J Math Chem (2009) 46:514–521
DOI 10.1007/s10910-008-9475-3

ORIGINAL PAPER

New upper bounds on Zagreb indices

Kinkar Ch. Das · Ivan Gutman · Bo Zhou

Received: 29 September 2008 / Accepted: 6 October 2008 / Published online: 25 October 2008

Abstract The first Zagreb index $M_1(G)$ is equal to the sum of squares of the degrees of the vertices, and the second Zagreb index $M_2(G)$ is equal to the sum of the products of the degrees of pairs of adjacent vertices of the underlying molecular graph G. In this paper we obtain an upper bound on the first Zagreb index $M_1(G)$ of G in terms of the number of vertices (n), number of edges (m), maximum vertex degree (Δ_1), second maximum vertex degree (Δ_2) and minimum vertex degree (δ). Using this result we find an upper bound on $M_2(G)$. Moreover, we present upper bounds on $M_1(G) + M_1(\overline{G})$ and $M_2(G) + M_2(\overline{G})$ in terms of $n,\ m,\ \Delta_1,\ \Delta_2,\ \delta$, where $\overline{G}$ denotes the complement of G.

Keywords Zagreb index · Molecular graph · Degree (of vertex) · First Zagreb index · Second Zagreb index

1 Introduction

Let $G = (V, E)$ be a simple graph with vertex set $V(G)$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let $\overline{G}$ be the complement of G. We assume that the

K. Ch. Das
Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Republic of Korea
e-mail: kinkar@lycos.com

I. Gutman (✉)
Faculty of Science, University of Kragujevac, B.O. Box 60, Kragujevac 34000, Serbia
e-mail: gutman@kg.ac.yu

B. Zhou
Department of Mathematics, South China Normal University, Guangzhou 510631, People's Republic of China
e-mail: zhoubo@scnu.edu.cn

vertices of G are ordered so that $d_1 \geq d_2 \geq \cdots \geq d_n$, where d_i is the degree of the i-th vertex of G , $i = 1, 2, \ldots, n$. The minimum vertex degree is denoted by δ, the maximum by Δ_1 and the second maximum by Δ_2. We define a graph $S_{r,n-r}$ of order n such that r vertices are of degree $n-1$ and the remaining $n-r$ vertices are of degree δ.

The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ is defined as follows:

$$M_1(G) = \sum_{i \in V} d_i^2$$

and

$$M_2(G) = \sum_{ij \in E(G)} d_i\, d_j.$$

The Zagreb indices $M_1(G)$ and $M_2(G)$ were introduced in [1] and elaborated in [2]. The main properties of $M_1(G)$ and $M_2(G)$ were summarized in [3,4]. Some recent results on the Zagreb indices are reported in [4–16], where also references to the previous mathematical research in this area can be found. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure-descriptors [17,18].

In this paper we obtain an upper bound on the first Zagreb index in terms of n, m, Δ_1, Δ_2, and δ. Using this result we find an upper bound on the second Zagreb index. Moreover, we present analogous upper bounds on $M_1(G) + M_1(\overline{G})$ and $M_2(G) + M_2(\overline{G})$.

2 Main results

In [5] the following two upper bounds for $M_1(G)$ were established:

Lemma 2.1 *Let G be a graph of order n with m edges, maximum degree Δ_1 and minimum degree δ. Then*

$$M_1(G) \leq 2m(\Delta_1 + \delta) - n\,\Delta_1\,\delta \tag{1}$$

with equality holding if and only if G has only two type of degrees Δ_1 and δ.

Lemma 2.2 *Let G be same as in Lemma 2.1. Then*

$$M_1(G) \leq \frac{4m^2 + 2m(n-1)(\Delta_1 - \delta)}{n + \Delta_1 - \delta} \tag{2}$$

with equality holding if and only if G is a regular graph or G is an $S_{\delta,n-\delta}$ or G is the vertex-disjoint union of $n - \Delta_1 - 1$ isolated vertices and the complete graph on $\Delta_1 + 1$ vertices.

We now state another upper bound on the first Zagreb index $M_1(G)$ in terms of n, m, Δ_1, Δ_2, δ, and characterize the graphs for which equality is attained.

Theorem 2.3 *Let G be a graph with n $(n > 1)$ vertices, m edges, maximum degree Δ_1, second maximum degree Δ_2 and minimum degree δ. Then*

$$M_1(G) \le \frac{(2m-\Delta_1)^2}{n-1} + \Delta_1^2 + \frac{(n-1)}{4}(\Delta_2-\delta)^2. \tag{3}$$

Equality holds in (3) if and only if G is isomorphic to a graph H_1 such that $d_2(H_1) = d_3(H_1) = \cdots = d_n(H_1) = \delta$ or G is isomorphic to a graph H_2 such that $d_2(H_2) = d_3(H_2) = \cdots = d_{p+1}(H_2) = \Delta_2$ and $d_{p+2}(H_2) = d_{p+3}(H_2) = \cdots = d_{2p+1}(H_2) = \delta$, $n = 2p+1$.

Proof For K_2, $\overline{K_2}$, K_3, $\overline{K_3}$, P_3, and $\overline{P_3}$ we easily see that the equality in (3) holds. Now we assume that $n \ge 4$ and that the numbers $p_3, p_4, \ldots, p_{n-1}\,; q_3, q_4, \ldots, q_{n-1}$ are defined by the equations

$$d_i^2 = p_i\,\Delta_2^2 + q_i\,\delta^2, \quad p_i + q_i = 1,\ i = 3, 4, \ldots, n-1. \tag{4}$$

Thus,

$$M_1(G) = \sum_{i=1}^{n} d_i^2 = \Delta_1^2 + p\Delta_2^2 + q\delta^2, \quad p + q = n-1$$

where

$$p = 1 + \sum_{i=3}^{n-1} p_i, \quad q = 1 + \sum_{i=3}^{n-1} q_i.$$

Now, $d_i^2 = (p_i\,\Delta_2^2 + q_i\,\delta^2)(p_i + q_i)$, from which

$$d_i \ge p_i\,\Delta_2 + q_i\,\delta, \quad i = 3, 4, \ldots, n-1 \tag{5}$$

and thus

$$\sum_{i=2}^{n} d_i \ge p\,\Delta_2 + q\,\delta.$$

Now,

$$\begin{aligned}(n-1)M_1(G) - \left(\sum_{i=2}^{n} d_i\right)^2 &\le (n-1)\Delta_1^2 + (p\,\Delta_2^2 + q\,\delta^2)(p+q) - (p\,\Delta_2 + q\,\delta)^2\\ &= (n-1)\Delta_1^2 + p\,q\,(\Delta_2-\delta)^2\\ &\le (n-1)\Delta_1^2 + \frac{(n-1)^2}{4}(\Delta_2-\delta)^2 \end{aligned} \tag{6}$$

since $p\,q \le (n-1)^2/4$.

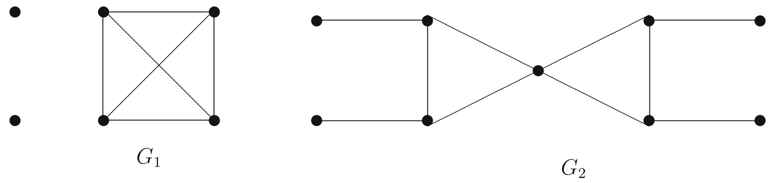

Fig. 1 Examples illustrating the mutual relations of the bounds (1), (2), and (3), cf. Remarks 2.4 and 2.6

From (6), we get (3), which completes the first part of the proof.

Now suppose that equality holds in (3). Then all inequalities in the above argument must be equalities. Thus from equality in (5), we get

$$p_i\, q_i(\Delta_2-\delta)^2=0, \quad i=3,4,\ldots,n-1. \tag{7}$$

From equality in (6), we get

$$(p-q)(\Delta_2-\delta)=0. \tag{8}$$

If $\Delta_2=\delta$, then G is isomorphic to a graph H_1 such that $d_2(H_1)=d_3(H_1)=\cdots=d_n(H_1)=\delta$. Otherwise, $\Delta_2\neq\delta$. From (7), we conclude that either $p_i=0$ or $q_i=0$ for $i=3,4,\ldots,n-1$. Since $p_i+q_i=1$, it must be $p_i=1$ or $q_i=1$.

From (8) follows that $p=q$ and therefore $n=2p+1$. Thus from (4),

$$d_2=d_3=\cdots=d_{p+1}=\Delta_2,\ d_{p+2}=d_{p+3}=\cdots=d_{2p+1}=\delta\ ,\ n=2p+1.$$

Hence G is isomorphic to a graph H, such that $d_2(H)=\cdots=d_{p+1}(H)=\Delta_2$ and $d_{p+2}(H)=d_{p+3}(H)=\cdots=d_{2p+1}(H)=\delta$, $n=2p+1$.

Conversely, let G be isomorphic to a graph H_1, such that $d_2(H_1)=d_3(H_1)=\cdots=d_n(H_1)=\delta$ or let G be isomorphic to a graph H_2, such that $d_2(H_2)=d_3(H_2)=\cdots=d_{p+1}(H_2)=\Delta_2$ and $d_{p+2}(H_2)=d_{p+3}(H_2)=\cdots=d_{2p+1}(H_2)=\delta$, $n=2p+1$. For both cases we can easily verify that the equality in (3) holds. □

Remark 2.4 For the graph G_2 depicted in Fig. 1, the upper bound given by (3) (= 56) is better than the upper bound given by (1) (= 64) and (2) (= 73.3). But for graph G_1, the upper bound given by (1) (=36) and (2) (= 36) is better than the upper bound given by (3) (= 36.45). Thus our bound given by (3) is not always better than (1) and (2).

Theorem 2.3 can be somewhat improved:

Theorem 2.5 *Let G be the same graph as in Theorem 2.3. Then*

$$M_1(G)\le\Delta_1^2+(\Delta_2+\delta)(2m-\Delta_1)-(n-1)\Delta_2\,\delta. \tag{9}$$

Equality holds in (9) if and only if G is isomorphic to a graph H such that $d_2(H)=d_3(H)=\cdots=d_p(H)=\Delta_2$ *and* $d_{p+1}(H)=d_{p+2}(H_2)=\cdots=d_n(H)=\delta$, $2\le p\le n$.

Proof For $i = 2, 3, \ldots, n$, we have $(d_i - \Delta_2)(d_i - \delta) \leq 0$, and thus

$$\sum_{i=2}^{n} d_i^2 \leq (\Delta_2 + \delta)(2m - \Delta_1) - (n-1)\Delta_2\,\delta$$

with equality if and only if $d_i = \Delta_2$ or $d_i = \delta$ for $i = 2, 3, \ldots, n$. So the result follows. □

Remark 2.6 Also in the case of Theorem 2.5 the upper bound (9) for the graph G_2 (=56) is better than the upper bounds (1) and (2). On the other hand, for the graph G_1, the upper bounds (1) and (2) give the same result (=36) as (9).

Remark 2.7 The bound (9) is always better than (1). In order to see this note that

$$\begin{aligned}
&2m(\Delta_1 + \delta) - n\Delta_1\,\delta \geq \Delta_1^2 + (2m - \Delta_1)(\Delta_2 + \delta) - (n-1)\Delta_2\,\delta \\
&\quad \Leftrightarrow 2m(\Delta_1 - \Delta_2) + \Delta_1(\Delta_2 + \delta) - \Delta_1^2 - n\,\delta\,(\Delta_1 - \Delta_2) - \Delta_2\,\delta \geq 0 \\
&\quad \Leftrightarrow (2m - \Delta_1 - n\delta + \delta)(\Delta_1 - \Delta_2) \geq 0 \\
&\quad \Leftrightarrow \sum_{i=2}^{n} (d_i - \delta)(\Delta_1 - \Delta_2) \geq 0
\end{aligned}$$

which, evidently, is always obeyed.

Remark 2.8 The bound (9) is also better than (3). To see this note that

$$\begin{aligned}
&(\Delta_2 + \delta)(2m - \Delta_1) - (n-1)\Delta_2\,\delta \leq \frac{(2m - \Delta_1)^2}{n-1} + \frac{(n-1)}{4}\,(\Delta_2 - \delta)^2 \\
&\quad \Leftrightarrow (\Delta_2 + \delta)(2m - \Delta_1) \leq \frac{(2m - \Delta_1)^2}{n-1} + \frac{(n-1)}{4}\,(\Delta_2 + \delta)^2 \\
&\quad \Leftrightarrow [2(2m - \Delta_1) - (n-1)(\Delta_2 + \delta)]^2 \geq 0
\end{aligned}$$

which, evidently, is always obeyed.

In [8] the following upper bound for $M_1(G) + M_1(\overline{G})$ was established, in terms of n only:

$$M_1(G) + M_1(\overline{G}) \leq n(n-1)^2.$$

Using Theorem 2.3, we deduce an upper bound on $M_1(G) + M_1(\overline{G})$ in terms of n, m, Δ_1, Δ_2, and δ.

Theorem 2.9 *Let G be a graph with n vertices, m edges, maximum degree Δ_1, second maximum degree Δ_2 and minimum degree δ. Then*

$$M_1(G)+M_1(\overline{G}) \le \frac{\left(n(n-2)-2m+\delta+1\right)^2+(2m-\Delta_1)^2}{n-1}+\Delta_1^2+(n-1-\delta)^2$$
$$+\frac{n-1}{4}\left[\left(\Delta_1-\delta\right)^2+(\Delta_2-\delta)^2\right]. \quad (10)$$

Equality holds in (10) *if and only if* G *is the path* P_3 *or* G *is a regular graph.*

Proof If G (or $\overline{G}$) is K_2, P_3 or K_3, we can easily check that the equality in (3) holds. Assume therefore that $n \ge 4$. We then have

$$M_1(G) \le \frac{(2m-\Delta_1)^2}{n-1}+\Delta_1^2+\frac{n-1}{4}(\Delta_2-\delta)^2$$

and

$$M_1(\overline{G}) \le \frac{\left(n(n-2)-2m+\delta+1\right)^2}{n-1}+(n-1-\delta)^2+\frac{n-1}{4}(\Delta_1-\delta)^2.$$

From this we get

$$M_1(G)+M_1(\overline{G}) \le \frac{\left(n(n-2)-2m+\delta+1\right)^2+(2m-\Delta_1)^2}{n-1}+\Delta_1^2+(n-1-\delta)^2$$
$$+\frac{n-1}{4}\left[\left(\Delta_1-\delta\right)^2+(\Delta_2-\delta)^2\right].$$

Using Theorem 2.3 we get the required result. □

We now deduce an upper bound on $M_2(G)$ using Theorem 2.3.

Theorem 2.10 *Let* G *be a graph with* n *vertices,* m *edges, maximum degree* Δ_1, *second maximum degree* Δ_2 *and minimum degree* δ. *Then*

$$M_2(G) \le 2m^2-(n-1)m\delta+\frac{1}{2}(\delta-1)\left[\frac{(2m-\Delta_1)^2}{n-1}+\Delta_1^2+\frac{(n-1)}{4}(\Delta_2-\delta)^2\right]. \quad (11)$$

Equality holds in (11) *if and only if* G *is a regular graph or* $G \cong S_{1,n-1}$ *or* $G \cong S_{p+1,p}$, $n=2p+1$.

Proof From [6] we have

$$M_2(G)=\frac{1}{2}\sum_{i=1}^{n} d_i^2\, m_i \le \frac{1}{2}\sum_{i=1}^{n} d_i\left[2m-d_i-(n-d_i-1)\delta\right] \quad (12)$$
$$=2m^2-(n-1)m\,\delta+\frac{1}{2}(\delta-1)M_1(G).$$

Inequality (11) follows now from Theorem 2.3.

Equality in (12) holds if and only if either $d_i = n-1$ or $d_j = \delta$ for all $i, ij \notin E(G)$, which implies that either (a) G is a regular graph, or (b) G is a bi-degreed graph in which each vertex is of degree either δ or $n-1$. By Theorem 2.3, the equality holds in (11) if and only if G is a regular graph or $G \cong S_{1,n-1}$ or $G \cong S_{p+1,p}$, $n = 2p+1$. □

In [8] the following upper bound for $M_2(G) + M_2(\overline{G})$ was established:

$$M_2(G) + M_2(\overline{G}) \le \frac{n(n-1)^3}{2}.$$

Using Theorem 2.3 we deduce:

Theorem 2.11 *Let G be a graph with n vertices, m edges, maximum degree Δ_1, second maximum degree Δ_2 and minimum degree δ. Then*

$$M_2(G) + M_2(\overline{G}) \le \frac{n(n-1)^3}{2} + 2m^2 - 3m(n-1)^2 + \left(n - \frac{3}{2}\right)\left[\frac{(2m-\Delta_1)^2}{n-1} + \Delta_1^2 + \frac{(n-1)}{4}(\Delta_2 - \delta)^2\right].$$

Equality holds if and only if G is isomorphic to a graph H_1, such that $d_2(H_1) = d_3(H_1) = \cdots = d_n(H_1) = \delta$ or G is isomorphic to a graph H_2, such that $d_2(H_2) = d_3(H_2) = \cdots = d_{p+1}(H_2) = \Delta_2$ and $d_{p+2}(H_2) = d_{p+3}(H_2) = \cdots = d_{2p+1}(H_2) = \delta$, $n = 2p+1$.

Proof From [6] we have

$$M_2(G) + M_2(\overline{G}) = \frac{n(n-1)^3}{2} + 2m^2 - 3m(n-1)^2 + \left(n - \frac{3}{2}\right) M_1(G).$$

Using Theorem 2.3 in the above relation, we get the required result. □

Acknowledgments K. Ch. D., I. G., and B. Z. thank, respectively, for support by Sungkyunkwan University BK21 Project, BK21 Math Modeling HRD Div.Sungkyunkwan University, Suwon, Republic of Korea, Serbian Ministry of Science (Grant No. 144015G), and the Guangdong Provincial Natural Science Foundation of China (Grant No. 8151063101000026).

References

1. I. Gutman, N. Trinajstić, Chem. Phys. Lett. **17**, 535 (1972)
2. I. Gutman, B. Ruščić, N. Trinajstić, C.F. Wilcox, J. Chem. Phys. **62**, 3399 (1975)
3. S. Nikolić, G. Kovačević, A. Milićević, N. Trinajstić, Croat. Chem. Acta. **76**, 113 (2003)
4. S. Chen, F. Xia, MATCH Commun. Math. Comput. Chem. **58**, 663 (2007)
5. K.C. Das, Discr. Math. 285, **57** (2004)
6. K.C. Das, I. Gutman, MATCH Commun. Math. Comput. Chem. **52**, 103 (2004)
7. B. Zhou, MATCH Commun. Math. Comput. Chem. **52**, 113 (2004)
8. L. Zhang, B. Wu, MATCH Commun. Math. Comput. Chem. **54**, 189 (2005)

9. B. Zhou, I. Gutman, MATCH Commun. Math. Comput. Chem. **54**, 233 (2005)
10. V. Kumar, A.K. Madan, J. Math. Chem. **42**, 925 (2007)
11. B. Zhou, MATCH Commun. Math. Comput. Chem. **57**, 591 (2007)
12. H. Deng, MATCH Commun. Math. Comput. Chem. **57**, 597 (2007)
13. B. Zhou, Int. J. Quantum Chem. **107**, 875 (2007)
14. Z. Yan, H. Liu, H. Liu, J. Math. Chem. **42**, 565 (2007)
15. E. Estrada, A. R. Matamala, J. Math. Chem. **43**, 508 (2008)
16. B. Zhou, N. Trinajstić, J. Math. Chem. **44**, 235 (2008)
17. A.T. Balaban, I. Motoc, D. Bonchev, O. Mekenyan, Topics Curr. Chem. **114**, 21 (1983)
18. R. Todeschini, V. Consonni *Handbook of Molecular Descriptors* (Wiley–VCH, Weinheim, 2000)