The Hosoya indices and Merrifield–Simmons indices of graphs with connectivity at most \( k \)

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\begin{abstract}

The Hosoya index and the Merrifield–Simmons index of a graph are defined as the total number of the matchings (including the empty edge set) and the total number of the independent vertex sets (including the empty vertex set) of the graph, respectively. Let \( V_{n,k} \) be the set of connected \( n \)-vertex graphs with connectivity at most \( k \). In this note, we characterize the extremal (maximal and minimal) graphs from \( V_{n,k} \) with respect to the Hosoya index and the Merrifield–Simmons index, respectively.

\end{abstract}

1. Introduction

The Hosoya index and the Merrifield–Simmons index of a graph \( G \) are two well-known topological indices in combinatorial chemistry. The former, denoted by \( z(G) \), is defined as the total number of the matchings (independent edge subsets), including the empty edge set, of the graph, and the latter, denoted by \( i(G) \), is defined as the total number of the independent vertex sets, including the empty vertex set, of the graph.

The Hosoya index was introduced by Hosoya \cite{1} in 1971. Since its first introduction the Hosoya index has received much attention (see \cite{2–9}). This index plays an important role in studying the relation between molecular structure and physical and chemical properties of certain hydrocarbon compounds. Moreover, it is connected with various physico-chemical properties of alkanes, for example, the boiling point, entropy, and heat of vaporization. There is an example in \cite{10} which shows the high correlation between the Hosoya index and the boiling points of acyclic alkanes. Details of chemical applications can be found in \cite{11,12–14}. In particular, the Hosoya index of general graphs (having loops or multi-edges) was considered in \cite{13}. The Merrifield–Simmons index is the other topological index introduced by Merrifield and Simmons \cite{15} in 1989. In \cite{16} Gutman first named this index the Merrifield–Simmons index, whose mathematical properties can be found in some detail \cite{17,18,5,9}. Many chemical applications can be found in \cite{15,19}. For example, in \cite{15} it was shown that \( i(G) \) is correlated with boiling points.

It is of significant interest to determine the extremal (maximal or minimal) graphs with respect to these two indices. Already, many nice results can be found in \cite{2,16,15,18,9} concerning the extremal graphs with respect to these two indices. For example, trees, unicyclic graphs, and so on, are of major interest. In particular, Wagner \cite{18} characterized the extremal trees having a given maximum degree and with maximal Hosoya index and minimal Merrifield–Simmons

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index. Deng and Chen [2] determined all the extremal unicyclic graphs with respect to these two indices. Xu and Xu [5] characterized all the unicyclic graphs of order \( n \) and with given maximum degree \( \Delta \) maximizing the Hosoya index and minimizing the Merrifield–Simmons index. Yu and Tian [9] characterized the graphs with minimal Hosoya indices and maximal Merrifield–Simmons indices among the connected graphs with given cyclomatic number and edge-independence number.

All graphs considered in this work are finite and simple. Let \( G \) be a graph with vertex set \( V(G) \) and edge set \( E(G) \). For a vertex \( v \in V(G) \), we denote by \( N_G(v) \) the neighbors of \( v \) in \( G \), and \( N_G[v] = \{v\} \cup N_G(v) \). \( d_G(v) = |N_G(v)| \) is called the degree of \( v \) in \( G \) and is written as \( d(v) \) for short. If \( e \notin E(G) \), we use \( G + e \) to denote the graph obtained by adding \( e \) to \( G \).

For a graph \( G \), the complete graph on \( n \) vertices, we refer to [20].

For \( k \geq 1 \), a graph \( G \) is called \( k \)-connected if either \( G \) is a complete graph \( K_{k+1} \) or else it has at least \( k + 2 \) vertices and has no \((k - 1)\)-vertex cut. Similarly, we call a graph \( k \)-edge-connected if it has at least two vertices and does not contain a \((k - 1)\)-edge cut. The maximum value of \( k \) such that a connected graph \( G \) is \( k \)-connected is the connectivity of \( G \) and it is denoted by \( \kappa(G) \). For a disconnected graph \( G \) we define \( \kappa(G) = 0 \). The \( k \)-edge-connectivity \( \kappa_k(G) \) of graph \( G \) is defined analogously. For a graph \( G \) with \( n \) vertices, we have the following remarks.

1. \( \kappa(G) \leq \kappa_k(G) \leq n - 1 \); 2. \( \kappa(G) = n - 1, \kappa_k(G) = n - 1 \) and \( G \cong K_n \) are equivalent.

Let \( \mathcal{V}_{n,k} \) (\( \mathcal{E}_{n,k} \)) be the set of all graphs of order \( n \) with connectivity (edge-connectivity) at most \( k \leq n - 1 \). Let \( K^k_n \) (shown in Fig. 1) be the graph obtained by joining \( k \) edges from \( k \) vertices of \( K_{n-1} \) to an isolated vertex. Recently Li et al. [21] proved that the graph from \( \mathcal{V}_{n,k} \) with maximal index (spectral radius) is uniquely \( K^k_n \). Motivated by their results, we will show that \( K^k_n \) is a unique graph from \( \mathcal{V}_{n,k} \) with maximal Hosoya index as well as the unique one from \( \mathcal{V}_{n,k} \), minimizing the Merrifield–Simmons index. And the minimal Hosoya index and maximal Merrifield–Simmons index of graphs from \( \mathcal{V}_{n,k} \) are uniquely attained at \( S_n \).

2. Lemmas and results

Before proving our main results, we first list the following lemmas and introduce some new definitions as some necessary preliminaries. From the definitions of the Hosoya index and Merrifield–Simmons index, it is not difficult to deduce the two lemmas below.

**Lemma 2.1** ([3]). Let \( G \) be a graph. Then:

1. If \( uv \in E(G) \), we have \( z(G) = z(G - uv) + z(G - \{u, v\}) \).
2. If \( v \in V(G) \), we have \( z(G) = z(G - v) + \sum_{w \in N_G(v)} z(G - \{w, v\}) \).
3. If \( G_1, G_2, \ldots, G_t \) are the components of graph \( G \), we have \( z(G) = \prod_{k=1}^t z(G_k) \).

**Lemma 2.2**. Let \( G \) be a graph. Then:

1. If \( uv \in E(G) \), we have \( i(G) = i(G - uv) + i(G - \{u, v\}) \).
2. If \( v \in V(G) \), we have \( i(G) = i(G - v) + i(G - \{N_G(v)\}) \).
3. If \( G_1, G_2, \ldots, G_t \) are the components of graph \( G \), we have \( i(G) = \prod_{k=1}^t i(G_k) \).

From Lemmas 2.1 and 2.2, the following corollary is easily obtained.

**Corollary 2.1.** Let \( G \) be a graph with \( e \notin E(G) \). Then we have:

1. \( z(G + e) > z(G) \).
2. \( i(G + e) < i(G) \).

**Lemma 2.3**. Let \( z(K_n) = z_n \) and \( i(K_n) = i_n \). Then we have \( 1 \leq z_1 = z_{n-1} + (n - 1)z_{n-2} \) where \( z_1 = 1 \) and \( z_2 = 2 \) and \( 2 \leq i_n = n + 1 \).

**Proof.** Applying Lemma 2.1(2) to any one vertex of graph \( K_n \), we have \( z_n = z_{n-1} + (n - 1)z_{n-2} \). From the definition of the Hosoya index, it is clear that \( z_1 = 1 \) and \( z_2 = 2 \).

In \( K_n \), any two vertices are adjacent. Therefore \( K_n \) does not contain an independent vertex set with more than one vertex. Thus \( i(K_n) \) is the order of \( K_n \) plus 1, that is, \( i_n = n + 1 \), which completes the proof of this lemma. □
From the definition of graph $K^k_n$, we find that $K^k_n$ can be viewed as a graph obtained by deleting all the edges of $K_{1,n-k-1}$ from the complete graph $K_n$. Generally, we introduce a graph $K^k_{n_1,n_2}$, which is obtained by deleting all the edges of $K_{n_1,n_2}$ from the complete graph $K_{n_1+n_2+k}$ where $K_{n_1,n_2}$ is a subgraph of $K_{n_1+n_2+k}$. As an example, the graph $K^2_{3,4}$ is shown in Fig. 2. Clearly, $K^k_{1,n-k-1}$ is just $K^k_n$.

In the following the Hosoya index of graph $K^k_{n_1,n_2}$ will be written as $z(n_1, n_2, k)$ for short; the Merrifield–Simmons index of $K^k_{n_1,n_2}$ will be similarly denoted by $i(n_1, n_2, k)$.

**Lemma 2.4.** Let $n_1$, $n_2$ be two positive integers such that $n_2 \geq n_1 \geq 2$ and $n_1 + n_2 = n - k$. Then we have $z(n_1 - 1, n_2 + 1, k) > z(n_1, n_2, k)$.

**Proof.** We will prove this lemma by induction on $n_1$.

When $n_1 = 2$, we get $n_2 = n - k - 2$. Note that $z(0, n - k - 2, k) = z_{n-2}$. From Lemmas 2.1(2) and 2.3(1), we have

$$z(n_1 - 1, n_2 + 1, k) = z(n_1 - 1, n_2, k) + kz(n_1 - 1, n_2, k - 1) + n_2 z(n_1 - 1, n_2 - 1, k),$$

and

$$z(n_1, n_2, k) = z(n_1 - 1, n_2, k) + k z(n_1 - 1, n_2, k - 1) + (n_1 - 1) z(n_1 - 2, n_2, k),$$

and

$$z(n_1 - 1, n_2 + 1, k) - z(n_1, n_2, k) = n_2 z(n_1 - 1, n_2 - 1, k) - (n_1 - 1) z(n_1 - 2, n_2, k) - (n - k - 2) z(n_1 - 2, n_2 - 2, k).$$

Note that the first inequality holds since $n - k - 2 = n_1 + n_2 - 2 \geq 2 > 1$.

Now we assume that the equality in this lemma holds for all the integers less than $n_1 \geq 3$. Set $A = z(n_1 - 1, n_2 + 1, k) - z(n_1, n_2, k)$. Similarly, we have

$$A = n_2 z(n_1 - 1, n_2 - 1, k) - (n_1 - 1) z(n_1 - 2, n_2, k)$$

and

$$A = z(n_1 - 1, n_2 - 1, k) - (n_1 - 1) z(n_1 - 2, n_2 - 2, k).$$

Considering the induction assumption, the last inequality follows immediately. So this proof is completed. □
Lemma 2.5 ([3,22]). Let $T$ be a tree with $n$ vertices. If $T$ is different from $S_n$, then we have $z(T) > z(S_n) = n$ and $i(T) < i(S_n) = 2^{n-1} + 1$.

Next we turn to determining the maximal Hosoya index and minimal Merrifield–Simmons index of graphs from $V_{n,k}$. When $k = n - 1$, only one graph $K_n$ belongs to $V_{n,k}$ and there is nothing to prove. If $k = n - 2$, by Corollary 2.1, the unique graph from $V_{n,k}$ with maximal Hosoya index is $K_{n-2}^k$, and the minimal Merrifield–Simmons index of graphs from this set is uniquely attained at $K_{n-2}^k$, too. For the case when $k = n - 3$, similarly, we find that $K_{n-3}^k$ is the only one graph from $V_{n,k}$ with maximal Hosoya index and with minimal Merrifield–Simmons index. Therefore, in the following, we always assume that $1 \leq k < n - 3$ in $V_{n,k}$.

Theorem 2.1. Let $G \in V_{n,k}$. Then we have $z(G) \leq z(K_n^k) = zn_{-1} + kzn_{-2}$ with the equality holding if and only if $G \cong K_n^k$.

Proof. Let $G^*$ with $V(G^*) = \{v_1, v_2, \ldots, v_n\}$ be the graph with maximal Hosoya index in $V_{n,k}$. Without loss of generality, we assume that $V_1 = \{v_1, v_2, \ldots, v_k\}$ is a $k$-vertex cut of $G^*$. By Corollary 2.1(1), the subgraph of $G^*$ induced by $V_1$ must be a complete graph $K_k$. In the next step, we will prove the following three claims.

Claim 1. There are exactly two components in $G^* - V_1$.

To the contrary, we suppose that $G^* - V_1$ contains three components $G_1, G_2$ and $G_3$. Let $u \in V(G_1)$ and $v \in V(G_2)$. Clearly, $V_1$ is still a $k$-vertex cut of $G^* + uv \in V_{n,k}$. From Corollary 2.1(1), we have $z(G^* + uv) > z(G^*)$. This is a contradiction to the choice of $G^*$.

Therefore, $G^* - V_1$ has exactly two components, $G_1$ and $G_2$.

Claim 2. Each subgraph of $G^*$ induced by $V(G_i) \cup V_1$, for $i = 1, 2$ is a clique.

Otherwise, there are two nonadjacent vertices $u, v \in V(G_i) \cup V_1$ for $i = 1$ or $2$. Obviously, $G^* + uv \in V_{n,k}$. From Corollary 2.1(1), we have $z(G^* + uv) > z(G^*)$. This is a contradiction to the choice of $G^*$ again.

From Claim 2, $G_1$ and $G_2$ are all cliques too. Next we write $K_n$ instead of $G_i$ for $i = 1$ or $2$ where $n_i = |V(G_i)|$. From the definition of graph $K_n^k$, we find that $G^* \cong K_{n_1, n_2}^k$.

Claim 3. Either $n_1 = 1 = n_2$.

If not, we have $n_1 \geq 2$ and $n_2 \geq 2$. Without loss of generality, we assume that $n_2 \geq n_1 \geq 2$. Thanks to Lemma 2.4, we have $z^a(n_1 - 1, n_1 + 2) = z^b(n_1, n_2)$, that is, $z(K_{n_1-1, n_2+1}^k) > z(K_{n_1, n_2}^k)$. Note that $K_{n_1-1, n_2+1}^k$ still belongs to $V_{n,k}$. This contradicts the fact that $z(K_{n_1, n_2}^k)$ attains the maximum of the Hosoya index of graphs from $V_{n,k}$.

Now we have found that $G^* \cong K_{1, n-k+1}^k$. In view of Lemma 2.1(2), we have $z(K^k_n) = zn_{-1} + kzn_{-2}$, which ends the proof of this theorem. □

Theorem 2.2. Let $G \in V_{n,k}$. Then we have $i(G) \geq i(K_n^k) = 2n - k$ with the equality holding if and only if $G \cong K_n^k$.

Proof. Assume that $G^* \in V_{n,k}$ is a graph minimizing the Merrifield–Simmons index. On the basis of Corollary 2.1(2), by a similar reasoning to that in the proof of Theorem 2.1, we find that $G^*$ must be of the form $K_{n_1, n_2}^k$ with $n_1 + n_2 + k = n$. Then it suffices to prove the following claim.

Claim. Either $n_1 = 1$ or $n_2 = 1$.

Otherwise, we have $n_1 \geq 2$ and $n_2 \geq 2$. Without loss of generality, we assume that $n_2 \geq n_1 \geq 2$. By Lemmas 2.2(2) and 2.3(2), we have

\[ i(n_1, n_2, k) = i(n_1 - 1, n_2, k) + n_2, i(n_1 - 1, n_2 + 1, k) = i(n_1 - 1, n_2, k) + n_1 - 1, \] and

\[ i(n_1, n_2, k) - i(n_1 - 1, n_2 + 1, k) = n_2 - n_1 - 1 > 0. \]

Therefore, $i(K_{n_1-1, n_2+1}^k) < i(K_{n_1, n_2}^k)$. But this is impossible because of the minimality of $i(G^*) = i(K_{n_1, n_2}^k)$. By now we find that $G^* \cong K_{1, n-k+1}^k$. Applying Lemma 2.2(2) to the vertex of degree $k$ in $K_{n_1, n_2}^k$, by Lemma 2.3(2), we get $i(K_{n_1}^k) = 2n - k$, which completes the proof of this theorem. □

Since $K_{n_1}^k \in E_{n,k} \subseteq V_{n,k}$, the following corollary is obvious.

Corollary 2.2. Let $G \in E_{n,k}$. Then we have:

(1) $z(G) \leq z(K_{n_1}^k) = zn_{-1} + kzn_{-2}$ with the equality holding if and only if $G \cong K_{n_1}^k$.

(2) $i(G) \geq i(K_{n_1}^k) = 2n - k$ with the equality holding if and only if $G \cong K_{n_1}^k$.

From Corollary 2.1, the corollary below follows immediately.
Corollary 2.3. Let $G$ be a graph with $e \in E(G)$. Then we have:

1. $z(G - e) < z(G)$.
2. $i(G - e) > i(G)$.

Note that for any $e \in E(G)$ where $G \in V_{n,k}$ (resp. $E_{n,k}$), $G - e$ also belongs to $V_{n,k}$ (resp. $E_{n,k}$). Combining Lemma 2.5 and Corollary 2.3, we have the following two results, which will finish this work.

Corollary 2.4. Let $G \in V_{n,k}$. Then we have:

1. $z(G) \geq z(S_n) = n$ with the equality holding if and only if $G \cong S_n$.
2. $i(G) \leq i(S_n) = 2^{n-1} + 1$ with the equality holding if and only if $G \cong S_n$.

Corollary 2.5. Let $G \in E_{n,k}$. Then we have:

1. $z(G) \geq z(S_n) = n$ with the equality holding if and only if $G \cong S_n$.
2. $i(G) \leq i(S_n) = 2^{n-1} + 1$ with the equality holding if and only if $G \cong S_n$.

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