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General Trinajstić Index

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Abstract: In memory of the outstanding theoretical chemist Nenad Trinajstić, Furtula introduced a new distance-based molecular structure descriptor "Trinajstić index" in chemical graph theory. In this paper, we propose the general Trinajstić index, and give the calculation formula of the general Trinajstić index for double-star graphs, double brooms, Kragujevac trees, firefly graphs and wheel graphs. As an application, we calculate the general Trinajstić index for some hydrocarbons.

Keywords: general Trinajstić index, distance-based indices, tree.

INTRODUCTION

IN chemical graph theory, molecular structure descriptors (also called topological indices) are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds.[1] The oldest and most important molecular structure descriptors is the Wiener index, introduced by Wiener in 1947,[2] which is defined as the sum of distances between all pairs of vertices of the (molecular) graph. Let G be a simple connected graph with the vertex set $V(G)$ and edge set $E(G)$. In the seminal paper, the Wiener index of acyclic alkanes (trees T) can be calculated by the following formula

$$W(T) = \sum_{uv \in E(T)} n_u \cdot n_v ,$$

where n_u is the number of vertices that are closer to the vertex u (including the vertex u) than to vertex v. Therefore, n_u becomes the basic quantity for generating topological index in chemical graph theory. In particular, Trinajstić has made great contributions to the research of this quantity.[3–5]

Based on the quantity, scholars have established many distance-based molecular structure descriptors, such as the modified Wiener index,[4] the Szeged index,[6] the hyper-Szeged index,[7] the revised Szeged index,[8] the vertex PI index,[9] a class of modified Wiener indices[10] and so on.

From the perspective of distance-balanced of graphs, Došlić et al.[11] proposed the Mostar index as follows:

$$Mo(G) = \sum_{uv \in E(G)} | n_u - n_v |,$$

which attracted considerable attention in the researchers' cycles.[12]

In 2022, a novel topological index, Trinajstić index, was introduced by Furtula,[13] defined as

$$NT(G) = \sum_{\{u,v\} \in V(G)} (n_u - n_v)^2 ,$$

which can also be used as a measure of unbalancedness of a graph such as the total Mostar index.[14] Moreover, this index can be regarded as Euclidean distance between any two vertices in a graph.

On this basis, for a positive real number α, we propose the general Trinajstić index as follows:

$$NT_\alpha(G) = \sum_{\{u,v\} \in V(G)} | n_u - n_v |^\alpha ,$$

which can be regarded as Minkowski distance between any two vertices in G.

In this paper, the calculation formula of the general Trinajstić index for double-star graphs, double brooms, Kragujevac trees, firefly graphs and wheel graphs are obtained. As an application, the values of general Trinajstić index of some hydrocarbons are given.

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PRELIMINARIES

The path on n vertices is denoted by P_n.

n_u^+ is the number of vertices to the right of vertex u that are closer to vertex u (excluding vertex u) than vertex v, and n_u^- is the number of vertices to the left of vertex u that are closer to vertex (excluding vertex u) than vertex v the number of vertices for u. $n_{[u]}^+$ is the number of vertices to the right of vertex u that are closer to vertex u (including vertex u) than vertex v, and $n_{[u]}^-$ is the number of vertices to the left of vertex u that are closer to vertex (including vertex u) than vertex v the number of vertices for u.

THE GENERAL TRINAJSTIĆ INDEX OF SOME TREES

The double star $S(a,b)$ is the tree obtained from P_2 by attaching a pendant edges to a vertex and b pendant edges to the other, shown in Figure 1.

Theorem 3.1. Let $S(a,b)$ $(a \geq b)$ be a double star graph with $a+b+2$ vertices. Then

$$NT_\alpha(S_{a,b}) = (a+b)^{\alpha+1} + ab^\alpha + ba^\alpha + (ab+1)(a-b)^\alpha.$$

Proof. Let $S(a,b)$ be a double star graph with $a+b+2$ vertices and $\{u,v\} \in V(S_{a,b})$, shown in Figure 1. By the definition of the general Trinajstić index, we will calculate the following Cases two by the positional relationship between u and v, which, put together, will get our proof.

Case 1. $uv \in E(S_{a,b})$. The graphs (a) and (b) satisfy this case, shown in Figure 1.

For (a), all vertices except u are less distant from v than from u, so, $n_u=1$, $n_v=a+b+1$, and $|n_u-n_v|=a+b$, it can be easily obtained that there are $a+b$ pairs of vertices that conform to the positional relationship of u and v.

For (b), the distance from the vertex in the left hand of the double star to u is less than the distance from v, and the distance from the vertex in the right hand of the double star to v is less than the distance from u, thus, $n_u=a+1$ and $n_v=b+1$, and then $|n_u-n_v|=a-b$, and (b) satisfies only one pair of vertices as shown in the (b).

Case 2. $uv \notin E(S_{a,b})$. The graphs (c) and (d) satisfy this case, shown in Figure 1.

For (c), the vertices on the left hand of the double star, except u, have n_u-n_v, and the distance from the vertices on the right hand of the double star to v is less than the distance to u, so, $n_u=1$, $n_v=b+1$ (or $n_u=1$, $n_v=a+1$), and $|n_u-n_v|=b$ (or $|n_u-n_v|=a$) and it can be easily obtained that there are $a+b$ pairs of vertices that conform to the positional relationship of u and v, and there are a (or b) pairs of vertices that conform to the positional relationship of u and v.

For (d), the distance from the vertex in the left hand of the double star to u is less than the distance from v, and the distance from the vertex in the right hand of the double star to v is less than the distance from u, thus, $n_u=a+1$, $n_v=b+1$, and $|n_u-n_v|=a-b$, and (d) satisfies ab pair of vertices.

Summing up the results of Cases 1 and 2, we have

$$\begin{aligned} NT_\alpha(S_{a,b}) &= (a+b)|a+b|^\alpha + a\,|b|^\alpha + b\,|a|^\alpha + ab|a-b|^\alpha + |a-b|^\alpha \\ &= (a+b)^{\alpha+1} + ab^\alpha + ba^\alpha + (ab+1)(a-b)^\alpha. \end{aligned}$$

This completes the proof.

The double broom $B_{s,w,t}$ is a pair of stars S_s and S_t whose central vertices are joined by a path with w edges, shown in Figure 2.

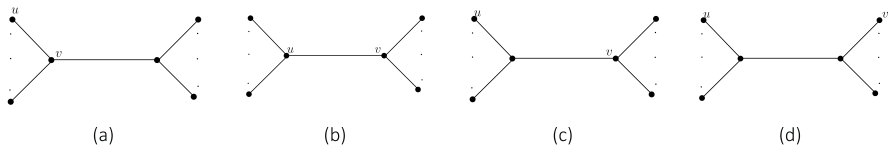

Figure 1. The position relation of any two vertices in $S(a,b)$.

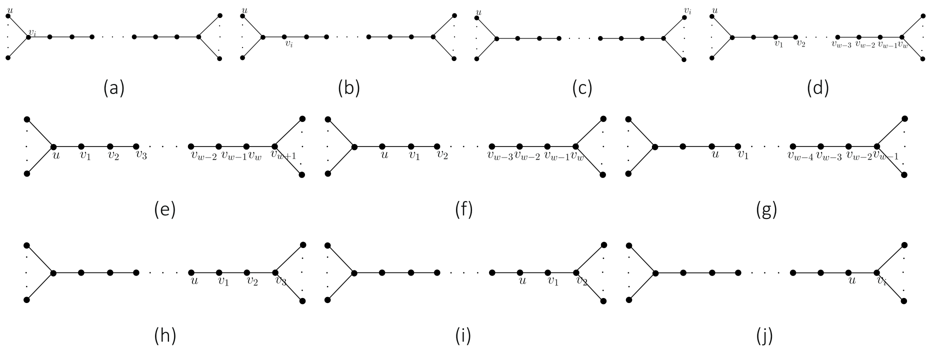

Figure 2. The position relation of any two vertices in $B_{s,w,t}$.

Theorem 3.2. Let $B_{s,w,t}$ be a double broom. Then

$$\begin{aligned}NT_\alpha(B_{s,w,t}) &= (s+t-2)(s+w+t-2)^\alpha + (s-1)(w+t-1)^\alpha \\ &+(t-1)(w+s-1)^\alpha + (s-1)(t-1)\,|s-t|^\alpha \\ &+\sum_{i=1}^{w}[(s-1)\,|s-1-w-t+i\,|^\alpha \\ &+(t-1)\,|t-1-w-s+i\,|^\alpha] \\ &+\sum_{j=-1}^{w-1}\sum_{i=1}^{w-j}|w+t-s-i-2j-1\,|^\alpha .\end{aligned}$$

Proof. Let $u, v_i \in V(B_{s,w,t})$, for a double broom $B_{s,w,t}$ with $s+w+t$ vertices and the positional relationship between u and v_i is shown in Figure 2. By the definition of the general Trinajstić index, we will calculate the following Cases 1–4 by the positional relationship between u and v_i, which, put together, will get our proof.

Case 1. As shown in (a) and (b), we have n_u=1. For (a), we have $n_{v_i} = s+w+t-1$. For (b), obviously $n_{v_i} = w+t$ for $u \in S_s$ or $n_{v_i} = w+s$ for $u \in S_t$. Thus

$$\begin{aligned}NT_\alpha(B_{s,w,t}^{(a+b)}) &= (s+t-2)(s+w+t-2)^\alpha \\ &+ (s-1)(w+t-1)^\alpha + (t-1)(w+s-1)^\alpha .\end{aligned}$$

Case 2. As shown in (c), u is located on the pendant vertices of S_s, and v_i is located on the pendant vertices of S_t, so $|\,n_u - n_{v_i}\,| = |\,s-t\,|$. Thus we have

$$NT_\alpha(B_{s,w,t}^{(c)}) = (s-1)(t-1)\,|\,s-t\,|^\alpha .$$

Case 3. As shown in (d), we fix the position of u so that $n_u^- = 0$, then the position of v_i will have w cases in Figure 2. The distance from the vertex in S_s (or S_t) to u is always less than the distance to v_i, so $n_{[u]}^+ - n_{[v_i]}^- = s-1$ (or $n_u^+ - n_{v_i}^- = t-1$), Therefore, if want to calculate the value of $|\,n_u - n_{v_i}\,|^\alpha$, only need to calculate the value of $|\,s-1+n_{[u]}^- - n_{[v_i]}^+\,|^\alpha$ (or $|\,t-1+n_{[u]}^- - n_{[v_i]}^+\,|^\alpha$). And it's easy to see that $n_{[v_i]}^+ = w+t-i, i \in 1,2,\ldots,w$ (or $n_{[v_i]}^+ = w+s-i,\ i \in 1,2,\ldots,w$). Thus

$$NT_\alpha(B_{s,w,t}^{(d)}) = \sum_{i=1}^{w}[(s-1)|s-1-w-t+i\,|^\alpha + (t-1)|\,t-1-w-s+i\,|^\alpha].$$

Case 4. As shown in (e)–(j), we have $|\,n_u - n_{v_i}\,|^\alpha = |\,n_{[u]}^- - n_{[v_i]}^+\,|^\alpha$. By induction $n_{[u]}^-$ and $n_{[v_i]}^+$, the value of $|\,n_{[u]}^- - n_{[v_i]}^+\,|^\alpha$ can be obtained as shown in the Table 1.

Thus we obtain

$$\begin{aligned}NT_\alpha(B_{s,w,t}^{(e+\cdots+j)}) &= \sum_{\{u,v\}\in V(G)} |\,n_u - n_v\,|^\alpha \\ &= \sum_{\{u,v_i\}\in V(G)} |\,n_{[u]}^- - n_{[v_i]}^+\,|^\alpha \\ &= \sum_{i=1}^{w+1}|\,w+t-s-i+1\,|^\alpha + \cdots \\ &+\sum_{i=1}^{w-j}|\,w+t-s-i-2j-1\,|^\alpha + \cdots \\ &+|\,s+w-t\,|^\alpha \\ &= \sum_{j=-1}^{w-1}\sum_{i=1}^{w-j}|\,w+t-s-i-2j-1\,|^\alpha .\end{aligned}$$

Summing up the results of Cases 1–4, we have

$$\begin{aligned}NT_\alpha(B_{s,w,t}) &= NT_\alpha(B_{s,w,t}^{(a+b)}) + NT_\alpha(B_{s,w,t}^{(c)}2) + NT_\alpha(B_{s,w,t}^{(d)}) \\ &+ NT_\alpha(B_{s,w,t}^{(e+\cdots+j)}) = (s+t-2)(s+w+t-2)^\alpha \\ &+ (s-1)(w+t-1)^\alpha + (t-1)(w+s-1)^\alpha \\ &+ (s-1)(t-1)(s-t)^\alpha \\ &+ \sum_{i=1}^{w}[(s-1)\,|\,s-1-w-t+i\,|^\alpha \\ &+ (t-1)\,|\,t-1-w-s+i\,|^\alpha] \\ &+ \sum_{j=-1}^{w-1}\sum_{i=1}^{w-j}|\,w+t-s-i-2j-1\,|^\alpha .\end{aligned}$$

This completes the proof.

By Theorem 3.2, we can obtain the following corollaries.

Corollary 3.1. Let P_n be a path graph with n vertices. Then

$$NT_\alpha(P_n) = \sum_{j=1}^{n-1}\sum_{i=1}^{n-j}(n-i-2j+1)^\alpha .$$

Table 1.

$n_{[u]}^-$	$n_{[v_i]}^+$	$\{\|\,n_{[u]}^- - n_{[v_i]}^+\,\|^\alpha\}$
s	$w+t-i+1$	$\{\|\,w+t-s-i+1\,\|^\alpha \mid i \in 1,2,\ldots,w+1\}$
$s+1$	$w+t-i$	$\{\|\,w+t-s-i-1\,\|^\alpha \mid i \in 1,2,\ldots,w\}$
$s+2$	$w+t-i-1$	$\{\|\,w+t-s-i-3\,\|^\alpha \mid i \in 1,2,\ldots,w-1\}$
⋮	⋮	⋮
$s+w-2$	$t+3-i$	$\{\|\,s+w-t+i-5\,\|^\alpha \mid i \in 1,2,3\}$
$s+w-1$	$t+2-i$	$\{\|\,s+w-t+i-3\,\|^\alpha \mid i \in 1,2\}$
$s+w$	t	$\|\,s+w-t\,\|^\alpha$

Corollary 3.2. Let $B_{a,b}$ be a broom graph, which have a pendant vertices and a path with b vertices. Then

$$\begin{aligned} NT_\alpha(G) &= a(a+b-2)^\alpha + a(b-2)^\alpha \\ &+\sum_{i=1}^{b-2} a\,|\,a-b+i+1\,|^\alpha \\ &+\sum_{j=1}^{b-1}\sum_{i=1}^{b-j} |\,b-a-i-2j+1\,|^\alpha . \end{aligned}$$

Let P_3 be the 3-vertex path, rooted at one of its terminal vertices, see Figure 3. For $i = 1,2,\ldots$, construct the rooted tree B_i by identifying the roots of i copies of P_3. The vertex obtained by identifying the roots of P_3 is the root of B_i. A Kragujevac tree is a tree possessing a central vertex, to which branches of the form B_1 and/or B_2 and/or B_3 and/or ... are attached, shown in Figure 3. The subgraphs B_i is the branch of Kragujevac tree.

Theorem 3.5. Let KT be a Kragujevac tree with n vertics and k branchs. Then

$$\begin{aligned} NT_\alpha(KT) &= \frac{n-k-1}{2}[(n-2)^\alpha + (n-3)^\alpha] \\ &+[n-k-1+\sum_{i=2}^{k}\frac{i!}{(i-2)!}x_i]\,(n-4)^\alpha \\ &+\sum_{i=1}^{k} x_i[i+i(k-1)]\,(n-2i-3)^\alpha \\ &+\sum_{i=1}^{k} i\,x_i(\frac{n-k-1}{2}-i+k-1)(n-4i-2)^\alpha \\ &+3\sum_{i=1}^{k}\sum_{j=1}^{k} x_i\,x_j(2j-2i)^\alpha , \end{aligned}$$

where x_1 is the number of P_3, and x_i is the number of B_i for $i = 2,\ldots, k$.

Proof. It is easy to see that KT has $\frac{n-k-1}{2}$ pendent edges. According to the structure of Kragujevac tree, we only need to consider two types of graphs: one is (a)–(f) and the other is (g)–(l), shown in Figure 3. By the definition of the general Trinajstić index, we will calculate the following Cases 1–3 by n_u, which, put together, will get our proof.

Case 1. $n_u = 1$. The graphs (a) and (b) satisfy this case.

For (a), the distance from all vertices to v except u is less than u, so $n_v = n-1$, that is, $|\,n_u - n_v\,| = n-2$.
For (b), we get $|\,n_u - n_v\,| = |\,n_u^- - n_v^+\,| = n-3$.
Thus, we have

$$NT_\alpha(KT^{(a+b)}) = \frac{n-k-1}{2}[(n-2)^\alpha + (n-3)^\alpha].$$

Case 2. $n_u = 2$. The graphs (c)–(g) satisfy this case.

For (c), (d) and (e), the distance from all vertices to v except u and its neighbors is less than u, so $n_v = n-2$, that is, $|\,n_u - n_v\,| = n-4$.
Thus we have

$$NT_\alpha(KT^{(c+d+e)}) = [n-k-1+\sum_{i=2}^{k}\frac{i!}{(i-2)!}x_i](n-4)^\alpha .$$

For (f), except for u itself and an adjacent pendent edge, the distances from other vertices to u are equal to the distance to v, so we can get $n_v = n-2i-1$, and there are i pairs of vertices that conform to this positional relationship. Thus we have

$$NT_\alpha(KT^{(f)}) = \sum_{i=1}^{k} x_i i(n-2i-3)^\alpha .$$

For (g), except for B_i, the distances from other vertices to v are less than the distance to u, so $n_v = n-2i-1$ and there are $i(k-1)$ pairs of vertices that conform to this positional relationship. Thus we have

$$NT_\alpha(KT^{(g)}) = \sum_{i=1}^{k} x_i i(k-1)(n-2i-3)^\alpha .$$

Case 3. $n_u = 2i+1$. The graphs (h)–(l) satisfy this case.
For (h) and (i), except for B_i, the distances from other vertices to v are less than the distance to u, so $n_v = n-2i-1$. And (h) is $i(\frac{n-k-1}{2}-i)$ and (i) is $i(k-1)$ pairs of vertices that conform to this positional relationship can be easily obtained. Thus we have

$$\begin{aligned} NT_\alpha(KT^{(h+i)}) &= \sum_{i=1}^{k} x_i\, i(\frac{n-k-1}{2}-i)\,(n-4i-2)^\alpha \\ &+\sum_{i=1}^{k} x_i\, i(k-1)\,(n-4i-2)^\alpha \\ &=\sum_{i} i(\frac{n-k-1}{2}-i+k-1)\,(n-4i-2)^\alpha . \end{aligned}$$

For (j), (k) and (l),except for B_i and B_j, all the vertices are the same distance from u and v, so, $n_v = 2j+1$, that is $|\,n_u - n_v\,| = 2j-2i$. Thus we have

$$NT_\alpha(KT^{(j+k+l)}) = 3\sum_{i=1}^{k}\sum_{j=1}^{k} x_i j_i (2j-2i)^\alpha .$$

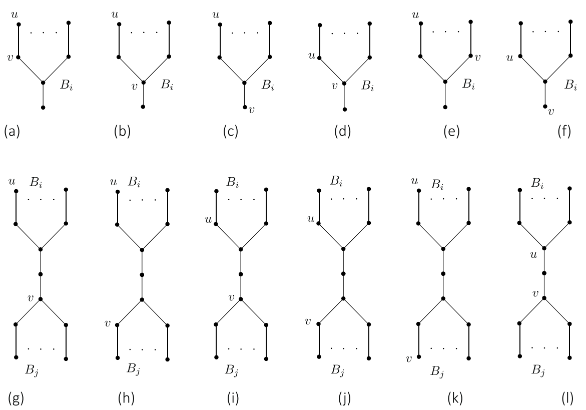

Figure 3. The position relation of any two vertices in KT.

Summing up the results of Cases 1–3, we obtain

$$
\begin{aligned}
NT_\alpha(KT) &= NT_\alpha(KT^{(a+b)}) + NT_\alpha(KT^{(c+d+e)}) \\
&+ NT_\alpha(KT^{(f)}) + NT_\alpha(KT^{(g)}) + NT_\alpha(KT^{(h+i)}) + NT_\alpha(KT^{(j+k+l)}) \\
&= \frac{n-k-1}{2}[(n-2)^\alpha + (n-3)^\alpha] \\
&+ [n-k-1+\sum_i \frac{i!}{(i-2)!}]\ (n-4)^\alpha \\
&+ \sum_i [i + i(k-1)]\ (n-2i-3)^\alpha \\
&+ \sum_i i(\frac{n-k-1}{2} - i + k - 1)\ (n-4i-2)^\alpha \\
&+ 3\sum_i \sum_j (2j-2i)^\alpha .
\end{aligned}
$$

This completes the proof.

THE GENERAL TRINAJSTIĆ INDEX OF FIREFLY GRAPH AND WHEEL GRAPH

The firefly graph $F_{s,t,p}$ ($s \geq 0$, $t \geq 0$, $p \geq 0$) is a graph that consists of s triangles, t pendent paths of length 2 and p pendent edges, sharing a common vertex, see Figure 4.

Theorem 4.1. Let $F_{s,t,p}$ be a firefly graph. If $t \geq 2$, then

$$
\begin{aligned}
NT_\alpha(F_{s,t,p}) &= tp + 2sp + (t+p)(2s+2t+p-1)^\alpha \\
&+ (2s+t)(2s+2t+p-2)^\alpha \\
&+ (\frac{t!}{(t-2)!} + tp + 2st + t)(2s+2t+p-3)^\alpha .
\end{aligned}
$$

If $t < 2$, then

$$
\begin{aligned}
NT_\alpha(F_{s,t,p}) &= tp + 2sp + (t+p)(2s+2t+p-1)^\alpha \\
&+ (2s+t)(2s+2t+p-2)^\alpha \\
&+ (tp + 2st + t)(2s+2t+p-3)^\alpha .
\end{aligned}
$$

Proof. According to the positional relationship of u and v, we have (a)–(k) types, shown in Figure 4.

By the definition of the general Trinajstić index, we will calculate the following Cases 1–3 by n_u, which, put together, will get our proof.

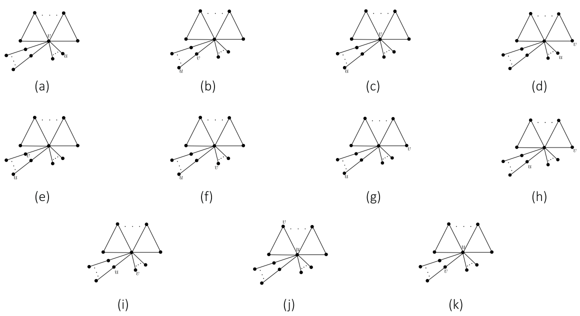

Figure 4. The position relation of any two vertices in $F_{s,t,p}$.

Case 1. $n_u = 1$. As shown in (a) and (b), we have $n_v = 2s + 2t + p$, then

$$NT_\alpha(F_{s,t,p}^{(a+b)}) = (t+p)\ (2s+2t+p-1)^\alpha .$$

As shown in (c), we have $n_v = 2s + 2t + p + 1 - 2$, then

$$NT_\alpha(F_{s,t,p}^{(c)}) = \sum | n_u - n_v |^\alpha = t(2s+2t+p-2)^\alpha .$$

As shown in (d), we have $n_v = 2$, then

$$NT_\alpha(F_{s,t,p}^{(d)}) = \sum | n_u - n_v |^\alpha = 2sp.$$

Case 2. $n_u = 2$. As shown in (e), (f), (g), we have $n_v = 2s + 2t + p + 1 - 2$, then

$$
\begin{aligned}
NT_\alpha(F_{s,t,p}^{(e+f+g)}) &= \sum | n_u - n_v |^\alpha \\
&= (\frac{t!}{(t-2)!} + tp + 2st)\ [2-(2s+2t+p+1-2)]^\alpha \\
&= (\frac{t!}{(t-2)!} + tp + 2st)\ (2s+2t+p-3)^\alpha , \quad (t \geq 2).
\end{aligned}
$$

If $t < 2$, obviously, (e) does not exist, so it is 0, therefore,

$$NT_\alpha(F_{s,t,p}^{(e+f+g)}) = (tp + 2st)(2s+2t+p-3)^\alpha .$$

As shown in (h) and (i), we have $n_v = 2$ and $n_v = 1$, respectively, then

$$NT_\alpha(F_{s,t,p}^{(h+i)}) = \sum | n_u - n_v |^\alpha = 2st\ | 2-2 |^\alpha + tp\ | 2-1 |^\alpha = tp.$$

Case 3. $n_u = 2s + 2t + p - 1$. As shown in (j) and (k), we have $n_v = 1$ and $n_v = 2$, respectively, then

$$NT_\alpha(F_{s,t,p}^{(j+k)}) = 2s(2s+2t+p-2)^\alpha + t(2s+2t+p-3)^\alpha .$$

Summing up the results of Cases 1–3, we obtain

$$
\begin{aligned}
NT_\alpha(F_{s,t,p}) &= NT_\alpha(F_{s,t,p}^{(a+b)}) + NT_\alpha(F_{s,t,p}^{(c)}) + NT_\alpha(F_{s,t,p}^{(d)}) \\
&+ NT_\alpha(F_{s,t,p}^{(e+f+g)}) + NT_\alpha(F_{s,t,p}^{(h+i)}) + NT_\alpha(F_{s,t,p}^{(j+k)}) \\
&= (t+p)\ (2s+2t+p-1)^\alpha + t(2s+2t+p-2)^\alpha \\
&+ 2sp + (\frac{t!}{(t-2)!} + tp + 2st)\ (2s+2t+p-3)^\alpha \\
&+ (tp + 2st)\ (2s+2t+p-3)^\alpha + tp \\
&+ 2s(2s+2t+p-2)^\alpha + t(2s+2t+p-3)^\alpha \\
&= tp + 2sp + (t+p)\ (2s+2t+p-1)^\alpha \\
&+ (2s+t)\ (2s+2t+p-2)^\alpha \\
&+ (\frac{t!}{(t-2)!} + tp + 2st + t)\ (2s+2t+p-3)^\alpha .
\end{aligned}
$$

for $t \geq 2$.

$$
\begin{aligned}
NT_\alpha(F_{s,t,p}) &= NT_\alpha(F_{s,t,p}^{(a+b)}) + NT_\alpha(F_{s,t,p}^{(c)}) + NT_\alpha(F_{s,t,p}^{(d)}) \\
&+ NT_\alpha(F_{s,t,p}^{(e+f+g)}) + NT_\alpha(F_{s,t,p}^{(h+i)}) + NT_\alpha(F_{s,t,p}^{(j+k)}) \\
&= (t+p)(2s+2t+p-1)^\alpha + t(2s+2t+p-2)^\alpha \\
&+ 2sp + (tp+2st)(2s+2t+p-3)^\alpha \\
&+ (tp+2st)(2s+2t+p-3)^\alpha + tp \\
&+ 2s(2s+2t+p-2)^\alpha + t(2s+2t+p-3)^\alpha \\
&= tp + 2sp + (t+p)(2s+2t+p-1)^\alpha \\
&+ (2s+t)(2s+2t+p-2)^\alpha \\
&+ (tp+2st+t)(2s+2t+p-3)^\alpha .
\end{aligned}
$$

for $t < 2$. This completes the proof.

A wheel graph has a distinguished (inner) vertex which is connected to all other (outer) vertices, and it can be drawn such that all outer vertices lie on a circle centered at the inner vertex.

Theorem 4.2. For a wheel graph W_n, we have

$$NT_\alpha(W_n) = (n-1)(n-4)^\alpha .$$

Proof. If u and v are on the outer cycle, then $n_u = n_v$, that is, $|n_u - n_v| = 0$. If u is the center vertex and v is on the outer cycle, then $n_u = n-3$ and $n_v = 1$, that is, $|n_u - n_v| = n-4$.

Thus $NT_\alpha(W_n) = (n-1)(n-4)^\alpha$. This completes the proof.

THE GENERAL TRINAJSTIĆ INDEX OF SOME HYDROCARBONS

The general Trinajstić index can be calculated for various chemically relevant chemical structures (Figure 5.) such as branched (a–i), cyclic (n–r) or branched cyclic (j–m) hydrocarbons, and their values are given in Table 2.

These are real chemical structures such as aromatic structures (o–r, Figure 5.), which attract the interest of scientists in studying their properties such as resonance energies, topological or circuit resonance energies, currents and aromaticity.[15] Moreover, different variants of the general Trinajstić index can be applied to simplified skeletons (hydrogen-suppressed graphs) of other heteroatomic compounds in which heteroatoms (which are not carbon) are weighted differently[16] or they can be treated as a carbon atom, which is common in quantitative structure-activity-property models.[17] Therefore, the general Trinajstić index could be used in modelling in chemistry as well as other topological indices.[16,17]

CONCLUSIONS

In this paper, we propose the general Trinajstić index of graphs, and obtain the general Trinajstić index of double-star graphs, double brooms, Kragujevac trees, firefly

Table 2. Values of different variants of the general Trinajstić index (for α = 1/2; 1; 3/2; 2; 3) calculated for some branched and cyclic hydrocarbons.

Alkane name	$NT_{1/2}$	NT_1	$NT_{3/2}$	NT_2	NT_3
2,3-Dimethylbutane	25.0892	54	119.3585	270	1458
2,2,3-Trimethylbutane	44.4484	86	187.4264	440	2714
2,2,3,3-Tetramethylbutane	38.6274	96	245.0193	640	4608
2,4-Dimethylpentane	21.8724	38	71.5059	142	614
2,2,4-Trimethylpentane	32.6862	60	120.5584	258	1320
2,5-Dimethylhexane	37.1116	64	121.4151	248	1192
3,5-Diethylheptane	93.0627	206	506.7527	1318	9614
3,3,5-Triethylheptane	129.9230	267	622.3656	1623	13689
3,3,5,5-Tetraethylheptane	124.8141	392	1283.5216	4280	48812
1-Ethyl-1-Methylcyclopropane	17.8530	28	45.9021	78	244
1,1-Diethylcyclopropane	26.3285	50	95.9298	186	722
1,1-Dimethylcyclopropane	8.2925	12	18.0491	28	72
Ethylcyclohexane	40.1414	63	104.7889	185	681
Benzene	0	0	0	0	0
Housane	6	6	6	6	6
Naphthalene	59.7989	104	187.5979	348	1268
1,1'-Biphenyl	134.7108	284	625.0593	1416	7652
Biphenylene	95.2901	196	416.1322	908	4612

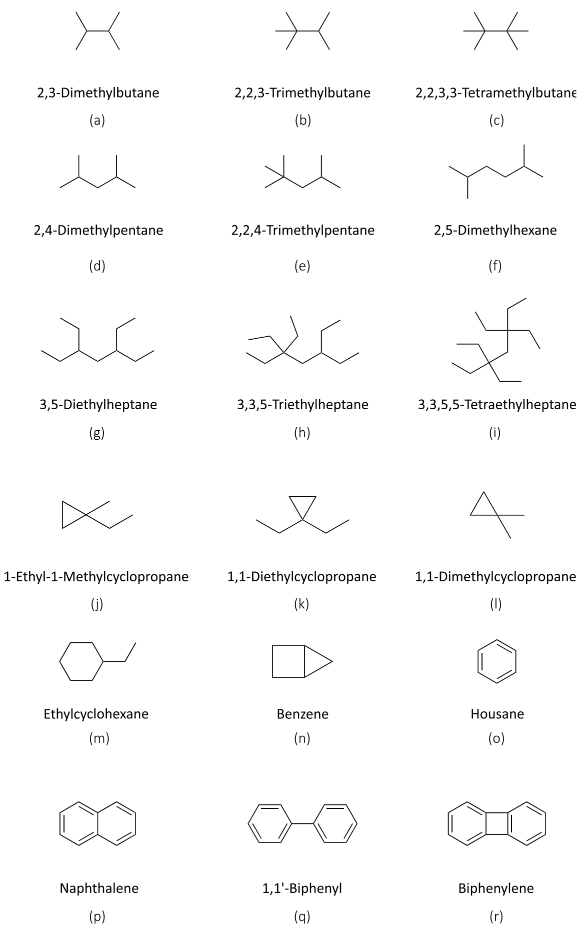

Figure 5. Some branched and cyclic hydrocarbons.

graphs, wheel graphs and some hydrocarbons. Moreover, the results of the this paper may be used in the computation of the general Trinajstić index of different networks.

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