www.toc.ui.ac.ir

Transactions on Combinatorics
ISSN (print): 2251-8657, ISSN (on-line): 2251-8665
Vol. 10 No. 2 (2021), pp. 97-106.
© 2021 University of Isfahan

www.ui.ac.ir

EXPONENTIAL SECOND ZAGREB INDEX OF CHEMICAL TREES

SELVARAJ BALACHANDRAN* AND TOMÁŠ VETRÍK

Abstract. Cruz, Monsalve and Rada [Extremal values of vertex-degree-based topological indices of chemical trees, Appl. Math. Comput. 380 (2020) 125281] posed an open problem to find the maximum value of the exponential second Zagreb index for chemical trees of given order. In this paper, we solve the open problem completely.

1. Introduction

Cruz, Monsalve and Rada [4] studied bounds on degree-based topological indices for chemical trees. In their Table 1, they posed three open problems on upper bounds for exponential degree-based indices (exponential second Zagreb index, exponential augmented Zagreb index and exponential atom-bond connectivity index) of chemical trees. Chemical trees with the largest exponential atom-bond connectivity index were found in [5]. In this paper, we extend the method used for the classical Zagreb indices in [9] and present sharp upper bounds on the exponential second Zagreb index for chemical trees of given order.

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The order is the number of vertices of G. The degree $d_G(v)$ of a vertex $v \in V(G)$ is the number of vertices adjacent to v. A leaf is a vertex of degree one. A tree is a connected acyclic graph. A chemical tree is a tree which does not have a vertex of degree greater than 4. We denote the path and the star of order n by P_n and S_n, respectively.

Communicated by Ali Reza Ashrafi
Manuscript Type: Research Paper.
MSC(2010): Primary: 05C05; Secondary: 05C07.
Keywords: Topological index, degree, extremal graph theory.
Received: 22 September 2020, Accepted: 01 November 2020.
*Corresponding author.

http://dx.doi.org/10.22108/toc.2020.125047.1764

.

For any real number $a > 1$, we study the exponential second Zagreb index of a graph G,

$$a^{M_2}(G) = \sum_{uv \in E(G)} a^{d_G(u) d_G(v)}.$$

This index is the exponential version of the well-known second Zagreb index

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

Degree-based indices have been studied due to their extensive applications. Exponential degree-based indices were investigated for example in [4], [5] and [8] and some other degree-based indices in [1], [2], [3], [6] and [7].

2. Results

It is very easy to prove the following lemma, which will be used in the proofs of Lemmas 2.2, 2.3, 2.4 and Theorem 2.5.

Lemma 2.1. *Let x, y, a, c be real numbers such that $x < y$, $a > 1$ and $c > 0$. Then $a^{x+c} - a^x < a^{y+c} - a^y$.*

Proof. We consider the function $f(x) = a^{x+c} - a^x$. The derivative of $f(x)$ is

$$f'(x) = (a^{x+c} - a^x)\ln a = a^x(a^c - 1)\ln a > 0.$$

So $f(x)$ is strictly increasing. Thus for $x < y$, we get $f(x) < f(y)$ which means that $a^{x+c} - a^x < a^{y+c} - a^y$. □

In Lemmas 2.2, 2.3 and 2.4, we bound the number of vertices of degree 2 and 3 in a chemical tree having the largest exponential second Zagreb index.

Lemma 2.2. *Let G' be a chemical tree of order $n \geq 5$ having the largest a^{M_2} index. Then G' has at most one vertex of degree 2.*

Proof. Assume to the contrary that G' contains (at least) two vertices x and y such that $d_{G'}(x) = d_{G'}(y) = 2$. We denote by x_1, x_2 and y_1, y_2 the neighbors of x and y in G', respectively. We can assume that the path between x and y contains the vertices x_1 and y_1 (if that path has exactly one edge, then $x = y_1$ and $y = x_1$). Without loss of generality, suppose that $d_{G'}(x_1) \leq d_{G'}(y_1)$.

We define G'' with $V(G'') = V(G')$ and $E(G'') = \{yx_2\} \cup E(G') \setminus \{xx_2\}$. Note that $d_{G''}(x) = 1$, $d_{G''}(y) = 3$ and $d_{G''}(z) = d_{G'}(z)$ for all $z \in V(G') \setminus \{x, y\}$. We consider two cases.

Case 1: $xy \notin E(G')$.

Then

$$\begin{aligned} a^{M_2}(G') - a^{M_2}(G'') &= (a^{d_{G'}(x)d_{G'}(x_1)} - a^{d_{G''}(x)d_{G''}(x_1)}) + (a^{d_{G'}(x)d_{G'}(x_2)} - a^{d_{G''}(y)d_{G''}(x_2)}) \\ &\quad + (a^{d_{G'}(y)d_{G'}(y_1)} - a^{d_{G''}(y)d_{G''}(y_1)}) + (a^{d_{G'}(y)d_{G'}(y_2)} - a^{d_{G''}(y)d_{G''}(y_2)}) \\ &= (a^{2d_{G'}(x_1)} - a^{d_{G'}(x_1)}) + (a^{2d_{G'}(x_2)} - a^{3d_{G'}(x_2)}) \\ &\quad + (a^{2d_{G'}(y_1)} - a^{3d_{G'}(y_1)}) + (a^{2d_{G'}(y_2)} - a^{3d_{G'}(y_2)}) \\ &< (a^{2d_{G'}(x_1)} - a^{d_{G'}(x_1)}) + (a^{2d_{G'}(y_1)} - a^{3d_{G'}(y_1)}) \\ &\le (a^{d_{G'}(x_1)+d_{G'}(y_1)} - a^{d_{G'}(x_1)}) + (a^{2d_{G'}(y_1)} - a^{3d_{G'}(y_1)}) \\ &< 0, \end{aligned}$$

since by Lemma 2.1, we have

$$a^{d_{G'}(x_1)+d_{G'}(y_1)} - a^{d_{G'}(x_1)} < a^{3d_{G'}(y_1)} - a^{2d_{G'}(y_1)}.$$

So, $a^{M_2}(G') < a^{M_2}(G'')$.

Case 2: $xy \in E(G')$.

Then $x = y_1$ and $y = x_1$. Since $n \ge 5$, at least one of $d_{G'}(x_2)$, $d_{G'}(y_2)$ is greater than 1. We can assume that $d_{G'}(x_2) \ge 2$. Then

$$\begin{aligned} a^{M_2}(G') - a^{M_2}(G'') &= (a^{d_{G'}(x)d_{G'}(y)} - a^{d_{G''}(x)d_{G''}(y)}) + (a^{d_{G'}(x)d_{G'}(x_2)} - a^{d_{G''}(y)d_{G''}(x_2)}) \\ &\quad + (a^{d_{G'}(y)d_{G'}(y_2)} - a^{d_{G''}(y)d_{G''}(y_2)}) \\ &= (a^4 - a^3) + (a^{2d_{G'}(x_2)} - a^{3d_{G'}(x_2)}) + (a^{2d_{G'}(y_2)} - a^{3d_{G'}(y_2)}) \\ &< (a^4 - a^3) + (a^{2d_{G'}(x_2)} - a^{3d_{G'}(x_2)}) \\ &< (a^4 - a^3) + (a^{3d_{G'}(x_2)-1} - a^{3d_{G'}(x_2)}) \\ &< 0, \end{aligned}$$

since by Lemma 2.1, we have

$$a^4 - a^3 < a^{3d_{G'}(x_2)} - a^{3d_{G'}(x_2)-1}.$$

Hence $a^{M_2}(G') < a^{M_2}(G'')$. So G' does not have the largest a^{M_2} index, which is a contradiction. □

Lemma 2.3. *Let G' be a chemical tree of order $n \ge 7$ having the largest a^{M_2} index. Then G' has at most one vertex of degree* 3.

Proof. Assume to the contrary that G' contains (at least) two vertices x and y such that $d_{G'}(x) = d_{G'}(y) = 3$. We denote by x_1, x_2, x_3 and y_1, y_2, y_3 the neighbors of x and y in G', respectively. We can assume that the path between x and y contains the vertices x_1 and y_1 (if that path has exactly one edge, then $x = y_1$ and $y = x_1$). We consider two cases.

Case 1: $xy \notin E(G')$.

Without loss of generality, suppose that $d_{G'}(x_1) \le d_{G'}(y_1)$ and $d_{G'}(x_2) \le d_{G'}(x_3)$. We define G'' with $V(G'') = V(G')$ and $E(G'') = \{yx_3\} \cup E(G') \setminus \{xx_3\}$. Note that $d_{G''}(x) = 2$, $d_{G''}(y) = 4$ and $d_{G''}(z) = d_{G'}(z)$ for all $z \in V(G') \setminus \{x, y\}$. Then

$$\begin{aligned}
a^{M_2}(G') - a^{M_2}(G'') &= (a^{d_{G'}(x)d_{G'}(x_1)} - a^{d_{G''}(x)d_{G''}(x_1)}) + (a^{d_{G'}(x)d_{G'}(x_2)} - a^{d_{G''}(x)d_{G''}(x_2)}) \\
&\quad + (a^{d_{G'}(x)d_{G'}(x_3)} - a^{d_{G''}(y)d_{G''}(x_3)}) + (a^{d_{G'}(y)d_{G'}(y_1)} - a^{d_{G''}(y)d_{G''}(y_1)}) \\
&\quad + (a^{d_{G'}(y)d_{G'}(y_2)} - a^{d_{G''}(y)d_{G''}(y_2)}) + (a^{d_{G'}(y)d_{G'}(y_3)} - a^{d_{G''}(y)d_{G''}(y_3)}) \\
&= (a^{3d_{G'}(x_1)} - a^{2d_{G'}(x_1)}) + (a^{3d_{G'}(x_2)} - a^{2d_{G'}(x_2)}) \\
&\quad + (a^{3d_{G'}(x_3)} - a^{4d_{G'}(x_3)}) + (a^{3d_{G'}(y_1)} - a^{4d_{G'}(y_1)}) \\
&\quad + (a^{3d_{G'}(y_2)} - a^{4d_{G'}(y_2)}) + (a^{3d_{G'}(y_3)} - a^{4d_{G'}(y_3)}) \\
&< (a^{3d_{G'}(x_1)} - a^{2d_{G'}(x_1)}) + (a^{3d_{G'}(y_1)} - a^{4d_{G'}(y_1)}) \\
&\quad + (a^{3d_{G'}(x_2)} - a^{2d_{G'}(x_2)}) + (a^{3d_{G'}(x_3)} - a^{4d_{G'}(x_3)}) \\
&\le (a^{2d_{G'}(x_1)+d_{G'}(y_1)} - a^{2d_{G'}(x_1)}) + (a^{3d_{G'}(y_1)} - a^{4d_{G'}(y_1)}) \\
&\quad + (a^{2d_{G'}(x_2)+d_{G'}(x_3)} - a^{2d_{G'}(x_2)}) + (a^{3d_{G'}(x_3)} - a^{4d_{G'}(x_3)}) \\
&< 0.
\end{aligned}$$

since by Lemma 2.1, we have

$$a^{2d_{G'}(x_1)+d_{G'}(y_1)} - a^{2d_{G'}(x_1)} < a^{4d_{G'}(y_1)} - a^{3d_{G'}(y_1)}$$

and

$$a^{2d_{G'}(x_2)+d_{G'}(x_3)} - a^{2d_{G'}(x_2)} < a^{4d_{G'}(x_3)} - a^{3d_{G'}(x_3)}.$$

So $a^{M_2}(G') < a^{M_2}(G'')$.

Case 2: $xy \in E(G')$.

Then $x = y_1$ and $y = x_1$. Without the loss of generality, assume that x_2 has the smallest degree and y_3 has the largest degree among the degrees of the vertices x_2, x_3, y_2, y_3 in G'. Since $n \ge 7$, we have $d_{G'}(y_3) \ge 2$.

Case 2.1: $d_{G'}(y_3) \ge 3$.

We use the graph G'' defined in Case 1. We obtain

$$\begin{aligned}
a^{M_2}(G') - a^{M_2}(G'') &= (a^9 - a^8) + (a^{3d_{G'}(x_2)} - a^{2d_{G'}(x_2)}) + (a^{3d_{G'}(x_3)} - a^{4d_{G'}(x_3)}) \\
&\quad + (a^{3d_{G'}(y_2)} - a^{4d_{G'}(y_2)}) + (a^{3d_{G'}(y_3)} - a^{4d_{G'}(y_3)}) \\
&< (a^9 - a^8) + (a^{3d_{G'}(y_3)} - a^{4d_{G'}(y_3)}) \\
&\quad + (a^{3d_{G'}(x_2)} - a^{2d_{G'}(x_2)}) + (a^{3d_{G'}(x_3)} - a^{4d_{G'}(x_3)}) \\
&< (a^9 - a^8) + (a^{4d_{G'}(y_3)-1} - a^{4d_{G'}(y_3)}) \\
&\quad + (a^{2d_{G'}(x_2)+d_{G'}(x_3)} - a^{2d_{G'}(x_2)}) + (a^{3d_{G'}(x_3)} - a^{4d_{G'}(x_3)}) \\
&< 0,
\end{aligned}$$

http://dx.doi.org/10.22108/toc.2020.125047.1764

since by Lemma 2.1, we have

$$a^9 - a^8 < a^{4d_{G'}(y_3)} - a^{4d_{G'}(y_3)-1}$$

and

$$a^{2d_{G'}(x_2)+d_{G'}(x_3)} - a^{2d_{G'}(x_2)} < a^{4d_{G'}(x_3)} - a^{3d_{G'}(x_3)}.$$

So $a^{M_2}(G') < a^{M_2}(G'')$.

Case 2.2: $d_{G'}(y_3) = 2$.

We have $yy_3 \in E(G')$. Let us denote the other vertex adjacent to y_3 in G' by y'. We define G''' with $V(G''') = V(G')$ and $E(G''') = \{yy'\} \cup E(G') \setminus \{y_3y'\}$. Then $d_{G'''}(y) = 4$, $d_{G'''}(y_3) = 1$ and $d_{G'''}(z) = d_{G'}(z)$ for all $z \in V(G') \setminus \{y, y_3\}$. We obtain

$$\begin{aligned} a^{M_2}(G') - a^{M_2}(G''') &= (a^{d_{G'}(x)d_{G'}(y)} - a^{d_{G'''}(x)d_{G'''}(y)}) + (a^{d_{G'}(y)d_{G'}(y_2)} - a^{d_{G'''}(y)d_{G'''}(y_2)}) \\ &\quad + (a^{d_{G'}(y)d_{G'}(y_3)} - a^{d_{G'''}(y)d_{G'''}(y_3)}) + (a^{d_{G'}(y')d_{G'}(y_3)} - a^{d_{G'''}(y)d_{G'''}(y')}) \\ &= (a^9 - a^{12}) + (a^{3d_{G'}(y_2)} - a^{4d_{G'}(y_2)}) + (a^6 - a^4) + (a^{2d_{G'}(y')} - a^{4d_{G'}(y')}) \\ &< (a^9 - a^{12}) + (a^6 - a^4) \\ &< (a^{10} - a^{12}) + (a^6 - a^4) \\ &< 0, \end{aligned}$$

since by Lemma 2.1, we have $a^6 - a^4 < a^{12} - a^{10}$. Hence $a^{M_2}(G') < a^{M_2}(G''')$. So G' does not have the largest a^{M_2} index, which is a contradiction. □

Lemma 2.4. *Let G' be a chemical tree of order $n \geq 7$ having the largest a^{M_2} index. Then G' does not contain exactly one vertex of degree 2 and one vertex of degree 3.*

Proof. Assume to the contrary that G' contains exactly one vertex x of degree 2 and one vertex y of degree 3. So $d_{G'}(x) = 2$ and $d_{G'}(y) = 3$. We denote by x_1, x_2 and y_1, y_2, y_3 the neighbors of x and y in G', respectively. We can assume that the path between x and y contains the vertices x_1 and y_1 (if that path has exactly one edge, then $x = y_1$ and $y = x_1$). We consider two cases.

Case 1: $xy \notin E(G')$.

We define G'' with $V(G'') = V(G')$ and $E(G'') = \{yx_2\} \cup E(G') \setminus \{xx_2\}$. Note that x and y are the only vertices of degree 2 and 3 in G', respectively. Thus $d_{G'}(x_1) = d_{G''}(x_1) = d_{G'}(y_1) = d_{G''}(y_1) = 4$.

http://dx.doi.org/10.22108/toc.2020.125047.1764

We have $d_{G''}(x) = 1$, $d_{G''}(y) = 4$ and $d_{G''}(z) = d_{G'}(z)$ for all $z \in V(G') \setminus \{x, y\}$. Then

$$\begin{aligned} a^{M_2}(G') - a^{M_2}(G'') &= (a^{d_{G'}(x)d_{G'}(x_1)} - a^{d_{G''}(x)d_{G''}(x_1)}) + (a^{d_{G'}(x)d_{G'}(x_2)} - a^{d_{G''}(y)d_{G''}(x_2)}) \\ &\quad + (a^{d_{G'}(y)d_{G'}(y_1)} - a^{d_{G''}(y)d_{G''}(y_1)}) + (a^{d_{G'}(y)d_{G'}(y_2)} - a^{d_{G''}(y)d_{G''}(y_2)}) \\ &\quad + (a^{d_{G'}(y)d_{G'}(y_3)} - a^{d_{G''}(y)d_{G''}(y_3)}) \\ &= (a^8 - a^4) + (a^{2d_{G'}(x_2)} - a^{4d_{G'}(x_2)}) + (a^{12} - a^{16}) + (a^{3d_{G'}(y_2)} - a^{4d_{G'}(y_2)}) \\ &\quad + (a^{3d_{G'}(y_3)} - a^{4d_{G'}(y_3)}) \\ &< (a^8 - a^4) + (a^{12} - a^{16}) \\ &< 0, \end{aligned}$$

since by Lemma 2.1, we have $a^8 - a^4 < a^{16} - a^{12}$. Thus $a^{M_2}(G') < a^{M_2}(G'')$.

Case 2: $xy \in E(G')$.

Then $x = y_1$ and $y = x_1$. Since $n \geq 7$, the degree of at least one of x_2, y_2, y_3 must be greater than 1 in G'. We can assume that $d_{G'}(y_3) > 1$ which implies that $d_{G'}(y_3) = 4$. We use the graph G'' defined in Case 1, so $E(G'') = \{yx_2\} \cup E(G') \setminus \{xx_2\}$. Then

$$\begin{aligned} a^{M_2}(G') - a^{M_2}(G'') &= (a^{d_{G'}(x)d_{G'}(y)} - a^{d_{G''}(x)d_{G''}(y)}) + (a^{d_{G'}(x)d_{G'}(x_2)} - a^{d_{G''}(y)d_{G''}(x_2)}) \\ &\quad + (a^{d_{G'}(y)d_{G'}(y_2)} - a^{d_{G''}(y)d_{G''}(y_2)}) + (a^{d_{G'}(y)d_{G'}(y_3)} - a^{d_{G''}(y)d_{G''}(y_3)}) \\ &= (a^6 - a^4) + (a^{2d_{G'}(x_2)} - a^{4d_{G''}(x_2)}) + (a^{3d_{G'}(y_2)} - a^{4d_{G''}(y_2)}) + (a^{12} - a^{16}) \\ &< (a^6 - a^4) + (a^{12} - a^{16}) \\ &< (a^8 - a^4) + (a^{12} - a^{16}) \\ &< 0, \end{aligned}$$

since by Lemma 2.1, we have $a^8 - a^4 < a^{16} - a^{12}$. Hence $a^{M_2}(G') < a^{M_2}(G'')$ which means that G' does not have the largest a^{M_2} index. □

Now, we present the main result of this paper.

Theorem 2.5. *Let G be any chemical tree of order $n \geq 7$. Then*

$$a^{M_2}(G) \leq \begin{cases} \left(\frac{n}{3} - 2\right) a^{16} + a^8 + \left(\frac{2n}{3} - 1\right) a^4 + a^2 & \text{if } n \equiv 0 \ (mod\ 3) \\ \left(\frac{n-7}{3}\right) a^{16} + a^{12} + \left(\frac{2n-5}{3}\right) a^4 + 2a^3 & \text{if } n \equiv 1 \ (mod\ 3) \\ \left(\frac{n-5}{3}\right) a^{16} + \left(\frac{2n+2}{3}\right) a^4 & \text{if } n \equiv 2 \ (mod\ 3) \end{cases}$$

Proof. For $i \in \{1, 2, 3, 4\}$, we denote by n_i the number of vertices of degree i in G. Since every vertex of G has degree at most 4, we obtain

$$n_1 + n_2 + n_3 + n_4 = n. \tag{2.1}$$

http://dx.doi.org/10.22108/toc.2020.125047.1764

Since $\sum_{v\in V(G)} d_G(v) = 2m$, where m is the number of edges of G, we get

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1). \tag{2.2}$$

From (2.1) and (2.2), we obtain

$$n_2 + 2n_3 + 3n_4 = n - 2. \tag{2.3}$$

Let G' be a chemical tree with n vertices having the largest a^{M_2} index. From Lemmas 2.2. 2.3, 2.4, we know that G' contains at most one vertex having degree different from 1 and 4. So $n_i = 0$ or 1 for $i = 2, 3$, but not both n_2 and n_3 are equal to 1. We consider three cases.

Case 1: $n \equiv 0 \pmod 3$.
From (2.3), we have $n_2 + 2n_3 \equiv 1 \pmod 3$ which implies that $n_2 = 1$ and $n_3 = 0$. Then by (2.3), we get $n_4 = \frac{n}{3} - 1$ and from (2.1), we obtain $n_1 = n - n_2 - n_4 = \frac{2n}{3}$.

If the vertex of degree 2 is adjacent to two vertices of degree 4, then all the $\frac{2n}{3}$ leaves are adjacent to vertices of degree 4. Then G' contains $n - 1 - \frac{2n}{3} - 2 = \frac{n}{3} - 3$ edges incident only with vertices of degree 4 and

$$a^{M_2}(G') = \left(\frac{n}{3} - 3\right) a^{16} + 2a^8 + \left(\frac{2n}{3}\right) a^4 = S_1.$$

If the vertex of degree 2 is adjacent to one vertex of degree 4 and one leaf, then the other $\frac{2n}{3} - 1$ leaves are adjacent to vertices of degree 4. Then G' contains $n - 1 - (\frac{2n}{3} - 1) - 2 = \frac{n}{3} - 2$ edges incident only with vertices of degree 4 and

$$a^{M_2}(G') = \left(\frac{n}{3} - 2\right) a^{16} + a^8 + \left(\frac{2n}{3} - 1\right) a^4 + a^2 = S_2.$$

We obtain

$$S_2 - S_1 = a^{16} - a^8 - a^4 + a^2 > a^{10} - a^8 - a^4 + a^2 > 0,$$

since by Lemma 2.1, we have $a^4 - a^2 < a^{10} - a^8$. So $S_2 > S_1$ and

$$a^{M_2}(G') = \left(\frac{n}{3} - 2\right) a^{16} + a^8 + \left(\frac{2n}{3} - 1\right) a^4 + a^2.$$

Case 2: $n \equiv 1 \pmod 3$.
From (2.3), we have $n_2 + 2n_3 \equiv 2 \pmod 3$ which implies that $n_2 = 0$ and $n_3 = 1$. Then by (2.3), we get $n_4 = \frac{n-4}{3}$ and from (2.1), we obtain $n_1 = n - n_3 - n_4 = \frac{2n+1}{3}$.

If the vertex of degree 3 is adjacent to three vertices of degree 4, then all the $\frac{2n+1}{3}$ leaves are adjacent to vertices of degree 4. Then G' contains $n - 1 - \frac{2n+1}{3} - 3 = \frac{n-13}{3}$ edges incident only with vertices of degree 4 and

$$a^{M_2}(G') = \left(\frac{n-13}{3}\right) a^{16} + 3a^{12} + \left(\frac{2n+1}{3}\right) a^4 = S_1.$$

If the vertex of degree 3 is adjacent to two vertices of degree 4 and one leaf, then the other $\frac{2n+1}{3} - 1 = \frac{2n-2}{3}$ leaves are adjacent to vertices of degree 4. Then G' contains $n - 1 - \frac{2n-2}{3} - 3 = \frac{n-10}{3}$

edges incident only with vertices of degree 4 and

$$a^{M_2}(G') = \left(\frac{n-10}{3}\right) a^{16} + 2a^{12} + \left(\frac{2n-2}{3}\right) a^4 + a^3 = S_2.$$

If the vertex of degree 3 is adjacent to one vertex of degree 4 and two leaves, then the other $\frac{2n+1}{3} - 2 = \frac{2n-5}{3}$ leaves are adjacent to vertices of degree 4. Then G' contains $n - 1 - \frac{2n-5}{3} - 3 = \frac{n-7}{3}$ edges incident only with vertices of degree 4 and

$$a^{M_2}(G') = \left(\frac{n-7}{3}\right) a^{16} + a^{12} + \left(\frac{2n-5}{3}\right) a^4 + 2a^3 = S_3.$$

We obtain

$$S_3 - S_2 = S_2 - S_1 = a^{16} - a^{12} - a^4 + a^3 > a^{13} - a^{12} - a^4 + a^3 > 0,$$

since by Lemma 2.1, we have $a^4 - a^3 < a^{13} - a^{12}$. Therefore $S_3 > S_2 > S_1$ and

$$a^{M_2}(G') = \left(\frac{n-7}{3}\right) a^{16} + a^{12} + \left(\frac{2n-5}{3}\right) a^4 + 2a^3.$$

Case 3: $n \equiv 2 \pmod 3$.
From (2.3), we have $n_2 + 2n_3 \equiv 0 \pmod 3$ which implies that $n_2 = n_3 = 0$. Then by (2.3), we get $n_4 = \frac{n-2}{3}$ and from (2.1), we obtain $n_1 = \frac{2n+2}{3}$. All the $\frac{2n+2}{3}$ leaves are adjacent to vertices of degree 4. The graph G' has $n-1$ edges, thus G' contains $n-1-\frac{2n+2}{3} = \frac{n-5}{3}$ edges incident only with vertices of degree 4. Hence

$$a^{M_2}(G') = \left(\frac{n-5}{3}\right) a^{16} + \left(\frac{2n+2}{3}\right) a^4.$$

□

Since Theorem 2.5 holds for $a > 1$, we obtain the following corollary which solves the open problem on the e^{M_2} index stated in [4] for $n \geq 7$.

Corollary 2.6. *Let G be any chemical tree of order $n \geq 7$. Then*

$$e^{M_2}(G) \leq \begin{cases} \left(\frac{n}{3} - 2\right) e^{16} + e^8 + \left(\frac{2n}{3} - 1\right) e^4 + e^2 & \text{if } n \equiv 0 \ (mod\ 3) \\ \left(\frac{n-7}{3}\right) e^{16} + e^{12} + \left(\frac{2n-5}{3}\right) e^4 + 2e^3 & \text{if } n \equiv 1 \ (mod\ 3) \\ \left(\frac{n-5}{3}\right) e^{16} + \left(\frac{2n+2}{3}\right) e^4 & \text{if } n \equiv 2 \ (mod\ 3) \end{cases}$$

In the proof of Theorem 2.5 we showed that if $n \equiv 0 \pmod 3$, then an extremal tree G' is any tree with $\frac{n}{3} - 1$ vertices of degree 4, $\frac{2n}{3}$ leaves and one vertex of degree 2 which is adjacent to one vertex of degree 4 and one leaf,

If $n \equiv 1 \pmod 3$, then G' is any tree with $\frac{n-4}{3}$ vertices of degree 4, $\frac{2n+1}{3}$ leaves and one vertex of degree 3 which is adjacent to one vertex of degree 4 and two leaves,

If $n \equiv 2 \pmod 3$, then an extremal tree G' is any tree with $\frac{n-2}{3}$ vertices of degree 4 and $\frac{2n+2}{3}$ leaves.

Theorem 2.5 and Corollary 2.6 hold for $n \geq 7$, so it remains to solve the problem for $n \leq 6$. The paths P_2 and P_3 are the only trees of order 2 and 3, respectively.

There are two trees of order 4: the star S_4 and the path P_4. Let us compare their a^{M_2} indices. We have $a^{M_2}(S_4) = 3a^3$ and $a^{M_2}(P_4) = a^4 + 2a^2$. Then

$$a^{M_2}(P_4) - a^{M_2}(S_4) = a^4 - 3a^3 + 2a^2 = a^2(a-1)(a-2).$$

Thus $a^{M_2}(P_4) > a^{M_2}(S_4)$ for $a > 2$, $a^{M_2}(P_4) < a^{M_2}(S_4)$ for $1 < a < 2$ and $a^{M_2}(P_4) = a^{M_2}(S_4)$ for $a = 2$. Hence, if G is a chemical tree of order 4, then

$$e^{M_2}(G) \leq e^4 + 2e^2$$

and the equality holds only if G is P_4.

Let us consider trees of order 5. There are three trees with 5 vertices: P_5, S_5 and the tree of diameter 3 with the central vertices having degrees 2 and 3. We denote that tree by $T_{2,3}$. By Lemma 2.2, P_5 does not have the largest a^{M_2} index. We have $a^{M_2}(S_5) = 4a^4$ and $a^{M_2}(T_{2,3}) = a^6 + 2a^3 + a^2$. Then

$$a^{M_2}(T_{2,3}) - a^{M_2}(S_4) = a^6 - 4a^4 + 2a^3 + a^2$$

has only one root greater than 1 which is $a' \approx 1.48$. We get $a^{M_2}(T_{2,3}) > a^{M_2}(S_4)$ for $a > a'$ and $a^{M_2}(T_{2,3}) < a^{M_2}(S_4)$ for $1 < a < a'$. Thus, if G is a chemical tree of order 5, then

$$e^{M_2}(G) \leq e^6 + 2e^3 + e^2$$

and the equality holds only if G is $T_{2,3}$.

Finally, we consider trees of order 6. There are five chemical trees with 6 vertices: P_6, two trees of diameter 4 and two trees of diameter 3; one of them with the central vertices having degrees 2 and 4 and the other one with the central vertices having degrees 3 and 3. We denote those trees by $T_{2,4}$ and $T_{3,3}$, respectively. The trees of order 6 with diameter 4 and P_6 have at least two vertices of degree 2, thus by Lemma 2.2, they do not have the largest a^{M_2} index. Let us compare the a^{M_2} indices of $T_{2,4}$ and $T_{3,3}$. We have $a^{M_2}(T_{2,4}) = a^8 + 3a^4 + a^2$ and $a^{M_2}(T_{3,3}) = a^9 + 4a^3$. Then

$$a^{M_2}(T_{3,3}) - a^{M_2}(T_{2,4}) = a^9 - a^8 - 3a^4 + 4a^3 - a^2$$

has only one root greater than 1 which is $a'' \approx 1.16$. We get $a^{M_2}(T_{3,3}) > a^{M_2}(T_{2,4})$ for $a > a''$ and $a^{M_2}(T_{3,3}) < a^{M_2}(T_{2,4})$ for $1 < a < a''$. Hence, if G is a chemical tree of order 6, then

$$e^{M_2}(G) \leq e^9 + 4e^3$$

and the equality holds only if G is $T_{3,3}$.

Acknowledgments

The work of T. Vetrík is based on the research supported by the National Research Foundation of South Africa (Grant Number 126894).

References

[1] M. Aghel, A. Erfanian and A. R. Ashrafi, On the first and second Zagreb indices of quasi unicyclic graphs, *Trans. Comb.*, **8** no. 3 (2019) 29–38.

[2] A. R. Ashrafi, T. Došlić and A. Hamzeh, Extremal graphs with respect to the Zagreb coindices, *MATCH Commun. Math. Comput. Chem.*, **65** no. 1 (2011) 85–92.

[3] M. Azari, Generalized Zagreb index of product graphs, *Trans. Comb.*, **8** no. 4 (2019) 35–48.

[4] R. Cruz, J. Monsalve and J. Rada, Extremal values of vertex-degree-based topological indices of chemical trees, *Appl. Math. Comput.*, **380** (2020) 125–281.

[5] R. Cruz, J. Monsalve and J. Rada, On chemical trees that maximize atom-bond connectivity index, its exponential version, and minimize exponential geometricarithmetic index, *MATCH Commun. Math. Comput. Chem.*, **84** (2020) 691–718.

[6] K. C. Das and A. Ali, On a conjecture about the second Zagreb index, *Discrete Math. Lett.*, **2** (2019) 38–43.

[7] M. Liang, B. Cheng and J. Liu, Solution to the minimum harmonic index of graphs with given minimum degree, *Trans. Comb.*, **7** no. 2 (2018) 25–33.

[8] J. Rada, Exponential vertex-degree-based topological indices and discrimination, *MATCH Commun. Math. Comput. Chem.*, **82** no. 1 (2019) 29–41.

[9] Ž. K. Vukićević and G. Popivoda, Chemical trees with extreme values of Zagreb indices and coindices, *Iran. J. Math. Chem.*, **5** no. 1 (2014) 19–29.

Selvaraj Balachandran

Department of Mathematics and Applied Mathematics, University of the Free State, P. O. Box 339, Bloemfontein, 9300, South Africa, and

Department of Mathematics, School of Arts, Sciences and Humanities, SASTRA Deemed University, Thanjavur, 613401, India Email: bala_maths@rediffmail.com

Tomáš Vetrík

Department of Mathematics and Applied Mathematics, University of the Free State, P. O. Box 339, Bloemfontein, 9300, South Africa

Email: vetrikt@ufs.ac.za

http://dx.doi.org/10.22108/toc.2020.125047.1764