Second Order Randić Index of Benzenoid Systems

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Abstract

Given S a benzenoid system, we find an expression of the second order Randić index, denoted by ${}^2\chi(S)$, in terms of inlet features of S. As a consequence, we classify benzenoid systems with equal ${}^2\chi$ and then find the minimal and maximal value over the set of catacondensed systems.

1 Introduction

The connectivity index (or Randić index) of a graph G, denoted by $\chi(G)$, was introduced by Randić [16] in the study of branching properties of alkanes. It is defined as

$$\chi(G) = \sum_{uv} \frac{1}{\sqrt{\delta_u \delta_v}}$$

where δ_u denotes the degree of the vertex u and the summation is taken over all pairs of adjacent vertices of the graph G.

A part of the current research in the mathematical properties of the connectivity index, involves the problem of finding minimal and maximal values of χ over significant classes of graphs. For instance (see [1],[2] and [8]), among all graphs without isolated vertices, the star has minimal connectivity index and the graph in which all components are regular graphs has maximal connectivity index. Restricting to the set of all trees with a fixed number of vertices, Caporossi et al. [3] proved that the path tree has maximal connectivity index. Other publications related to this problem can be found in the literature ([4],[7],[9] and [17]).

With the intention of extending the applicability of the connectivity index, Randić, Kier, Hall and co-workers ([10] and [11]) considered the higher-order connectivity indices of a general graph G as

$$^h\chi(G) = \sum_{u_1 u_2 \cdots u_{h+1}} \frac{1}{\sqrt{\delta_{u_1} \cdots \delta_{u_{h+1}}}}$$

where the summation is taken over all possible paths of length h of G (we do not distinguish between the paths $u_1u_2\cdots u_{h+1}$ and $u_{h+1}u_h\cdots u_1$). This new approach has been applied successfully to an impressive variety of physical, chemical and biological properties (boiling points, solubilities, densities, anesthesic, narcotic, toxicities etc.) which have appeared in several hundred scientific publications and in two books ([10] and [12]). Results related to the mathematical properties of these indices have been reported in the literature ([1] and [14]).

Our main concern is the class of benzenoid systems, graph representations of benzenoid hydrocarbons which are of great importance in chemistry. A benzenoid system is a finite connected plane graph without cut vertices, in which all interior regions are mutually congruent regular hexagons (we exclude the hollow coronoid species from the class of benzenoid systems). More details on this class of graphs can be found in [6].

Following the terminology proposed by Cyvin and Gutman ([5] and [6]), an hexagon of a benzenoid system can be classified according to the number and position of edges shared with the adjacent hexagons. Figure 1 shows the 12 different types of hexagons that can occur in a benzenoid system with more than one hexagon.

Figure 1

We can associate to each path $u_1u_2\cdots u_{h+1}$ of length h of a benzenoid system S, the vertex degree sequence $(\delta_{u_1},\delta_{u_2},\cdots\delta_{u_{h+1}})$. If one goes along the perimeter of S, then a fissure, bay, cove and fjord, are respectively, paths of degree sequences $(2,3,2)$, $(2,3,3,2)$, $(2,3,3,3,2)$ and $(2,3,3,3,3,2)$ (see Figure 1). The number of fissures, bays, coves and fjords are denoted, respectively, by $f(S)$, $B(S)$, $C(S)$ and $F(S)$.

A new parameter $r(S) = f(S) + B(S) + C(S) + F(S)$, called the number of inlets of S, was introduced in [13] and a simple relation with the connectivity index was established; namely,

$$\chi(S) = \frac{n(S)}{2} - \frac{5-2\sqrt{6}}{6}r(S), \qquad (1)$$

where $n(S)$ is the number of vertices of S. If we restrict ourselves to the class of catacondensed systems, i.e. benzenoid systems with no internal vertices or, equivalently, benzenoid systems which posseses only hexagons of the type L_1, L_2, A_2 and A_3, then equation 1 can be used to find the minimal and maximal value of χ over the set of all catacondensed systems with a fixed number of hexagons [15].

In this work we derive an expression for ${}^2\chi(S)$ in terms of structural features of S. Since all vertices in a benzenoid system S have degrees equal to 2 or 3, the paths of length 2 of S have degree sequences $(2,2,2)$, $(2,3,2)$, $(2,2,3)$, $(2,3,3)$, $(3,2,3)$ and $(3,3,3)$. It follows that

$${}^2\chi(S) = \frac{1}{\sqrt{8}}m_{222} + \frac{1}{\sqrt{12}}(m_{232} + m_{223}) + \frac{1}{\sqrt{18}}(m_{233} + m_{323}) + \frac{1}{\sqrt{27}}m_{333}, \qquad (2)$$

where m_{ijk} denotes the number of paths with degree sequence (i, j, k). In Theorem 2, we show that the second order connectivity index of S is completely determined by the number of vertices $n(S)$, hexagons $h(S)$, inlets $r(S)$, fissures $f(S)$ and adjacent inlets $a(S)$ (i.e., number of pairs of inlets that have a common vertex of degree 2). As a consequence, in Corollary 3 we classify benzenoid systems with equal second order connectiviy index.

The expression obtained for $^2\chi$ in terms of inlet features is applied in Theorem 6 to prove that, among all catacondensed systems with h hexagons, the linear polyacene L_h has maximal and the ladder-type catacondensed system E_h has minimal second order connectivity index.

2 Second order Randić index of benzenoid systems

In order to express the second order connectivity index of a general benzenoid system in terms of the number of inlets, we begin by proving two reduction formulas. But first, let us introduce the notation which we use in the sequel. If S is a benzenoid system with n vertices, m edges and h hexagons, then

n_j = number of vertices of degree j ($j = 2, 3$);
n_i = number of internal vertices;
m_e = number of external edges (i.e., edges lying on the perimeter of S);
m_i = number of internal edges (i.e., non-external edges of S).

Relations between these structural invariants of benzenoid systems can be found in [6]. Of particular interest in our next results are the relations $m = n + h - 1$, $n_3 = 2(h-1)$ and $n_i = 4h + 2 - n$.

Lemma 1 *Let S be a benzenoid system with n vertices and h hexagons ($h \geq 2$). Then*

1. $m_{33} + 2m_{323} + 3m_{3223} + 4m_{32223} + 5m_{322223} = n + h - 1$;
2. $m_{33} + m_{323} + m_{3223} + m_{32223} + m_{322223} = 3(h-1)$;

   where $m_{32\cdots23}$ represents the number of paths of degree sequence $(3, 2, \ldots, 2, 3)$ in S.

Proof. 1. We know that

$$m = m_i + m_e = m_{33} + \sum_{i=1}^{4} (i+1)\, m_{3,\underbrace{2,\ldots,2}_{i},3}$$

since each path of S of degree sequence $\left(3, \underbrace{2, \ldots, 2}_{i}, 3\right)$ has $i+1$ (external) edges.
The result follows from the relation $m = n + h - 1$.

2. It is clear that

$$n_2 = \sum_{i=1}^{4} i \cdot \left(m_{3,\underbrace{2,\ldots,2}_{i},3} \right) = n - n_3$$

since every path of S of degree sequence $\left(3,\underbrace{2,\ldots,2}_{i},3\right)$ has i vertices of degree 2. Hence, by the equation of part 1 and bearing in mind that $n_3 = 2(h-1)$, we conclude that

$$\begin{aligned}\sum_{i=0}^{4} m_{3,\underbrace{2,\ldots,2}_{i},3} &= \sum_{i=0}^{4} (i+1)\, m_{3,\underbrace{2,\ldots,2}_{i},3} - \sum_{i=1}^{4} i \cdot \left(m_{3,\underbrace{2,\ldots,2}_{i},3} \right) \\ &= (n+h-1) - (n-n_3) = 3(h-1)\end{aligned}$$

■

Theorem 2 *Let S be a benzenoid system with n vertices, h hexagons, r inlets, f fissures and a adjacent inlets. Then*

$$^2\chi(S) = \alpha n + \beta h + \gamma r + \delta f + \epsilon a + \eta$$

where $\alpha = \frac{\sqrt{2}}{4}$, $\beta = \frac{4\sqrt{3}-3\sqrt{2}}{6}$, $\gamma = \frac{3\sqrt{2}-2\sqrt{3}}{18}$, $\delta = \frac{5\sqrt{3}-6\sqrt{2}}{18}$, $\epsilon = \frac{5\sqrt{2}-4\sqrt{3}}{12}$ *and* $\eta = \frac{3\sqrt{2}-4\sqrt{3}}{6}$.

Proof. Using the equations of Lemma 1 and the relation $m_{33} = 3h - r - 3$ [13, Lemma 1], we express each of the m_{ijk} of equation (2) in terms of n, h, r, f and a. First of all, it is clear that $m_{323} = a$ and $m_{232} = f$. Furthermore,

$$\begin{aligned}m_{222} &= m_{32223} + 2m_{322223} \\ &= (4-3)m_{32223} + (5-3)m_{322223} \\ &= (4m_{32223} + 5m_{322223}) - 3(m_{32223} + m_{322223}) \\ &= [(n+h-1) - (m_{33} + 2m_{323} + 3m_{3223})] \\ &\quad -3[3(h-1) - (m_{33} + m_{323} + m_{3223})] \\ &= n - 8h + 2m_{33} + m_{323} + 8 \\ &= n - 8h + 2(3h - r - 3) + a + 8 \\ &= n - 2h - 2r + a + 2;\end{aligned}$$

$$\begin{aligned}m_{223} &= 2m_{3223} + 2m_{32223} + 2m_{322223} \\ &= 2(m_{3223} + m_{32223} + m_{322223}) \\ &= 2[3(h-1) - (m_{33} + m_{323})] \\ &= 6h - 2m_{33} - 2m_{323} - 6 \\ &= 6h - 2(3h - r - 3) - 2a - 6 \\ &= 2(r - a);\end{aligned}$$

and

$$\begin{aligned} m_{233} &= 2f + 4(B + C + F) \\ &= 2f + 4(r - f) \\ &= 4r - 2f. \end{aligned}$$

To find m_{333} we use the fact that every path in S of the form $(3,3,3)$ has all its edges in the same hexagon unless they belong to a cove or a fjord. Hence,

$$m_{333} = 6h - 6m_{322223} - 5m_{32223} - 4m_{3223} - 3m_{323} + C + 2F.$$

But

$$\begin{aligned} -6m_{322223}-5m_{32223}-4m_{3223}-3m_{323} &= -(5m_{322223} + 4m_{32223} + 3m_{3223} + 2m_{323}) \\ &\quad -(m_{322223} + m_{32223} + m_{3223} + m_{323}) \\ &= -(n + h - 1 - m_{33}) - [3(h - 1) - m_{33}] \\ &= -n - 4h + 2m_{33} + 4 \\ &= -n - 4h + 2(3h - r - 3) + 4 \\ &= 2h - n - 2r - 2. \end{aligned}$$

In order to calculate $C + 2F$, we first note that the number of external vertices of degree 3 is given by the expression $4F + 3C + 2B + f$. Consequently,

$$4F + 3C + 2B + f = n_3 - n_i.$$

Since $n_3 = 2(h - 1)$ and $n_i = 4h + 2 - n$ we deduce that

$$4F + 3C + 2B + f = n - 2h - 4.$$

By definition of the number of inlets

$$F + C + B + f = r$$

and so from these two last relations we obtain

$$C + 2F = n - 2h - 2r + f - 4.$$

Therefore,

$$\begin{aligned} m_{333} &= 6h + (2h - n - 2r - 2) + (n - 2h - 2r + f - 4) \\ &= 6h - 4r + f - 6. \end{aligned}$$

Now the result follows by substituting the values of m_{ijk} obtained above in equation (2). ■

Our next result classifies benzenoid systems that have equal second order Randić index.

Corollary 3 *Let S and S' be benzenoid systems such that $n(S) = n(S')$ and $h(S) = h(S')$. The following conditions are equivalent:*

(i) ${}^2\chi(S) = {}^2\chi(S')$;

(ii) $-2[r(S) - r(S')] = f(S) - f(S') = a(S) - a(S')$.

Proof. Let $u = r(S) - r(S')$, $v = f(S) - f(S')$ and $w = a(S) - a(S')$. Since $n(S) = n(S')$ and $h(S) = h(S')$, we know by Theorem 2 that

$$\begin{aligned} 36\left({}^2\chi(S) - {}^2\chi(S')\right) &= 2\left(3\sqrt{2} - 2\sqrt{3}\right)u + 2\left(5\sqrt{3} - 6\sqrt{2}\right)v \\ &\quad +3\left(5\sqrt{2} - 4\sqrt{3}\right)w \\ &= (6u - 12v + 15w)\sqrt{2} + (-4u + 10v - 12w)\sqrt{3}. \end{aligned}$$

The fact that $\left\{\sqrt{2}, \sqrt{3}\right\}$ is a linearly independent set over $\mathbb{Q}$ implies that ${}^2\chi(S) = {}^2\chi(S')$ if, and only if,

$$\begin{aligned} 2u - 4v + 5w &= 0 \\ -2u + 5v - 6w &= 0 \end{aligned}$$

and the solution for this system is $-2u = v = w$. ■

Example 4 *Consider the benzenoid systems*

Figure 2

Note that $r(S) = r(S') = 5$, $f(S) = f(S') = 2$ and $a(S) = a(S') = 0$. Consequently, ${}^2\chi(S) = {}^2\chi(S')$.

The following example illustrates the situation in which $r(T) \neq r(T')$, $f(T) \neq f(T')$ and $a(T) \neq a(T')$, but still ${}^2\chi(T) = {}^2\chi(T')$.

Example 5 *Consider the benzenoid systems*

Figure 3

Note that $h(T) = h(T') = 16$ and $n(T) = n(T') = 66$. Moreover, $a(T) = 2$, $f(T) = 6$, $r(T) = 17$ and $a(T') = 4$, $f(T') = 8$, $r(T') = 16$. Then condition (ii) of Corollary 3 is satisfied and consequently, ${}^2\chi(T) = {}^2\chi(T')$.

In Theorem 2 we reduced the number of parameters that occur in ${}^2\chi(S)$ from 6 (equation 1) to 5 (Theorem 2). Actually, we can reduce it to 4 when considering catacondensed systems. In this type of systems we have the relation

$$n = 4h + 2$$

which gives

$${}^2\chi(S) = \mu h + \gamma r + \delta f + \epsilon a + \rho \tag{3}$$

where $\mu = \frac{3\sqrt{2}+4\sqrt{3}}{6}$, $\rho = \frac{3\sqrt{2}-2\sqrt{3}}{3}$ and γ,δ,ϵ as in Theorem 2. We will now use this relation to find the minimal and maximal value of ${}^2\chi$ over $\mathbb{C}_h$, the set of all catacondensed systems with h hexagons.

For a positive integer k, let $H(k)$ denote the catacondensed ladder system, as shown in Figure 4

Figure 4

We can use $H(k)$ as the basic structure to construct catacondensed systems with minimal number of inlets, fissures and adjacent inlets as follows: let E_4 be as in Figure 5 and if $h \geq 6$ is even, let E_h be the catacondensed system obtained from $H(\frac{h-2}{2})$ by adding two hexagons, one to the A_2 hexagon on the top and the other to the A_2 hexagon on the bottom

Figure 5

In the odd case, E_3, E_5 and E_7 are shown in Figure 6 and if $h \geq 9$ is odd, let E_h be the catacondensed system constructed from $H(\frac{h-5}{2})$ by adding E_4 to the A_2 hexagon of the bottom and an hexagon to the A_2 hexagon of the top

Figure 6

The following table contains information related to the inlet counts in each of the catacondensed systems defined above:

	f	r	a
L_h $(h \geq 2)$	$2(h-1)$	$2(h-1)$	$2(h-2)$
E_h $(h \geq 6)$	0	$\lceil\frac{h+3}{2}\rceil$	0

where $\lfloor x \rfloor$ is the integer part of x.

Theorem 6 *For all $h \geq 3$, if $S \in \mathbb{C}_h$ then*

$$ {}^2\chi(E_h) \leq {}^2\chi(S) \leq {}^2\chi(L_h). $$

Proof. It was shown in [15, Propositions 1 and 3], that if $S \in \mathbb{C}_h$ and $h \geq 3$ then

$$ r(E_h) = \left\lceil \frac{h+3}{2} \right\rceil \leq r(S) \leq r(L_h). $$

Moreover,

$$ f(E_h) = 0 \leq f(S) \leq r(S) \leq r(L_h) = f(L_h) $$

for $h = 4$ and $h \geq 6$. Finally, since S is a catacondensed system, it follows that $a(S) = 2l_2$ and $l_1 \geq 2$, where l_1 and l_2 denote the number of L_1 and L_2 hexagons in S. Consequently,

$$ a(E_h) = 0 \leq a(S) = 2l_2 \leq 2(h-l_1) \leq 2(h-2) = a(L_h). $$

This implies that ${}^2\chi(E_h) \leq {}^2\chi(S) \leq {}^2\chi(L_h)$ for $h = 4$ and $h \geq 6$, in view of relation (3); and the remaining cases when $h = 3$ or 5 can easily be checked seperately. ■

Remark 7 *Note that if we define* $E_1 = L_1$ *and* $E_2 = L_2$ *then Theorem 6 holds trivially for* $h = 1$ *and* 2, *since* $\mathbb{C}_1 = \{L_1\}$ *and* $\mathbb{C}_2 = \{L_2\}$.

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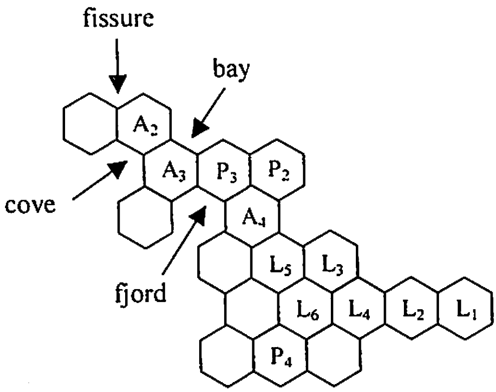


Figure 1

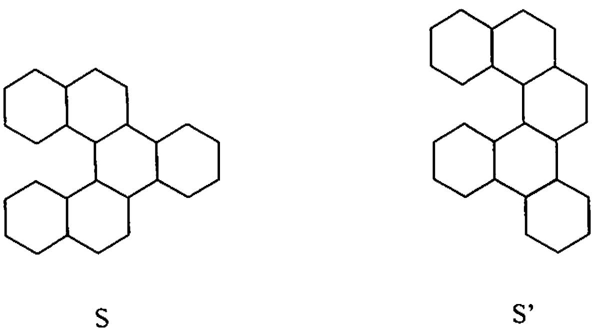
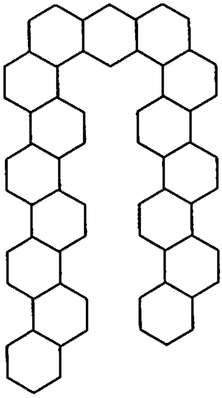


Figure 2



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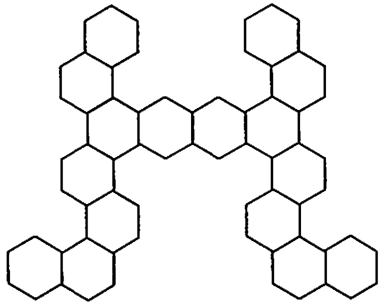

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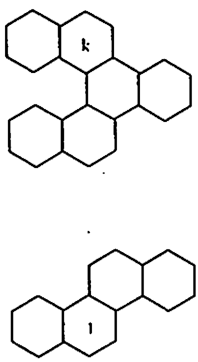
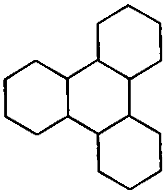
Figure 3

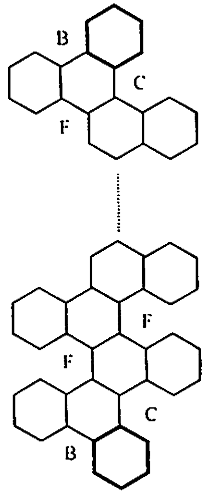


H(k)

Figure 4

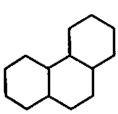


E_4

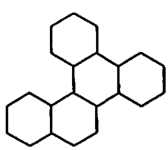


E_h

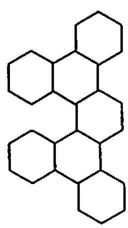
Figure 5



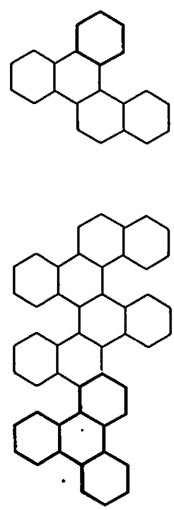
E_3



E_5



E_7



E_h

Figure 6