Temperature indices for a Non-Kekulean benzenoid graph

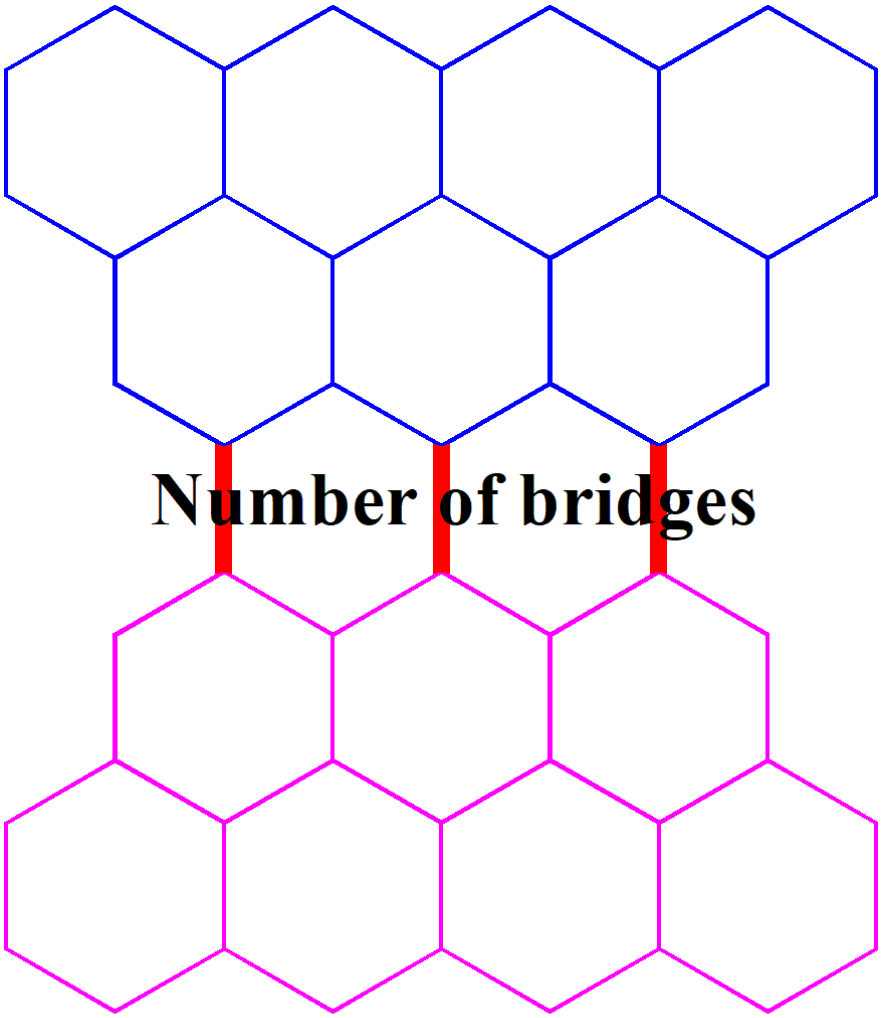
Jia-bao Liu[1], Muhammad Ghani[2], ABDUL RAUF KHAN[2], Murat Cancan[3], and Hafiz Muhammad Asif[4]

[1]Anhui Xinhua University
[2]Khwaja Fareed University of Engineering & Information Technology
[3]Van Yuzuncu Yil University Faculty of Education
[4]Bahauddin Zakariya University

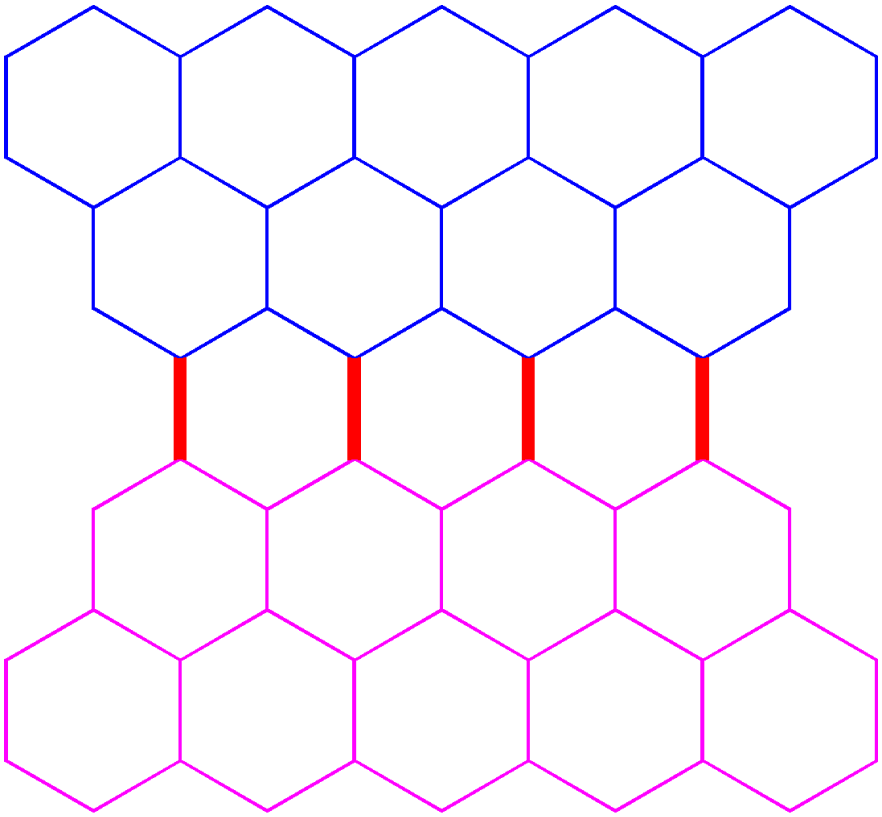
April 05, 2024

Abstract

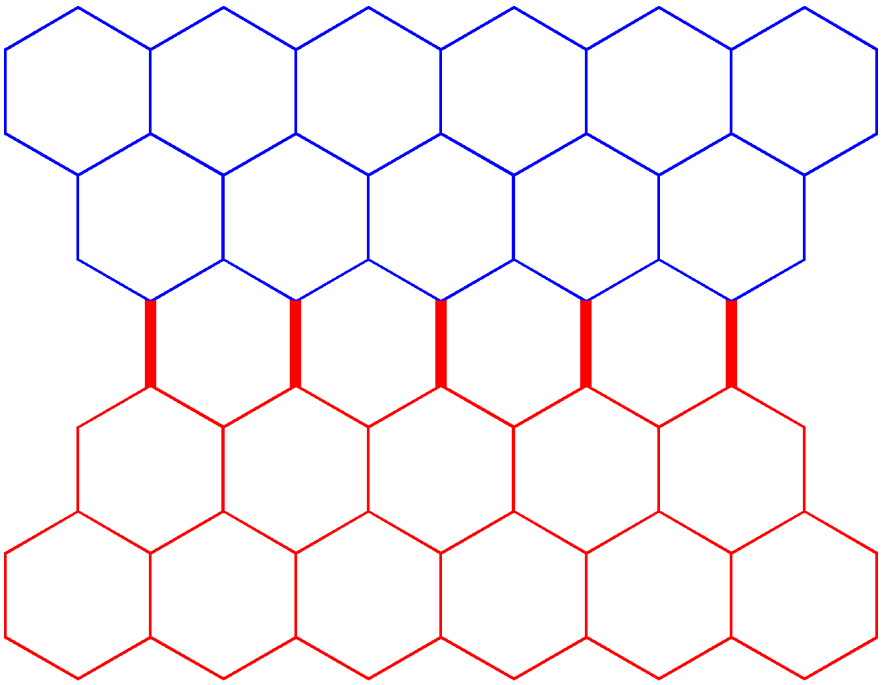
A molecular descriptor, also known as a topological graph index, is a mathematical formula that may be implemented to any network that reflects a molecule structure. This index can be used to explore some physical aspects of a molecule and examine mathematical values. As a consequence, it is a better solution for costly and time-consuming laboratory experiments. In this work, we calculate the first temperature index, the second temperature index, the first hyper temperature index, the second hyper temperature index, the sum temperature index, the product temperature index, the reciprocal product temperature index and the F-temperature index. These defined indices are computed for the Non-KuKulean benzenoid graph.



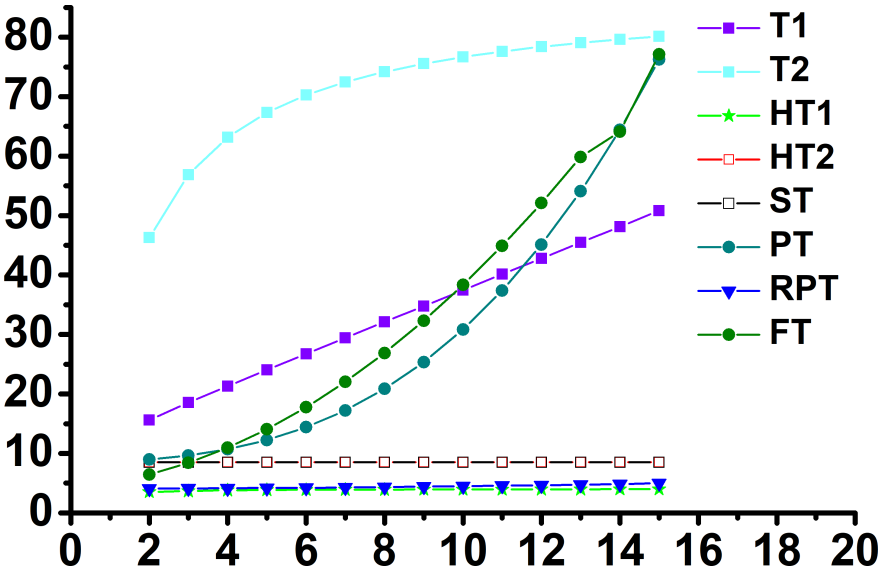
K3

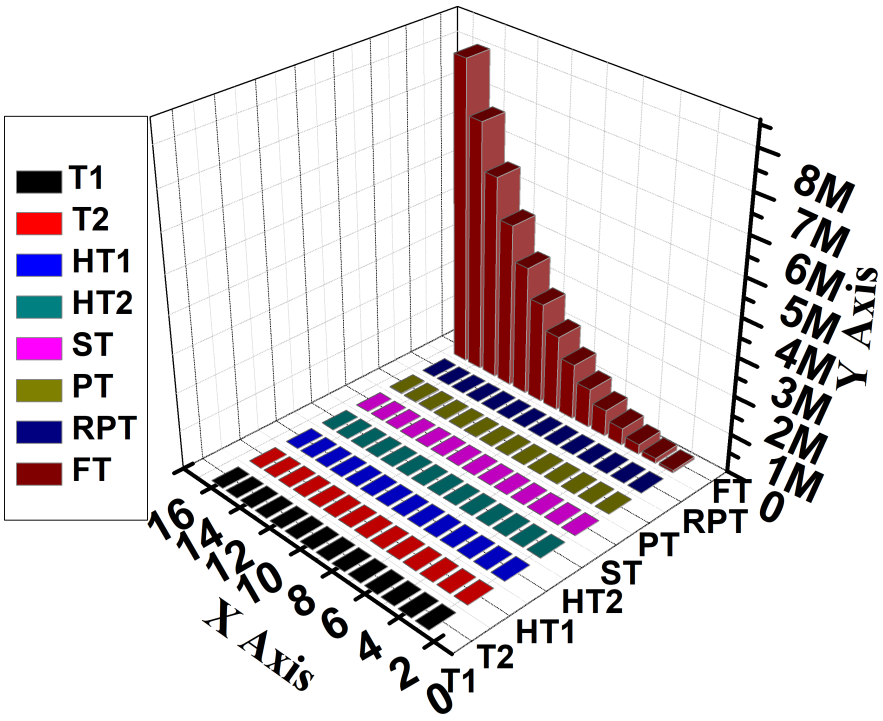


K4



K5





Temperature indices for a Non-Kekulean benzenoid graph

Jia-Bao Liu[1], Muhammad Usman Ghani[2], Abdul Rauf Khan[3*], Murat Cancan[4] and Hafiz Muhammad Asif[5]

[1]School of Mathematics and Physics, Anhui Jianzhu University, Hefei 230601, P.R. China.

Email: liujiabaoad@163.com

[2,3]Department of Mathematics, Khawaja Fareed University of Engineering & Information Technology, 64200, Rahim Yar Khan, Punjab, Pakistan.

Email: usmanghani85a@gmail.com, khankts@gmail.com*

[3]Faculty of Education, Yuzuncu Yil University, Van, Turkey.

Email: mcancan@yyu.edu.tr

[5]Institute of Chemical Sciences, Bahauddin Zakariya University, 60800, Multan, Pakistan.

Email: hmasifc@gmail.com

*†‡

Abstract

A molecular descriptor, also known as a topological graph index, is a mathematical formula that may be implemented to any network that reflects a molecule structure. This index can be used to explore some physical aspects of a molecule and examine mathematical values. As a consequence, it is a better solution for costly and time-consuming laboratory experiments. In this work, we calculate the first temperature index, the second temperature index, the first hyper temperature index, the second

*Corresponding author: khankts@gmail.com

†*Keywords:* Temperature indices, Non-Kekulean benzenoid graph

‡2020 AMS Mathematics Subject Classification: 05C07, 05C09, 05C31, 05C76, 05C99

hyper temperature index, the sum temperature index, the product temperature index, the reciprocal product temperature index and the F-temperature index. These defined indices are computed for the Non-KuKulean benzenoid graph.

1 Introduction

Using chemical graph theory, one can determine a wide range of characteristics of chemical networks such as physical, chemical, thermal properties, biological activity, and chemical activity [10]. Topological indices, which are molecular descriptors, can characterize these features and specific graphs [7]. In chemical graph theory, vertices represent atoms and edges represent chemical bonding between the atoms [3]. The topological index of a chemical composition is a numerical value or a continuation of a given structure under discussion, which indicates chemical, physical and biological properties of a structure of chemical compound [6, 9, 16].
Mathematical chemistry explains how to use polynomials and functions to provide instructions hidden in the symmetry of molecular graphs, and graph theory has many applications in modern chemistry, particularly organic chemistry. Many applications of topological indices are used in theoretical chemistry, particularly QSPR/QSAR research. Many well-known researchers have investigated topological indices in order to learn more about various graph families [13, 15]. In Qualitative Structure Property Relationships and Qualitative Structure Activity Relationships, topological indices are used directly as simple numerical descriptors in comparison with physical, biological, or chemical parameters of molecules, which is an advantage of chemical industry. Many researchers have worked on various chemical compounds and computed topological descriptors of various molecular graphs over the last few decades [10, 17].

In chemical graph theory, the molecular graph is a simple connected graph which contains atoms and bonds, which are often known as vertices and edges, respectively and there must be linkage among the vertices set V_G and edges set E_G. If two atoms have an atom-bond then it is denoted by $u_i \sim v_j$ for all u_i, v_j contain in E_G, the valency of every atom of G is actually the total number of atoms connected to v_j of G and it is denoted by d_{v_j} [12].
Fajtlowicz defined the temperature of a every vertex u_i of a graph G in [4] as

$$T_{u_i} = \frac{d_{u_i}}{|V_G| - d_{u_i}} \qquad where \qquad \forall \ \ u_i \in V_G \tag{1}$$

The first temperature index [19] is defined as follows:

$$T_1(G) = \sum_{u_i \sim v_j} \left(T_{u_i} + T_{v_j}\right) \tag{2}$$

In 2020, Kulli introduced second temperature index [8], which is defined as follows:

$$T_2(G) = \sum_{u_i \sim v_j} \left(T_{u_i} \times T_{v_j}\right) \tag{3}$$

Kulli introduced the first and second hyper temperature indices in [8], which are defined as

$$HT_1(G) = \sum_{u_i \sim v_j} \left(T_{u_i} + T_{v_j}\right)^2 \tag{4}$$

$$HT_2(G) = \sum_{u_i \sim v_j} \left(T_{u_i} \times T_{v_j}\right)^2 \tag{5}$$

Also introduced in the same paper [8] were the sum connectivity temperature index, the product connectivity temperature index, and the reciprocal product connectivity index, which are defined as

$$ST(G) = \sum_{u_i \sim v_j} \frac{1}{\sqrt{\left(T_{u_i} + T_{v_j}\right)}} \tag{6}$$

$$PT(G) = \sum_{u_i \sim v_j} \frac{1}{\sqrt{\left(T_{u_i} \times T_{v_j}\right)}} \tag{7}$$

$$RPT(G) = \sum_{u_i \sim v_j} \sqrt{\left(T_{u_i} \times T_{v_j}\right)} \tag{8}$$

Kulli introduced the F-temperature index and general temperature index of a graph G in [8], and they are defined as

$$FT(G) = \sum_{u_i \sim v_j} \left(T_{u_i}^2 + T_{v_j}^2\right) \tag{9}$$

By using the above equations from (2) to (9) and manufactured by the atom-bond partition of Non-Kekulean benzenoid graph, we compute the first temperature index, second temperature index, first and second hyper temperature index, sum temperature index, product temperature index, reciprocal product temperature index, and F-temperature index. These indices are helpful in comparison of certain physio-chemical properties like strain energy, boiling point, stability etc [11, 14, 18].

2 Non-Kekulean benzenoid graph $\mathcal{K}_n$

The Kekulean and Non-kekulean structures of benzene are real and distinct due to the presence of rings in the benzenoid form. The specific arrangement of rings in the benzenoid system provides the transformation in series of benzenoid structures of the benzenoid graph thats way the structures are changed. In the series of concealed Non-Kekulean benzenoid graph $\mathcal{K}_n$ [1, 2, 5], where n shows the number of bridges [20] in the center of $\mathcal{K}_n$, as shown in Figure 1. Similarly for $n = k$, there are k bridges. Here in the Non-Kekulean benzenoid graph $\mathcal{K}_n$, we observed that there are three type of atom-bonds on the bases of valency of every atom. Therefore by observing this concept of atom-bonds, there are two types of atoms v_i and v_j such that $d_{v_i} = 2$ and $d_{v_j} = 3$, where d_{v_i} and d_{v_j} means the valency of atoms $\forall$ $v_i, v_j \in \mathcal{K}_n$. The order and size of Non-Kekulean benzenoid graphs $\mathcal{K}_n$ is [5]:

$$|V(\mathcal{K}_n)| = 2(6n + 7) \qquad and \qquad |E(\mathcal{K}_n)| = 17n + 14 \tag{10}$$

Following are the three figures of Non-Kekulean benzenoid graphs K_3, K_4 and K_5:

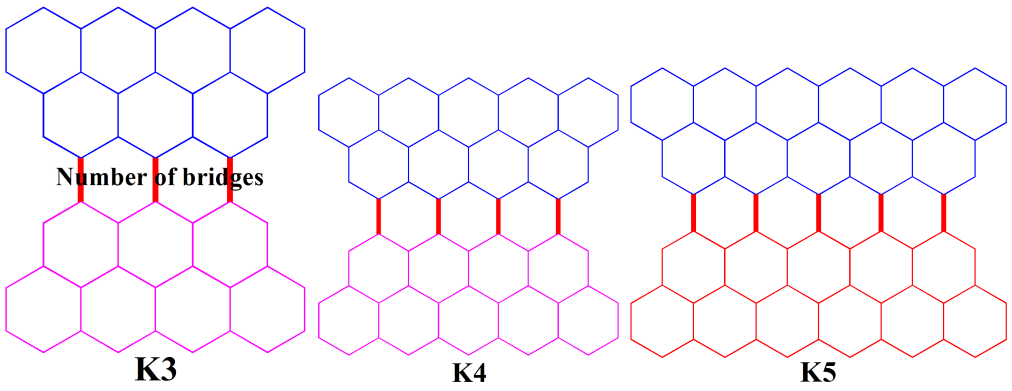


Figure 1: Non-Kekulean benzenoid Graphs $\mathcal{K}_n$ [5]

According to the degree of the atoms, there are three types of atom-bonds in $\mathcal{K}_n$: $(2 \sim 2)$, $(2 \sim 3)$ and $(3 \sim 3)$. The atom-bonds partition of $\mathcal{K}_n$ is shown as [5]:

$$\begin{aligned}
E_{2\sim2} &= \Big\{e = u \sim v, \forall\, u, v \in V(\mathcal{K}_n)\Big| d_u = 2, d_v = 2\Big\},\ |E_{2\sim2}| = 8 \\
E_{2\sim3} &= \Big\{e = u \sim v, \forall\, u, v \in V(\mathcal{K}_n)\Big| d_u = 2, d_v = 3\Big\},\ |E_{2\sim3}| = 4(n + 3) \\
E_{3\sim3} &= \Big\{e = u \sim v, \forall\, u, v \in V(\mathcal{K}_n)\Big| d_u = 3, d_v = 3\Big\},\ |E_{3\sim3}| = 13n - 6.
\end{aligned}$$

Table 1 shows three types of edges based on the temperature of end vertices of each edge using equation (1) and the above division of $\mathcal{K}_n$.

Table 1: Atom-bonds based partition of each atom of $\mathcal{K}_n$

(T_{u_i}, T_{v_j})	$\left(\frac{2}{2(6n+7)-2}, \frac{3}{2(6n+7)-3}\right)$	$\left(\frac{2}{2(6n+7)-2}, \frac{6}{2(6n+7)-6}\right)$	$\left(\frac{6}{2(6n+7)-6}, \frac{6}{2(6n+7)-6}\right)$
Frequency	8	$4(n+3)$	$(13n-6)$

2.1 Results and discussion

In this section, we investigate some temperature indices for Non-Kekulean benzenoid graph.

Theorem 2.1. *Let $\mathcal{K}_n$ be a Non-Kekulean benzenoid graph. Then the first temperature index is $\frac{8}{3}(n+1) + \frac{2(30n^2+119n+87)}{3(12n^2+23n+11)} + \frac{6(13n-6)}{12n+11}$.*

Proof. Using the atom-bonds partition from Table 1 in the formula of the first temperature index (2), we obtain

$$\begin{aligned} T_1(\mathcal{K}_n) &= \sum_{E_{2\sim 2}} (T_2 + T_2) + \sum_{E_{2\sim 3}} (T_2 + T_3) + \sum_{E_{3\sim 3}} (T_3 + T_3) \\ &= 8\left[\frac{2}{2(6n+7)-2} + \frac{2}{2(6n+7)-2}\right] \\ &+ 4(n+3)\left[\frac{2}{2(6n+7)-2} + \frac{3}{2(6n+7)-3}\right] \\ &+ (13n-6)\left[\frac{3}{2(6n+7)-3} + \frac{3}{2(6n+7)-3}\right] \end{aligned}$$

After simplification, we get

$$T_1(\mathcal{K}_n) = \frac{8}{3}(n+1) + \frac{2(30n^2+119n+87)}{3(12n^2+23n+11)} + \frac{6(13n-6)}{12n+11}. \tag{11}$$

□

Theorem 2.2. *Let $\mathcal{K}_n$ be a Non-Kekulean benzenoid graph. Then the second temperature index is $\frac{2}{9(n+1)^2} + \frac{2(n+3)}{12n^2+23n+11} + \frac{9(13n-6)}{(12n+11)^2}$.*

Proof. Using the atom-bonds partition from Table 1 in the formula of the second temperature index (3), we obtain

$$\begin{aligned} T_2(\mathcal{K}_n) &= \sum_{E_{2\sim 2}} (T_2 \times T_2) + \sum_{E_{2\sim 3}} (T_2 \times T_3) + \sum_{E_{3\sim 3}} (T_3 \times T_3) \\ &= 8\left[\frac{2}{2(6n+7)-2} \times \frac{2}{2(6n+7)-2}\right] \\ &+ 4(n+3)\left[\frac{2}{2(6n+7)-2} \times \frac{3}{2(6n+7)-3}\right] \\ &+ (13n-6)\left[\frac{3}{2(6n+7)-3} \times \frac{3}{2(6n+7)-3}\right] \end{aligned}$$

After simplification, we get

$$T_2(\mathcal{K}_n) = \frac{2}{9(n+1)^2} + \frac{2(n+3)}{12n^2+23n+11} + \frac{9(13n-6)}{(12n+11)^2}. \tag{12}$$

□

Theorem 2.3. *Let $\mathcal{K}_n$ be a Non-Kekulean benzenoid graph. Then the first hyper temperature index is $\frac{8(n+1)^2}{9} + \frac{(n+3)(30n+29)^2}{36(n+1)^2(12n+11)^2} + \frac{36(13n-6)}{(12n+11)^2}$.*

Proof. Using the atom-bonds partition from Table 1 in the formula of the first hyper temperature index (4), we obtain

$$\begin{aligned} HT_1(\mathcal{K}_n) &= \sum_{E_{2\sim 2}} (T_2 + T_2)^2 + \sum_{E_{(2,3)}} (T_2 + T_3)^2 + \sum_{E_{3\sim 3}} (T_3 + T_3)^2 \\ &= 8\left[\frac{2}{2(6n+7)-2} + \frac{2}{2(6n+7)-2}\right]^2 \\ &+ 4(n+3)\left[\frac{2}{2(6n+7)-2} + \frac{3}{2(6n+7)-3}\right]^2 \\ &+ (13n-6)\left[\frac{3}{2(6n+7)-3} + \frac{3}{2(6n+7)-3}\right]^2 \end{aligned}$$

After simplification, we get

$$HT_1(\mathcal{K}_n) = \frac{8(n+1)^2}{9} + \frac{(n+3)(30n+29)^2}{36(n+1)^2(12n+11)^2} + \frac{36(13n-6)}{(12n+11)^2}. \tag{13}$$

□

Theorem 2.4. *Let $\mathcal{K}_n$ be a Non-Kekulean benzenoid graph. Then the second hyper temperature index is .*

Proof. Using the atom-bonds partition from Table 1 in the formula of the second temperature index (5), we obtain

$$\begin{aligned} HT_2(\mathcal{K}_n) &= \sum_{E_{2\sim 2}} (T_2 \times T_2)^2 + \sum_{E_{2\sim 3}} (T_2 \times T_3)^2 + \sum_{E_{3\sim 3}} (T_3 \times T_3)^2 \\ &= 8\left[\frac{2}{2(6n+7)-2} \times \frac{2}{2(6n+7)-2}\right]^2 \\ &+ 4(n+3)\left[\frac{2}{2(6n+7)-2} \times \frac{3}{2(6n+7)-3}\right]^2 \\ &+ (13n-6)\left[\frac{3}{2(6n+7)-3} \times \frac{3}{2(6n+7)-3}\right]^2 \end{aligned}$$

After simplification, we get

$$HT_2(\mathcal{K}_n) = \frac{1}{162(n+1)^4} + \frac{n+3}{(n+1)^2(12n+11)^2} + \frac{81(13n-6)}{12n+11}. \tag{14}$$

□

Theorem 2.5. *Let $\mathcal{K}_n$ be a Non-Kekulean benzenoid graph, then the sum connectivity temperature index is $\frac{8\sqrt{3}}{\sqrt{n+1}} + 4(n+3)\sqrt{\frac{12n^2+23n+11}{6(30n^2+119n+87)}} + \frac{(13n-6)\sqrt{12n+11}}{6}$.*

Proof. Using the atom-bonds partition from Table 1 in the formula of the sum connectivity temperature index (6), we obtain

$$\begin{aligned} ST(\mathcal{K}_n) &= \sum_{E_{2\sim 2}} \frac{1}{\sqrt{(T_3+T_2)}} + \sum_{E_{2\sim 3}} \frac{1}{\sqrt{(T_2+T_3)}} + \sum_{E_{3\sim 3}} \frac{1}{\sqrt{(T_3+T_3)}} \\ &= 8\frac{1}{\sqrt{\left[\frac{2}{2(6n+7)-2} + \frac{2}{2(6n+7)-2}\right]}} \\ &+ 4(n+3)\frac{1}{\sqrt{\left[\frac{2}{2(6n+7)-2} + \frac{3}{2(6n+7)-3}\right]}} \\ &+ (13n-6)\frac{1}{\sqrt{\left[\frac{3}{2(6n+7)-3} + \frac{3}{2(6n+7)-3}\right]}} \end{aligned}$$

After simplification, we get

$$ST(\mathcal{K}_n) = \frac{8\sqrt{3}}{\sqrt{n+1}} + 4(n+3)\sqrt{\frac{12n^2+23n+11}{6(30n^2+119n+87)}} + \frac{(13n-6)\sqrt{12n+11}}{6}. \tag{15}$$

□

Theorem 2.6. *Let $\mathcal{K}_n$ be a Non-Kekulean Benzenoid graph. Then the product connectivity temperature index is* $24(n+1)+4(n+3)\sqrt{2(12n^2+23n+11)}+\frac{(13n-6)(12n+11)}{3}$.

Proof. Using the atom-bond s partition from Table 1 in the formula of the product connectivity temperature index (7), we obtain

$$\begin{aligned} PT(\mathcal{K}_n) &= \sum_{E_{2\sim 2}} \frac{1}{\sqrt{(T_2\times T_2)}} + \sum_{E_{2\sim 3}} \frac{1}{\sqrt{(T_3\times T_3)}} + \sum_{E_{3\sim 3}} \frac{1}{\sqrt{(T_3\times T_3)}} \\ &= 8\frac{1}{\sqrt{\left[\frac{2}{2(6n+7)-2}\times\frac{2}{2(6n+7)-2}\right]}} \\ &+ 4(n+3)\frac{1}{\sqrt{\left[\frac{2}{2(6n+7)-2}\times\frac{3}{2(6n+7)-3}\right]}} \\ &+ (13n-6)\frac{1}{\sqrt{\left[\frac{3}{2(6n+7)-3}\times\frac{3}{2(6n+7)-3}\right]}} \end{aligned}$$

After simplification, we get

$$PT(\mathcal{K}_n) = 24(n+1)+4(n+3)\sqrt{2(12n^2+23n+11)}+\frac{(13n-6)(12n+11)}{3}. \qquad (16)$$

□

Theorem 2.7. *Let $\mathcal{K}_n$ be a Non-Kekulean benzenoid graph. Then the reciprocal product temperature index is* $\frac{4}{3(n+1)}+\frac{4(n+3)}{\sqrt{2(12n^2+23n+11)}}+\frac{3(13n-6)}{12n+11}$.

Proof. Using the atom-bonds partition from Table 1 in the formula of the second temperature index (3), we obtain

$$\begin{aligned} RPT(\mathcal{K}_n) &= \sum_{E_{2\sim 2}} (T_2\times T_2) + \sum_{E_{2\sim 3}} (T_2\times T_3) + \sum_{E_{3\sim 3}} (T_3\times T_3) \\ &= 8\left[\frac{2}{2(6n+7)-2}\times\frac{2}{2(6n+7)-2}\right] \\ &+ 4(n+3)\left[\frac{2}{2(6n+7)-2}\times\frac{3}{2(6n+7)-3}\right] \\ &+ (13n-6)\left[\frac{3}{2(6n+7)-3}\times\frac{3}{2(6n+7)-3}\right] \end{aligned}$$

After simplification, we get

$$RPT(\mathcal{K}_n) = \frac{4}{3(n+1)} + \frac{4(n+3)}{\sqrt{2(12n^2+23n+11)}} + \frac{3(13n-6)}{12n+11}. \tag{17}$$

□

Theorem 2.8. *Let $\mathcal{K}_n$ be a Non-Kekulean benzenoid graph. Then the F-temperature index is $\frac{4}{9(n+1)^2} + 4(n+3)(468n^2+328n+445) + \frac{18(13n-6)}{(12n+11)^2}$.*

Proof. Using the atom-bonds partition from Table 1 in the formula of the F-temperature index (9), we obtain

$$\begin{aligned} FT(\mathcal{K}_n) &= \sum_{E_{2\sim 2}} \left(T_2^2 + T_2^2\right) + \sum_{E_{2\sim 3}} \left(T_2^2 + T_3^2\right) + \sum_{E_{3\sim 3}} \left(T_3^2 + T_3^2\right) \\ &= 8\left[\left\{\frac{2}{2(6n+7)-2}\right\}^2 + \left\{\frac{2}{2(6n+7)-2}\right\}^2\right] \\ &+ 4(n+3)\left[\left\{\frac{2}{2(6n+7)-2}\right\}^2 + \left\{\frac{3}{2(6n+7)-3}\right\}^2\right] \\ &+ (13n-6)\left[\left\{\frac{3}{2(6n+7)-3}\right\}^2 + \left\{\frac{3}{2(6n+7)-3}\right\}^2\right] \end{aligned}$$

After simplification, we get

$$FT(\mathcal{K}_n) = \frac{4}{9(n+1)^2} + 4(n+3)(468n^2+328n+445) + \frac{18(13n-6)}{(12n+11)^2}. \tag{18}$$

□

2.2 Numerical and graphical comparison temperature indices for $\mathcal{K}_n$

In this section, we present a numerical and graphical comparison temperature indices for $p = 2, 3, 4, ..., 15$ of Non-Kekulean benzenoid graph $\mathcal{K}_n$.

Table 2: Temperature indices of Non-Kekulean benzenoid graph $\mathcal{K}_n$ for $n \geq 2$

p	T_1	T_2	HT_1	HT_2	ST	PT	RPT	FT
2	15.63	0.27	8.69	46.29	28.63	595.16	3.54	59460
3	18.55	0.21	14.83	56.87	45.41	1078.38	3.67	135384
4	21.32	0.18	22.75	63.15	65.94	1704.78	3.81	258860
5	24.04	0.15	32.46	67.31	89.58	2474.38	3.85	441120
6	26.74	0.13	43.96	70.27	115.03	3387.17	3.88	693396
7	29.43	0.11	57.25	72.47	144.72	4443.15	3.9	1026920
8	32.1	0.1	72.33	74.18	174.18	5642.33	3.92	1452924
9	34.79	0.09	89.19	75.55	208.81	6984.69	3.93	1982640
10	37.46	0.084	107.83	76.67	243.83	8470.25	3.94	2627300
11	40.13	0.08	128.26	77.6	280.69	10099	3.95	3398136
12	42.8	0.072	150.46	78.39	319.28	11871	3.96	4306380
13	45.47	0.067	174.45	79.06	359.53	13786	3.97	5363264
14	48.14	0.063	200.21	79.64	401.38	14844	3.98	6580020
15	50.81	0.059	227.75	80.15	444.75	18046	3.99	7967880

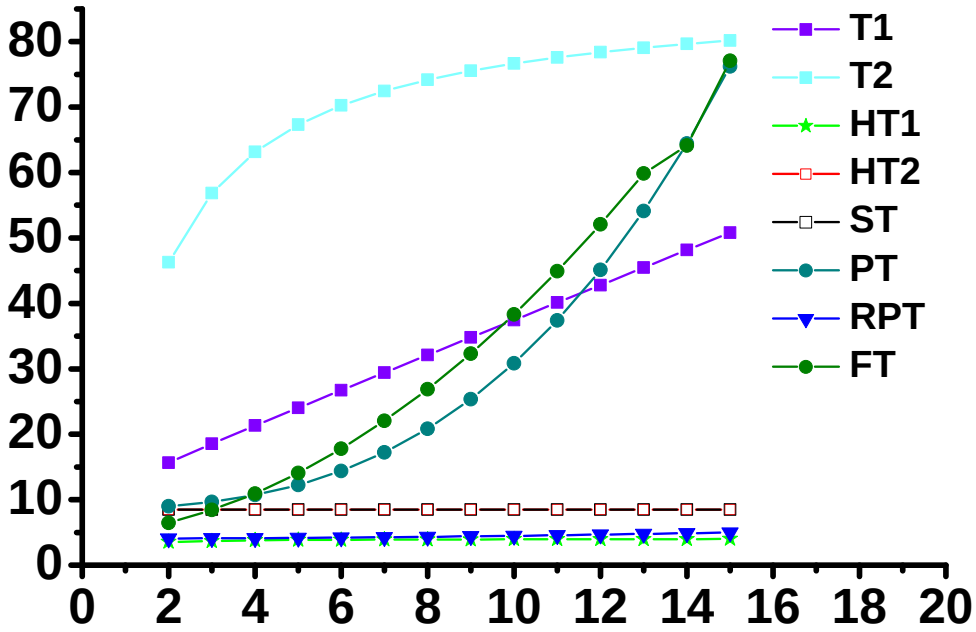


Figure 2: 2D-graphical comparison of temperature indices of $\mathcal{K}_n$

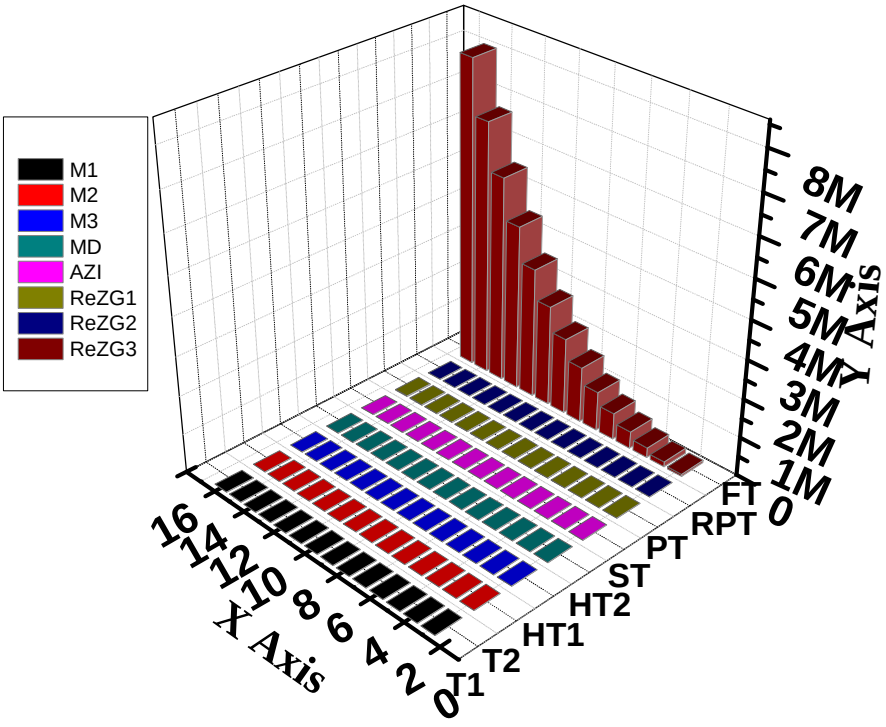


Figure 3: 3D-graphical comparison of temperature indices of $\mathcal{K}_n$

3 Conclusion

In this article, we propose computing the first temperature index, second temperature index, first hyper temperature index, second hyper temperature index, sum temperature index, product temperature, reciprocal product temperature index, and F-temperature index of a Non-Kekulean benzenoid graph $\mathcal{K}_n$, which correlates well with entropy, acentric factor, enthalpy of vaporisation, and standard enthalpy of vaporisation.

References

[1] S. Cyvins and I. Gutman, *Topological properties of benzenoid hydrocarbons: Part xliv. obvious and concealed non-kekuléan benzenoids*, Journal of Molecular Structure:

THEOCHEM **150** (1987), no. 1-2, 157–169.

[2] J. R. Dias and G. C. Cash, *Determining the number of resonance structures in concealed non-kekulean benzenoid hydrocarbons*, Journal of chemical information and computer sciences **41** (2001), no. 1, 129–133.

[3] S. Ding, M. I. Qureshi, S. F. Shah, A. Fahad, M. K. Jamil, and J. B. Liu, *Face index of nanotubes and regular hexagonal lattices*, International Journal of Quantum Chemistry (2021), e26761.

[4] S. Fajtlowicz, *On conjectures of graffiti*, Annals of Discrete Mathematics, vol. 38, Elsevier, 1988, pp. 113–118.

[5] M. Ibrahim, N. Zahra, and M. K. Siddiqui, *On ve-degree and ev-degree based topological indices for the series of benzenoid graphs*, Polycyclic Aromatic Compounds (2021), 1–10.

[6] M. Irfan, H. U. Rehman, H. Almusawa, S. Rasheed, and I. A. Baloch, *M-polynomials and topological indices for line graphs of chain silicate network and h-naphtalenic nanotubes*, Journal of Mathematics **2021** (2021).

[7] C. Kan, Y. Tan, J. B. Liu, and B. H. Xing, *Some chemistry indices of clique-inserted graph of a strongly regular graph*, Complexity **2021** (2021).

[8] V. Kulli, *The (a, b)-ka temperature indices of tetrameric 1, 3-adamantane*.

[9] J. B. Liu, S. Akram, M. Javaid, A. Raheem, and R. Hasni, *Bounds of degree-based molecular descriptors for generalized-sum graphs*, Discrete Dynamics in Nature and Society **2021** (2021).

[10] J. B. Liu, M. Arockiaraj, M. Arulperumjothi, and S. Prabhu, *Distance based and bond additive topological indices of certain repurposed antiviral drug compounds tested for treating covid-19*, International Journal of Quantum Chemistry **121** (2021), no. 10, e26617.

[11] J. B. Liu, W. Gao, M. K. Siddiqui, and M. R. Farahani, *Computing three topological indices for titania nanotubes tio2 [m, n]*, AKCE International Journal of Graphs and Combinatorics **13** (2016), no. 3, 255–260.

[12] J. B. Liu, I. Khalid, M. T. Rahim, M. U. Rehman, F. Ali, and M. Salman, *Eccentric topological properties of a graph associated to a finite dimensional vector space*, Main Group Metal Chemistry **43** (2020), no. 1, 164–176.

[13] J. B. Liu, X. F. Pan, F. T. Hu, and F. F. Hu, *Asymptotic laplacian-energy-like invariant of lattices*, Applied mathematics and computation **253** (2015), 205–214.

[14] J. B. Liu, H. M. A. Siddiqui, M. F. Nadeem, and M. A. Binyamin, *Some topological properties of uniform subdivision of sierpiński graphs*, Main Group Metal Chemistry **44** (2021), no. 1, 218–227.

[15] J. B. Liu, S. Wang, C. Wang, and S. Hayat, *Further results on computation of topological indices of certain networks*, IET Control Theory & Applications **11** (2017), no. 13, 2065–2071.

[16] J. B. Liu, T. Zhang, and S. Hayat, *The calculations of topological indices on certain networks*, Journal of Mathematics **2021** (2021).

[17] J. B. Liu, J. Zhao, H. He, and Z. Shao, *Valency-based topological descriptors and structural property of the generalized sierpiński networks*, Journal of statistical physics **177** (2019), no. 6, 1131–1147.

[18] J. A. Manalo, J. Matsumoto, H. G. Takahashi, M. Q. Villafuerte, L. M. Olaguera, G. Ren, and T. Cinco, *The effect of urbanization on temperature indices in the philippines*, International Journal of Climatology.

[19] K. P. Narayankar, A. T. Kahsay, and D. Selvan, *Harmonic temperature index of certain nanostructures*.

[20] T. Pisanski and M. Randic, *Bridges between geometry and graph theory*, University of Ljubljana, Inst. of Mathematics, Physics and Mechanics , 1998.