Bounds on Hosoya Index Involving Some Other Topological Indices*

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Abstract

For a graph G, its Hosoya index is defined as the total number of matchings in it, including the empty set. The Hosoya index is one of the oldest and well-studied molecular topological descriptors. Almost all results concerning Hosoya index in the existing literatures deal with its extremal properties, and there exists no results revealing the relations between this index and other topological indices so far. In this note, we establish some sharp lower bounds for Hosoya index in terms of some other topological indices.

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $V(G)$. For a graph G, we let $d_G(v)$ be the degree of a vertex v in G and let $d_G(u, v)$ denote the distance between vertices u and v in G. Denote by $ec_G(v)$ the *eccentricity* of a vertex v in G.

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A graph invariant is a function defined on a graph which is independent of the labeling of its vertices. Till now, hundreds of different graph invariants have been employed in QSAR/QSPR studies, some of which have been proved to be successful (see [27]). Among those successful invariants, there are some invariants worth noting. We mention here some of them relevant to the topics of our paper. There are the *Hosoya index* (see [10–17,25,26,30] and [31] for a survey), the *first Zagreb index* and the *second Zagreb index* (see [4, 9, 23, 24, 32–34]).

The *Hosoya index* of a graph G is defined as

$$Z(G) = \sum_{k \geq 0} m(G; k),$$

where $m(G; k)$ is the number of k-matchings in G for $k \geq 1$, and $m(G; 0) = 1$.

The first Zagreb index and second Zagreb index are defined, respectively, as

$$M_1(G) = \sum_{u \in V(G)} (d_G(u))^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

Evidently, one can rewrite the first Zagreb index as

$$M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v)). \tag{1}$$

Noticing that the contribution of nonadjacent vertex pairs should be taken into account when computing the weighted Wiener polynomials of certain composite graphs (see [6]). Ashrafi et al. [1, 2] introduced the *first Zagreb coindex* (corresponding to the form in the equation (1)) and *second Zagreb coindex*, which are defined as

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} (d_G(u) + d_G(v)) \text{ and } \overline{M}_2(G) = \sum_{uv \notin E(G)} d_G(u) d_G(v),$$

respectively.

The *eccentric connectivity index* (see [3, 21, 22]) of a connected graph G, denoted by $\xi^c(G)$, is defined as

$$\xi^c(G) = \sum_{u \in V(G)} ec_G(u) d_G(u). \tag{2}$$

The *degree distance or schultz index* of a connected graph G is defined [8] as

$$D'(G) = \sum_{x \in V(G)} d_G(x) D_G(x), \tag{3}$$

where $D_G(x)$ is the sum of distances between x and all other vertices in G. For recent results on degree distance, see [7, 18, 20, 28, 29].

The *reverse degree distance* of a connected graph G with n vertices, m edges and diameter d is defined [35] as

$$^{r}D'(G) = 2(n-1)md - D'(G). \tag{4}$$

In this note, we establish some sharp lower bounds for Hosoya index in terms of some other topological indices including the first Zagreb index, the first Zagreb coindex, the eccentric connectivity index, the degree distance and the reverse degree distance.

Since the contribution of each vertex u in G to $\overline{M}_1(G)$ is exactly $(n - d_G(u) - 1)d_G(u)$, we rewrite (as in [19])

$$\overline{M}_1(G) = \sum_{u \in V(G)} (n - d_G(u) - 1) d_G(u). \tag{5}$$

2 Bounds for Hosoya index

In this section, we establish relationships between Hosoya index and other topological indices. More precisely, we provide some lower bounds for Hosoya index in terms of some other topological indices.

A *matching* M of the graph G is a subset of $E(G)$ such that no two edges in M share a common vertex. A matching M of G is said to be a *maximum matching*, if for any other matching $\overline{M}$ of G, $|\overline{M}| \leq |M|$. The *matching number* of G is the number of edges of a maximum matching in G.

Lemma 2.1 *Let G be a non-trivial and non-complete graph of size m. Then*

$$m(G; 2) = \frac{1}{2} m(m+1) - \frac{1}{2} M_1(G). \tag{6}$$

Proof. By the definition of $m(G;k)$,

$$m(G;2) = \frac{1}{2}\sum_{uv\in E(G)}[m-(d_G(u)+d_G(v)-2)-1]$$
$$= \frac{1}{2}m(m+1) - \frac{1}{2}\sum_{uv\in E(G)}(d_G(u)+d_G(v))$$
$$= \frac{1}{2}m(m+1) - \frac{1}{2}\sum_{u\in V(G)}(d_G(u))^2$$
$$= \frac{1}{2}m(m+1) - \frac{1}{2}M_1(G),$$

as claimed. ∎

Proposition 2.1 *Let G be a non-trivial and non-complete graph of order n and size m. Then*

$$Z(G) \geq -\frac{1}{2}M_1(G) + \frac{1}{2}(m+1)(m+2),$$

with equality if and only if the matching number of G is 2.

Proof. Note that for any non-trivial and non-complete graph G of size m,

$$Z(G) \geq 1 + m + m(G;2) \tag{7}$$

with equality if and only if the matching number of G is 2.

By Eq.(6) and Ineq. (7), we have

$$\frac{1}{2}m(m+1) - \frac{1}{2}M_1(G) \leq Z(G) - 1 - m,$$

that is,

$$Z(G) \geq -\frac{1}{2}M_1(G) + \frac{1}{2}(m+1)(m+2),$$

with equality if and only if the matching number of G is 2.

This completes the proof. ∎

Proposition 2.2 *Let G be a non-trivial and non-complete graph of order n and size m. Then*

$$Z(G) \geq \frac{1}{2}\overline{M}_1(G) + \frac{1}{2}(m+1)(m+2) - m(n-1),$$

with equality if and only if the matching number of G is 2.

Proof. In view of Eq.(5), we have

$$\begin{aligned}\overline{M}_1(G) &= \sum_{u\in V(G)} (n - d_G(u) - 1)d_G(u) \\ &= 2m(n-1) - \sum_{u\in V(G)} (d_G(u))^2 \\ &= 2m(n-1) - M_1(G).\end{aligned}$$

Combining this fact with Proposition 2.1, we obtain

$$Z(G) \geq -\frac{1}{2}[2m(n-1) - \overline{M}_1(G)] + \frac{1}{2}(m+1)(m+2),$$

that is,

$$Z(G) \geq \frac{1}{2}\overline{M}_1(G) + \frac{1}{2}(m+1)(m+2) - m(n-1),$$

with equality if and only if the matching number of G is 2.

This proves our desired result. ∎

We summarize here a result of [19] as the following lemma.

Lemma 2.2 *Let G be a non-trivial connected graph of order n. For each vertex v_i in G, it holds*

$$ec_G(v_i) \leq n - d_G(v_i).$$

For $i = 1, \ldots, n$, all equalities hold together if and only if $G \cong P_4$ or $K_n - iK_2\,(0 \leq i \leq \lfloor\frac{n}{2}\rfloor)$, where $K_n - iK_2$ denotes the graph obtained by removing i independent edges from G.

Proposition 2.3 *Let G be a non-trivial and non-complete connected graph of order n and size m. Then*

$$Z(G) \geq \frac{1}{2}\xi^c(G) + \frac{1}{2}m^2 - mn + \frac{3}{2}m + 1,$$

with equality if and only if $G \cong P_4$ or $K_n - iK_2\,(0 \leq i \leq \lfloor\frac{n}{2}\rfloor)$, $n = 4, 5$.

Proof. For each vertex v in G, we clearly have $ec_G(v) \leq n - d_G(v)$.

According to Eq.(2), we have

$$\begin{aligned}\xi^c(G) &= \sum_{v\in V(G)} ec_G(v)d_G(v)\\ &\le \sum_{v\in V(G)} (n-d_G(v))d_G(v)\\ &= 2mn - M_1(G),\end{aligned}$$

with equality if and only if $ec_G(v) = n - d_G(v)$ holds for each vertex v in G, that is, $G \cong P_4$ or $K_n - iK_2\,(0 \le i \le \lfloor \frac{n}{2} \rfloor)$ by Lemma 2.2.

Hence,

$$-M_1(G) \ge \xi^c(G) - 2mn, \tag{8}$$

with equality if and only if $G \cong P_4$ or $K_n - iK_2\,(0 \le i \le \lfloor \frac{n}{2} \rfloor)$.

Note that if $n \ge 6$, then for $0 \le i \le \lfloor \frac{n}{2} \rfloor$, the matching number of $K_n - iK_2$ is at least 3.

By Eq. (6), Ineqs. (7) and (8), we have

$$\begin{aligned}Z(G) &\ge 1 + m + m(G;2)\\ &\ge 1 + m + \frac{1}{2}m(m+1) + \frac{1}{2}(\xi^c(G) - 2mn)\\ &= \frac{1}{2}\xi^c(G) + \frac{1}{2}m^2 - mn + \frac{3}{2}m + 1,\end{aligned}$$

with equality if and only if $G \cong P_4$ or $K_n - iK_2\,(0 \le i \le \lfloor \frac{n}{2} \rfloor)$, $n = 4, 5$.

This completes the proof. ∎

Proposition 2.4 *Let G be a non-trivial and non-complete connected graph of order n, size m and diameter d. Then*

$$Z(G) \ge \frac{1}{2(d-1)}D'(G) - \frac{(n-1)dm}{d-1} + \frac{1}{2}m^2 + \frac{3}{2}m + 1,$$

with equality if and only if both the diameter and the matching number of G are equal to 2.

Proof. Note that $G \not\cong K_n$. Thus, $d \geq 2$. By means of Eq. (3),

$$\begin{aligned} D'(G) &= \sum_{x\in V(G)} d_G(x)D_G(x) \\ &= \sum_{x\in V(G)} (d_G(x))^2 + \sum_{x\in V(G)} d_G(x) \sum_{y\in V(G)\setminus N_G[x]} d_G(x, y) \\ &\leq \sum_{x\in V(G)} (d_G(x))^2 + \sum_{x\in V(G)} d\cdot d_G(x)(n - d_G(x) - 1) \\ &= 2(n-1)dm - (d-1)M_1(G), \end{aligned}$$

with equality if and only if for each x in G and any $y \in V(G) \setminus N_G[x]$, $d_G(x, y) = d$, that is, $d \leq 2$.

So,

$$-M_1(G) \geq \frac{1}{d-1}D'(G) - \frac{2(n-1)dm}{d-1}. \tag{9}$$

with equality if and only if $d = 2$.

By Eq. (6), Ineqs. (7) and (9), we have

$$\begin{aligned} Z(G) &\geq 1 + m + m(G; 2) \\ &\geq 1 + m + \frac{1}{2}m(m+1) + \frac{1}{2(d-1)}D'(G) - \frac{2(n-1)dm}{2(d-1)} \\ &= \frac{1}{2(d-1)}D'(G) - \frac{(n-1)dm}{d-1} + \frac{1}{2}m^2 + \frac{3}{2}m + 1, \end{aligned}$$

with equality if and only if both the diameter and the matching number of G are equal to 2. ∎

Proposition 2.5 *Let G be a non-trivial and non-complete connected graph of order n, size m and diameter d. Then*

$$Z(G) \geq -\frac{1}{2(d-1)} \cdot^{r} D'(G) + \frac{1}{2}m^2 + \frac{3}{2}m + 1,$$

with equality if and only if both the diameter and the matching number of G are equal to 2.

Proof. According to Eq. (4) and Proposition 2.4, we immediately have the following consequence. ∎

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