

Multiplicative (a, b) -KA Temperature Indices of Certain Nanostructure

V.R.Kulli

Department of Mathematics, Gulbarga University, Gulbarga 585106, India

Abstract: In Chemical Graph Theory, graph indices are applied to measure the chemical characteristics of chemical compounds. In this study, we introduce the first and second multiplicative (a, b) -KA temperature indices of a chemical graph. Furthermore, we compute these indices for tetrameric 1,3-adamantane. Also we establish some other multiplicative temperature indices directly as a special case of multiplicative (a, b) -KA temperature indices for some special values of a and b .

Keywords: Chemical graph, temperature of a vertex, first and second multiplicative (a, b) -KA indices, tetrameric 1,3-adamantane.

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I. Introduction

In this paper, G denotes a finite, simple, connected graph, $V(G)$ and $E(G)$ denote the vertex set and edge set of G . The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u . We refer [1] for undefined term and notation.

A chemical graph is a graph whose vertices correspond to the atoms and the edges to the bonds. Graph indices have their applications in various disciplines of Science and Technology, see [2, 3]. For more information about graph indices, see [4]. Recently, some new graph indices were studied in [5, 6, 7, 8, 9, 10, 11, 12, 13].

The temperature of a vertex u of a graph G is defined by Faitlowicz in [14] as

$$T(u) = \frac{d_G(u)}{1 - d_G(u)}, \quad \text{where } |V(G)| = n.$$

The multiplicative first and second temperature indices and multiplicative first and second hyper temperature indices were introduced by Kulli in [15] and they are defined as

$$\begin{aligned} TH_1(G) &= \prod_{uv \in E(G)} [T(u) + T(v)], & TH_2(G) &= \prod_{uv \in E(G)} T(u)T(v). \\ HTH_1(G) &= \prod_{uv \in E(G)} [T(u) + T(v)]^2, & HTH_2(G) &= \prod_{uv \in E(G)} [T(u)T(v)]^2. \end{aligned}$$

Recently, some new variants of temperature indices were studied such as first temperature index [16], first and second hyper temperature indices [17], (a, b) - temperature index [18], harmonic temperature index [19], atom bond connectivity temperature index [20].

In [15], Kulli introduced the general multiplicative first and second temperature indices of a graph G and they are defined as

$$TH_1^a(G) = \prod_{uv \in E(G)} [T(u) + T(v)]^a, \quad TH_2^a(G) = \prod_{uv \in E(G)} [T(u)T(v)]^a.$$

where a is a real number.

Also in the same paper [15], the multiplicative sum and product connectivity temperature indices and multiplicative reciprocal product connectivity temperature index were defined as

$$\begin{aligned} STH(G) &= \prod_{uv \in E(G)} \frac{1}{\sqrt{T(u) + T(v)}}. \\ PTH(G) &= \prod_{uv \in E(G)} \frac{1}{\sqrt{T(u)T(v)}}. \end{aligned}$$

$$RPTII(G) = \prod_{uv \in E(G)} \sqrt{T(u)T(v)}.$$

Recently some new connectivity indices were studied in [21, 22, 23, 24, 25].

The multiplicative F -temperature index and general multiplicative temperature index were introduced in [15] and they are defined as

$$FTII(G) = \prod_{uv \in E(G)} [T(u)^2 + T(v)^2], \quad TH_a(G) = \prod_{uv \in E(G)} [T(u)^a + T(v)^a].$$

We now propose the modified multiplicative first and second temperature indices of a graph G , defined as

$${}^mT_1II(G) = \prod_{uv \in E(G)} \frac{1}{T(u) + T(v)}, \quad {}^mT_2II(G) = \prod_{uv \in E(G)} \frac{1}{T(u)T(v)}.$$

We introduce the multiplicative first and second (a, b) -KA temperature indices of a graph G , defined as

$$KAT_{a,b}^1II(G) = \prod_{uv \in E(G)} [T(u)^a + T(v)^a]^b, \quad KAT_{a,b}^2II(G) = \prod_{uv \in E(G)} [T(u)^a T(v)^a]^b,$$

where a, b are real numbers.

Recently, some (a, b) -KA indices were studied in [26, 27, 28].

In this paper, the first and second multiplicative (a, b) -KA temperature indices for tetrameric 1,3-adamantane are computed.

II. Observations

We observe the following

1. $TH_1(G) = KAT_{1,1}^1II(G).$
2. $HTH_1(G) = KAT_{1,2}^1II(G).$
3. ${}^mT_1II(G) = KAT_{1,-1}^1II(G).$
4. $TH_1^a(G) = KAT_{1,a}^1II(G).$
5. $STII(G) = KAT_{1,-\frac{1}{2}}^1II(G).$
6. $FTII(G) = KAT_{2,1}^1II(G).$
7. $TH_a(G) = KAT_{a,1}^1II(G).$

We also observe that

1. $TH_2(G) = KAT_{1,1}^2II(G).$
2. $HTH_2(G) = KAT_{1,2}^2II(G).$
3. ${}^mT_2II(G) = KAT_{1,-1}^2II(G).$
4. $TH_2^a(G) = KAT_{1,a}^2II(G).$
5. $PTII(G) = KAT_{1,-\frac{1}{2}}^2II(G).$
6. $RPTII(G) = KAT_{1,\frac{1}{2}}^2II(G).$

Clearly, we obtain some other multiplicative temperature indices directly as a special case of multiplicative (a, b) -KA temperature indices for some special values of a and b .

III. Results for Tetrameric 1,3-Adamantane

In Chemistry, diamondoids are variants of the carbon cage known as adamantane $C_{10}H_{16}$, the smallest unit cage structure of the diamond crystal lattice. We focus on the molecular graph structure of the family of the tetrameric 1,3-adamantane, symbolized by $TA[n]$. The graph of tetrameric 1,3-adamantane $TA[4]$ is shown in Figure 1.

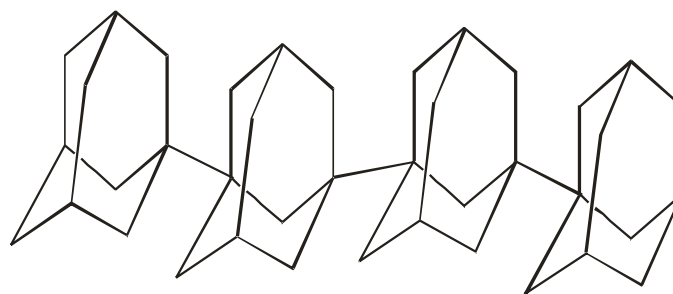


Figure 1.

Let G be the graph of tetrameric 1,3-adamantane $TA[n]$. By calculation, G has $10n$ vertices and $13n - 1$ edges.

By calculation, we obtain three types of edges based on the degrees of the end vertices of each edge as follows:

$$E_1 = \{uv \in E(G) \mid d_G(u)=2, d_G(v)=3\}, \quad |E_1| = 6n + 6.$$

$$E_2 = \{uv \in E(G) \mid d_G(u)=2, d_G(v)=4\}, \quad |E_2| = 6n - 6.$$

$$E_3 = \{uv \in E(G) \mid d_G(u)=d_G(v) = 4\}, \quad |E_3| = n - 1.$$

Thus in $TA[n]$, there are three types of edges based on the temperature of end vertices of each edge as given in Table 1.

$T(u), T(v) \setminus uv \in E(G)$	$\left(\frac{2}{10n-2}, \frac{3}{10n-3}\right)$	$\left(\frac{2}{10n-2}, \frac{4}{10n-4}\right)$	$\left(\frac{4}{10n-4}, \frac{4}{10n-4}\right)$
Number of edges	$6n + 6$	$6n - 6$	$n - 1$

Table 1. Temperature edge partition of G

Theorem 1. The multiplicative first (a, b) -KA temperature index of a tetrameric 1,3-adamantane $TA[n]$ is

$$KAT_{a,b}^1(TA[n]) = \left[\left(\frac{1}{5n-1}\right)^a + \left(\frac{3}{10n-3}\right)^a \right]^{b(6n+6)} \times \left[\left(\frac{1}{5n-1}\right)^a + \left(\frac{2}{5n-2}\right)^a \right]^{b(6n-6)} \times \left[2\left(\frac{2}{5n-2}\right)^a \right]^{b(n-1)}.$$

Proof: By definition and by using Table 1, we deduce

$$\begin{aligned} KAT_{a,b}^1 II(G) &= \prod_{uv \in E(G)} [T(u)^a + T(v)^a]^b \\ &= \left[\left(\frac{2}{10n-2}\right)^a + \left(\frac{3}{10n-3}\right)^a \right]^{b(6n+6)} \times \left[\left(\frac{2}{10n-2}\right)^a + \left(\frac{4}{10n-4}\right)^a \right]^{b(6n-6)} \\ &\quad \times \left[\left(\frac{4}{10n-4}\right)^a + \left(\frac{4}{10n-4}\right)^a \right]^{b(n-1)} \\ &= \left[\left(\frac{1}{5n-1}\right)^a + \left(\frac{3}{10n-3}\right)^a \right]^{b(6n+6)} \times \left[\left(\frac{1}{5n-1}\right)^a + \left(\frac{2}{5n-2}\right)^a \right]^{b(6n-6)} \times \left[2\left(\frac{2}{5n-2}\right)^a \right]^{b(n-1)}. \end{aligned}$$

By using observations and from Theorem 1, we obtain the following results.

Corollary 1.1. The multiplicative first temperature index of $TA[n]$ is

$$\begin{aligned} TH_1(TA[n]) &= KAT_{1,1}^1 II(TA[n]) \\ &= \left[\frac{25n-6}{(5n-1)(10n-3)} \right]^{(6n+6)} \times \left[\frac{15n-4}{(5n-1)(5n-2)} \right]^{(6n-6)} \times \left(\frac{4}{5n-2}\right)^{(n-1)} \end{aligned}$$

Corollary 1.2. The multiplicative first hyper temperature index of $TA[n]$ is

$$HTH_1(TA[n]) = KAT_{1,2}^1 II(TA[n])$$

$$= \left[\frac{25n-6}{(5n-1)(10n-3)} \right]^{(12n+12)} \times \left[\frac{15n-4}{(5n-1)(5n-2)} \right]^{(12n-12)} \times \left(\frac{4}{5n-2} \right)^{(2n-2)}$$

Corollary 1.3. The modified multiplicative first temperature index of $TA[n]$ is

$${}^m T_1 II(TA[n]) = KAT_{1,-1}^1 II(TA[n]) \\ = \left[\frac{25n-6}{(5n-1)(10n-3)} \right]^{-(6n+6)} \times \left[\frac{15n-4}{(5n-1)(5n-2)} \right]^{-(6n-6)} \times \left(\frac{4}{5n-2} \right)^{-(n-1)}$$

Corollary 1.4. The general multiplicative first temperature index of $TA[n]$ is

$$TII_1^a(TA[n]) = KAT_{1,a}^1 II(TA[n]) \\ = \left[\frac{25n-6}{(5n-1)(10n-3)} \right]^{a(6n+6)} \times \left[\frac{15n-4}{(5n-1)(5n-2)} \right]^{a(6n-6)} \times \left(\frac{4}{5n-2} \right)^{a(n-1)}$$

Corollary 1.5. The multiplicative sum connectivity temperature index of $TA[n]$ is

$$STII(TA[n]) = KAT_{1,-\frac{1}{2}}^1 II(TA[n]) \\ = \left[\frac{25n-6}{(5n-1)(10n-3)} \right]^{-(3n+3)} \times \left[\frac{15n-4}{(5n-1)(5n-2)} \right]^{-(3n-3)} \times \left(\frac{4}{5n-2} \right)^{\frac{1}{2}(n-1)}$$

Corollary 1.6. The multiplicative F -temperature index of $TA[n]$ is

$$FTII(TA[n]) = KAT_{2,1}^1 II(TA[n]) \\ = \left[\frac{1}{(5n-1)^2} + \frac{9}{(10n-3)^2} \right]^{6n+6} \times \left[\frac{1}{(5n-1)^2} + \frac{4}{(5n-1)^2} \right]^{6n-6} \times \left(\frac{4}{(5n-2)^2} \right)^{n-1}$$

Corollary 1.7. The general multiplicative temperature index of $TA[n]$ is

$$TII_a(TA[n]) = KAT_{a,1}^1 II(TA[n]) \\ = \left[\left(\frac{1}{5n-1} \right)^a + \left(\frac{3}{10n-3} \right)^a \right]^{6n+6} \times \left[\left(\frac{1}{5n-1} \right)^a + \left(\frac{2}{5n-2} \right)^a \right]^{6n-6} \times \left[2 \left(\frac{2}{5n-2} \right)^a \right]^{n-1}$$

Theorem 2. The multiplicative second (a, b) -KA temperature index a tetrameric 1,3-adamantane $TA[n]$ is

$$KAT_{a,b}^2(TA[n]) = \left[\left(\frac{1}{5n-1} \right)^a \left(\frac{3}{10n-3} \right)^a \right]^{b(6n+6)} \times \left[\left(\frac{1}{5n-1} \right)^a \left(\frac{2}{5n-2} \right)^a \right]^{b(6n-6)} \times \left(\frac{2}{5n-2} \right)^{2ab(n-1)}$$

Proof: To compute $KAT_{a,b}^2 II(TA[n])$, we see that

$$KAT_{a,b}^2 II(G) = \prod_{uv \in E(G)} [T(u)^a T(v)^a]^b \\ = \left[\left(\frac{2}{10n-2} \right)^a \times \left(\frac{3}{10n-3} \right)^a \right]^{b(6n+6)} \times \left[\left(\frac{2}{10n-2} \right)^a \times \left(\frac{4}{10n-4} \right)^a \right]^{b(6n-6)} \\ \times \left[\left(\frac{4}{10n-4} \right)^a \times \left(\frac{4}{10n-4} \right)^a \right]^{b(n-1)} \\ = \left[\left(\frac{1}{5n-1} \right)^a \times \left(\frac{3}{10n-3} \right)^a \right]^{b(6n+6)} \times \left[\left(\frac{1}{5n-1} \right)^a \times \left(\frac{2}{5n-2} \right)^a \right]^{b(6n-6)} \times \left(\frac{2}{5n-2} \right)^{2ab(n-1)}$$

From Theorem 2 and observations, we establish the following results.

Corollary 2.1. The multiplicative second temperature index of $TA[n]$ is

$$T_2 II(TA[n]) = KAT_{1,1}^2 II(TA[n])$$

$$= \left[\frac{3}{(5n-1)(10n-3)} \right]^{(6n+6)} \times \left[\frac{2}{(5n-1)(5n-2)} \right]^{(6n-6)} \times \left(\frac{2}{5n-2} \right)^{2(n-1)}.$$

Corollary 2.2. The multiplicative second hyper temperature index of $TA[n]$ is

$$HT_2 II(TA[n]) = KAT_{1,2}^2 II(TA[n])$$

$$= \left[\frac{3}{(5n-1)(10n-3)} \right]^{12n+12} \times \left[\frac{2}{(5n-1)(5n-2)} \right]^{12n-12} \times \left(\frac{2}{5n-2} \right)^{4(n-1)}$$

Corollary 2.3. The modified multiplicative second temperature index of $TA[n]$ is

$${}^m T_2 II(TA[n]) = KAT_{1,-1}^2 II(TA[n])$$

$$= \left[\frac{3}{(5n-1)(10n-3)} \right]^{-(6n+6)} \times \left[\frac{2}{(5n-1)(5n-2)} \right]^{-(6n-6)} \times \left(\frac{2}{5n-2} \right)^{-2(n-1)}.$$

Corollary 2.4. The general multiplicative second temperature index of $TA[n]$ is

$$T_2^a II(TA[n]) = KAT_{1,a}^2 II(TA[n])$$

$$= \left[\frac{3}{(5n-1)(10n-3)} \right]^{a(6n+6)} \times \left[\frac{2}{(5n-1)(5n-2)} \right]^{a(6n-6)} \times \left(\frac{2}{5n-2} \right)^{2a(n-1)}.$$

Corollary 2.5. The multiplicative product connectivity temperature index of $TA[n]$ is

$$PTII(TA[n]) = KAT_{1,-\frac{1}{2}}^2 II(TA[n])$$

$$= \left[\frac{3}{(5n-1)(10n-3)} \right]^{-(3n+3)} \times \left[\frac{2}{(5n-1)(5n-2)} \right]^{-(3n-3)} \times \left(\frac{2}{5n-2} \right)^{-(n-1)}.$$

Corollary 2.6. The multiplicative reciprocal product connectivity temperature index $TA[n]$ is

$$RPTII(TA[n]) = KAT_{1,\frac{1}{2}}^2 II(TA[n])$$

$$= \left[\frac{3}{(5n-1)(10n-3)} \right]^{3n+3} \times \left[\frac{2}{(5n-1)(5n-2)} \right]^{3n-3} \times \left(\frac{2}{5n-2} \right)^{n-1}.$$

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