Iranian J. Math. Chem. 13 (2) June (2022) 99 – 108

IRANIAN JOURNAL OF
Mathematical Chemistry
Journal homepage: ijmc.kashanu.ac.ir

Original Scientific Paper

Another Approach to a Conjecture about the Exponential Reduced Sombor Index of Molecular Trees

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ARTICLE INFO

Article History:

Received: 12 June 2022
Accepted: 28 June 2022
Published online: 30 June 2022
Academic Editor: Akbar Ali

Keywords:

Sombor index
Exponential reduced Sombor index
Degree
Tree

ABSTRACT

For a graph G, the exponential reduced Sombor index (ERSI), denoted by $\mathrm{e}^{SO_{red}}$, is $\sum_{uv\in E(G)} \mathrm{e}^{\sqrt{(d_G(v)-1)^2+(d_G(u)-1)^2}}$, where $d_G(v)$ is the degree of vertex v. The authors in [On the reduced Sombor index and its applications, *MATCH Commun. Math. Comput. Chem.* 86 (2021) 729–753] conjectured that for each molecular tree T of order n, $\mathrm{e}^{SO_{red}}(T) \leq \frac{2}{3}(n+1)\mathrm{e}^3 + \frac{1}{3}(n-5)\mathrm{e}^{3\sqrt{2}}$ where $n \equiv 2 \pmod 3$, $\mathrm{e}^{SO_{red}}(T) \leq \frac{1}{3}(2n+1)\mathrm{e}^3 + \frac{1}{3}(n-13)\mathrm{e}^{3\sqrt{2}} + 3\mathrm{e}^{\sqrt{13}}$ where $n \equiv 1 \pmod 3$ and $\mathrm{e}^{SO_{red}}(T) \leq \frac{2}{3}n\mathrm{e}^3 + \frac{1}{3}(n-9)\mathrm{e}^{3\sqrt{2}} + 2\mathrm{e}^{\sqrt{10}}$ where $n \equiv 0 \pmod 3$. Recently, Hamza and Ali [On a conjecture regarding the exponential reduced Sombor index of chemical trees. *Discrete Math. Lett.* 9 (2022) 107–110] proved the modified version of this conjecture. In this paper, we adopt another method to prove it.

1. INTRODUCTION

In this paper, we consider finite, simple and connected graphs. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. Let $v \in V(G)$. Then $N_G(v)$ and

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DOI: 10.22052/IJMC.2022.246488.1632

$d_G(v)$ are the open neighbourhood and degree of vertex v in G, respectively. We denote the set of degrees of vertices G by $D(G)$.

Let $M \subseteq E(G)$ be a subset of edges of G. Then graph $G - M$ obtained of G by removing edges in M. Let $u,v \in V(G)$ and $uv \not\in E(G)$. Then graph $G + uv$ obtained of G by adding edge uv.

Graphs were first used in 1947 as a tool for approaching chemical problems. Until now, several formulas have been proposed as topological indices. For instance, Sombor-type indices are the vertex-degree-based topological indices introduced by Gutman [11] as a geometric approach to degree-based topological indices. We refer interested readers to study references [1-12,14-33] for more details on Sombor-type indices and their applications. Recently, a new Sombor-type index was defined as $\mathrm{e}^{SO_{red}}(G) = \sum_{uv\in E(G)} \mathrm{e}^{\sqrt{(d_G(v)-1)^2+(d_G(u)-1)^2}}$, and named as the exponential reduced Sombor index in [22]. In this work, the authors posed the following conjecture on exponential reduced Sombor index.

Conjecture 1.1. *Let $\mathcal{CT}_n$ be the set of molecular trees of order n. For $n \geq 5$, if $T \in \mathcal{CT}_n$, then*

$$\mathrm{e}^{SO_{red}}(T) \leq \begin{cases} \frac{2}{3}n\mathrm{e}^3 + \frac{1}{3}(n-9)\mathrm{e}^{3\sqrt{2}} + 2\mathrm{e}^{\sqrt{10}}, & n \equiv 0(\mathrm{mod}3), \\ \frac{1}{3}(2n+1)\mathrm{e}^3 + \frac{1}{3}(n-13)\mathrm{e}^{3\sqrt{2}} + 3\mathrm{e}^{\sqrt{13}}, & n \equiv 1(\mathrm{mod}3), \\ \frac{2}{3}(n+1)\mathrm{e}^3 + \frac{1}{3}(n-5)\mathrm{e}^{3\sqrt{2}}, & n \equiv 2(\mathrm{mod}3). \end{cases}$$

In this paper, we show that cases $n \equiv 1(\mathrm{mod}3)$ and $n \equiv 0(\mathrm{mod}3)$ of this conjecture are not true. Then we prove the revised form of this conjecture; Infact we prove that if $n \geq 5$ and $T \in \mathcal{CT}_n$, then

$$\mathrm{e}^{SO_{red}}(T) \leq \begin{cases} \mathrm{e} + \left(\frac{2n-3}{3}\right)\mathrm{e}^3 + \mathrm{e}^{\sqrt{10}} + \left(\frac{n-6}{3}\right)\mathrm{e}^{3\sqrt{2}}, & n \equiv 0(\mathrm{mod}3), \\ 2\,\mathrm{e}^2 + \left(\frac{2n-5}{3}\right)\mathrm{e}^3 + \mathrm{e}^{\sqrt{13}} + \left(\frac{n-7}{3}\right)\mathrm{e}^{3\sqrt{2}}, & n \equiv 1(\mathrm{mod}3), \\ \left(\frac{2n+2}{3}\right)\mathrm{e}^3 + \left(\frac{n-5}{3}\right)\mathrm{e}^{3\sqrt{2}}, & n \equiv 2(\mathrm{mod}3). \end{cases}$$

We also characterize the molecular trees that achieve the equalities of above relation. It is worthy to mention here that this conjecture was also proved by a different method in [13].

2. MAIN RESULTS

Let G be a gaph of order n and for $1 \leq i \leq j \leq n-1$ let $n_i = n_i(G) = |\{v: v \in V(G) \text{ and } d_G(v) = i\}|$ and $m_{i,j} = m_{i,j}(G) = |\{uv: uv \in E(G) \text{ and } \{d_G(u),d_G(v)\} = \{i,j\}\}|$. Then by definitions of $\mathrm{e}^{SO_{red}}$ and $m_{i,j}$ we can write

$$\mathrm{e}^{SO_{red}}(G) = \textstyle\sum_{1\leq i\leq j\leq n-1} m_{i,j}\mathrm{e}^{\sqrt{(i-1)^2+(j-1)^2}}. \tag{1}$$

Let $T \in \mathcal{CT}_n$. Then by Equation (1), one can see that

$$\begin{aligned}\mathrm{e}^{SO_{red}}(G) = m_{1,2}\mathrm{e} + m_{1,3}\mathrm{e}^2 + m_{1,4}\mathrm{e}^3 + m_{2,2}\mathrm{e}^{\sqrt{2}} + m_{2,3}\mathrm{e}^{\sqrt{5}} + m_{2,4}\mathrm{e}^{\sqrt{10}}\\ + m_{3,3}\mathrm{e}^{2\sqrt{2}} + m_{3,4}\mathrm{e}^{\sqrt{13}} + m_{4,4}\mathrm{e}^{3\sqrt{2}}.\end{aligned} \tag{2}$$

As a consequence of Equations (1) and (2), we have the following proposition.

Proposition 2.1. *Let G be a graph without isolated edges of order n and size m. Then* $n_1\mathrm{e} + (m-n_1)\mathrm{e}^{\sqrt{2}} \leq \mathrm{e}^{SO_{red}}(G) \leq n_1\mathrm{e}^{\Delta-1} + (m-n_1)\mathrm{e}^{(\Delta-1)\sqrt{2}}$. The equality on the left side holds if and only if $D(G) \subseteq \{1,2\}$ and the equality on the right side occurs if and only $D(G) \subseteq \{1,\Delta\}$.

Proof. Since G do not have isolated edges, one can see that $\sum_{i=2}^{\Delta} m_{1,i} = n_1$ and $\sum_{2\leq i\leq j\leq n-1} m_{i,j} = m - n_1$. Thus by Equation (1) we conclude that

$$\mathrm{e}^{SO_{red}}(G) \geq \textstyle\sum_{i=2}^{n} m_{1,i}\mathrm{e} + \sum_{2\leq i\leq j\leq n-1} m_{i,j}\mathrm{e}^{\sqrt{2}} = n_1\mathrm{e} + (m-n_1)\mathrm{e}^{\sqrt{2}},$$

and the equality holds if and only if $D(G) \subseteq \{1,2\}$. And also

$$\mathrm{e}^{SO_{red}}(G) \leq \textstyle\sum_{i=2}^{n} m_{1,i}\mathrm{e}^{\Delta-1} + \sum_{2\leq i\leq j\leq n-1} m_{i,j}\mathrm{e}^{(\Delta-1)\sqrt{2}} = n_1\mathrm{e}^{\Delta-1} + (m-n_1)\mathrm{e}^{(\Delta-1)\sqrt{2}},$$

and the equality occurs if and only if $D(G) \subseteq \{1,\Delta\}$. ■

Corollary 2.2. *Let G be a molecular graph without isolated edges of order n and size m. Then* $n_1\mathrm{e} + (m-n_1)\mathrm{e}^{\sqrt{2}} \leq \mathrm{e}^{SO_{red}}(G) \leq n_1\mathrm{e}^3 + (m-n_1)\mathrm{e}^{3\sqrt{2}}$. The equality on the left side holds if and only if $D(G) \subseteq \{1,2\}$ and the equality on the right side occurs if and only $D(G) \subseteq \{1,4\}$.

Let $n \geq 2$ and $T \in \mathcal{CT}_n$. Then by this fact that $\sum_{v\in V(G)} d_G(v) = 2|E(G)|$, we have $n_1 + n_2 + n_3 + n_4 = n$ and $n_1 + 2n_2 + 3n_3 + 4n_4 = 2n - 2$. Thus it is not difficult to check that

$$n_2 = n - 2 - 2n_3 - 3n_4. \tag{3}$$

$$n_1 = n_3 + 2n_4 + 2. \tag{4}$$

Let $n \geq 5$ be an integer number. Set

$$\mathcal{CT}_n^0 = \left\{T \in \mathcal{CT}_n: n_4 = \frac{n-3}{3}, n_3 = 0, n_2 = 1, n_1 = \frac{2n}{3}\right\},$$

$$\mathcal{CT}_n^1 = \left\{T \in \mathcal{CT}_n: n_4 = \frac{n-4}{3}, n_3 = 1, n_2 = 0, n_1 = \frac{2n+1}{3}\right\},$$

$$\mathcal{CT}_n^2 = \left\{T \in \mathcal{CT}_n : n_4 = \frac{n-2}{3}, n_3 = 0, n_2 = 0, n_1 = \frac{2n+2}{3}\right\},$$
$$\mathcal{ECT}_n^0 = \left\{T \in \mathcal{CT}_n^0 : m_{4,4} = \frac{n-6}{3}, m_{2,4} = 1, m_{1,2} = 1, m_{1,4} = \frac{2n-3}{3}\right\},$$
$$\mathcal{ECT}_n^1 = \left\{T \in \mathcal{CT}_n^1 : m_{4,4} = \frac{n-7}{3}, m_{3,4} = 1, m_{1,3} = 2, m_{1,4} = \frac{2n-5}{3}\right\},$$
$$\mathcal{ECT}_n^2 = \left\{T \in \mathcal{CT}_n^2 : m_{4,4} = \frac{n-5}{3}, m_{1,4} = \frac{2n+2}{3}\right\}.$$

Since n_i, for $1 \leq i \leq 4$, is an integer number, then $\mathcal{ECT}_n^j$ is non-empty for $j \in \{0,1,2\}$ if and only if $n \equiv j \pmod 3$. Also, using relation (2), we conclude that if $T^0 \in \mathcal{ECT}_n^0$, $T^1 \in \mathcal{ECT}_n^1$ and $T^2 \in \mathcal{ECT}_n^2$, then

$$\mathrm{e}^{SO_{red}}(T^0) = \mathrm{e} + \left(\frac{2n-3}{3}\right)\mathrm{e}^3 + \mathrm{e}^{\sqrt{10}} + \left(\frac{n-6}{3}\right)\mathrm{e}^{3\sqrt{2}}, \tag{5}$$

$$\mathrm{e}^{SO_{red}}(T^1) = 2\,\mathrm{e}^2 + \left(\frac{2n-5}{3}\right)\mathrm{e}^3 + \mathrm{e}^{\sqrt{13}} + \left(\frac{n-7}{3}\right)\mathrm{e}^{3\sqrt{2}}, \tag{6}$$

$$\mathrm{e}^{SO_{red}}(T^2) = \left(\frac{2n+2}{3}\right)\mathrm{e}^3 + \left(\frac{n-5}{3}\right)\mathrm{e}^{3\sqrt{2}}. \tag{7}$$

Thus

$$\mathrm{e}^{SO_{red}}(T^0) > \frac{2}{3}n\mathrm{e}^3 + \frac{1}{3}(n-9)\mathrm{e}^{3\sqrt{2}} + 2\mathrm{e}^{\sqrt{10}},$$
$$\mathrm{e}^{SO_{red}}(T^1) > \frac{1}{3}(2n+1)\mathrm{e}^3 + \frac{1}{3}(n-13)\mathrm{e}^{3\sqrt{2}} + 3\mathrm{e}^{\sqrt{13}}.$$

These yield that Conjecture 1.1 for cases $n \equiv 0$ or $1 \pmod 3$ is not valid. In the following we show that if $n \geq 5$ and $T \in \mathcal{CT}_n$, then

$$\mathrm{e}^{SO_{red}}(T) \leq \begin{cases} \mathrm{e} + \left(\frac{2n-3}{3}\right)\mathrm{e}^3 + \mathrm{e}^{\sqrt{10}} + \left(\frac{n-6}{3}\right)\mathrm{e}^{3\sqrt{2}}, & n \equiv 0 \pmod 3, \\ 2\,\mathrm{e}^2 + \left(\frac{2n-5}{3}\right)\mathrm{e}^3 + \mathrm{e}^{\sqrt{13}} + \left(\frac{n-7}{3}\right)\mathrm{e}^{3\sqrt{2}}, & n \equiv 1 \pmod 3, \\ \left(\frac{2n+2}{3}\right)\mathrm{e}^3 + \left(\frac{n-5}{3}\right)\mathrm{e}^{3\sqrt{2}}, & n \equiv 2 \pmod 3, \end{cases}$$

with equality in the first case if and only if $T \in \mathcal{ECT}_n^0$, and equality in the second case if and only if $T \in \mathcal{ECT}_n^1$, and equality in the third case if and only if $T \in \mathcal{ECT}_n^2$.

Lemma 2.3. *If T has maximum value of ERSI among all members of $\mathcal{CT}_n$, then $m_{2,2}(T) = 0$.*

Proof. Assume, to the contrary, that u and v are two vertices of T such that $d_T(u) = d_T(v) = 2$ and $uv \in E(T)$. Let $N_T(u)\backslash\{v\} = u_1$ and $N_T(v)\backslash\{u\} = v_1$. Set $T_1 = (T - u_1u) + u_1v$. Then $T_1 \in \mathcal{CT}_n$, $T_1 \ncong T$. Thus, if $\Upsilon_1 = \mathrm{e}^{SO_{red}}(T) - \mathrm{e}^{SO_{red}}(T_1)$, then by the sructures of T and T_1, we have $\Upsilon_1 = \mathrm{e}^{\sqrt{(d_T(v_1)-1)^2+1}} + \mathrm{e}^{\sqrt{(d_T(u_1)-1)^2+1}} + \mathrm{e}^{\sqrt{2}} -$

$e^{\sqrt{(d_T(v_1)-1)^2+4}} - e^{\sqrt{(d_T(u_1)-1)^2+4}} - e^2 < 0$. Therefore, $e^{SO_{red}}(T) < e^{SO_{red}}(T_1)$, which is contrary to our assumption. ■

Lemma 2.4. *If T has maximum value of ERSI among all members of $\mathcal{CT}_n$, then $m_{1,2}(T) \leq 1$.*

Proof. Suppose, by way of contradiction, that uv and xy are two pendant edges of T such that $d_T(u) = d_T(x) = 2$, $d_T(v) = d_T(y) = 1$, $N_T(u)\backslash\{v\} = u_1$, $N_T(x)\backslash\{y\} = x_1$ and $d_T(x_1) \geq d_T(u_1)$. Set $T_2 = (T - uv) + xv$. Thus $T_2 \in \mathcal{CT}_n$ and $T_2 \ncong T$. Also, if $\Upsilon_2 = e^{SO_{red}}(T) - e^{SO_{red}}(T_2)$, then according to the sructures of T and T_2, we reach to

$$\Upsilon_2 = 2e + e^{\sqrt{(d_T(u_1)-1)^2+1}} + e^{\sqrt{(d_T(x_1)-1)^2+1}} - 2e^2 - e^{d_T(u_1)-1} - e^{\sqrt{(d_T(x_1)-1)^2+4}} < 0.$$

Therefore, $e^{SO_{red}}(T) < e^{SO_{red}}(T_1)$, which is contrary to the hypothesis. ■

Lemma 2.5. *If T has maximum value of ERSI among all members of $\mathcal{CT}_n$, then $m_{2,3}(T) = 0$.*

Proof. Assume, to the contrary, that uv is an edge of T such that $d_T(u) = 2$, $d_T(v) = 3$, $N_T(u)\backslash\{v\} = u_1$ and $N_T(v)\backslash\{u\} = \{v_1,v_2\}$. Set $T_3 = (T - u_1u) + u_1v$. Thus $T_3 \in \mathcal{CT}_n$, $T_3 \ncong T$. Also, if $\Upsilon_3 = e^{SO_{red}}(T) - e^{SO_{red}}(T_3)$, then the sructures of T and T_3 lead to

$$\Upsilon_3 = e^{\sqrt{(d_T(u_1)-1)^2+1}} + e^{\sqrt{5}} + e^{\sqrt{(d_T(v_1)-1)^2+4}} + e^{\sqrt{(d_T(v_2)-1)^2+4}} - e^{\sqrt{(d_T(u_1)-1)^2+9}} - e^4 - e^{\sqrt{(d_T(v_1)-1)^2+9}} - e^{\sqrt{(d_T(v_2)-1)^2+9}} < 0.$$

Therefore, $e^{SO_{red}}(T) < e^{SO_{red}}(T_3)$, a contradiction. ■

Lemma 2.6. *Let T have maximum value of ERSI among all members of $\mathcal{CT}_n$. Then $m_{2,4}(T) \leq 1$.*

Proof. By contradiction. Let $m_{2,4}(T) \geq 2$. Then using Lemmas 2.3, 2.4 and 2.5 conclude that there exists set $\{u,v,w,x,y\} \subseteq V(T)$ such that $\{uw,wv,xy\} \subseteq E(T)$, $d_T(u) = d_T(v) = 4$, $d_T(x) = 3$ or 4, $d_T(w) = 2$ and $d_T(y) = 1$.

Set $T_4 = (T - \{uw,wv\}) + \{uv,yw\}$. Thus $T_4 \in \mathcal{CT}_n$, $T_4 \ncong T$. Also, if $\Upsilon_4 = e^{SO_{red}}(T) - e^{SO_{red}}(T_4)$, then by the sructures of T and T_4 we have $\Upsilon_4 = 2e^{\sqrt{10}} + e^{d_T(x)-1} - e^{3\sqrt{2}} - e^{\sqrt{(d_T(x)-1)^2+1}} - e < 0$. Therefore, $e^{SO_{red}}(T) < e^{SO_{red}}(T_4)$, which is contrary to our assumption. ■

Lemma 2.7. *If T has maximum value of ERSI among all members of $\in \mathcal{CT}_n$ then $m_{3,3}(T) = 0$.*

Proof. Assume, to the contrary, that uv is an edge of T such that $d_T(u) = d_T(v) = 3$, $N_T(u)\backslash\{v\} = \{u_1,u_2\}$ and $N_T(v)\backslash\{u\} = \{v_1,v_2\}$. Set $T_5 = (T - u_1u) + u_1v$. Thus $T_5 \in \mathcal{CT}_n$ and $T_5 \ncong T$. Also, if $\Upsilon_5 = \mathrm{e}^{SO_{red}}(T) - \mathrm{e}^{SO_{red}}(T_5)$, then clearly

$$\begin{aligned}\Upsilon_5 &= \mathrm{e}^{2\sqrt{2}} + \mathrm{e}^{\sqrt{(d_T(u_1)-1)^2+4}} + \mathrm{e}^{\sqrt{(d_T(u_2)-1)^2+4}} + \mathrm{e}^{\sqrt{(d_T(v_1)-1)^2+4}} \\ &+ \mathrm{e}^{\sqrt{(d_T(v_2)-1)^2+4}} - \mathrm{e}^{\sqrt{10}} - \mathrm{e}^{\sqrt{(d_T(u_1)-1)^2+9}} - \mathrm{e}^{\sqrt{(d_T(u_2)-1)^2+1}} \\ &- \mathrm{e}^{3\sqrt{2}} - \mathrm{e}^{\sqrt{(d_T(v_2)-1)^2+9}} < 0.\end{aligned}$$

This yields that $\mathrm{e}^{SO_{red}}(T) < \mathrm{e}^{SO_{red}}(T_5)$, a contradiction. ∎

Lemma 2.8. *Let T have maximum value of ERSI among all members of $\mathcal{CT}_n$. Then $n_2(T) \leq 1$.*

Proof. By contradiction. Let $n_2(T) \geq 2$. Thus we have three below cases for vertices of degree 2:

(i) There exist two adjacent vertices u and v of degree 2. This case is contrary to Lemma 2.3.

(ii) There exist two adjacent vertices u and v of degree 2 and 3, respectively. But this is contrary to Lemma 2.5.

(iii) Each vertex of degree 2 is adjacent to a vertex of degree 4. This leads to a contradiction to Lemma 2.6.

Using cases (i)-(iii) we conclude that $n_2(T) \leq 1$. ∎

Lemma 2.9. *If T has maximum value of ERSI among all members of $\mathcal{CT}_n$, then $n_3(T) \leq 1$.*

Proof. By contradiction. Let $n_3(T) \geq 2$. Now, we consider three possible cases for vertices of degree 3 as below:

(i) There exist two adjacent vertices of degree 3. This case is contradiction to Lemma 2.7.

(ii) There exist two adjacent vertices u and v of degree 2 and 3, respectively. But this is contrary to Lemma 2.5.

(iii) There exist two vertices u and v of degree 3 such that $d_T(x) = 1$ or 4 for each $x \in N_T(u) \cup N_T(v)$. Without loss of generality, we may suppose that $N_T(u) = \{u_1,u_2,u_3\}$, $N_T(v) = \{v_1,v_2,v_3\}$, $u_1 \notin N_T(u) \cap N_T(v)$ and set $T_6 = (T - u_1u) + u_1v$. Thus $T_6 \in \mathcal{CT}_n$ and $T_6 \ncong T$. Also, if $\Upsilon_6 = \mathrm{e}^{SO_{red}}(T) - \mathrm{e}^{SO_{red}}(T_6)$, then clearly

$$\begin{aligned}\Upsilon_6 &= \mathrm{e}^{\sqrt{(d_T(u_1)-1)^2+4}} + \mathrm{e}^{\sqrt{(d_T(u_2)-1)^2+4}} + \mathrm{e}^{\sqrt{(d_T(u_3)-1)^2+4}} \\ &+ \mathrm{e}^{\sqrt{(d_T(v_1)-1)^2+4}} + \mathrm{e}^{\sqrt{(d_T(v_2)-1)^2+4}} + \mathrm{e}^{\sqrt{(d_T(v_3)-1)^2+4}} \\ &- \mathrm{e}^{\sqrt{(d_T(u_1)-1)^2+9}} - \mathrm{e}^{\sqrt{(d_T(u_2)-1)^2+1}} - \mathrm{e}^{\sqrt{(d_T(u_3)-1)^2+1}} \\ &- \mathrm{e}^{\sqrt{(d_T(v_1)-1)^2+9}} - \mathrm{e}^{\sqrt{(d_T(v_2)-1)^2+9}} - \mathrm{e}^{\sqrt{(d_T(v_3)-1)^2+9}} < 0.\end{aligned}$$

Therefore, $e^{SO_{red}}(T) < e^{SO_{red}}(T_6)$, a contradiction. Cases (i–iii) contradict the choice of T and hence $n_3(T) \leq 1$. ■

Lemma 2.10. *Let T have maximum value of ERSI among all members of $\mathcal{CT}_n$. Then $m_{3,4}(T) \leq 1$.*

Proof. Suppose, by way of contradiction, that $m_{3,4}(T) \geq 2$. Using Lemmas 2.5, 2.8 and 2.9 yields that there exits subset $\{u,v,w,x,y,z\}$ of $V(T)$ such that $\{uw,wv,wz,xy\} \subseteq E(T)$, $d_T(u) = d_T(v) = d_T(x) = 4$, $d_T(w) = 3$ and $d_T(y) = 1$. Without loss of generality, we may suppose that $z \neq x$. Set $T_7 = (T - \{uw,wv,wz\}) + \{uv,yw,yz\}$. Thus $T_7 \in \mathcal{CT}_n$ and $T_7 \ncong T$. Also, if $\Upsilon_7 = e^{SO_{red}}(T) - e^{SO_{red}}(T_7)$, Then $\Upsilon_7 = e^{\sqrt{13}} + e^3 - e^{3\sqrt{2}} - e^2 < 0$. Hence $e^{SO_{red}}(T) < e^{SO_{red}}(T_7)$, which is contrary to our assumption. ■

Lemma 2.11. *If T has maximum value of ERSI among all members of $\mathcal{CT}_n$, then $n_2(T) + n_3(T) \leq 1$.*

Proof. By contradiction. Let $n_2(T) + n_3(T) \geq 2$. Thus there are three below cases for vertices of degrees 2 and 3.

(i) $n_2(T) \geq 2$. This is a contradiction to Lemma 2.8.

(ii) $n_3(T) \geq 2$. This case leads to a contradiction to Lemma 2.9.

(iii) $n_2(T) = 1$ and $n_3(T) = 1$. Let u be a vertex of degree 2 and let v be a vertex of degree 3. By Lemma 2.5, $uv \notin E(T)$. In this case, without loss of generality, we may suppose that $N_T(u) = \{u_1,u_2\}$, $N_T(v) = \{v_1,v_2,v_3\}$, $d_T(u_1) \geq d_T(u_2)$ and $d_T(v_1) \geq d_T(v_2) \geq d_T(v_3)$. Then $d_T(u_1) = 4$, $d_T(u_2) = 1$ by Lemma 2.6, and also $d_T(v_1) = 4$, $d_T(v_2) = d_T(v_3) = 1$ by Lemma 2.10. Set $T_8 = (T - u_2u) + u_2v$. Thus $T_8 \in \mathcal{CT}_n$ and $T_8 \ncong T$. Also, if $\Upsilon_8 = e^{SO_{red}}(T) - e^{SO_{red}}(T_8)$, then obviously $\Upsilon_8 = e + e^{\sqrt{10}} + e^{\sqrt{13}} + 2e^2 - 4e^3 - e^{3\sqrt{2}} < 0$. Therefore, $e^{SO_{red}}(T) < e^{SO_{red}}(T_8)$, a contradiction to our assumption.

Using cases (i)-(iii) we conclude that $n_2(T) + n_3(T) \geq 2$ is not true. ■

Theorem 2.12. *Let $n \geq 5$ and let T have maximum value of ERSI among all members of $\mathcal{CT}_n$. Then below assertions are valid:*

(i) If $n \equiv 0(\text{mod}3)$, then $T \in \mathcal{ECT}_n^0$.

(ii) If $n \equiv 1(\text{mod}3)$, then $T \in \mathcal{ECT}_n^1$.

(iii) If $n \equiv 2(\text{mod}3)$, then $T \in \mathcal{ECT}_n^2$.

Proof. (i) If $T \in \mathcal{CT}_n^0$, then by Lemma 2.6 we reach to the assertion. If $n_3 = n_2 = 0$, then by relation (3) we have $n_4 = \frac{n-2}{3}$, which is contradiction because n_4 is an integer number. Otherwise, by Lemma 2.11, we have $n_3 = 1$ and $n_2 = 0$, and consequently by relation (3), $n_4 = \frac{n-4}{3}$, which is a contradiction to this fact that n_4 is an integer number. Therefore, the first assertion is true. (ii) If $T \in \mathcal{CT}_n^1$, then by Lemma 2.10 we have the assertion. If $n_3 = n_2 = 0$, then by relation (3) we conclude that $n_4 = \frac{n-2}{3}$; but this is contrary to this fact that n_4 is an integer number. Otherwise, by Lemma 2.11, we lead to $n_3 = 0$ and $n_2 = 1$. Thus by relation (3), we have $n_4 = \frac{n-3}{3}$, which is a contradiction to this fact that n_4 is an integer number. (iii) If $T \in \mathcal{CT}_n^2$, then $\mathcal{ECT}_n^2 = \mathcal{CT}_n^2$ and so the assertion is valid. Otherwise, by Lemma 2.11, $(n_3 = 1,\, n_2 = 0)$ or $(n_3 = 0,\, n_2 = 1)$. Now, if $n_3 = 1$ and $n_2 = 0$, then from relation (3) we conclude that $n_4 = \frac{n-4}{3}$, a contradiction. Also, if $n_3 = 0$ and $n_2 = 1$, then by relation (3), we reach to $n_4 = \frac{n-3}{3}$, which is a contradiction. ■

The next result is the revised form of Conjecture 1.1.

Corollary 2.13. *If $n \geq 5$ and $T \in \mathcal{CT}_n$, then*

$$\mathrm{e}^{SO_{red}}(T) \leq \begin{cases} \mathrm{e} + \left(\frac{2n-3}{3}\right)\mathrm{e}^3 + \mathrm{e}^{\sqrt{10}} + \left(\frac{n-6}{3}\right)\mathrm{e}^{3\sqrt{2}}, & n \equiv 0 (\mathrm{mod}\, 3), \\ 2\,\mathrm{e}^2 + \left(\frac{2n-5}{3}\right)\mathrm{e}^3 + \mathrm{e}^{\sqrt{13}} + \left(\frac{n-7}{3}\right)\mathrm{e}^{3\sqrt{2}}, & n \equiv 1 (\mathrm{mod}\, 3), \\ \left(\frac{2n+2}{3}\right)\mathrm{e}^3 + \left(\frac{n-5}{3}\right)\mathrm{e}^{3\sqrt{2}}, & n \equiv 2 (\mathrm{mod}\, 3). \end{cases}$$

The equality in the first case holds if and only if $T \in \mathcal{ECT}_n^0$; the equality in the second case holds if and only if $T \in \mathcal{ECT}_n^1$; the equality in the third case holds if and only if $T \in \mathcal{ECT}_n^2$.

Proof. The assertion follows almost immediately from relations (5–7) and Theorem 2.12. ■

ACKNOWLEDGEMENTS. The authors are grateful to the referees for helpful suggestions.

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