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RESEARCH

On the Computation of Temperature Indices of Silicates, with Strong Potential to Predict the Boiling Point of Hydrocarbons

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Abstract
The molecular graph of a chemical compound can be measured using a topological index, which helps us to understand its physical and chemical characteristics. Topological indices play a crucial role in characterizing the different chemical properties of substances, such as $Si\,O_4$, within the field of chemical graph theory. $Si\,O_4$ is an important compound owing to its versatility, accessibility, and quantifiability. In this study, we developed the methodology for calculating various temperature indices for a linear molecular graph of $Si\,O_4$. We compare and find the correlation of temperature indices of silicate chain. In the last section of the paper, we present an application of benzenoid hydrocarbons to elucidate the significance of temperature indices.

Keywords Topological indices · Temperature indices · $Si\,O_4$ embedded in a chain · Benzenoid hydrocarbons · Correlation

1 Introduction

Mathematical chemistry uses functions and polynomials to find symmetrical patterns within molecular graphs, which has important implications in multiple domains of modern chemistry, especially in organic chemistry. Topological indices are widely used in theoretical chemistry, specifically in the study of relationships between molecular structure and the characteristics or activities of molecules (QSPR/QSAR). Several well-known researchers have extensively studied topological indices to understand different properties of graphs [1, 2]. Topological indices, employed in QSPR and QSAR are quantitative measures that assess a molecule's biological, physical, and chemical characteristics. These indices play a vital role in the chemical industry. Recently, some researchers have examined a wide range of chemical substances and calculated topological indices for different molecular graphs [3–6]. The primary impetus for this paper stems from two recent publications [7, 8].

A graph invariant, frequently known as a topological invariant, is a numerical measure that captures the relationship between the molecular structure of a molecule and its physical, biological, and chemical properties. Scholars have investigated multiple topological features to forecast the chirality and complexity. For a more comprehensive understanding of the applications of topological indices, we refer the book [9].

Let G be a simple, connected and undirected graph. The distance between vertices x and y in G, represented as $d(x, y)$, is the minimum number of edges in a shortest path between x and y. The neighbourhood set is defined as the set of vertices, denoted as N_x, in G that are next to vertex x, meaning they have a distance of 1 from x. The degree (d_x) of a vertex is the cardinality of the neighbourhood set of x. Let $\Phi(d_u, d_v)$ be a real-valued function. For a graph G, the degree-based topological index (or graphical function-index) $TI(G)$ with edge-weight function $\Phi(d_u, d_v)$ is defined as

$$TI(G) := \sum_{uv \in E(G)} \Phi(d_u, d_v), \tag{1}$$

where d_u and d_v represent the degrees of vertices u and v correspondingly.

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Several topological indices based on degrees have already been defined, and some of them are shown in Table 1.

In the paper [10], Fajtlowicz defined the temperature of a vertex as, for a graph G having n vertices, the temperature of a vertex u is defined as

$$T_u = \frac{d_u}{n - d_u}, \tag{2}$$

Temperature-based topological indices can be defined using Eq. 2. For example, the harmonic temperature (HT) index of a graph G can be defined as

$$HT(G) = \sum_{uv \in E(G)} \frac{2}{T_u + T_v}, \tag{3}$$

where T_u and T_v represent the temperatures of u and v correspondingly.

Some more temperature based topological indices are shown in Table 2.

In this paper, we discuss the construction of the temperature-based indices (Table 2) based on the Si and O atoms degrees-dependent atom-bonds partition of a silicate chain SC_q^p. Applying the atom-bonds partition to the molecular structure of silicates, we also examine the silicon tetrahedron $Si\,O_4$ in a complicated structure and find the exact formulas for various important temperature-based indices. Regarding temperature indices, we consult [16]. We will determine the methodology for calculating various temperature indices for a linear molecular graph of $Si\,O_4$. Moreover, we will give a comparison and a correlation of temperature indices of the silicate chain. In the last section of the paper, we will give an application of benzenoid hydrocarbons to understand the significance of temperature indices.

2 Chain of Silicates SC_q^p

In this section, we will discuss the structure of the SC_q^p. The formula $Si\,O_4$, which has tetrahedron geometry, empirically represents the fundamental unit of silicates [17]. The $Si\,O_4$ tetrahedron is present in almost all silicates. From a chemical perspective, a tetrahedron $Si\,O_4$, as shown in Fig. 1, has silicon atoms bound to evenly spaced oxygen atoms at each corner of the tetrahedron. A single chain of silicates is formed from the resulting $Si\,O_4$, and a silicate tetrahedron links with other $Si\,O_4$ horizontally. Likewise, when two $Si\,O_4$ molecules unite corner to corner, as shown in Fig. 1, each $Si\,O_4$ shares its oxygen atoms with the other $Si\,O_4$ molecule. Once this sharing procedure is done, these two $Si\,O_4$ molecules can be connected with two more molecules. The silicate chain SC_q^p is now obtained; here, p and q denote the number of silicate chains created and the total number of $Si\,O_4$ in a single silicate chain, respectively. Here, pq number of tetrahedron $Si\,O_4$ is employed in a chain of silicates SC_q^p; see Fig. 1.

Here, we have three different kinds of atom bonding on the valency bases of each SC_q^p atom in the chain of silicates SC_q^p. We can create three distinct sets based on the valencies. Let E_{ij} represent the collection of all edges where each edge has a degree of i at one end and j at the other. For SC_q^p, we have

$$E_{33} = \{uv \in E(G) | d_u = d_v = 3\},$$
$$E_{36} = \{uv \in E(G) | d_u = 3, d_v = 6\},$$
$$E_{66} = \{uv \in E(G) | d_u = d_v = 6\}.$$

From Fig. 1, it is clear $|E_{33}| = 3p+2$, $|E_{36}| = 3q\,(p+1)-4$ and $|E_{33}| = 3q\,(p-2)+2$ also $\left|V\left(SC_q^p\right)\right| = p\,(3p-1)$ and $\left|E\left(SC_q^p\right)\right| = 3p\,(2q+1)-q$.

3 Temperature Based Indices for SC_q^p

In this section, we will compute the temperature indices mentioned in Table 2 for the SC_q^p when $p = q$. Therefore, we will now refer to it as SC_p^p.

Theorem 1 *Let SC_p^p be a chain of silicates. Then the harmonic temperature index is* $\frac{p^2\left(3p\left(12+p\left(63p^2-6p-209\right)\right)+488\right)}{18(p+1)(3p-4)}$.

Table 1 Some degree based topological indices

Name	Symbol	Edge weighted function	Reference
Harmonic index	H	$\frac{2}{d_u+d_v}$	[11]
Inverse sum indeg index	ISI	$\frac{d_u d_v}{d_u+d_v}$	[12]
First Gourava index	GO_1	$d_u + d_v + d_u d_v$	[13]
Second Gourava index	GO_2	$(d_u + d_v)\, d_u d_v$	[13]
Sombor index	SO	$\sqrt{d_u^2 + d_v^2}$	[14]
Geometric-arithmetic index	GA	$\frac{2\sqrt{d_u d_v}}{d_u+d_v}$	[15]
Arithmetic-geometric index	AG	$\frac{d_u+d_v}{2\sqrt{d_u d_v}}$	[15]

Table 2 Some temperature based topological indices

Name	Symbol	Edge weighted function
Inverse sum indeg temperature	$ISIT$	$\frac{T_u T_v}{T_u+T_v}$
First Gourava temperature index	GO_1T	$T_u + T_v + T_u T_v$
Second Gourava temperature index	GO_2T	$(T_u + T_v)\, T_u T_v$
Sombor temperature index	SOT	$\sqrt{T_u^2 + T_v^2}$
Geometric-arithmetic temperature index	GAT	$\frac{2\sqrt{T_u T_v}}{T_u+T_v}$
Arithmetic-geometric temperature index	AGT	$\frac{T_u+T_v}{2\sqrt{T_u T_v}}$

Proof Using the bond partition from Table 3 in the formula of the harmonic temperature index, we obtain

$$HT(SC_p^p) = \sum_{uv\in E_{33}} \left(\frac{2}{T_u+T_v}\right) + \sum_{uv\in E_{36}} \left(\frac{2}{T_u+T_v}\right) + \sum_{uv\in E_{66}} \left(\frac{2}{T_u+T_v}\right) = (3p+2)\left(\frac{2}{\frac{3}{3p^2-p-3}+\frac{3}{3p^2-p-3}}\right) + \left(3p^2+3p-4\right)\left(\frac{2}{\frac{3}{3p^2-p-3}+\frac{6}{3p^2-p-6}}\right) + \left(3p^2-6p+2\right)\left(\frac{2}{\frac{6}{3p^2-p-6}+\frac{6}{3p^2-p-6}}\right).$$

After some simple steps of calculations, we get

$$HT(SC_p^p) = \frac{p^2\left(3p\left(12+p\left(63p^2-6p-209\right)\right)+488\right)}{18\,(p+1)\,(3p-4)}.$$

□

Theorem 2 *Let SC_p^p be a chain of silicates. Then the inverse sum indeg temperature index is* $5 + \frac{9p-6}{6p^2-2p-6} + \frac{32}{7(3p-4)} + \frac{8}{7(p+1)} - \frac{24-15p}{p-3p^2+6}$.

Proof Using the bond partition from Table 3 in the formula of the inverse sum indeg temperature index, we obtain

$$ISIT(SC_p^p) = \sum_{uv\in E_{33}} \left(\frac{T_u T_v}{T_u+T_v}\right) + \sum_{uv\in E_{36}} \left(\frac{T_u T_v}{T_u+T_v}\right) + \sum_{uv\in E_{66}} \left(\frac{T_u T_v}{T_u+T_v}\right) = (3p+2)\left(\frac{\left(\frac{3}{3p^2-p-3}\right)\left(\frac{3}{3p^2-p-3}\right)}{\left(\frac{3}{3p^2-p-3}\right)+\left(\frac{3}{3p^2-p-3}\right)}\right) + \left(3p^2+3p-4\right)\left(\frac{\left(\frac{3}{3p^2-p-3}\right)\left(\frac{6}{3p^2-p-6}\right)}{\left(\frac{3}{3p^2-p-3}\right)+\left(\frac{6}{3p^2-p-6}\right)}\right) + \left(3p^2-6p+2\right)\left(\frac{\left(\frac{6}{3p^2-p-6}\right)\left(\frac{6}{3p^2-p-6}\right)}{\left(\frac{6}{3p^2-p-6}\right)+\left(\frac{6}{3p^2-p-6}\right)}\right).$$

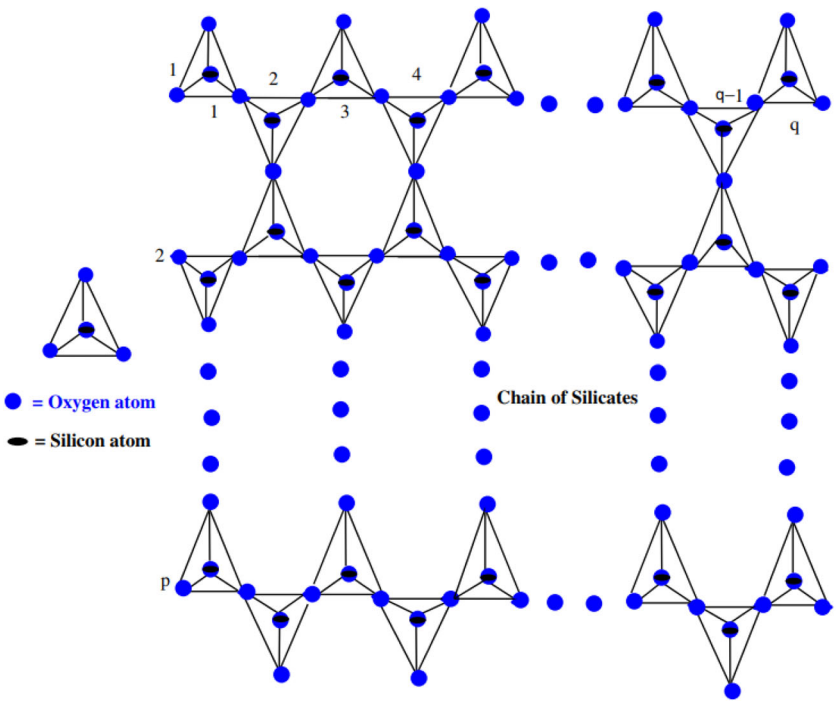

Fig. 1 Schematic representation of chain of silicates

Table 3 Atomic-bond separation of SC_q^p, for $p = q$

(T_u, T_v)	$\left(\frac{3}{3p^2-p-3}, \frac{3}{3p^2-p-3}\right)$	$\left(\frac{3}{3p^2-p-3}, \frac{6}{3p^2-p-6}\right)$	$\left(\frac{6}{3p^2-p-6}, \frac{6}{3p^2-p-6}\right)$
Frequency	$3p+2$	$3p^2+3p-4$	$3p^2-6p+2$

After some simple steps of calculations, we get

$$ISIT(SC_p^p) = 5 + \frac{9p-6}{6p^2-2p-6} + \frac{32}{7(3p-4)} + \frac{8}{7(p+1)} - \frac{24-15p}{p-3p^2+6}.$$

□

Theorem 3 *Let SC_p^p be a chain of silicates. Then the first Gourava temperature index for SC_p^p is* $\frac{9p^2(-214+p(-216+p(528+p(488+9p(-53+3p(-10+7p))))))}{(18+p(9+p(-26-6p+9p^2)))^2}$.

Proof Using the bond partition from Table 3 in the formula of the first Gourava temperature index, we obtain

$$\begin{aligned}GO_1T(SC_p^p) &= \sum_{uv\in E_{33}} (T_u + T_v + T_uT_v) + \sum_{uv\in E_{36}} (T_u + T_v + T_uT_v) \\ &+ \sum_{uv\in E_{66}} (T_u + T_v + T_uT_v) = (3p+2)\left(\frac{3}{3p^2-p-3}\right. \\ &+ \frac{3}{3p^2-p-3} + \left(\frac{3}{3p^2-p-3}\right)\left(\frac{3}{3p^2-p-3}\right)\Bigg) \\ &+ (3p^2+3p-4)\left(\frac{3}{3p^2-p-3} + \frac{6}{3p^2-p-6}\right. \\ &+ \left.\left(\frac{3}{3p^2-p-3}\right)\left(\frac{6}{3p^2-p-6}\right)\right) \\ &+ (3p^2-6p+2)\left(\frac{6}{3p^2-p-6} + \frac{6}{3p^2-p-6}\right. \\ &+ \left.\left(\frac{6}{3p^2-p-6}\right)\left(\frac{6}{3p^2-p-6}\right)\right).\end{aligned}$$

After some simple steps of calculations, we get

$$GO_1T(SC_p^p) = \frac{9p^2(-214+p(-216+p(528+p(488+9p(-53+3p(-10+7p))))))}{(18+p(9+p(-26-6p+9p^2)))^2}.$$

□

Theorem 4 *Let SC_p^p be a chain of silicates. Then the second Gourava temperature index for SC_p^p is* $\frac{162p^2(-278+p(-731+p(459+p(1276+9p(-58-69p+33p^2)))))}{(18+p(9+p(-26-6p+9p^2)))^3}$.

Proof Using the bond partition from Table 3 in the formula of the second Gourava temperature index, we obtain

$$\begin{aligned}GO_2T(SC_p^p) &= \sum_{uv\in E_{33}} (T_u + T_v)\,T_uT_v + \sum_{uv\in E_{36}} (T_u + T_v)\,T_uT_v \\ &+ \sum_{uv\in E_{66}} (T_u + T_v)\,T_uT_v = (3p+2)\left(\left(\frac{3}{3p^2-p-3}\right.\right. \\ &+ \left.\left.\frac{3}{3p^2-p-3}\right)\frac{3}{3p^2-p-3}\frac{3}{3p^2-p-3}\right) \\ &+ (3p^2+3p-4)\left(\left(\frac{3}{3p^2-p-3} + \frac{6}{3p^2-p-6}\right)\right. \\ &\times \left.\frac{3}{3p^2-p-3}\frac{6}{3p^2-p-6}\right) + (3p^2-6p+2) \\ &\times \left(\left(\frac{6}{3p^2-p-6} + \frac{6}{3p^2-p-6}\right)\right. \\ &\times \left.\frac{6}{3p^2-p-6}\frac{6}{3p^2-p-6}\right).\end{aligned}$$

After some simple steps of calculations, we get

$$GO_2T(SC_p^p) = \frac{162p^2(-278+p(-731+p(459+p(1276+9p(-58-69p+33p^2)))))}{(18+p(9+p(-26-6p+9p^2)))^3}.$$

□

Theorem 5 *Let SC_p^p be a chain of silicates. Then the sombor temperature index for SC_p^p is*

$$\begin{aligned}&3\sqrt{2}(2+3p)\sqrt{\frac{1}{(3+p-3p^2)^2}} + 6\sqrt{2}(2+3p(-2+p)) \\ &\sqrt{\frac{1}{(6+p-3p^2)^2}} + 3(3p(p+1)-4) \\ &\sqrt{\frac{1}{(p-3p^2+3)^2} + \frac{4}{(p-3p^2+6)^2}}.\end{aligned}$$

Proof Using the bond partition from Table 3 in the formula of the sombor temperature index, we obtain

$$\begin{aligned}SOT(SC_p^p) &= \sum_{uv\in E_{33}} \sqrt{T_u^2+T_v^2} + \sum_{uv\in E_{36}} \sqrt{T_u^2+T_v^2} + \sum_{uv\in E_{66}} \sqrt{T_u^2+T_v^2} \\ &= (3p+2)\sqrt{\left(\frac{3}{3p^2-p-3}\right)^2 + \left(\frac{3}{3p^2-p-3}\right)^2}\end{aligned}$$

$$+\left(3p^2+3p-4\right)\sqrt{\left(\frac{3}{3p^2-p-3}\right)^2+\left(\frac{6}{3p^2-p-6}\right)^2}$$
$$+\left(3p^2-6p+2\right)\sqrt{\left(\frac{6}{3p^2-p-6}\right)^2+\left(\frac{6}{3p^2-p-6}\right)^2}.$$

After some simple steps of calculations, we get

$$SOT(SC_p^p)=3\sqrt{2}\,(2+3p)\sqrt{\frac{1}{\left(3+p-3p^2\right)^2}}$$
$$+6\sqrt{2}\,(2+3p\,(-2+p))\sqrt{\frac{1}{\left(6+p-3p^2\right)^2}}$$
$$+3\,(3p\,(p+1)-4)\sqrt{\frac{1}{\left(p-3p^2+3\right)^2}+\frac{4}{\left(p-3p^2+6\right)^2}}.$$

□

Theorem 6 *Let SC_p^p be a chain of silicates. Then the geometric-arithmetic temperature index for SC_p^p is*

$$\left(-12+34-6p^2-21p^3+9p^4\right)\sqrt{\frac{1}{\left(6+p-3p^2\right)^2}}$$
$$+\left(-6-11p+3p^2+9p^3\right)\sqrt{\frac{1}{\left(3+p-3p^2\right)^2}}$$
$$+\frac{2\,(-4+3p\,(1+p))}{3\,(1+p)\,(-4+3p)\sqrt{\frac{1}{36+2p(9+p(-26-6p+9p^2))}}}.$$

Proof Using the bond partition from Table 3 in the formula of geometric-arithmetic temperature index, we obtain

$$GAT(SC_p^p)=\sum_{uv\in E_{33}}\frac{2\sqrt{T_uT_v}}{T_u+T_v}+\sum_{uv\in E_{36}}\frac{2\sqrt{T_uT_v}}{T_u+T_v}+\sum_{uv\in E_{66}}\frac{2\sqrt{T_uT_v}}{T_u+T_v}$$
$$=(3p+2)\frac{2\sqrt{\left(\frac{3}{3p^2-p-3}\right)\left(\frac{3}{3p^2-p-3}\right)}}{\frac{3}{3p^2-p-3}+\frac{3}{3p^2-p-3}}$$
$$+\left(3p^2+3p-4\right)\frac{2\sqrt{\left(\frac{3}{3p^2-p-3}\right)\left(\frac{6}{3p^2-p-6}\right)}}{\frac{3}{3p^2-p-3}+\frac{6}{3p^2-p-6}}$$
$$+\left(3p^2-6p+2\right)\frac{2\sqrt{\left(\frac{6}{3p^2-p-6}\right)\left(\frac{6}{3p^2-p-6}\right)}}{\frac{6}{3p^2-p-6}+\frac{6}{3p^2-p-6}}.$$

After some simple steps of calculations, we get

$$GAT(SC_p^p)=\left(-12+34-6p^2-21p^3+9p^4\right)\sqrt{\frac{1}{\left(6+p-3p^2\right)^2}}$$
$$+\left(-6-11p+3p^2+9p^3\right)\sqrt{\frac{1}{\left(3+p-3p^2\right)^2}}$$
$$+\frac{2\,(-4+3p\,(1+p))}{3\,(1+p)\,(-4+3p)\sqrt{\frac{1}{36+2p(9+p(-26-6p+9p^2))}}}.$$

□

Theorem 7 *Let SC_p^p be a chain of silicates. Then the arithmetic-geometric temperature index for SC_p^p is*

$$\left(-12+34p-6p^2-21p^3-9p^4\right)\sqrt{\frac{1}{\left(6+p-3p^2\right)^2}}$$
$$+\left(-6-11p+3p^2+9p^3\right)\sqrt{\frac{1}{\left(3+p-3p^2\right)^2}}$$
$$+\frac{3}{2}\left(16-8p-27p^2+6p^3+9p^4\right)$$
$$\sqrt{\frac{1}{36+2p\left(9+p\left(-26-6p+9p^2\right)\right)}}.$$

Proof Using the bond partition from Table 3 in the formula of the arithmetic-geometric temperature index, we obtain

$$AGT(SC_p^p)=\sum_{uv\in E_{33}}\frac{T_u+T_v}{2\sqrt{T_uT_v}}+\sum_{uv\in E_{36}}\frac{T_u+T_v}{2\sqrt{T_uT_v}}$$
$$+\sum_{uv\in E_{66}}\frac{T_u+T_v}{2\sqrt{T_uT_v}}=(3p+2)$$
$$\times\frac{\frac{3}{3p^2-p-3}+\frac{3}{3p^2-p-3}}{2\sqrt{\frac{3}{3p^2-p-3}\frac{3}{3p^2-p-3}}}+\left(3p^2+3p-4\right)$$
$$\times\frac{\frac{3}{3p^2-p-3}+\frac{6}{3p^2-p-6}}{2\sqrt{\frac{3}{3p^2-p-3}\frac{6}{3p^2-p-6}}}+\left(3p^2-6p+2\right)$$
$$\times\frac{\frac{6}{3p^2-p-6}+\frac{6}{3p^2-p-6}}{2\sqrt{\frac{6}{3p^2-p-6}\frac{6}{3p^2-p-6}}}.$$

After some simple steps of calculations, we get

$$AGT(SC_p^p)=\left(-12+34p-6p^2-21p^3-9p^4\right)$$
$$\times\sqrt{\frac{1}{\left(6+p-3p^2\right)^2}}+\left(-6-11p+3p^2+9p^3\right)$$
$$\times\sqrt{\frac{1}{\left(3+p-3p^2\right)^2}}+\frac{3}{2}\left(16-8p-27p^2+6p^3+9p^4\right)$$
$$\times\sqrt{\frac{1}{36+2p\left(9+p\left(-26-6p+9p^2\right)\right)}}.$$

□

4 Comparison and Correlation of Indices of SC_p^p

In this section, we will analyze the indices of the SC_p^p and observe their trend. Additionally, we will also identify a correlation among the indices. Table 4 displays the temperature indices of SC_p^p, allowing us to observe the trend. The indices

Table 4 Temperature indices of SC_p^p

p	$HT(SC_p^p)$	$ISIT(SC_p^p)$	$GO_1T(SC_p^p)$	$GO_2T(SC_p^p)$	$SOT(SC_p^p)$	$GAT(SC_p^p)$	$AGT(SC_p^p)$
2	34.5185	7.8810	54.8265	32.1166	30.9317	21.6407	26.8375
3	244.4000	5.8190	28.6848	1.6046	19.0128	51.3285	56.9149
4	840.7111	5.3648	24.5691	0.3652	16.9998	92.0997	100.1922
5	2122.6431	5.1898	23.0563	0.1305	16.2428	144.4462	155.9372
6	4473.2245	5.1053	22.3226	0.0587	15.8718	208.4223	224.0795
7	8359.4641	5.0591	21.9103	0.0304	15.6622	284.0428	304.6008
8	14332.3654	5.0317	21.6559	0.0174	15.5325	371.3133	397.4942
9	23026.9304	5.0145	21.4885	0.0107	15.4469	470.2367	502.7563
10	35162.1601	5.0033	21.3728	0.0069	15.3877	580.8142	620.3856
11	51541.0549	4.9958	21.2899	0.0047	15.3452	703.0467	750.3809
12	73050.6154	4.9906	21.2287	0.0033	15.3137	836.9348	892.7418
13	100661.8417	4.9871	21.1823	0.0024	15.2899	982.4787	1047.4677
14	135429.7341	4.9846	21.1465	0.0018	15.2714	1139.6787	1214.5585
15	178493.2927	4.9829	21.1185	0.0013	15.2570	1308.5350	1394.0140

HT, GAT, and AGT show an increasing trend, while all other indices show a decreasing trend.

The table displays the correlation coefficients, coefficients of determination, and standard errors of estimate for various pairs of temperature indices of the silicate chain when $p = q$. In the indices columns of Table 5, the index on the left indicates the dependent variable, while the index on the right represents the independent variable. For instance, in the case of $HT - ISIT$, HT is the dependent variable, and $ISIT$ is the independent variable. Table 5 shows that specific pairs of indices have highly significant positive correlations. The pairs $GO_1T - SOT$, $ISIT - GO_1T$, and $GAT - AGT$ have strong connection. The correlation coefficients R exhibit a value of one or go towards it, indicating a robust association.

Specific pairs exhibit a notably feeble association: $HT - ISIT$, $HT - GO_1T$, $HT - GO_2T$, and $HT - SOT$. These pairs have correlation coefficients (R values) that are extremely near zero, indicating a weak association between them. There are several moderate correlations, such as $HT - GAT$, $HT - AGT$, $ISIT - GO_2T$, and $SOT - GAT$, for these pairs have $0.4 \leq R \leq 0.6$ and $0.2 \leq R^2 \leq 0.4$. These correlations indicate a statistically significant moderate linear relationship.

Briefly, the conclusion: Silicate chain temperature indices range from highly strong to highly weak when $p = q$. Certain indices exhibit a high degree of similarity, whilst others demonstrate a high degree of independence. The correlation coefficients, coefficients of determination, and standard errors of estimation offer valuable insights into the magnitude, direction, and precision of the linear associations between the indices. Fig. 2 shows the linear fitting among the indices.

Table 5 R, R^2, SEE between temperature indices of SC_p^p

Indices	R	R^2	SEE	Indices	R	R^2	SEE
$HT - ISIT$	0.353	0.125	55513.75354	$GO_1T - GO_2T$	0.983	0.966	1.7021077
$HT - GO_1T$	0.330	0.109	56015.70969	$GO_1T - SOT$	1	1	0.1520726
$HT - GO_2T$	0242	0.059	57561.90518	$GO_1T - GAT$	0.465	0.216	8.2097650
$HT - SOT$	0.337	0.114	55852.88644	$GO_1T - AGT$	0.464	0.216	8.2129110
$HT - GAT$	0.963	0.927	16028.41765	$GO_2T - SOT$	0.9800	0.960	1.7761017
$HT - AGT$	0.963	0.927	16027.21639	$GO_2T - GAT$	0.357	0.127	8.3111612
$ISIT - GO_1T$	0.998	0.995	0.0543631	$GO_2T - AGT$	0.356	0.127	8.3136136
$ISIT - GO_2T$	0.968	0.938	0.2005317	$SOT - GAT$	0.474	0.225	3.7990858
$ISIT - SOT$	0.999	0.997	0.0414477	$SOT - AGT$	0.474	0.224	3.8005694
$ISIT - GAT$	0.495	0.245	0.6989952	$GAT - AGT$	1	1	0.3684196
$ISIT - AGT$	0.495	0.245	0.6992767				

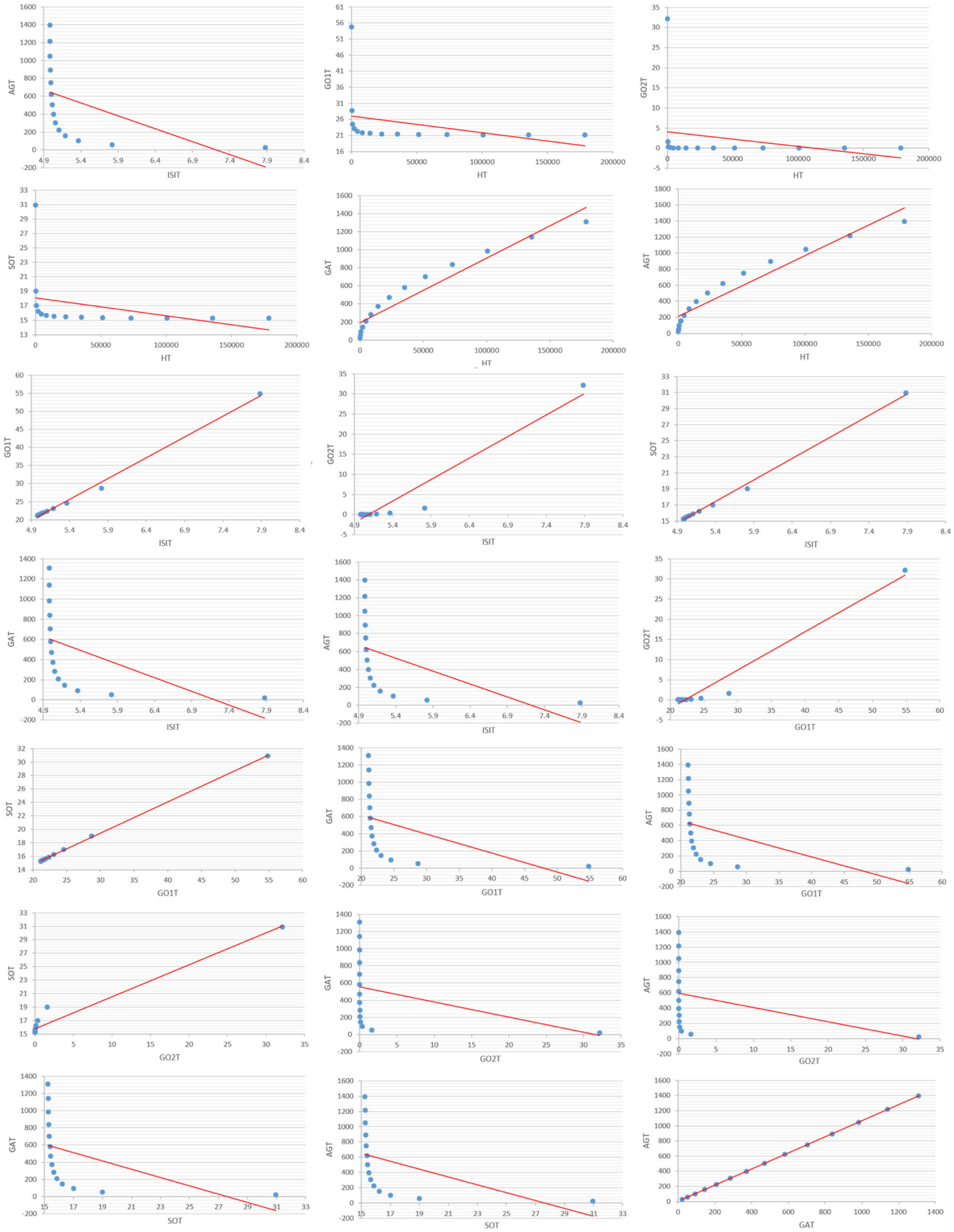

Fig. 2 Scatter plots between temperature indices

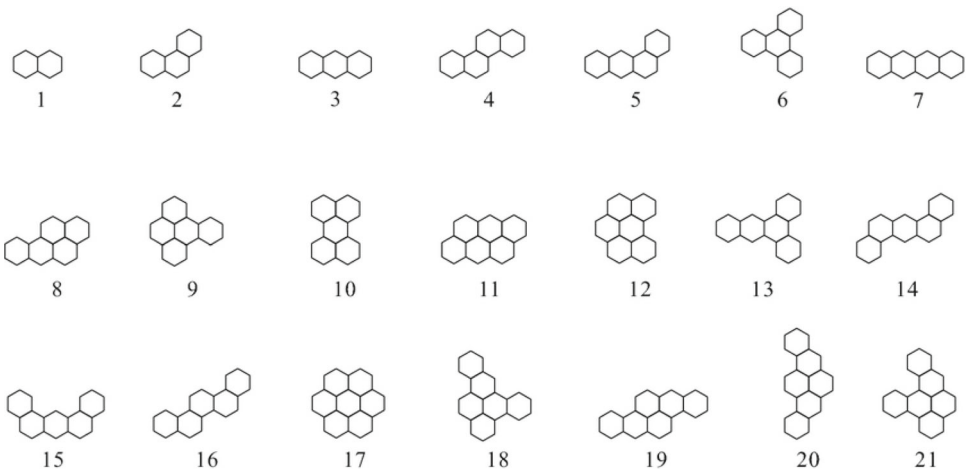

Fig. 3 Under consideration molecular graphs of benzenoid hydrocarbons

5 Application of Temperature Indices on Benzenoid Hydrocarbons

The primary aim of this article is to establish the relationship between temperature indices, π-electron energy E, and boiling point $(B.P(^{\circ}C))$ of specific benzenoid hydrocarbons.

The variable E is defined for a graph G

$$E(G) = \sum_{i=1}^{n} |\Upsilon_i| , \tag{4}$$

where $\Upsilon_1, \Upsilon_2, \Upsilon_3, \ldots, \Upsilon_n$ are the eigenvalues of adjacency matrix of G.

Table 6 The values of some temperature indices, E, and $B.P$ of 21 benzenoid hydrocarbons

Molecule (G)	$HT(G)$	$ISIT(G)$	$GO_1T(G)$	$GO_2T(G)$	$SOT(G)$	$GAT(G)$	$AGT(G)$	$E(G)$	$B.P(^{\circ}C)$
1	38.1228	1.5959	7.5587	0.6358	4.7120	10.8590	11.1461	8	218
2	80.3103	1.6131	7.2964	0.3064	4.7247	15.8226	16.1828	13.6832	338
3	79.7471	1.6003	7.2851	0.2965	4.7426	15.7634	16.2438	19.3137	340
4	138.2308	1.6154	7.1250	0.1763	4.7152	20.7841	21.2219	19.4483	431
5	137.5385	1.6067	7.1194	0.1726	4.7273	20.7301	21.2774	24.9308	425
6	138.9231	1.6240	7.1306	0.1799	4.7031	20.8381	21.1664	25.1875	429
7	136.8462	1.5981	7.1138	0.1689	4.7394	20.6761	21.3329	25.1012	440
8	172.2121	1.6884	7.4025	0.1525	4.9323	23.7383	24.2687	25.1922	496
9	172.9697	1.6958	7.4067	0.1550	4.9219	23.7906	24.2150	25.2745	493
10	172.9697	1.6958	7.4067	0.1550	4.9219	23.7906	24.2150	22.5055	497
11	210.0612	1.7452	7.6107	0.1317	5.1010	26.6937	27.3143	30.5440	547
12	210.8844	1.7517	7.6140	0.1334	5.0919	26.7448	27.2619	30.7255	542
13	211.8844	1.6149	7.0119	0.1138	4.7048	25.7448	26.2619	30.8805	535
14	211.0612	1.6084	7.0085	0.1121	4.7139	25.6937	26.3143	30.8795	536
15	211.0612	1.6084	7.0085	0.1121	4.7139	25.6937	26.3143	30.7627	531
16	211.8844	1.6149	7.0119	0.1138	4.7048	25.7448	26.2619	30.9990	519
17	252.6667	1.7965	7.7750	0.1154	5.2277	29.7000	30.3077	30.9362	590
18	254.5556	1.6789	7.2395	0.1022	4.8707	28.7500	29.2565	30.9386	592
19	249.6667	1.6991	7.3528	0.1053	4.9522	28.7000	29.3077	30.9432	596
20	253.6667	1.6732	7.2368	0.1009	4.8788	28.7000	29.3077	30.8390	594
21	254.5556	1.6789	7.2395	0.1022	4.8707	28.7500	29.2565	30.9418	595

Table 7 R, R^2, and SEE between E and temperature indices

Pair	R	R^2	SEE
$E - HT(G)$	0.925	0.856	2.5208619
$E - ISIT(G)$	0.445	0.198	5.9478613
$E - GO_1T(G)$	0.153	0.024	6.5642452
$E - GO_2T(G)$	0.896	0.802	2.9560980
$E - SOT(G)$	0.391	0.153	6.1146432
$E - GAT(G)$	0.936	0.877	2.3308281
$E - AGT(G)$	0.939	0.881	2.2873682

Benzenoid hydrocarbons are a group of chemical compounds that have at least one benzene ring in their structure. Benzenoid hydrocarbons are highly prized for their distinct physical and chemical properties, making them useful in several commercial and scientific fields. One can analyze the structure-activity relationship of benzenoid hydrocarbons and their derivatives by utilizing E throughout chemistry, biology, and mathematics. Benzenoid hydrocarbons are essential compounds used in various research and technological applications. Refer to the book [18] for additional information. Fig. 3 shows 21 benzenoid hydrocarbons.

One might calculate the indices in Table 6 using the benzonid hydrocarbons' chemical graphs illustrated in Fig. 3. We took data for E from the paper [19, 20], and data for $B.P$ from reference [21].

Table 7 shows the relation of E with indices and Fig. 4 shows the linear fitting of E with the temperature indices.

$$E(G) = 0.095\ (\pm 0.009)\ HT(G) + 8.942\ (\pm 1.705)\ .$$
$$E(G) = 49.035\ (\pm 22.617)\ ISIT(G) - 55.169\ (\pm 37.506).$$
$$E(G) = -4.462\ (\pm 6.590)\ GO_1T(G) + 58.595\ (\pm 48.021).$$
$$E(G) = -48.219\ (\pm 5.497)\ GO_2T(G) + 34.459\ (\pm 1.151).$$
$$E(G) = 16.259\ (\pm 8.785)\ SOT(G) - 52.622\ (\pm 42.555)\ .$$
$$E(G) = 1.217\ (\pm 0.105)\ GAT(G) - 2.754\ (\pm 2.532)\ .$$
$$E(G) = 1.204\ (\pm 0.101)\ AGT(G) - 3.050\ (\pm 2.503)\ .$$

The temperature indices that have a substantial association with E are HT, GO_2T, GAT, and AGT. The relationship between $ISIT$ and E is moderate, while SOT has a weak link and GO_1T has a fragile association with E.

Table 8 shows the relation of $B.P$ with indices and Fig. 5 shows the linear fitting of E with the temperature indices.

$$B.P(G) = 1.561\ (\pm 0.058)\ HT(G) + 207.187\ (\pm 10.996)\ .$$
$$B.P(G) = 1016.437\ (\pm 312.414)\ ISIT(G) - 1194\ (\pm 518.079)\ .$$

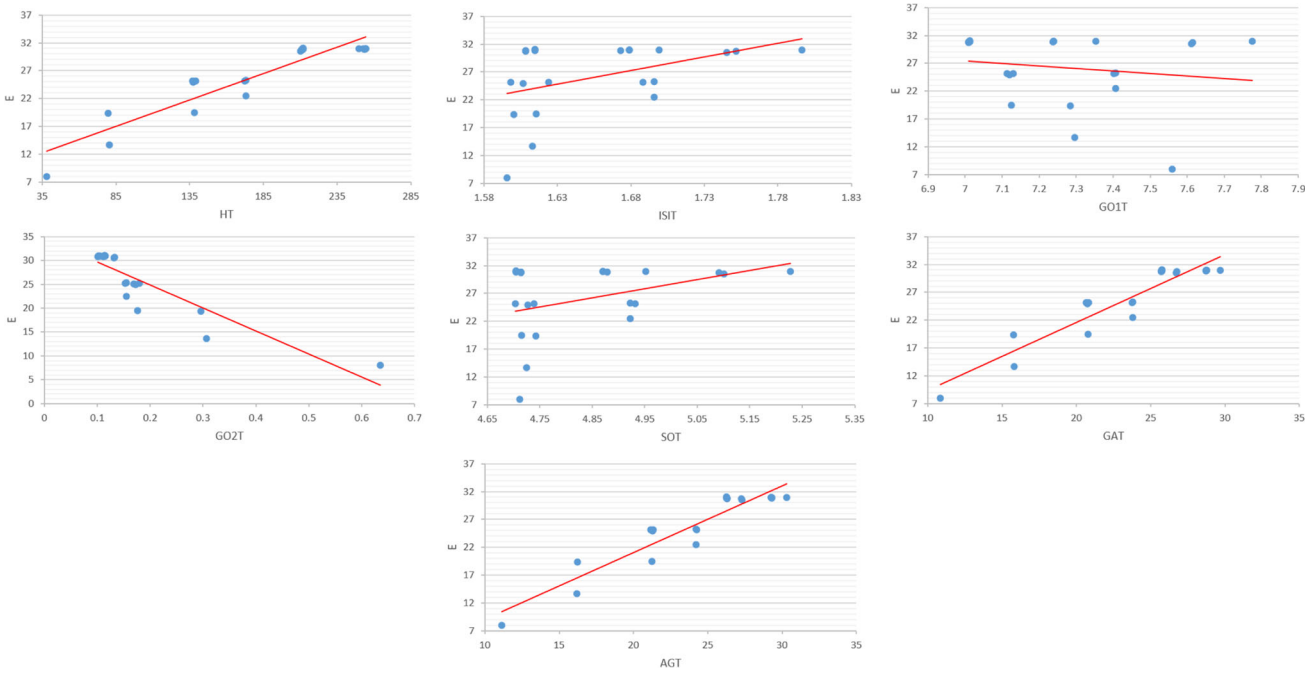

Fig. 4 Scatter plots between E and temperature indices

Table 8 R, R^2, and SEE between $B.P$ and temperature indices

Pair	R	R^2	SEE
$B.P - HT(G)$	0.987	0.975	16.2552084
$B.P - ISIT(G)$	0.568	0.358	82.1592661
$B.P - GO_1T(G)$	0.007	0.000	102.5197291
$B.P - GO_2T(G)$	0.893	0.797	46.1872748
$B.P - SOT(G)$	0.529	0.280	87.0186147
$B.P - GAT(G)$	0.997	0.993	8.2739494
$B.P - AGT(G)$	0.997	0.994	8.0045471

$$B.P(G) = -2.958\ (\pm 102.925)\ GO_1T(G) + 511.262\ (\pm 749.987)\ .$$
$$B.P(G) = -741.885\ (\pm 85.887)\ GO_2T(G) + 618.371\ (\pm 17.984)\ .$$
$$B.P(G) = 339.493\ (\pm 125.026)\ SOT(G) - 1153.928\ (\pm 605.609)\ .$$
$$B.P(G) = 19.997\ (\pm 0.371)\ GAT(G) + 15.778\ (\pm 8.987)\ .$$
$$B.P(G) = 19.729\ (\pm 0.354)\ AGT(G) + 12.056\ (\pm 8.758)\ .$$

Indices HT and GO_2T exhibit a strong correlation with $B.P$, while indices $ISIT$ and SOT have a moderate relationship with $B.P$. GO_1T does not exhibit any correlation with $B.P$. The correlation coefficient value (R) is almost 1 for the indices GAT and AGT, indicating their potential use in predicting the future boiling point of benzenoid hydrocarbons.

6 Conclusions

This paper determined the methodology for calculating various temperature indices for a linear molecular graph of $Si\,O_4$. Additionally, we did a comparison and found correlation of the temperature indices of the silicate chain. At the end of the paper, we gave an application of benzenoid hydrocarbons to elucidate the significance of temperature indices. We demonstrated that the temperature geometric-arithmetic index and temperature arithmetic-geometric index can forecast the boiling points of benzoniode hydrocarbons.

Open Problem

The following unresolved issues are interesting for the characterization of the silicate chain.

1. Do the temperature indices change when p and q are either even or odd, when one is even and the other is odd, and when p is less than q?
2. How does the situation change when p is greater than or equal to q?

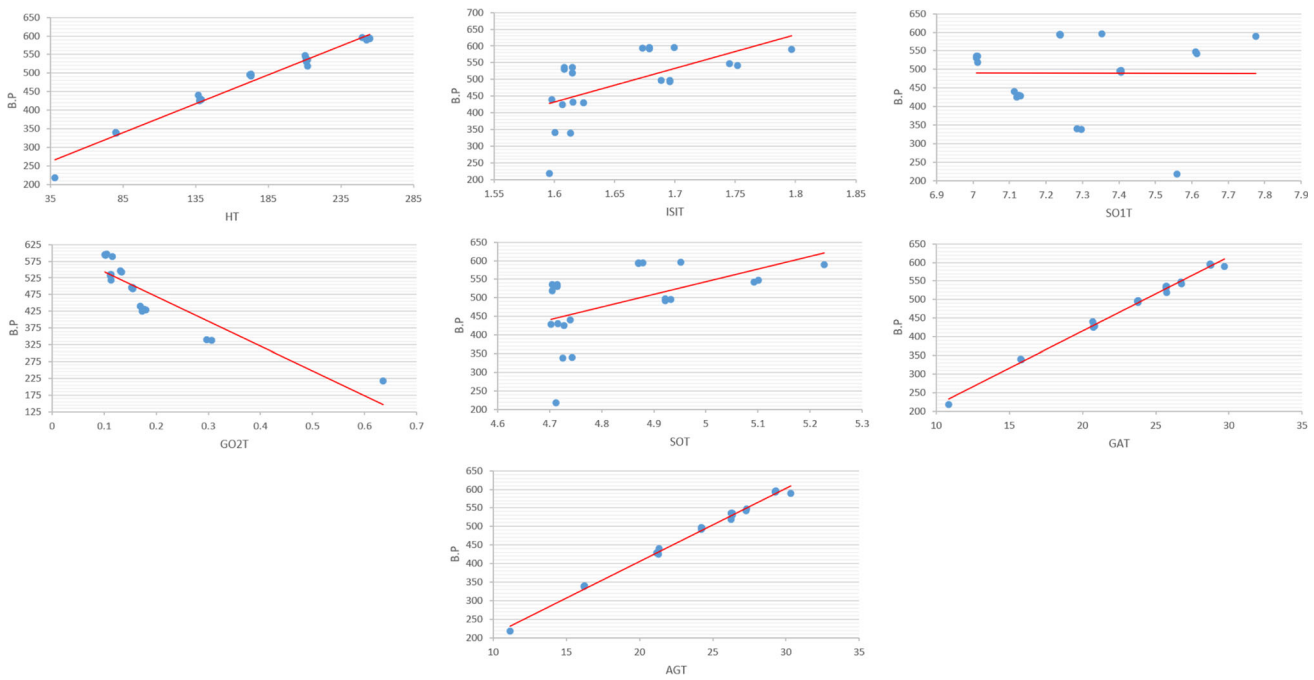

Fig. 5 Scatter plots between $B.P$ and temperature indices

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Author Contributions All authors contributed equally.

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Data Availability No datasets were generated or analysed during the current study.

Declarations

Competing interests The authors declare no competing interests.

Conflict of interest We declare that we have no conflicts of interest.

Ethics approval Not applicable. This study did not involve human participants, animals, or data that required ethical approval.

Consent to participate Yes, informed consent was obtained from all individual participants involved in the study.

Consent to publication Yes, consent for publication was obtained from all participants whose identifiable information is included in this study.

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