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Ordering chemical graphs by Randić and sum-connectivity numbers

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ABSTRACT

Let G be a graph with edge set $E(G)$. The Randić and sum-connectivity indices of G are defined as $R(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{deg_G(u)deg_G(v)}}$ and $SCI(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{deg_G(u)+deg_G(v)}}$, respectively, where $deg_G(u)$ denotes the vertex degree of u in G. In this paper, the extremal Randić and sum-connectivity index among all n-vertex chemical trees, $n\geq 13$, connected chemical unicyclic graphs, $n\geq 7$, connected chemical bicyclic graphs, $n\geq 6$ and connected chemical tricyclic graphs, $n\geq 8$, were presented.

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1. Definitions and notations

In this section, we fix our notations and recall some basic definitions that will be used later. All graphs considered in this note are finite, undirected, loopless and without multiple edges. Undefined terms and notations can be found in [10,12]. Let G be such a graph with vertex and edge sets $V(G)$ and $E(G)$, respectively.

The degree of a vertex v in G, $deg_G(v)$ ($deg(v)$ for short), is the number of edges incident to v and $N[v,G]$ denotes the set of all vertices adjacent to v. A vertex with degree one is called a *pendent vertex*. The notations $\Delta=\Delta(G)$ and $n_i=n_i(G)$ are denoted the maximum degree and the number of vertices of degree i in G, respectively. Note that $\sum_{i=1}^{\Delta(G)} n_i=|V(G)|$. The number of edges connecting a vertex of degree i with a vertex of degree j in G is denoted by $m_{i,j}(G)$. We label the vertex set $V(G)=\{v_1,\ldots,v_n\}$ in such a way that $deg_G(v_1)\geq deg_G(v_2)\geq\cdots deg_G(v_n)$ and define $d_k(G)=deg_G(v_k)$, $1\leq k\leq n$. The sequence $D(G)=(d_1,d_2,\ldots,d_n)$ is called the *degree sequence* of G. If $\{deg_G(v_1),\ldots,deg_G(v_n)\}=\{x_1,\ldots,x_t\}$, $x_1>x_2\cdots x_t$, and G has exactly a_1 vertex of degree x_1, a_2 vertex of degree x_2, …, a_t vertex of degree x_t then we use the following compact notation for degree sequence of G:

$$D(G)=(\overbrace{x_1,\ldots,x_1}^{a_1\ times},\overbrace{x_2,\ldots,x_2}^{a_2\ times},\ldots,\overbrace{x_t,\ldots,x_t}^{a_t\ times})=(x_1^{a_1},x_2^{a_2},\ldots,x_t^{a_t}).$$

Notice that $a_1+a_2+\ldots+a_t=n$.

If $W\subseteq V(G)$ then $G-W$ will be the subgraph of G obtained by deleting the vertices of W and similarly, for a subset F of $E(G)$, the subgraph obtained by deleting all edges in F is denoted by $G-F$. In the case that $W=\{v\}$ or $F=\{xy\}$, the subgraphs $G-W$ and $G-F$ will shortly be written as $G-v$ or $G-xy$, respectively. Moreover, for two nonadjacent vertices x and y in G, the notation $G+xy$ is used for the graph obtained from G by adding an edge xy.

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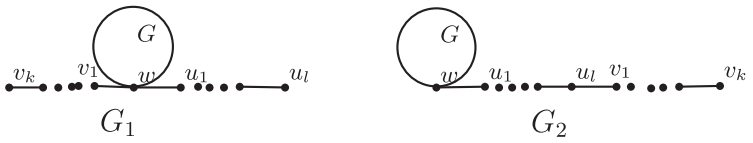

Fig. 1. The graphs G, P, Q, G_1 and G_2 in Transformation A.

A *chemical graph* is a graph having maximum degree at most four and if the graph is a tree, then the word *chemical tree* will be used. The set of all $n-$vertex chemical trees will be denoted by $\tau(n)$, see [7,11]. In this paper, the path and the star graphs with exactly n vertices are denoted by P_n and S_n, respectively. In this paper, we continue our earlier works on ordering chemical trees by some topological indices [1,8]. For some other related works see [2,3,17,18].

2. Randić and sum-connectivity indices of chemical graphs

Suppose G is an undirected simple graph. The Randić and sum-connectivity indices of G are defined as $R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{deg_G(u)deg_G(v)}}$ and $SCI(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{deg_G(u)+deg_G(v)}}$, respectively, where $deg_G(u)$ denotes the vertex degree of u in G. The Randić index was proposed by Randić [14] and most of its mathematical properties were presented in [10,12]. Motivated by the work of Randić, the notion of sum-connectivity index was presented by Zhou and Trinajstić [19]. The aim of this paper is to improve earlier results on ordering chemical trees by these graph invariants.

In the following, we first briefly review the literature on ordering graphs with Randić and sum-connectivity index. To do this, we fix our notation. An $n-$vertex graph G is called unicyclic, bicyclic, tricyclic or tetracyclic, if it has $n+c$ edges such that $c = 0, 1, 2, 3,$ respectively. On of the present authors (ARA) [5,6] computed the the first and second maximum of Randić index in the class of all $n-$vertex tricyclic and tetracyclic graphs, respectively. Shiu and Zhang [16] found the maximum Randić index of chemical trees for $n < 3k-2$. They also constructed examples of chemical trees corresponding to the maximum Randić index. Shi [15] obtained among others some results for chemical trees with respect to two generalizations of Randić index. We refer also to [13] for a complete survey on the topic of Randić index.

Zhou and Trinajstić [19], were determined the unique tree with fixed numbers of vertices and pendent vertices with the minimum value of the sum-connectivity index, and trees with the minimum, second minimum, third minimum, the maximum, second maximum and third maximum values of the sum-connectivity index. Das and Dehmer [4] presented an upper bound for the sum-connectivity index of graphs. They also proved that the Randić index is greater than the sum-connectivity index for trees.

3. Some graph transformations

In this section, some graph transformations are presented by which we can increase the Randić and sum-connectivity indices of chemical graphs. By applying these graph operations, we identify the class of chemical trees, chemical unicyclic graphs and chemical bi-cyclic graphs with the extremal Randić and sum-connectivity numbers.

Transformation A. Suppose G is a graph with a given vertex w such that $deg_G(w) = 1$ or 2. In addition, we assume that $P := v_1v_2, \ldots, v_k$ and $Q := u_1u_2, \ldots, u_l$ are two paths with k and l vertices, respectively. Let G_1 be the graph obtained from G, P and Q by attaching edges v_1w and wu_1. Define $G_2 = G_1 - v_1w + u_kv_1$. The above referred graphs have been illustrated in Fig. 1.

Lemma 3.1. *Let G_1 and G_2 be two graphs as shown in Fig. 1. Then $R(G_2) > R(G_1)$ and $SCI(G_2) > SCI(G_1)$.*

Proof. Suppose $x = d_G(w)$, $N[w, G] = \{l_1, \ldots, l_x\}$, $d_G(l_i) = d_i$, $1 \le i \le x$, and $k, l \ge 2$. Since $x = 1$ or 2 and by definition,

$$\begin{aligned} R(G_2) - R(G_1) &= \left(\frac{1}{\sqrt{2(x+1)}} + 1 + \sum_{i=1}^{x} \frac{1}{\sqrt{d_i(x+1)}}\right) \\ &\quad - \left(\frac{2}{\sqrt{2(x+2)}} + \frac{1}{\sqrt{2}} + \sum_{i=1}^{x} \frac{1}{\sqrt{d_i(x+2)}}\right) \\ &> \left(\frac{1}{\sqrt{2(x+1)}} + 1\right) - \left(\frac{2}{\sqrt{2(x+2)}} + \frac{1}{\sqrt{2}}\right) > 0, \\ SCI(G_2) - SCI(G_1) &= \left(\frac{1}{\sqrt{x+3}} + 1 + \sum_{i=1}^{x} \frac{1}{\sqrt{d_i + x + 1}}\right) \end{aligned}$$

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