On General Sum-Connectivity Index of Benzenoid Systems and Phenylenes

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ABSTRACT

The general sum-connectivity index of a graph G, denoted by $\chi_a = \chi_a(G)$ is defined as $\chi_a = \sum_{uv \in E(G)} (d_u + d_v)^a$, where d_u (or d_v) is the degree of the vertex u (or v). Efficient formulas for calculating the general sum-connectivity index of benzenoid systems and their phenylenes are given, and a relation is established between the general sum-connectivity index of a phenylene and of the corresponding hexagonal squeeze in this paper.

Key words: general sum-connectivity index; benzenoid systems; phenylene; hexagonal squeeze.

1   INTRODUCTION

The well-known Randic index (connectivity index), introduced by chemist Randić [1] in 1975 under the name "*the branching index*", which is now also called " the Randic index" or " *the connectivity index*", is a graph-based molecular structure descriptor that is most frequently applied in quantitative structure-property and structure-activity studies [2−6]. It is defined as the sum over all edges of the (molecular) graph of the terms $(d_u d_v)^{-1/2}$, where u and v are the vertices of the edge $uv \in E(G)$, and d_u (or d_v) is the degree of the vertex u (or v), i.e.,

$$R = R(G) = \sum_{uv \in E(G)} (d_u d_v)^{-\frac{1}{2}} \qquad (1)$$

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The sum-connectivity index of the graph G, denoted by $\chi = \chi(G)$, is defined as [7]:

$$\chi = \chi(G) = \sum_{uv \in E(G)} (d_u + d_v)^{-\frac{1}{2}} \tag{2}$$

For convenience, we might sometimes call $R(G)$ the product-connectivity index of G. These two molecular descriptors are highly intercorrelated quantities [8]. In [7], the authors provided several basic properties for sum-connectivity index,

especially lower and upper bounds in terms of sum-connectivity index, determined the unique tree with given numbers of vertices and pendant vertices with the minimum value of the sum-connectivity index, and trees with the minimum, second minimum and third minimum, and with the maximum, second maximum and third maximum values of the sum-connectivity index, and discussed properties of the sum-connectivity index for a class of trees representing acyclic hydrocarbons. In [9], some properties of the sum-connectivity index for trees and unicyclic graphs with given matching number were obtained.

Motivated by the Randic index, in 1998 B. Bollobas and P. Erdos[10] introduced the general Randic index:

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha \tag{3}$$

where a is any real number, and $(d_u d_v)^\alpha$ is also called the *a weight* of the edge *uv*. The properties of the general Randic index may be found in [11−16].

Similar to the definition of the general Randic index, the general sum−connectivity index was defined in [17]:

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha \tag{4}$$

the general sum-connectivity index generalized both the ordinary sum-connectivity index and the first Zagreb index, and in [17], the authors gave some basic properties about the general sum-connectivity index.

In this report, we investigate the general sum−connectivity index of benzenoid systems and phenylenes.

2   PRELIMINARIES

Some basic concepts is necessary. A i−vertex denotes a vertex degree i, and a (j,k)−edge stands for an edge connecting a j−vertex with a k−vertex, and let n_i denote the number

of i−vertex, m_{jk} be the number of (j,k)−edge, respectively. Then, the general sum−connectivity index of any graph G with n vertices can be rewritten as

$$\chi_\alpha(G) = \sum_{1 \le j \le k \le n-1} m_{jk}(j+k)^\alpha \tag{5}$$

In the case of a benzenoid system S, which possesses only (2,2)−, (2,3)− and (2,3)−edges, the above formula reduces to

$$\chi_\alpha(G) = m_{22}4^\alpha + m_{23}5^\alpha + m_{33}6^\alpha \tag{6}$$

For the simplicity of the expression (6), we only need calculate m_{22}, m_{23} and m_{33}. Before our main results, we introduce some notions of the benzenoid systems.

As described in [18], we introduce the number of inlets, r, a novel parameter related in the manner to the structure of benzenoid systems and/or phenylenes proposed by Cyvin *et al* [19-21], and show that the general sum-connectivity index is the function of r. Thus,

B=number of simple bays; C=number of coves; F=number of fjords;
f=number of fissures; L=number of lagoons; b=number of regions.

Note that Bays, coves, and fjords, fissures and lagoons are structural characteristics of the perimeter of the benzenoid systems playing some role in their theory. An illustrative example is depicted in Figure 1.
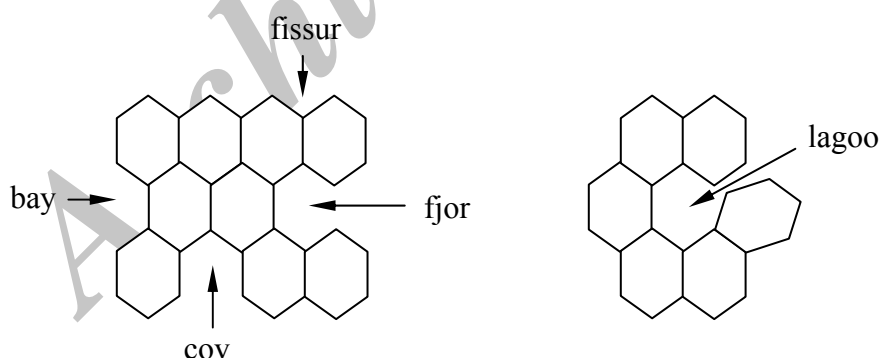
Figure 1. Types of inlets occurring on the perimeter of a benzenoid system.

Let r be the total number of inlets on the perimeters of a benzenoid system described above, it is easy to see that

$$b = B + 2C + 3F + 4L;$$
$$r = B + C + F + f + L.$$

3   THE GENERAL SUM-CONNECTIVITY INDEX OF BENZENOID SYSTEMS

Theorem 1. Let S be a benzenoid system with n vertices, h hexagons and r inlets. Then

$$\chi_\alpha(S) = (n - 2h - r + 2) \cdot 4^\alpha + 2r \cdot 5^\alpha + (3h - r - 3) \cdot 6^\alpha$$

Proof By the definition of an inlet, an inlet corresponds to a sequence of vertices on the perimeter, of which the first and the last are 2-vertices and all other 3-vertices, thus, we have

$$m_{23} = 2r \tag{7}$$

The number of 3-vertices in a benzenoid system S, is

$$n_3 = 2(h - 1) \tag{8}$$

and it follows that

$$m_{23} + m_{33} = 3n_3 = 6h - 6 \tag{9}$$

By combing (7) with (9), we have

$$m_{33} = 3h - r - 3 \tag{10}$$

In benzenoid systems,

$$m_{22} + m_{23} + m_{33} = m \tag{11}$$

is the total number of edges, and $m = n + h - 1$. Substituting relations (7) and (10) into (11), we arrive at

$$m_{22} = n - 2h - r + 2 \tag{12}$$

Substituting relations (7), (10) and (12) into equation (6), we directly obtain the desired result. This completes the proof.

Corollary 2. Let S be a benzenoid system with n vertices, h hexagons and r inlets. Then

$$\chi(S) = \frac{n}{2} - \frac{2-\sqrt{6}}{2}h - \frac{15-12\sqrt{5}+5\sqrt{6}}{30}r + \frac{2-\sqrt{6}}{2}$$

4   THE GENERAL SUM-CONNECTIVITY INDEX OF PHENYLENES

Phenylenes are a class of chemical compounds in which the carbon atoms form 6- and 4-membered cycles. Each 4-membered cycle(=square) is adjacent to two disjoint 6-membered cycles(=hexagons), and no two hexagons are adjacent[22]. By eliminating, "squeezing out", the squares from a phenylene, a catacondensed hexagonal system (which may be jammed) is obtained, called the hexagonal squeeze of the respective phenylene [23]. Clearly, there is a one-to-one correspondence between a phenylene (PH) and its hexagonal squeeze (HS). Both possess the same number (h) of hexagons. In addition, a phenylene with h hexagons possesses h-1 squares. The number of vertices of PH and HS are 6h and 4h+2, respectively; The number of edges of PH and HS are 8h-2 and 5h+1, respectively. An example of phenylene and its hexagonal squeeze is shown in Figure 2.

PH   HS
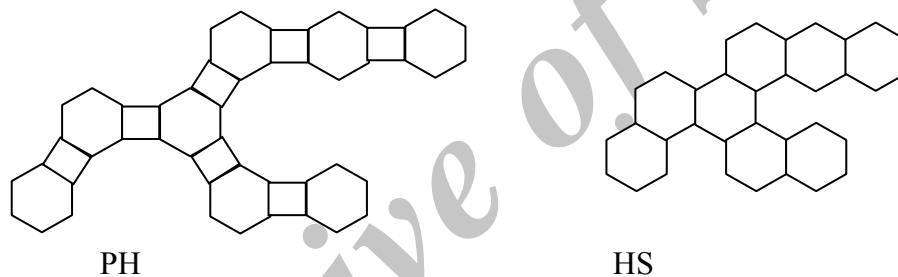
Figure 2. A phenylene (PH) and its hexagonal squeeze (HS).

In the case of phenylenes, a fissure, bay, cove, fjord, and lagoon are defined in full analogy to the benzenoid systems: A fissure (respectively. a bay, cove, fjord, or lagoon) corresponds to a sequence of four (*resp.* six, eight, ten, and twelve) consecutive vertices on the perimeter, of which the first and the last are 2-vertices and the rest are 3-vertices. Similar to the discussion of Theorem 1, we have

Theorem 3. Let PH be a phenylene with h hexagons and r inlets. Then

$$\chi_\alpha(PH) = (2h - r + 4)\cdot 4^\alpha + 2r\cdot 5^\alpha + (6h - r - 6)\cdot 6^\alpha$$

Proof The proof is analogous to the proof of Theorem 1.

The number of 3-vertice is $n_3 = 4(h-1)$, whereas the number of edge is $m = n + (2h-1) - 1 = 8h - 2$. Thus,

$$m_{22} = 2h - r + 4 \tag{13}$$

$$m_{23} = 2r \tag{14}$$

$$m_{33} = 6h - r - 6 \tag{15}$$

Substituting relations (13)–(15) into equation (6), we arrive at the result. Note that a phenylene with h hexagons has $6h$ vertices. Inserting relations (13)–(15) back into (2), we readily arrive at:

Corollary 4. Let PH be a phenylene with n vertices and r inlets. Then

$$\chi(PH) = (1 + \sqrt{6})h - \frac{15 - 12\sqrt{5} + 5\sqrt{6}}{30} r + 2 - \sqrt{6}$$

5   A R<small>ELATION OF THE</small> G<small>ENERAL</small> S<small>UM–</small>C<small>ONNECTIVITY</small> I<small>NDEX</small> B<small>ETWEEN</small> PH <small>AND</small> HS

In the following, we establish a relation between the general sum-connectivity index of a phenylene and of the corresponding hexagonal squeeze.

For the hexagonal squeeze HS of a phenylene, HS may be jammed (which possesses lagoons). Since a phenylene with n vertices has $n/6$ hexagons, its hexagonal squeeze has $4.(n/6) + 2$ vertices.

By comparing Theorem 2 with Theorem 4, we have:

Theorem 5. Let PH be a phenylene with h hexagons and HS its hexagonal squeeze. Then

$$\chi_\alpha(PH) = \chi_\alpha(HS) + 3(h-1) \cdot 6^\alpha$$

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