP}_n) | \zeta_x = 1 \text{ and } \zeta_y = 3\}, \tag{6}$$

$$\xi_2 = \{\varepsilon = xy \in \xi(\mathrm{NP}_n) | \zeta_x = 2 \text{ and } \zeta_y = 2\}, \tag{7}$$

$$\xi_3 = \{\varepsilon = xy \in \xi(\mathrm{NP}_n) | \zeta_x = 2 \text{ and } \zeta_y = 3\}, \tag{8}$$

$$\xi_4 = \{\varepsilon = xy \in \xi(\mathrm{NP}_n) | \zeta_x = 3 \text{ and } \zeta_y = 3\}. \tag{9}$$

It can be easily seen that $|\xi_1| = 2, |\xi_2| = 3, |\xi_3| = 6n-14$ and $|\xi_4| = 3(n-2)(n-3)/2$.

By applying the definitions and Equalities (6)–(9), we can write

$$\begin{aligned}
\psi_1^{\omega}(\mathrm{NP}_n) &= \sum_{xy\in\xi(\mathrm{NP}_n)} (\psi(x)+\psi(y))^{\omega} \\
&= \sum_{xy\in\xi_1(\mathrm{NP}_n)} (\psi(x)+\psi(y))^{\omega} + \sum_{xy\in\xi_2(\mathrm{NP}_n)} (\psi(x)+\psi(y))^{\omega} + \sum_{xy\in\xi_3(\mathrm{NP}_n)} (\psi(x)+\psi(y))^{\omega} + \sum_{xy\in\xi_4(\mathrm{NP}_n)} (\psi(x)+\psi(y))^{\omega} \\
&= 2\left(\frac{1}{n^2-1}+\frac{3}{n^2-3}\right)^{\omega} + 3\left(\frac{2}{n^2-2}+\frac{2}{n^2-2}\right)^{\omega} + (6n-14)\left(\frac{2}{n^2-2}+\frac{3}{n^2-3}\right)^{\omega} + \left(\frac{3(n-2)(n-3)}{2}\right)\left(\frac{3}{n^2-3}+\frac{3}{n^2-3}\right)^{\omega} \\
&= 2\left(\frac{1}{n^2-1}+\frac{3}{n^2-3}\right)^{\omega} + 3\left(\frac{4}{n^2-2}\right)^{\omega} + (6n-14) + \left(\frac{2}{n^2-2}+\frac{3}{n^2-3}\right)^{\omega} + \left(\frac{3(n-2)(n-3)}{2}\right)\left(\frac{6}{n^2-3}\right)^{\omega}.
\end{aligned} \tag{10}$$

□

Now, we compute the general second temperature index.

Theorem 2. *For NP_n network, we have*

$$\psi_2^{\omega}(\mathrm{NP}_n) = 2\left(\frac{3}{(n^2-1)(n^2-3)}\right)^{\omega} + 3\left(\frac{4}{(n^2-2)^2}\right)^{\omega} + (6n-14)\left(\frac{6}{(n^2-2)(n^2-3)}\right)^{\omega} + \left(\frac{3(n-2)(n-3)}{2}\right)\left(\frac{9}{(n^2-3)^2}\right)^{\omega}. \tag{11}$$

Proof. By applying the definitions and equalities (6)–(9), we have

$$
\begin{aligned}
\psi_2^{\omega}(\mathrm{NP}_n) &= \sum_{xy\in\xi(\mathrm{NP}_n)} (\psi(x)\times\psi(y))^{\omega}\\
&= \sum_{xy\in\xi_1(\mathrm{NP}_n)} (\psi(x)\times\psi(y))^{\omega} + \sum_{xy\in\xi_2(\mathrm{NP}_n)} (\psi(x)\times\psi(y))^{\omega} + \sum_{xy\in\xi_3(\mathrm{NP}_n)} (\psi(x)\times\psi(y))^{\omega} + \sum_{xy\in\xi_4(\mathrm{NP}_n)} (\psi(x)\times\psi(y))^{\omega}\\
&= 2\left(\frac{1}{n^2-1}\times\frac{3}{n^2-3}\right)^{\omega} + 3\left(\frac{2}{n^2-2}\times\frac{2}{n^2-2}\right)^{\omega} + (6n-14)\left(\frac{2}{n^2-2}\times\frac{3}{n^2-3}\right)^{\omega} + \left(\frac{3(n-2)(n-3)}{2}\right)\left(\frac{3}{n^2-3}\times\frac{3}{n^2-3}\right)^{\omega}\\
&= 2\left(\frac{3}{(n^2-1)(n^2-3)}\right)^{\omega} + 3\left(\frac{4}{(n^2-2)^2}\right)^{\omega} + (6n-14)\left(\frac{6}{(n^2-2)(n^2-3)}\right)^{\omega} + \left(\frac{3(n-2)(n-3)}{2}\right)\left(\frac{9}{(n^2-3)^2}\right)^{\omega}.
\end{aligned}
\tag{12}
$$

□

Here, we compute the general temperature index.

Theorem 3. *For NP_n network, we have*

$$
\psi_{\omega}(\mathrm{NP}_n) = 3n^2\left(\frac{3}{n^2-3}\right)^{\omega} + 6n\left(\frac{2}{n^2-2}\right)^{\omega} - 9n\left(\frac{3}{n^2-3}\right)^{\omega} + 2\left(\frac{1}{n^2-1}\right)^{\omega} + 6\left(\frac{3}{n^2-3}\right)^{\omega} - 8\left(\frac{2}{n^2-2}\right)^{\omega}.
\tag{13}
$$

Proof. By applying the definitions and Equalities (6)–(9), we can write

$$
\begin{aligned}
\psi_{\omega}(\mathrm{NP}_n) &= \sum_{xy\in\xi(\mathrm{NP}_n)} (\psi(x)^{\omega}+\psi(y)^{\omega})\\
&= \sum_{xy\in\xi_1(\mathrm{NP}_n)} (\psi(x)^{\omega}+\psi(y)^{\omega}) + \sum_{xy\in\xi_2(\mathrm{NP}_n)} (\psi(x)^{\omega}+\psi(y)^{\omega}) + \sum_{xy\in\xi_3(\mathrm{NP}_n)} (\psi(x)^{\omega}+\psi(y)^{\omega})\\
&\quad + \sum_{xy\in\xi_4(\mathrm{NP}_n)} (\psi(x)^{\omega}+\psi(y)^{\omega})\\
&= 2\left(\left(\frac{1}{n^2-1}\right)^{\omega} + \left(\frac{3}{n^2-3}\right)^{\omega}\right) + 3\left(\left(\frac{2}{n^2-2}\right)^{\omega} + \left(\frac{2}{n^2-2}\right)^{\omega}\right) + (6n-14)\left(\left(\frac{2}{n^2-2}\right)^{\omega} + \left(\frac{3}{n^2-3}\right)^{\omega}\right)\\
&\quad + \left(\frac{3(n-2)(n-3)}{2}\right)\left(\left(\frac{3}{n^2-3}\right)^{\omega} + \left(\frac{3}{n^2-3}\right)^{\omega}\right)\\
&= 3n^2\left(\frac{3}{n^2-3}\right)^{\omega} + 6n\left(\frac{2}{n^2-2}\right)^{\omega} - 9n\left(\frac{3}{n^2-3}\right)^{\omega} + 2\left(\frac{1}{n^2-1}\right)^{\omega} + 6\left(\frac{3}{n^2-3}\right)^{\omega} - 8\left(\frac{2}{n^2-2}\right)^{\omega}.
\end{aligned}
\tag{14}
$$

□

3. Results for NT_t Network

The OTIS (swapped) network NT_t is derived from the graph Υ, which a graph with vertex set $V(\mathrm{NT}_{\Upsilon}) = \langle z, x\rangle | z, x \in V(\Upsilon)$ and edge set $\xi(\mathrm{NT}_{\Upsilon}) = \langle z, x_1\rangle, \langle z, x_2\rangle z \in V(\Upsilon)$, $(x_1, x_2) \in \xi(\mathrm{NT}_{\Upsilon}) \cup (\langle z, x\rangle, \ \langle z, x, z\rangle) | z, x \in V(\Upsilon))$ and $z \neq x$, see Figure 2.

In this section, we obtaining new results for the OTIS networks NT_t.

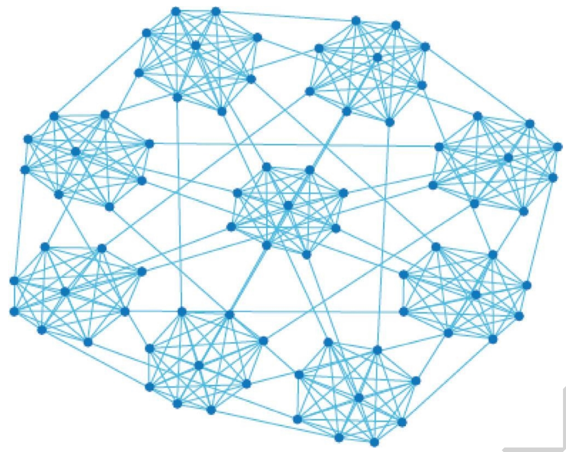

Figure 2: The graph NT_7.

Theorem 4. *For NT_t network, we have*

$$\psi_1^{\omega}(NT_t) = nt\left(\frac{t}{(n+2)^2 - t} + \frac{t+1}{(n+2)^2 - t - 1}\right)^{\omega} + \frac{2^{\omega-1}(t+1)^{\omega}\left(n^2(t+1) - n(2t+1)\right)}{\left((n+2)^2 - t - 1\right)^{\omega}}. \quad (15)$$

Proof. The NT_t has $(n+2)^2$ vertices and $n^3/2 + 3n^2 + 11n/2 + 3$ edges. Hence, there are two partitions, $V_{\{1\}} = \{y \in V(NT_t) | \zeta_y = t\}$ and $V_{\{2\}} = \{y \in V(NP_n) | \zeta_y = t+1\}$. Hence, we have the following equalities:

$$\xi_1 = \{\varepsilon = xy \in \xi(NT_t) | \zeta_x = t \text{ and } \zeta_y = t+1\}, \quad (16)$$

$$\xi_2 = \{\varepsilon = xy \in \xi(NT_t) | \zeta_x = t+1 \text{ and } \zeta_y = t+1\}. \quad (17)$$

It can be easily seen that $|\xi_1| = nt$ and $|\xi_2| = n^2(t+1) - n(2t+1)/2$.

By applying the definitions and equalities (16) and (17), we can write

$$\begin{aligned}
\psi_1^{\omega}(NT_t) &= \sum_{xy \in \xi(NT_t)} (\psi(x) + \psi(y))^{\omega} \\
&= \sum_{xy \in \xi_1(NT_t)} (\psi(x) + \psi(y))^{\omega} + \sum_{xy \in \xi_2(NT_t)} (\psi(x) + \psi(y))^{\omega} \\
&= nt\left(\frac{t}{(n+2)^2 - t} + \frac{t+1}{(n+2)^2 - t - 1}\right)^{\omega} + \left(\frac{n^2(t+1) - n(2t+1)}{2}\right)\left(\frac{t+1}{(n+2)^2 - t - 1} + \frac{t+1}{(n+2)^2 - t - 1}\right)^{\omega} \\
&= nt\left(\frac{t}{(n+2)^2 - t} + \frac{t+1}{(n+2)^2 - t - 1}\right)^{\omega} + \left(\frac{n^2(t+1) - n(2t+1)}{2}\right)\left(\frac{2(t+1)}{(n+2)^2 - t - 1}\right)^{\omega} \\
&= nt\left(\frac{t}{(n+2)^2 - t} + \frac{t+1}{(n+2)^2 - t - 1}\right)^{\omega} + \frac{2^{\omega-1}(t+1)^{\omega}\left(n^2(t+1) - n(2t+1)\right)}{\left((n+2)^2 - t - 1\right)^{\omega}}.
\end{aligned} \quad (18)$$

□

Theorem 5. *For NT_t network, we have*

$$\psi_2^{\omega}(NT_t) = nt\left(\frac{t(t+1)}{\left((n+2)^2 - t\right)\left((n+2)^2 - t - 1\right)}\right)^{\omega} + \left(\frac{n^2(t+1) - n(2t+1)}{2}\right)\left(\frac{t+1}{(n+2)^2 - t - 1}\right)^{2\omega}. \quad (19)$$

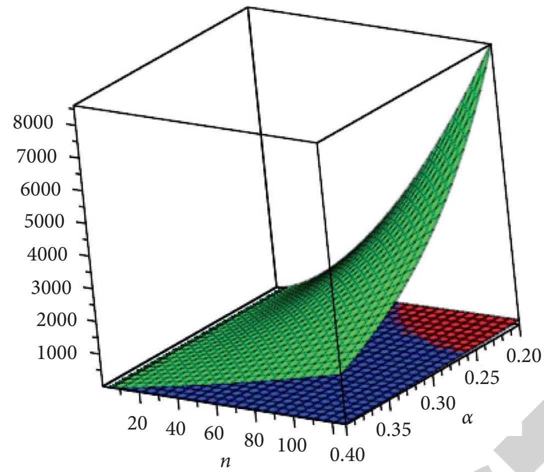

Figure 3: Comparison of $\psi_1^{\omega}, \psi_2^{\omega}$, and ψ_{ω} for NP_n.

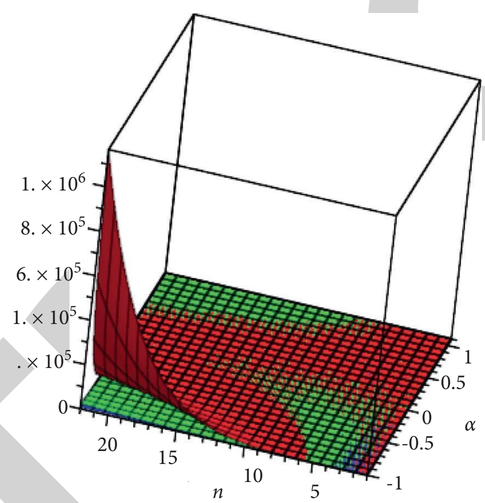

Figure 4: Comparison of $\psi_1^{\omega}, \psi_2^{\omega}$ and ψ_{ω} for NT_t.

Proof. By applying the definitions and equalities (16) and (17), we have

$$\begin{aligned}
\psi_2^{\omega}(NT_t) &= \sum_{xy\in\xi(NT_t)} (\psi(x)\times\psi(y))^{\omega} \\
&= \sum_{xy\in\xi_1(NT_t)} (\psi(x)\times\psi(y))^{\omega} + \sum_{xy\in\xi_2(NT_t)} (\psi(x)\times\psi(y))^{\omega} \\
&= nt\left(\frac{t}{(n+2)^2-t}\times\frac{t+1}{(n+2)^2-t-1}\right)^{\omega} + \left(\frac{n^2(t+1)-n(2t+1)}{2}\right)\left(\frac{t+1}{(n+2)^2-t-1}\times\frac{t+1}{(n+2)^2-t-1}\right)^{\omega} \\
&= nt\left(\frac{t}{(n+2)^2-t}\times\frac{t+1}{(n+2)^2-t-1}\right)^{\omega} + \left(\frac{n^2(t+1)-n(2t+1)}{2}\right)\left(\frac{(t+1)^2}{\left((n+2)^2-t-1\right)^2}\right)^{\omega} \\
&= nt\left(\frac{t(t+1)}{\left((n+2)^2-t\right)\left((n+2)^2-t-1\right)}\right)^{\omega} + \left(\frac{n^2(t+1)-n(2t+1)}{2}\right)\left(\frac{t+1}{(n+2)^2-t-1}\right)^{2\omega}.
\end{aligned} \tag{20}$$

□

Theorem 6. *For NT_t network, we have*

$$\psi_\omega(\mathrm{NT}_t) = nt\left(\left(\frac{t}{(n+2)^2 - t}\right)^\omega + \left(\frac{t+1}{(n+2)^2 - t - 1}\right)^\omega\right) + \left(n^2(t+1) - n(2t+1)\right)\left(\frac{t+1}{(n+2)^2 - t - 1}\right)^\omega. \tag{21}$$

Proof. By applying the definitions and equalities (16) and (17), we can write

$$\begin{aligned}
\psi_\omega(\mathrm{NT}_t) &= \sum_{xy\in\xi(\mathrm{NT}_t)} \left(\psi(x)^\omega + \psi(y)^\omega\right)\\
&= \sum_{xy\in\xi_1(\mathrm{NT}_t)} \left(\psi(x)^\omega + \psi(y)^\omega\right) + \sum_{xy\in\xi_2(\mathrm{NT}_t)} \left(\psi(x)^\omega + \psi(y)^\omega\right)\\
&= nt\left(\left(\frac{t}{(n+2)^2 - t}\right)^\omega + \left(\frac{t+1}{(n+2)^2 - t - 1}\right)^\omega\right) + \left(\frac{n^2(t+1) - n(2t+1)}{2}\right)\left(\left(\frac{t+1}{(n+2)^2 - t - 1}\right)^\omega + \left(\frac{t+1}{(n+2)^2 - t - 1}\right)^\omega\right)\\
&= nt\left(\left(\frac{t}{(n+2)^2 - t}\right)^\omega + \left(\frac{t+1}{(n+2)^2 - t - 1}\right)^\omega\right) + \left(n^2(t+1) - n(2t+1)\right)\left(\frac{t+1}{(n+2)^2 - t - 1}\right)^\omega.
\end{aligned} \tag{22}$$

□

4. Graphical Representation and Discussion

In this paper, we discussed physical properties of some OTIS networks in terms of topological indices. The study of graphs and networks through topological descriptors area unit necessary to grasp their underlying topologies. Hence, in this paper, we computed general topological temperature indices. The graphical representations of general temperature indices of NP_n and NT_t area unit are represented in Figures 3 and 4.

5. Conclusion

In medical science, chemical, medical, biological, and pharmaceutical properties of molecular structure are essential for drug design. These properties can be studied by the topological index calculation. Hence, we have computed general topological indices of some OTIS networks such as NP_n networks and NT_t networks. We obtained the closed formulas of the general first and second temperature indices and the general temperature index for these networks. Our results can help to guess the many physical and chemical properties of networks.

Data Availability

The data involved in the examples of our manuscript are included within the article.

Disclosure

We would like to declare that the work described was original research that has not been published previously. This work was in memoriam of Dr. Rana Khoeilar, the author died prior to the submission of this paper. This is one of the last works of her.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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