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Hosoya index of bridge and splice graphs

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ABSTRACT. The Hosoya index of a graph is defined as the total number of the matchings (including the empty edge set) of the graph. In this paper, explicit formulas are given for the Hosoya index of bridge and splice graphs.

Keywords: Hosoya index, bridge graphs, splices graphs.

1. INTRODUCTION

In this article, we are concerned with simple graphs that are finite and undirected graphs without loops and multiple edges. Let G be such a graph and $V(G)$ and $E(G)$ be its vertex set and edge set, respectively. An edge of G, connecting the vertices u and v will be denoted by uv. A molecular graph is a simple graph, such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted. Molecular descriptors play a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [9].

A topological index of a molecular graph G is a numeric quantity related to G which is invariant under the symmetry properties of G. The Hosoya index of a graph is a

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topological parameter to study the relation between molecular structure and physical and chemical properties of certain hydrocarbon compounds.

Two edges of a graph G are said to *be independent* if they possess no vertex in common. Let $E(G)$ be the edge set of graph G. Any subset of $E(G)$ containing no two mutually incident edges is called an independent edge set. The Hosoya index of a graph G is defined as the total number of independent edge sets of G, and denoted by $Z(G)$, that is,

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

where $m(G;k)$ denotes the number of ways in which k pairwise independent edges are selected in G; $k\geq 2$, in addition $m(G;0)=1$ and $m(G;1)=$ the number of edges of G.

For a molecular graph$G$, the Hosoya index $Z(G)$, or simply Z-index, is defined as the number of subsets of the edge set $E(G)$ in which no two edges are adjacent in G. In graph-theoretical terminology, $Z(G)$ is the total number of matching of G including the empty set.

The Hosoya index of a graph was introduced by Hosoya [5] in 1971 and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures [2,3,8].

For a vertex v of a graph G, we denote $N(v)=\{u| uv\in E(G)\}$ and if $W\subseteq V(G)$, we denote by $G-W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them. Similarly, if $E_0\subseteq E(G)$, we denote by $G-E_0$ the subgraph of G obtained by deleting the edges of E_0.

Suppose G_1 and G_2 are graphs with disjoint vertex sets. Following Došlić [4], for given vertices $x\in V(G_1)$ and $y\in V(G_2)$ a splice of G_1 and G_2 by vertices x and y, $(G_1\bullet G_2)(x,y)$, is defined by identifying the vertices x and y in the union of G_1 and G_2.

Let $\{G_i\}_{i=1}^{d}$ be a set of finite pairwise disjoint graphs with $v_i\in V(G_i)$. The *bridge graph*

$$B(G_1,G_2,...,G_d;v_1,v_2,...,v_d),$$

of with respect to the vertices $\{v_i\}_{i=1}^{d}$ is the graph obtained from the graphs $G_1,...,G_d$ by connecting the vertices v_i and v_{i+1} by an edge for all $i=1,2,...,d-1$. In the case that $i=2$, we denote $B(G_1,G_2;v_1,v_2)$, by $(G_1\sim G_2)(v_1,v_2)$.

Some topological indices of bridge and splice graphs are computed already [1,7]. In this paper we aim to compute the Hosoya index for these graphs.

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Lemma 1.1 ([6]). Let G be a graph with k components $G_1, G_2, ..., G_k$. Then

$$Z(G) = \prod_{i=1}^{k} Z(G_i).$$

Lemma 1.2 ([6]). Let G be a graph, and let $xy \in E(G)$ and $x \in V(G)$. Then

(i) $$Z(G) = Z(G - \{xy\}) + Z(G - \{x, y\});$$

(ii) $$Z(G) = Z(G - \{x\}) + \sum_{u \in N_G(x)} Z(G - \{u, x\}).$$

In particular, when x is a pendent vertex of G and u is the unique vertex adjacent to x, we have $Z(G) = Z(G - \{x\}) + Z(G - \{u, x\})$.

1. MAIN RESULT

In this section we give a formula for the Hosoya index of the bridge graph $(G_1 \sim G_2)(x, y)$ and the splice graph $G = G_1 \bullet G_2(x, y)$ in terms of the graphs G_i, $1 \le i \le 2$.

Theorem 2.1. Let G_1 and G_2 be graphs and $x \in E(G_1)$, $y \in E(G_2)$. Then

$$Z(G_1 \sim G_2(x, y)) = Z(G_1)Z(G_2) + Z(G_1 - \{x\})Z(G_2 - \{y\}).$$

Proof. Assuming that $G := G_1 \sim G_2(x, y)$ it is obvious that $G - \{xy\} = G_1 \bigcup G_2$ and

$$G - \{x, y\} = (G_1 - \{x\}) \bigcup (G_2 - \{y\}).$$

Therefore, by Lemma 1.1 we have:

$$\begin{aligned} Z(G - xy) &= Z(G_1)Z(G_2) \\ Z(G - \{x, y\}) &= Z(G_1 - \{x\})Z(G_2 - \{y\}). \end{aligned} \quad (1)$$

Thus by Lemma 1.2(i) and equation (1) we have:

$$\begin{aligned} Z(G) &= Z(G - xy) + Z(G - \{x, y\}) \\ &= Z(G_1)Z(G_2) + Z(G_1 - \{x\})Z(G_2 - \{y\}). \end{aligned}$$

Lemma 2.2. Let G_1 and G_2 be graphs and $x \in E(G_1)$, $y \in E(G_2)$. Assuming that $G = G_1 \bullet G_2(x, y)$ and $xu \in E(G)$. Then $Z(G - \{x, u\}) = Z(G_2 - \{y\})Z(G_1 - \{u, x\})$ if $u \in V(G_1)$; and $Z(G - \{x, u\}) = Z(G_1 - \{x\})Z(G_2 - \{u, y\})$ if $u \in V(G_2)$.

Proof. It is easy to see that $G-\{x,u\}=(G_2-\{y\})\bigcup(G_1-\{u,x\})$ if $u\in V(G_1)$. Then the result follows from Lemma 1.2 (ii).

Theorem 2.3. Let G_1 and G_2 be graphs and $x\in E(G_1), y\in E(G_2)$. Assuming that $G=G_1\bullet G_2(x,y)$ we have:

$$Z(G)=Z(G_1)Z(G_2-\{y\})+Z(G_2)Z(G_1-\{x\})-Z(G_1-\{x\})Z(G_2-\{y\})$$

Proof. It is clear that $G-\{x\}=G_1-\{x\}\bigcup G_2-\{y\}$ and so

$$Z(G-\{x\})=Z(G_1-\{x\})Z(G_2-\{y\}).$$

On the other hand, it follows from Lemma 2.2 that

$$\sum_{u\in N_G(x)} Z(G-\{u,x\})=\sum_{u\in N_{G_1}(x)}\left(Z(G_2-\{y\})Z(G_1-\{u,x\})\right)$$
$$+\sum_{u\hat{I}N_{G_2}(y)}\left(Z(G_1\text{-}\{x\})Z(G_2\text{-}\{u,y\})\right).$$

Hence by Lemma 1.2(ii) $Z(G)=Z(G-\{x\})+\sum_{u\in N_G(x)} Z(G-\{u,x\})$. By substituting $Z(G-\{x\})$ and $\sum_{u\in N_G(x)} Z(G-\{u,x\})$ in the above formula, we have:

$$Z(G)=Z(G_2-\{y\})\left(Z(G_1-\{x\})+\sum_{u\in N_{G_1}(x)} Z(G_1-\{u,x\})\right)+$$
$$Z(G_1-\{x\}\left(Z(G_2-\{y\}+\sum_{u\in N_{G_2}(y)}\left(Z(G_2-\{u,y\})\right)-Z(G_1-\{x\})\,Z(G_2-\{y\}).$$

It follows from Lemma 1.2(ii) that

$$Z(G)=Z(G_1)Z(G_2-\{y\})+Z(G_2)Z(G_1-\{x\})-Z(G_1-\{x\})Z(G_2-\{y\}).$$

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