A Novel/Old Modification of the First Zagreb Index
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Abstract: In the seminal paper [I. Gutman, N. Trinajstić, Chem. Phys. Lett. 1972, 17, 535–538], it was shown that total electron energy \( E_v \) of any alternant hydrocarbon depends on the sum of the squares of the degrees of the corresponding molecular graph. Nowadays, this sum is known as the first Zagreb index. In the same paper, another molecular descriptor was proved to influence \( E_v \), but that descriptor was never restudied explicitly. We call this descriptor as modified first Zagreb connection index and denote it by \( ZC_1^t \). In this paper, chemical applicability of the molecular descriptor \( ZC_1^t \) is tested for the octane isomers. Some basic properties of \( ZC_1^t \) are also established here. Furthermore, the alkanes with maximum and minimum \( ZC_1^t \) values are determined from the class of all alkanes having fixed number of carbon atoms.

Keywords: molecular descriptor · first Zagreb index · modified first Zagreb connection index · alkanes

1 Introduction

Throughout this paper, we consider only simple and finite graphs. Undefined notations and terminologies from (chemical) graph theory can be found in the books.[1–3]

It is well known fact that chemical compounds can be represented by graphs (known as molecular graphs) in which vertices correspond to the atoms while edges represent the covalent bonds between atoms.[1,4] In the present study, we consider only hydrogen-depleted molecular graphs, that is, the molecular graphs with hydrogen vertices deleted. In theoretical chemistry, the physicochemical properties of chemical compounds are often modeled by the molecular descriptors.[5,6] According to Todeschini and Consonni[7] molecular descriptor is the final result of a logical and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into an useful number or the result of some standardized experiment. In the paper,[7] it was shown that the following molecular descriptors appear in an approximate formula for total \( \pi \)-electron energy of any alternant hydrocarbon \( M_1 \):

\[
M_1(G) = \sum_{v \in V(G)} (d_v)^2, \quad ZC_1^t(G) = \sum_{v \in V(G)} d_v \tau_v,
\]

where \( G \) is the graph corresponding to the molecule \( M \), \( V(G) \) is the vertex set of \( G \), \( d_v \) is degree of the vertex it \( v \) and \( \tau_v \) is the connection number of \( v \) (that is, the number of vertices at distance 2 from \( v \), see[8]). The descriptor \( M_1 \) is known as the first Zagreb index. We call the molecular descriptor \( ZC_1^t \) as modified first Zagreb connection index (we reserve the name first Zagreb connection index for another related descriptor, considered in the last section). The following molecular descriptor, appeared within the study of molecular branching,[8] is called second Zagreb index:

\[
M_2(G) = \sum_{uv \in E(G)} d_ud_v,
\]

where \( E(G) \) is the edge set of the (molecular) graph \( G \) and \( uv \) is the edge between the vertices \( u, v \). The first Zagreb index and second Zagreb index are among the oldest and most studied topological indices. Several hundred papers have been devoted to these Zagreb indices, for example, see the reviews[9–11] published on the occasion of their 30th anniversary, recent surveys,[12–16] recent papers[17–24] and related references cited therein. In contrast, the modified first Zagreb connection index did not attract explicit attention in any of the numerous publications till 2016. The main purpose of the present study is to check whether the modified first Zagreb connection index has any chemical applicability or not, and to explore some basic properties as well as some extremal results of this descriptor.

2 Chemical Applicability and Some Properties of the Modified First Zagreb Connection Index

In order to test the chemical applicability of the molecular descriptor \( ZC_1^t \), the correlating ability of \( ZC_1^t \) is checked for the following thirteen physicochemical properties of octane isomers: boiling point, density, heat capacity at \( P \) constant, entropy, heat capacity at \( T \) constant, enthalpy of vaporization, acentric factor, standard enthalpy of vaporization,

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enthalpy of formation, octanol-water partition coefficient, standard enthalpy of formation, total surface area and molar volume. The experimental values of these properties are taken from the web site www.moleculardescriptors.eu which is suggested by the International Academy of Mathematical Chemistry. In the cases of entropy and acentric factor, we found that the absolute value of the correlation coefficient is greater than 0.8, or more precisely, it is approximately equal to 0.892 and 0.949, respectively. This gives a hope that the molecular descriptor \( ZC_1 \) may be useful in quantitative structure-property relationship and quantitative structure-activity relationship studies, and hence this descriptor may be considered for further investigations on the benchmark data sets containing molecules different from octane isomers.

Now, we establish some basic properties of the molecular descriptor \( ZC_1 \). Suppose that the graph \( G \) has \( n \) vertices with degree zero and let \( V_1(G) \) be the set of these vertices. In Reference[25] the following identity was derived:

\[
\sum_{u \in V(G)} d_f(u) = \sum_{u \in V(G)} (f(d_u) + f(d_v)),
\]

where \( f \) is a real-valued function defined on the set of vertex degrees of the graph \( G \). The proof technique used in establishing (1) also works for deriving the following more general identity:

\[
\sum_{u \in V(G)} d_g(u) = \sum_{u \in E(G)} (g(u) + g(v)),
\]

where \( g \) is a real-valued function defined on the vertex set \( V(G) \) of a (connected) graph. Hence, the molecular descriptor \( ZC_1 \) can be rewritten in the following form by setting \( g(u) = \tau_u \) in (2):

\[
ZC_1(G) = \sum_{u \in V(G)} (\tau_u + \tau_v).
\]

Došlić and Reti[26] derived an inequality (given in the next proposition), concerning the first Zagreb index \( M_1 \), where the the quantity \( \sum_{u \in V(G)} d_u \tau_u \) also appears.

**Proposition 2.1.** If \( G \) is a connected \((n,m)\)-graph different from complete graph, then

\[
M_1(G) + \sum_{u \in V(G)} d_u \tau_u \leq 2m(n-1),
\]

with equality if and only if \( G \) has diameter 2.

In 2008, Yamaguchi[27] derived a lower bound (given in the following proposition (see also[26])) on the second Zagreb index \( M_2 \), in which the quantity \( \sum_{u \in V(G)} d_u \tau_u \) also appears:

\[
M_2(G) \geq \frac{1}{2} \left( \sum_{u \in V(G)} d_u (d_u + \tau_u) \right).
\]

with equality if and only if \( G \) is a triangle- and quadrangle-free graph.

Hence, if the graph under consideration is triangle- and quadrangle-free then the molecular descriptor \( ZC_1 \) can be written as the linear combination of \( M_1 \) and \( M_2 \).

**Corollary 2.3.** If \( G \) is a triangle- and quadrangle-free graph, then

\[
ZC_1(G) = 2M_2(G) - M_1(G).
\]

Here, it needs to be mentioned that Xu *et al.*[28] considered the linear combination \( 2M_2(G) - M_1(G) \) for any connected graph \( G \).

As usual, the path graph, star graph and complete graph on \( n \) vertices will be denoted by \( P_n \), \( S_n \) and \( K_n \), respectively. As there are many (lower and upper) bounds as well as relations for the Zagreb indices \( M_i \) and \( M_j \) in the literature. Hence, several bounds for the molecular descriptor \( ZC_1 \) can be easily established using Eq. (6), in case of triangle- and quadrangle-free graphs. For instance, we derive an upper bound for \( ZC_1 \), using the following result, which was reported in References[9,29]

**Proposition 2.4.** If \( G \) is an \((n,m)\)-graph with minimum degree \( \delta \), then

\[
M_1(G) \leq 2m^2 - (n-1)m\delta + \frac{1}{2} (\delta - 1)M_1(G)
\]

with equality if and only if \( G \cong S_n \) or \( G \cong K_n \).

The upper bound on the molecular descriptor \( ZC_1 \), given in the following corollary, follows immediately from Proposition 2.2 and Proposition 2.4:

**Corollary 2.5.** If \( G \) is a triangle- and quadrangle-free graph with order \( n \), size \( m \) and minimum vertex degree \( \delta \) then

\[
ZC_1(G) \leq 4m^2 - 2(n-1)m\delta + (\delta - 2)M_1(G)
\]

with equality if and only if \( G \cong S_n \).

### 3 Modified First Zagreb Connection Index of Molecular Trees

Denote by \( \mathcal{MT}_n \) the collection of all \( n \)-vertex molecular trees (that is, the molecular graphs representing alkanes with \( n \) carbon atoms). This section is devoted to solve the problem of finding the molecular trees with minimum and maximum \( ZC_1 \) values among the collection \( \mathcal{MT}_n \), for \( n \geq 4 \).
All the non-isomorphic members of the collections \( MT_n \), \( MT_2 \) and \( MT_3 \) (together with vertex connection numbers) are depicted in Figure 1, and their \( ZC_i \) values are given in Table 1. As, the collection \( MT_4 \) consists of only two non-isomorphic trees and both of these trees have the same \( ZC_i \) value. Hence, the above mentioned problem make sense only for \( n \geq 5 \).

![Figure 1](image)

**Figure 1.** All the non-isomorphic molecular trees (together with vertex connection numbers) on (a) four vertices (b) five vertices (c) six vertices.

Table 1. The \( ZC_i \) values of the molecular trees depicted in Figure 1.

| Molecular tree \( T_i \) shown in Figure 1 | \( ZC_i \) value of \( T_i \) |
|-------------------------------------------|-----------------------------|
| \( T_1 \)                                  | 6                           |
| \( T_2 \)                                  | 6                           |
| \( T_3 \)                                  | 10                          |
| \( T_4 \)                                  | 12                          |
| \( T_5 \)                                  | 12                          |
| \( T_6 \)                                  | 14                          |
| \( T_7 \)                                  | 16                          |
| \( T_8 \)                                  | 18                          |
| \( T_9 \)                                  | 20                          |
| \( T_{10} \)                               | 20                          |

For a vertex \( u \in V(G) \), denote by \( N(u) \) (that is, the neighborhood of \( u \)) the set of all vertices adjacent with \( u \). A vertex having degree 1 is called pendant vertex. A pendant vertex adjacent with a vertex having degree greater than 2 is called star-type pendant vertex.

**Proposition 3.1.** For \( n \geq 5 \), only the path graph \( P_n \) has minimum \( ZC_i \) value among all the members of \( MT_n \).

**Proof.** Simple calculations yield \( ZC_i(P_n) = 4n - 10 \). The result will be proved by induction on \( n \). For \( n = 5 \), the desired result follows from Figure 1 and Table 1. Suppose that the result holds for all trees of order at most \( n - 1 \), where \( n \geq 6 \). Let \( T_n \) be an \( n \)-vertex tree and \( u \in V(T_n) \) be a pendant vertex adjacent to the vertex \( v \in V(T_n) \). Set \( d_v = x \) and \( N(v) = \{u = u_0, u_1, u_2, \ldots, u_{x - 1}, u_x\} \) where \( d_{u_i} = 1 \) for \( 0 \leq i \leq r - 1 \) and \( d_{u_i} \geq 2 \) for \( r \leq i \leq x - 1 \). As \( T_n \) is different from the star graph \( S_n \), so \( r_x \geq 1 \). Let \( T_{n-1} \) be the tree obtained from \( T_n \) by removing the vertex \( u \). Then

\[
ZC_i(T_n) = ZC_i(T_{n-1}) + \sum_{i=1}^{x-1} d_{u_i} + d_v + r_x - 1
\]

which is equivalent to

\[
ZC_i(T_n) = ZC_i(T_{n-1}) + \sum_{i=1}^{x-1} d_{u_i} + d_v + r_x - 1
\] (7)

Bearing in mind the facts \( r_x \geq 1 \), \( d_v \geq 2 \), \( \sum_{i=1}^{x-1} d_{u_i} \geq 2 \) and the inductive hypothesis, from Eq. (7) we have

\[
ZC_i(T_n) \geq ZC_i(T_{n-1}) + 4 \geq 4(n - 1) - 10 + 4 = ZC_i(P_n).
\]

We observe that the equality \( ZC_i(T_n) = ZC_i(P_n) \) holds if and only if \( r_x = 1 \), \( d_v = 2 \), \( d_{u_i} = 2 \) and \( T_{n-1} \cong P_{n-1} \). This completes the proof.

We note that the proof of Proposition 3.1 remains valid if we replace the collection \( MT_n \) with the collection of all \( n \)-vertex general trees different from the star graph \( S_n \), where \( n \geq 5 \). Moreover, \( ZC_i(P_n) = 4n - 10 < ZC_i(S_n) = (n - 1)(n - 2) \) for all \( n \geq 5 \). Hence, we have the following result.

**Corollary 3.2.** For \( n \geq 5 \), only the path \( P_n \) has minimum \( ZC_i \) value among all \( n \)-vertex trees.
Now, we solve the problem of finding the trees with maximum $ZC_i^*$ value among all the members of the collection $MIT_n$. For $n = 5, 6$, solution of this problem can be easily obtained from Figure 1, using Table 1. So, next, we assume $n \geq 7$. In the remaining part of this section, we will use the alternative formula of $ZC_i^*$, given in Eq. (6).

Let $T^*$ be a tree obtained from another tree $T$ by applying some graph transformation such that $V(T) = V(T^*)$. In the rest of paper, whenever such two trees are under discussion, by the vertex degree $d_v$, we always mean that it is the degree of the vertex $u$ in $T$.

Lemma 3.3. Let $u, v, w$ be three (different) vertices of a tree $T$ such that $uv \in E(T)$ and $uw \notin E(T)$. If $T' \cong T - uv + uw$ then

$$ZC_i^*(T) - ZC_i^*(T') = \sum_{x \in (N(v) \cup x = u)} (2d_x - 1) - \sum_{y \in (N(w) \cup y = v)} (2d_y - 1)$$

$$(2d_u - 1)(d_v - d_w - 1),$$

if $vw \notin E(T)$ and

$$ZC_i^*(T) - ZC_i^*(T') = \sum_{x \in (N(v) \cup x = u \neq w)} (2d_x - 1) - \sum_{y \in (N(w) \cup y \neq v)} (2d_y - 1)$$

$$(2d_u - 3)(d_v - d_w - 1),$$

if $vw \in E(T)$.

Proof. The proof is straightforward.

Lemma 3.4. For $n \geq 7$, if a tree $T^* \in MIT_n$ has the maximum $ZC_i^*$ value then $T^*$ contains at most one vertex of degree 2.

Proof. Suppose to the contrary that $u, v \in V(T^*)$ such that $d_u = d_v = 2$. Let $N(u) = \{u_1, u_2\}$ and $N(v) = \{v_1, v_2\}$. Suppose that the unique path connecting the vertices $u$ and $v$ contains the vertices $u_2, v_2$. Without loss of generality, we assume that $d_{u_2} + d_{v_2} \leq d_{u_1} + d_{v_1}$. Let $T^{(1)}$ be the tree obtained from $T^*$ by removing the edge $u_1, v_1$ and adding the edge $u, v$. We calculate the value of the difference $ZC_i^*(T^*) - ZC_i^*(T^{(1)})$ by using Lemma 3.3. There are two cases.

Case 1. The vertices $u$ and $v$ are adjacent. That is, $u_2 = v$ and $v_2 = u$.

If the vertex $u_1$ is pendant then the condition $n \geq 7$ guaranties that $d_{u_1} \geq 2$. Hence, whether the vertex $u_1$ is pendant or not, in either case, we have

$$ZC_i^*(T^*) - ZC_i^*(T^{(1)}) = 2(d_u - d_v - d_{u_1}) < 0,$$

a contradiction to the definition of $T^*$.

Case 2. The vertices $u$ and $v$ are not adjacent.

Bearing in mind the inequality $d_{u_2} + d_{v_2} \leq d_{u_1} + d_{v_1}$, we have

$$ZC_i^*(T^*) - ZC_i^*(T^{(1)}) = 2(d_u - d_v - d_{u_1} - d_{v_1} + 1) < 0,$$

again a contradiction.

In both cases, contradiction arises. Hence, $T^*$ contains at most one vertex of degree 2.

Lemma 3.5. For $n \geq 7$, if a tree $T^* \in MIT_n$ has the maximum $ZC_i^*$ value and $T^*$ contains a vertex “$u$” of degree 2 then one of the neighbors of “$u$” is pendant.

Proof. Suppose to the contrary that both the neighbors of $u$, say $u_1$ and $u_2$, are non-pendant. Then, Lemma 3.4 guaranties that both of the vertices $u_1, u_2$ have degree at least 3 and all the pendant vertices of $T^*$ are star-type pendant vertices. Let $w \in V(T^*)$ be a pendant vertex adjacent to a vertex $t \in V(T^*)$. The vertex $t$ may coincide with either of the vertices $u_1, u_2$. If this is the case, then without loss of generality we assume that $t = u_1$. Suppose that $T^{(1)}$ is the tree obtained from $T^*$ by removing the edges $u,t, u_1, u_2, w t$ and adding the edges $u, u_2, w, u_1, t$. We observe that both the trees $T^{(1)}$ and $T^*$ have same degree sequence. Whether $t = u_1$ or $t \neq u_1$, in either case, we have

$$ZC_i^*(T^*) - ZC_i^*(T^{(1)}) = 2(d_u + 2d_u - d_{u_1} d_{u_2} - 2 - d_t).$$

We note that $2d_u + 2d_u - d_{u_1} d_{u_2} - 2 - d_t < 0$, which implies that

$$ZC_i^*(T^*) - ZC_i^*(T^{(1)}) \leq 2(1 - d_t) < 0.$$

This contradicts the maximality of $ZC_i^*(T^*)$.

Lemma 3.6. For $n \geq 7$, if a tree $T^* \in MIT_n$ has the maximum $ZC_i^*$ value then $T^*$ contains at most one vertex of degree 3.

Proof. Suppose, contrarily, that $u, v \in V(T^*)$ such that $d_u = d_v = 3$. Let $N(u) = \{u_1, u_2, u_3\}$ and $N(v) = \{v_1, v_2, v_3\}$. Suppose that the unique path connecting the vertices $u$ and $v$ contains the vertices $u_1, v_1$. Without loss of generality, we also assume that $d_{u_1} + d_{v_1} \leq d_{u_2} + d_{v_2}$. Let $T^{(1)}$ be the tree obtained from $T^*$ by removing the edge $u_1, v_1$ and adding the edge $u, v$. By using Lemma 3.3, we calculate the value of the difference $ZC_i^*(T^*) - ZC_i^*(T^{(1)})$. There are two cases.

Case 1. The vertices $u$ and $v$ are adjacent. That is, $u_3 = v$ and $v_3 = u$.

If both the vertices $u_1$ and $u_2$ are pendant then the assumption $n \geq 7$ forces that at least one of the vertices $v_1, v_2$ must be non-pendant and hence

$$ZC_i^*(T^*) - ZC_i^*(T^{(1)}) = 2(2 + d_{u_1} - d_{v_1} - d_{u_2} - d_{v_2}) < 0,$$

which contradicts the maximality of $ZC_i^*(T^*)$.

If at least one of the vertices $u_1, u_2$ is non-pendant then $d_{u_1} \geq 2$ (because $d_{u_1} \geq d_{u_2}$) and hence we have
\[ ZC_i(T) - ZC_i(T^{(1)}) = 2(2 + du_u - du_v - du_d - du_v) \leq 2(du_u - du_v - du_v) < 0, \]

a contradiction.

**Case 2.** The vertices \( u \) and \( v \) are not adjacent. In this case, we have

\[ ZC_i(T) - ZC_i(T^{(1)}) = 2(1 - du_u + du_v - du_v - du_v - du_v). \tag{8} \]

From the inequality \( du_u + du_v < du_v + du_v + du_v \) and Eq. (8), it follows that

\[ ZC_i(T) - ZC_i(T^{(1)}) < 2(1 - 2du_u) < 0, \]

which is again a contradiction.

**Lemma 3.7.** For \( n \geq 7 \), if a tree \( T^* \in \mathcal{MT}_n \) has the maximum \( ZC_i \) value then \( T^* \) does not contain vertices of degrees 2 and 3 simultaneously.

**Proof.** Suppose to the contrary that \( u, v \in V(T^*) \) such that \( du_u = 2 \) and \( du_v = 3 \). Let \( N(u) = \{u_1, u_2\} \) and \( N(v) = \{v_1, v_2, v_3\} \). Suppose that the unique path connecting the vertices \( u \) and \( v \) contains the vertices \( u_2, v_3 \). Let \( T^{(1)} \) be the tree obtained from \( T^* \) by removing the edge \( u_2u \) and adding the edge \( u_2v_3 \). There are two cases.

**Case 1.** The vertices \( u \) and \( v \) are adjacent. That is, \( u_2 = v \) and \( v_3 = u \).

The assumption \( n \geq 7 \) implies that at least one of the vertices \( u_2, v_1, v_2 \) must be non-pendant and hence, by Lemma 3.3, it holds that

\[ ZC_i(T) - ZC_i(T^{(1)}) = 2(4 - 2du_u - du_v - du_v) < 0, \]

which is a contradiction.

**Case 2.** The vertices \( u \) and \( v \) are not adjacent. By Lemma 3.4 and Lemma 3.6, we have \( du_u = du_v = 4 \) and hence, again by Lemma 3, we have

\[ ZC_i(T) - ZC_i(T^{(1)}) = 2(2 - 2du_u - du_v - du_v) < 0, \]

again a contradiction.

**Lemma 3.8.** For \( n \geq 7 \), let \( T^* \in \mathcal{MT}_n \) be a tree with maximum \( ZC_i \) value. If \( T^* \) contains a vertex \( u \) of degree 3 then \( u \) has two pendant neighbors.

**Proof.** Contrarily, suppose that \( u_1, u_2 \) are non-pendant neighbors of \( u \) and let \( N(u) = \{u_1, u_2, u_3\} \). Due to Lemma 3.6 and Lemma 3.7, both the vertices \( u_1, u_2 \) have degree 4 and there must exist a vertex \( v \in V(T^*) \) of degree 4 such that three neighbors of \( v \) are pendant. The vertex \( v \) may coincide with any of the vertices \( u_1, u_2, u_3 \); if this is the case then, without loss of generality, we assume that \( v = u_1 \). Let \( w \) be a pendant neighbor of \( v \) and suppose that \( T^{(1)} \) is the tree obtained from \( T^* \) by removing the edge \( vw \) and adding the edge \( uw \). Whether \( v = u_1 \) or \( v \neq u_1 \), in either case, by using Lemma 3.3, we have

\[ ZC_i(T) - ZC_i(T^{(1)}) = -2(du_u + 2) < 0, \]

a contradiction.

Now, we are in position to state and prove the main result of this paper.

**Theorem 3.9.** If \( n \geq 7 \) and \( k \) is some integer greater than 1, then among all \( n \)-vertex molecular trees, the tree(s) with maximum \( ZC_i \) value contain(s)

(i) no vertex of degree 3 and contain(s) exactly one vertex of degree 2, which is adjacent to a pendant vertex and a vertex of degree 4 for \( n = 3k \);

(ii) no vertex of degree 2 and contain(s) exactly one vertex of degree 3, which is adjacent to two pendant vertices and one vertex of degree 4 for \( n = 3k + 1 \);

(iii) only vertices of degrees 1 and 4 for \( n = 3k + 2 \).

**Proof.** The proofs of all three parts are similar and thereby we only prove first part, and omit the proofs of remaining ones. Among all \( n \)-vertex molecular trees, suppose that the tree \( T^* \) has maximum \( ZC_i \) value, where \( n \geq 7 \). The following equations hold for \( T^* \):

\[ n_1 + n_2 + n_3 + n_4 = n, \tag{9} \]
\[ n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1), \tag{10} \]

where \( n_i \) is the number of vertices of degree \( i \) in \( T^* \). By eliminating \( n_1 \) from Eqs. (9) and (10), we have

\[ n_2 + 2n_3 + 3n_4 = n - 2. \tag{11} \]

From the assumption \( n = 3k \), where \( k \geq 3 \), and Eq. (11), it follows that \( n_2 + 2n_3 + 2 \) is a multiple of 3, which implies that \( n_3 = 1, n_4 = 0 \), because \( n_2 + n_1 \leq 1 \) by Lemmas 3.4, 3.6 and 3.7. Now, from Lemma 3.5, it follows that \( T^* \) has the desired property.

It is interesting to note that the trees having maximum \( M_2 \) value \(^{36} \) and maximum \( ZC_i \) value, among all \( n \)-vertex molecular trees, are same for \( n \geq 7 \) (it is, however, not true for general trees).

Denote by \( x_{a,b} \) the number of edges in a graph \( G \) connecting the vertices of degrees \( a \) and \( b \). The next result is an immediate consequence of Theorem 3.9.

**Corollary 3.10.** If \( k \) is an integer greater than 1, \( n \geq 7 \) and \( T \) is an \( n \)-vertex molecular tree, then

\[ ZC_i(T) \leq \begin{cases} 10(n - 4) & \text{if } n = 3k \text{ or } n = 3k + 1, \\ 2(5n - 19) & \text{otherwise}. \end{cases} \]

The equality sign in the first inequality holds if either \( T \) contains no vertex of degree 3 and it contains exactly one
The equality sign in the second inequality holds if $T$ contains only vertices of degrees 1 and 4.

Proof. By Theorem 3.9, we only need to calculate the $ZC_1$ value of the extremal trees mentioned in Theorem 3.9. Firstly, we assume that $T_{3k}$ is the extremal tree, specified in Theorem 3.9 for $n = 3k$ where $k \geq 3$. From the fact $n_2 = 1, n_3 = 0$ and from Eqs. (9), (10), it follows that $n_1 = 2k, n_4 = k - 1$. Also, we note that $x_{12} = x_{24} = 1$. The equations

\[ x_{12} + x_{13} + x_{14} = n_1, \]
\[ x_{14} + x_{24} + x_{34} + 2x_{44} = 4n_4, \]

give us $x_{14} = 2k - 1, x_{44} = k - 2$ and hence $ZC_1(T_{3k}) = 10(n - 4)$. In a similar way, one can easily verify that the $ZC_1$ value of the extremal trees, mentioned in Theorem 3.9, is $10(n - 4)$ for $n = 3k + 1$ and $2(5n - 19)$ for $n = 3k + 2$.

4 Concluding Remarks

In Section 2, it has been concluded that the molecular descriptor $ZC_1$ is well-correlated with the entropy and acentric factor of octane isomers. Hence, by using Proposition 3.1 and Theorem 3.9, one may predict the alkanes having minimum/maximum entropy and minimum/maximum acentric factor among all the alkanes with fixed number of carbon atoms.

We recall that the first Zagreb index $M_1$ can be rewritten as

\[ M_1(G) = \sum_{uv \in E(G)} (d_u + d_v). \]  

If we replace vertex degrees by vertex connection numbers in Eq. (12), we get the molecular descriptor $ZC_1$. Hence, it is natural to consider the following connection-number-based versions of the Zagreb indices $\sum_{uv \in V(G)} d_u^2$ and $\sum_{uv \in E(G)} d_u d_v$ for a connected graph $G$:

\[ ZC_1(G) = \sum_{uv \in V(G)} r_u^2 \] and \[ ZC_2(G) = \sum_{uv \in E(G)} t_u t_v, \]

respectively. We call $ZC_1$ as the first Zagreb connection index and $ZC_2$ as the second Zagreb connection index. Also, the following bond incident connection-number (BIC) indices may be considered as a generalization of the Zagreb connection indices:

\[ BIC(G) = \sum_{\phi_{ab}(G) \leq n-2} \gamma_{ab}(G) \cdot \phi_{ab}, \]  

where $\gamma_{ab}(G)$ is the number of edges in the connected graph $G$ connecting the vertices with connection numbers $a$ and $b$, and $\phi_{ab}$ is a non-negative real valued symmetric function which depends on $a$ and $b$. Furthermore, the BIC indices can be obtained from the following more general setting:

\[ \sum_{uv \in E(G)} \phi(k_{fu}, k_{fv}), \]  

where $k_{fu}$ is the number of vertices at distance $k$ from the vertex $u$ of the (connected) graph $G$, see, and $\phi$ is a non-negative real valued symmetric function depending on $k_{fu}$ and $k_{fv}$.

Conflict of Interest

None declared.

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