MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **72** (2014) 723-732

ISSN 0340 - 6253

On Reformulated Zagreb Indices with Respect to Acyclic, Unicyclic and Bicyclic Graphs*

Shengjin Ji[1], Xia Li[1], Bofeng Huo[2]

[1] *School of Science, Shangdong University of Technology, Zibo, Shandong 255049, China*

[2] *Department of Mathematics, Qinghai Normal University, Xining, Qinghai 810008, China*

jishengjin2013@163.com, summer08lixia@163.com, Huobofeng@mail.nankai.edu.cn

(Received June 21, 2014)

Abstract

The authors Miličević et al. introduced the reformulated Zagreb indices [19], which is a generalization of classical Zagreb indices of chemical graph theory. In the paper, we characterize the extremal properties of the first reformulated Zagreb index. We first introduce some graph operations which increase or decrease this index. Furthermore, we will determine the extremal acyclic and bicyclic graphs with minimum and maximum of the first Zagreb index by a unified method, respectively. Recently, Ilić and Zhou [18] characterized the extremal graph of unicyclic graphs with the first reformulated Zagreb index. We will provide a shorter proof.

1 Introduction

Topological indices are major invariants to characterize some properties of the graph of a molecule. One of the most important topological indices is the well-known Zagreb indices,

*The first author is supported by NNSFC (Nos. 11326216 and 11301306); and the last author is supported by NNSFC(No. 11261047) .

as a pair of molecular descriptors, introduced in [14, 22]. For a simple graph G, the first and second Zagreb indices, M_1 and M_2, respectively, are defined as:

$$M_1(G) = \sum_{v \in V} deg(v)^2, \quad M_2(G) = \sum_{uv \in E} deg(u) \cdot deg(v).$$

Zagreb indices, as a pair of molecular descriptors, first appeared in the topological formula for the total π-energy of conjugated molecules that has been derived in 1972 [14]. Soon after these indices have been used as branching indices [13]. Later the Zagreb indices found applications in QSPR and QSAR studies[1, 9, 22]. The latest related results refer to [6, 10, 11, 25, 28].

Since an edge of graph G corresponds to a vertex of the line graph $L(G)$. Motivated by the connection, Miličević et al. [19] in 2004 reformulated the Zagreb indices in terms of edge–degrees instead of vertex–degrees as:

$$EM_1(G) = \sum_{e \in E} deg(e)^2, \quad EM_2(G) = \sum_{e \sim f} deg(e) \cdot deg(f),$$

where $deg(e)$ denotes the degree of the edge e in G, which is defined by $deg(e) = deg(u) + deg(v) - 2$ with $e = uv$, and $e \sim f$ means that the edges e and f are adjacent, i.e., they share a common end–vertex in G. Recently, the upper and lower bounds on $EM_1(G)$ and $EM_2(G)$ were presented in [33, 18, 7]; Su et al. [21] characterize the extremal graph properties on $EM_1(G)$ with respect to given connectivity.

In order to exhibit our results, we introduce some graph-theoretical notations and terminology. For other undefined ones, see the book [2].

Let S_n, P_n and C_n be the star, path and cycle on n vertices, respectively. Let $G = (V; E)$ be a simple undirected graph. For $v \in V(G)$ and $e \in E(G)$, let $N_G(v)$ (or N(v) for short) be the set of all neighbors of v in G, $G - v$ be a subgraph of G by deleting vertex v, and $G - e$ be a sub graph of G by deleting edge e. Let G_0 be a nontrivial graph and u be its vertex. If G is obtained by G_0 fusing a tree T at u. Then we say that T is a *subtree* of G and u is its *root*. Let $u \circ v$ denote the fusing two vertices u and v of G.

In this paper we characterize the extremal properties of the first reformulated Zagreb index. In Section 2 we present some graph operations which increase or decrease EM_1. In Section 3, we determine the extremal acyclic, unicyclic and bicyclic graphs with minimum and maximum the first Zagreb index, respectively.

2 Some graph operations

In the section we will introduce some graph operations, which increase or decrease the first reformulated Zagreb index. In fact, these graph operations play an key role in determining the extremal graphs of the first reformulated Zagreb index among acyclic, unicyclic, bicyclic graphs, respectively.

Now we introduce a graph operation which strictly decreases the first reformulated Zagreb index of a graph.

Operation I. As shown in Fig. 1, Let G be a nontrivial connected graph and v is a given vertex in G. Let G_1 be a graph obtained from G by attaching at v two paths $P: vu_1u_2\cdots u_k$ of length k and $Q: vw_1w_2\cdots w_\ell$ of length ℓ. If $G_2 = G_1 - vw_1 + u_kw_1$, we say that G_2 is obtained from G_1 by *Operation I.*

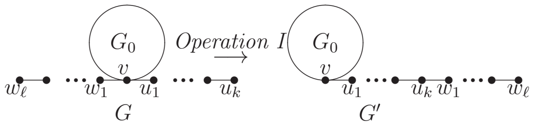

Fig. 1 Two graphs G and G' in Operation I.

Lemma 2.1. *If G' is obtained from G by Operation I as shown in Fig. 1, then*

$$EM_1(G') < EM_1(G).$$

Proof. In fact, the degree of v is decreased in Operation I. Meanwhile, the degree of $N_{G_0}(v)$ all keep the same values during the above proceeding. Hence,

$$\begin{aligned} EM_1(G) - EM_1(G') &> d_G^2(vw_1) + d_G^2(u_1v) + d_G^2(u_{k-1}u_k) \\ &\quad - [d_{G'}^2(u_kw_1) + d_{G'}^2(u_1v) + d_{G'}^2(u_{k-1}u_k)] \\ &= 2(2 + d_{G_0}(v))^2 + 1 - (1 + d_{G_0}(v))^2 - 8 \\ &= d_{G_0}^2(v) + 6d_{G_0}(v) > 0. \end{aligned}$$

The result thus holds. ∎

Operation II. As shown in Fig. 2, let uv be an edge of connected graph G with $d_G(v) \geq 2$. Suppose that $\{v, w_1, w_2, \ldots w_t\}$ are all the neighbors of vertex u while $w_1, w_2, \ldots$ w_t are pendent vertices. If $G' = G - \{uw_1, uw_2, \cdots uw_t\} + \{vw_1, vw_2, \ldots vw_t\}$, we say that G' is obtained from G by *Operation II.*

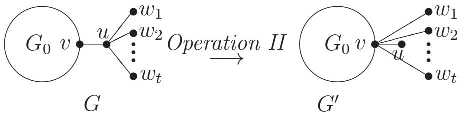

Fig. 2 Graphs G and G' in Operation II.

We now show that Operation II strictly increases the EM_1 of a graph.

Lemma 2.2. *If G' is obtained from G by Operation II as shown in Fig. 2, then*

$$EM_1(G) < EM_1(G').$$

Proof. Since $d_G(v) < d_{G'}(v)$ and $d(uv)$ is not changed during Operation II. So we have

$$\begin{aligned} EM_1(G') - EM_1(G) &> \sum_{i=1}^{t}[d^2_{G'}(vw_i) - d^2_G(uw_i)] + d^2_{G'}(uv) - d^2_G(uv) \\ &= \sum_{i=1}^{t}[d^2_{G'}(vw_i) - d^2_G(uw_i)] > 0. \end{aligned}$$

Hence, the result holds. ■

Operation III. As shown in Fig. 3, Let G be nontrivial connected graph G and u and v be two vertices of G. Let $P_\ell = v_1(= u)v_2 \cdots v_\ell(= v)$ is a nontrivial ℓ- length path of G connecting vertices u and v. If $G' = G - \{v_1v_2, v_2v_3, \cdots, v_{\ell-1}v_\ell\} + \{w(= u \circ v)v_1, wv_2, \cdots, wv_\ell\}$, we say that G' is obtained from G by *Operation III.*

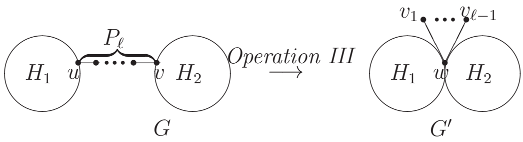

Fig. 3 The graphs G and G' in Operation III.

Lemma 2.3. *If G' is obtained from G by Operation III as shown in Fig. 2, then*

$$EM_1(G') > EM_1(G).$$

Proof. As shown in Figure 3, let $d_{H_1}(u) = x$ and $d_{H_2}(v) = y$ while w be the new vertex by fusing u and v with $d_{G'}(w) = x + y + \ell - 1$ with $\ell \geq 2$. If $\ell = 2$, Then, by means of the definition of EM_1, $EM_1(G') - EM_1(G) > d^2_{G'}(v_1w) - (x + y)^2 = (x + y)^2 - (x + y)^2 = 0$. We now consider the case $\ell \geq 3$. According to the definition of the first reformulated

Zagreb index, we have

$$\begin{aligned} EM_1(G_2) - EM_1(G_1) &> \sum_{i=1}^{\ell-1} d^2_{G'}(wv_i) - ((x+1)^2 + (y+1)^2 + (\ell-3)2^2) \\ &= (\ell-1)(x+y+\ell-2)^2 - (x+1)^2 - (y+1)^2 - 4(\ell-3)) \\ &> [(x+y+\ell-2)^2 - (x+1)^2] + [(x+y+\ell-2)^2 - (y+1)^2] \\ &> 0. \end{aligned}$$

Therefore, the proof is complete. ■

Operation IV. As shown in Fig. 4, let G_0 be a nontrivial subgraph(acyclic) of G with $|G_0| = t$ which is attached at u_1 in graph G, x and y be two neighbors of u_1 different from in G_0. If $G' = G - (G_0 - u_1) + u_1v_2 + v_2v_3 + \cdots + v_ty$, we say that G' is obtained from G by *Operation IV*.

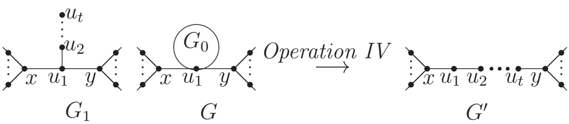

Fig. 4 Graphs G, G', G_1 in Operation IV.

Lemma 2.4. *Let G and G' be two graphs as shown in Fig. 4. Then we have*

$$EM_1(G) > EM_1(G')$$

Proof. In terms of Operation II, as shown in Fig. 4, there is a graph G_1 such that $EM_1(G) \geq EM_1(G_1)$. In order to show the conclusion, we now just to verify the following Inequality:

$$EM_1(G_1) > EM_1(G'). \tag{1}$$

By means of the definition of EM_1, we have

$$\begin{aligned} EM_1(G_1) - EM_1(G') &= d^2_{G_1}(u_{t-1}u_t) + d^2_{G_1}(u_1u_2) + d^2_{G_1}(xu_1) + d^2_{G_1}(yu_1) \\ &\quad - [d^2_{G'}(u_{t-1}u_t) + d^2_{G'}(u_1u_2) + d^2_{G'}(xu_1) + d^2_{G'}(yu_t)] \\ &= 10 + (x+1)^2 + (y+1)^2 - 8 - x^2 - y^2 > 0. \end{aligned}$$

Therefore, the Ineq. (1)holds. Then we finish the proof. ■

We now introduce some terminology which will be used in the following graph operation. Let G be a nontrivial connected graph and two given vertices u and v in G. If $G - u \cong G - v$. Then we say that u and v are *equivalent.* That is, if u and v are a pair of equivalent vertices in G, then $|N(u)| = |N(v)|$ and their neighborhoods have the same degree sequence.

Operation V. Let G_0 be a nontrivial connected graph and u and v are a pair of equivalent vertices in G_0 with $d_{G_0}(u) = d_{G_0}(v) = x$. Let G be the graph obtained by attaching S_{k+1} and $S_{\ell+1}$ at the vertices u and v of G_0 with $k \geq \ell$, respectively. If G' is the graph obtained by delating the ℓ pendent vertices at v in G and connecting them to u of G, respectively, see Fig. 5. We say that G' is obtained from G by *Operation V*.

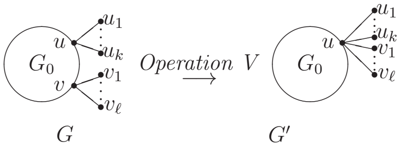

Fig. 5 Operation V.

Lemma 2.5. *If G' is obtained from G by Operation V as shown in Figure. 5. Then*

$$EM_1(G) < EM_1(G').$$

Proof. Note that $d_{G_0}(u) = d_{G_0}(v) = x > 0$ and $k \geq \ell \geq 1$. By the definition of EM_1, we have

$$\begin{aligned}
EM_1(G') - EM_1(G) &> \sum_{i=1}^{k} d_{G'}^2(uu_i) - \sum_{i=1}^{k} d_G^2(uu_i) + \sum_{i=1}^{\ell} d_{G'}^2(uv_i) - \sum_{i=1}^{\ell} d_G^2(vv_i) \\
&= \ell \sum_{i=1}^{k} (d_{G'}(uu_i) + d_G(uu_i)) + k \sum_{i=1}^{\ell} (d_{G'}(uv_i) + d_G(vv_i)) \\
&\geq \ell + k > 0.
\end{aligned}$$

So the result follows. ■

As the above shown, both Operation I and Operation IV strictly decrease the EM_1 of a graph; while all of Operation II, Operation III and Operation V strictly increase the EM_1 of a graph.

3 Main results

In the section, we will characterize the extremal graph with respect to EM_1 among acyclic, unicyclic, bicyclic graphs by a unified method.

For convenience, we first define some notations which will be using in the sequel. Denote by $\mathscr{B}_n$ the set of all connected bicyclic graphs with order n. We define three special classes of graphs. Let $P_n^{k,\ell,m}$ be the graph obtained by connecting two cycles C_k and C_m with a path P_ℓ with $k + \ell + m - 2 = n$, $C_n(p, q)$ be the graph just contains two cycles C_k and C_ℓ having a common vertex with $p+q-1=n$, and $C_n(r,\ell,t)$ be the graph obtained by fusing two triples of pendent vertices of three paths P_ℓ, P_r and P_t to two vertices with $\ell+r+t-4=n$.(without loss of generality, we set $2\le\ell\le r\le t$.) If a bicyclic graph G contains one of the three graphs $C_s(p,q)$ $P_s^{k,\ell,m}$ and $C_s(r,\ell,t)$ as its subgraph. Then we call it as a *brace* of G. By the way, we set $\mathscr{B}_n^1$, $\mathscr{B}_n^2$ and $\mathscr{B}_n^3$ be the set of all bicyclic graphs which include $C_s(p,q)$, $P_s^{k,\ell,m}$ and $C_s(r,\ell,t)$ as their brace, respectively. So the set $\mathscr{B}_n$ can be partitioned into three subsets $\mathscr{B}_n^1$, $\mathscr{B}_n^2$ and $\mathscr{B}_n^3$. In addition, we replace the sign "if and only if" by "iff" for short.

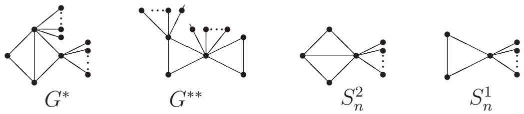

Fig. 6 Some graphs using in the later proof.

We next introduce the extremal graphs with respect to EM_1 on acyclic graphs. If G is an acyclic connected graph with order n, by using Lemma 2.1 and Lemma 2.2, it is easy to deduce the following result.

Theorem 3.1. *Let G be a acyclic connected graph with order n. Then*

$$EM_1(P_n)\le EM_1(G)\le EM_1(S_n)\,,$$

while the lower bound is attached iff $G\cong P_n$ and the upper bound is attached iff $G\cong S_n$.

Ilić and Zhou [18] obtained the next conclusion. Here we provide a shorter proof by utilizing some graph operations.

Theorem 3.2. *Let G be a unicyclic graph with n vertices. Then*

$$EM_1(C_n)\le EM_1(G)\le EM_1(S_n^1)\,,$$

while the lower bound is attached iff $G\cong C_n$ and the upper bound is attached iff $G\cong S_n^1$.

Proof. Since G is a unicyclic graph with n vertices. G contains a uniquely cycle C_ℓ. By Lemma 2.3, we can obtain the graph G' in which the length of the cycle is three and its EM_1 is increased strictly. Furthermore, by using Lemma 2.5, we can get the uniquely maximum graph S_n^1 with respect to EM_1.(see, Fig. 6.) Meanwhile, by Lemma 2.1 and Lemma 2.4, we deduce that the minimum graph is C_n. ■

Theorem 3.3. *Let G be a bicyclic graph with n vertices. Then*

$$4n + 34 \leq EM_1(G) \leq n^3 - 5n^2 + 16n + 4\,,$$

where the lower bound is attached iff $G \in \{P_n^{k,\ell,m} : \ell \geq 3\} \cup \{C_n(r,\ell,t) : \ell \geq 3\}$ *and the upper bound is attached iff* $G \cong S_n^2$.

Proof. We now first show the upper bound. If $G \cong S_n^2$, then $EM_1(G) = n^3 - 5n^2 + 16n + 4$ by simple calculation. Hence, we next verify that $EM_1(G) < EM_1(S_n^2)$ with $G \ncong S_n^2$.

Case 1. G contains $K_4 - e$ as its brace.

If G contains $K_4 - e$ as its brace, by using Lemma 2.2 and Lemma 2.5, we can obtain a new graph (bicyclic) G^* whose EM_1 is more than that of G, see Fig. 6. It is easy to check that $EM_1(G^*) \leq n^3 - 5n^2 + 16n + 4$, equality holds iff $G \cong S_n^2$.

Case 2. $K_4 - e$ is not the brace of G.

Although G does not include the subgraph $K_4 - e$. By Lemma 2.3, maybe there are a bicyclic graph whose EM_1 is more than that of G has the brace $K_4 - e$. So we need to discuss the following two subcases.

Subcase 2.1. $C_s(3,2,m)$ is the brace of G.

In view of Lemma 2.3, subcase 2.1 is converted to **Case 1**.

Subcase 2.2. $C_s(3,2,m)$ is not the brace of G.

By Lemma 2.2, Lemma 2.3 and Lemma 2.5, we get a new graph (bicyclic) G^{**} whose EM_1 is more than that of G, see Figure 6. It is not difficult to verify that $EM_1(G^{**}) < n^3 - 5n^2 + 16n + 4$.

Furthermore, we continue to show the lower bound of bicyclic graphs with respect to EM_1. Using Lemma 2.1, Lemma 2.2 and Lemma 2.4, we deduce that the extremal graph of the minimum EM_1 in bicyclic graphs must be the element which belongs to the set $\{C_n(p,q), P_n^{k,\ell,m}, C_n(r,\ell,t)\}$.

By simply calculation, we have that $EM_1(C_n(p,q)) = 4n + 52$; $EM_1(P_n^{k,\ell,m}) = 4n + 36$ if $\ell = 2$, $EM_1(P_n^{k,\ell,m}) = 4n + 34$, otherwise; $EM_1(C_n(r,\ell,t)) = 4n + 36$ if $\ell = 2$, $EM_1(C_n(r,\ell,t)) = 4n + 34$, otherwise.

So we verify the lower bound, and equality holds iff $G \in \{P_n^{k,\ell,m}, C_n(r,\ell,t), \ell \geq 3\}$.

Therefore, we complete the proof. ■

References

[1] A. T. Balaban, *From Chemical Topology to Three–Dimensional Geometry*, Plenum Press, New York, 1997.

[2] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, Berlin, 2008.

[3] K. C. Das, Maximizing the sum of the squares of the degrees of a graph, *Discr. Math.* **285** (2004) 57–66.

[4] K. C. Das, On comparing Zagreb indices of graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 433–440.

[5] K. C. Das, I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 581–593.

[6] K. C. Das, K. Xu, I. Gutman, On Zagreb and Harary indices, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 301–314.

[7] N. De, Some bounds of reformulated Zagreb indices, *Appl. Math. Sci.* **6** (2012) 5005–5012.

[8] H. Deng, A unified approach to the extremal Zagreb indices for tree, unicyclic graphs and bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 597–616.

[9] J. Devillers, A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon & Breach, Amsterdam, 1999.

[10] C. M. da Fonseca, D. Stevanović, Further properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 655–668.

[11] I. Gutman, B. Furtula, C. Elphick, Three new/old vertex-degree-based topological indices, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 617–632.

[12] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

[13] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Phys. Chem.* **62** (1975) 399–405.

[14] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals, III. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[15] P. Hansen, D. Vukičević, Comparing the Zagreb indices, *Croat. Chem. Acta.* **80** (2007) 165–168.

[16] A. Ilić, M. Ilić, B. Liu, On the upper bounds for the first Zagreb index, *Kragujevac J. Math.* **35** (2011) 173–182.

[17] A. Ilić, D. Stevanović, On comparing Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 681–687.

[18] A. Ilić, B. Zhou, On reformulated Zagreb indices, *Discr. Appl. Math.* **160** (2012) 204–209.

[19] A. Miličević, S. Nikolić, N. Trinajstić, On reformulated Zagreb indices, *Mol. Divers.* **8** (2004) 393–399.

[20] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta.* **76** (2003) 113–124.

[21] G. Su, L. Xiong, L. Xu, B. Ma, On the maximum and minimum first reformulated Zagreb index of graphs with connectivity at most k, *Filomat* **25** (2011) 75–83.

[22] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[23] D. Vukičević, I. Gutman, B. Furtula, V. Andova, D. Dimitrov, Some observations on comparing Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 627–645.

[24] D. Vukičević, N. Trinajstić, On the discriminatory power of the Zagreb indices for molecular graphs, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 111–138.

[25] K. Xu, K. C. Das, S. Balachandran, Maximizing the Zagreb indices of (n, m)-graphs, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 641–654.

[26] K. Xu, H. Hua, A unified approach to extremal multiplicative Zagreb indices for trees, unicyclic and bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 241–256.

[27] Z. Yan, H. Liu, H. Liu, Sharp bounds for the second Zagreb index of unicyclic graphs, *J. Math. Chem.* **42** (2007) 565–574.

[28] L. Zhong, K. Xu, Inequalities between vertex–degree–based topological indices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 627–642.

[29] B. Zhou, Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 113–118.

[30] B. Zhou, Remarks on Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 597–616.

[31] B. Zhou, I. Gutman, Further properties of Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 233–239.

[32] B. Zhou, D. Stevanović, A note on Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 571–578.

[33] B. Zhou, N. Trinajstić, Some properties of the reformulated Zagreb indices, *J. Math. Chem.* **48** (2010) 714–719.