Journal of Mathematical Chemistry, Vol. 42, No. 4, November 2007 (© 2006)
DOI: 10.1007/s10910-006-9150-5

Second order Randić index of phenylenes and their corresponding hexagonal squeezes

Jie Zhang, Hanyuan Deng* and Shubo Chen

College of Mathematics and Computer Science, Hunan Normal University, Changsha, Hunan 410081, P.R. China
E-mail: hydeng@hunnu.edu.cn

Received: 5 April 2006; revised 9 May 2006

Given PH a phenylene, and HS its corresponding hexagonal squeeze, their second-order Randić indices are denoted by ${}^2\chi(PH)$ and ${}^2\chi(HS)$, respectively. The expressions of both ${}^2\chi(PH)$ and ${}^2\chi(HS)$ in terms of their inlet features are found, and a simple relation is estabblished between the second order Randić index of a phenylene and of the corresponding hexagonal squeeze.

KEY WORDS: second-order Randić index, phenylenes, hexagonal squeeze

1. Introduction

The connectivity index (or Randić Index) of a graph G, denoted by $\chi(G)$, was introduced by Randić [1] 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. Some publications related to the connectivity index can be found in the literature [2–9].

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

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

where the summation is taken over all possible paths of length h of G (we do not distinguish between the paths $u_1 u_2, \ldots, u_{h+1}$ and $u_{h+1} u_h, \ldots, u_1$). This

* Corresponding author.

new approach has been applied successfully to an impressive variety of physical, chemical and biological properties (boiling points, solubilities, densities, anesthesic, narcotions, toxicities, etc.), which have appeared in many scientific publications and in two books ([10] and [12]). Results related to the mathematical properties of these indices have been reported in the literature([2] and [13]). Specifically, Rada [14] gave an expression of the second-order Randić index of benzenoid systems and found the minimal and maximal value over the set of catacondensed systems. And the Randić index of phenylenes has been discussed in [15], so our main concern is the second-order Randić index of Phenylenes and its corresponding hexagonal squeeze.

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. Their respective molecular graphs are also referred to as phenylenes.

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. 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.

An example of PH and its HS is shown in figure 1.

Throughout this paper, the notation and terminology are mainly taken from [14,15].

Let PH be a phenylene with n vertices, m edges and h hexagons. If one goes along the perimeter of HS, then a fissure, bay, cove, fjord and lagoon, are respectively, paths of degree sequences (2,3,2), (2,3,3,2), (2,3,3,3,2), (2,3,3,3,3,2) and (2,3,3,3,3,3,2). In the case of PH, a fissure, bay, cove, fjord and lagoon are defined in full analogy to HS: a fissure (resp. a bay, cove, fjord, or lagoon) corresponds to a sequence of four (resp. six, eight, 10, or 12) consecutive vertices on the perimeter, of which the first and the last are vertices of degree 2 and the rest are vertices of degree 3. (For examples see figures 1 and 2).

The number of fissures, bays, coves, fjords and lagoons are denoted, respectively, by f, B, C, F and L.

Fissures, bays, coves, fjords and lagoons are various types of inlets. The total number of inlets on the perimeter of PH or HS, $f+B+C+F+L$, will be denoted by r.

There is another parameter $b = B + 2C + 3F + 4L$, called the number of bay regions, will be usefull later.

Two inlets of a phenylene or of a hexagonal squeeze are said to be adjacent if they have a common vertex of degree 2.

The number of adjacent inlets is dented by a.

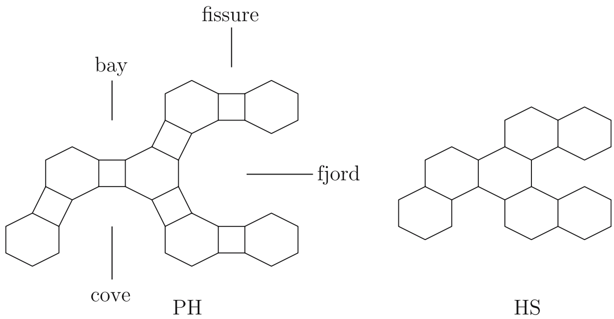

Figure 1. A PH and its HS.

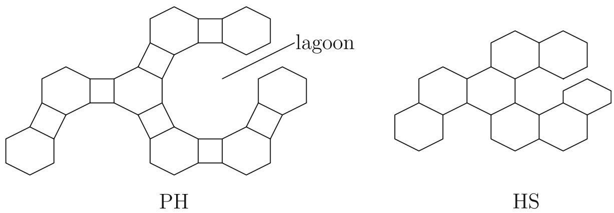

Figure 2. A PH which has a lagoon and its HS.

2. Second-order Randić index of PH and HS

First of all, since all vertices in a PH have degrees equal to 2 or 3, the paths of length 2 of PH have degree sequences (2,2,2), (2,2,3), (2,3,3), (3,2,3) and (3,3,3). It is easy to see that PH cannot possess the path of degree sequence (2,3,2). So it follows that

$$^2\chi(PH) = \frac{1}{\sqrt{8}}m_{222} + \frac{1}{\sqrt{12}}m_{223} + \frac{1}{\sqrt{18}}(m_{233} + m_{323}) + \frac{1}{\sqrt{27}}m_{333}. \tag{1}$$

If PH is a phenylene with n vertices, m edges and h hexagons, then

$$n = 6h.$$

Since $n - m + 2h = 2$, we have

$$m = 8h - 2$$

and

$$n_2 + n_3 = n,$$
$$2n_2 + 3n_3 = 2m,$$

where n_j is the number of vertices of degree $j (j = 2, 3)$, it can be shown that

$$n_2 = 2h + 4,$$
$$n_3 = 4h - 4.$$

Lemma 1. Let PH be a phenylene with n vertices and h hexagons ($h \geqslant 2$). Then

(1) $m_{33} + 2m_{323} + 3m_{3223} + 5m_{322223} = 8h - 2$;

(2) $m_{33} + m_{323} + m_{3223} + m_{322223} = 6h - 6$,

where $m_{3\underbrace{2,\ldots,2}_{i}3}$ represents the number of paths of degree sequence $(3, \underbrace{2, \ldots, 2}_{i}, 3)$ in PH.

Proof. (1) It is known that

$$m = \sum_{i=0}^{4} (i+1) m_{3\underbrace{2,\ldots,2}_{i}3}$$

since each path of PH of degree sequence $(3, \underbrace{2, \ldots, 2}_{i}, 3)$ has $i+1$ edges and PH has no path of degree sequence (3, 2, 2, 2, 3). The result follows from the relation $m = 8h - 2$.

(2) It is easy to see that

$$n_2 = \sum_{i=1}^{4} i \cdot m_{3\underbrace{2,\ldots,2}_{i}3} = 2h + 4$$

since every path of PH of degree sequence $(3, \underbrace{2, \ldots, 2}_{i}, 3)$ has i vertices of degree 2. By the equation of part (1), we conclude that

$$\begin{aligned}\sum_{i=0}^{4} m_{3\underbrace{2,\ldots,2}_{i}3} &= \sum_{i=0}^{4} (i+1) \cdot m_{3\underbrace{2,\ldots,2}_{i}3} - \sum_{i=1}^{4} i \cdot m_{3\underbrace{2,\ldots,2}_{i}3} \\ &= (8h - 2) - (2h + 4) \\ &= 6h - 6.\end{aligned}$$

Theorem 2. Let PH be a phenylene with h hexagons, r inlets and a adjacent inlets. Then

$$^{2}\chi(PH) = \frac{3\sqrt{2} + 8\sqrt{3}}{6} h + \frac{3\sqrt{2} - 2\sqrt{3}}{18} r + \frac{5\sqrt{2} - 4\sqrt{3}}{12} a + \left(\sqrt{2} - \frac{4}{3}\sqrt{3}\right). \quad (2)$$

Proof. First, we have $m_{33} = 6h - r - 6$ since

$$m_{23} = 2r,$$
$$m_{23} + 2m_{33} = 3n_3.$$

(Or,

$$\begin{aligned} m_{33} &= (f + 3B + 5C + 7F + 9L) + 2(h - 1) \\ &= (r + 2b) + 2(h - 1) \end{aligned}$$

since every path of degree sequence (3, 3) in PH has its edge lying on the perimeter or lying in the internal of PH. Note that

$$b + r = f + 2B + 3C + 4F + 5L = \frac{1}{2}n_3 = 2h - 2,$$

we also have

$$m_{33} = r + 2(2h - r - 2) + 2(h - 1) = 6h - r - 6.)$$

Second, it is clear that $m_{323} = a$. Using the equations of lemma 1 and m_{33} and m_{323}, we conclude that

$$m_{3223} = 2r - h - \tfrac{3}{2}a - 2,$$
$$m_{322223} = h - r + \tfrac{1}{2}a + 2$$

and

$$m_{222} = 2m_{322223} = 2h - 2r + a + 4,$$
$$m_{223} = 2m_{3223} + 2m_{322223} = 2(r - a).$$

Furthermore, because every inlet of PH has four paths of degree sequence (2, 3, 3), we have

$$m_{233} = 4r.$$

To find out m_{333}, we should note that every path of degree sequence (3, 3, 3) in PH has its edges all in the same hexagon, or all in the same square, or one in a hexagon and another in a square, it follows that

$$\begin{aligned} m_{333} &= 6h - 6m_{322223} - 4m_{3223} - 3m_{323} + 4(h - 1) + 2B + 4C + 6F + 8L \\ &= 8h - 2r + 2b - 8 \\ &= 12h - 4r - 12. \end{aligned}$$

Now theorem 2 follows by substituting the values of m_{ijk} obtained above in equation (1).

Let S be a benzenoid system with n vertices, h hexagons, r inlets, f fissures and a adjacent inlets, Rada [14] has proven that

$$
\begin{aligned}
{}^{2}\chi(S) = {} & \frac{\sqrt{2}}{4}n + \frac{4\sqrt{3}-3\sqrt{2}}{6}h + \frac{3\sqrt{2}-2\sqrt{3}}{18}r + \frac{5\sqrt{3}-6\sqrt{2}}{18}f \\
& + \frac{5\sqrt{2}-4\sqrt{3}}{12}a + \frac{3\sqrt{2}-4\sqrt{3}}{3}.
\end{aligned} \tag{3}
$$

For the hexagonal squeeze HS of a phenylene, HS may be jammed (which possesses lagoons), equation (3) also holds for HS by modifying Rada's proof slightly.

Lemma 3 ([14]). Let HS be the hexagonal squeeze of a phenylene with h hexagons, r inlets, f fissures and a adjacent inlets. Then

$$
\begin{aligned}
{}^{2}\chi(HS) = {} & \frac{3\sqrt{2}+4\sqrt{3}}{6}h + \frac{3\sqrt{2}-2\sqrt{3}}{18}r + \frac{5\sqrt{2}-4\sqrt{3}}{12}a \\
& + \frac{5\sqrt{3}-6\sqrt{2}}{18}f + \left(\sqrt{2} - \frac{2\sqrt{3}}{3}\right).
\end{aligned} \tag{4}
$$

The equation is obtained from (3) since $n = 4h + 2$ in HS.

Comparing with theorem 2, we have

Corollary 4. The second-order Randić index of a phenylene PH with h hexagons, f fissures and its hexagonal squeeze HS are related as

$$
{}^{2}\chi(PH) = {}^{2}\chi(HS) + \frac{2\sqrt{3}}{3}h - \frac{5\sqrt{3}-6\sqrt{2}}{18}f - \frac{2\sqrt{3}}{3}.
$$

Acknowledgments

Project 10471037 supported by National Natural Science Foundation of China and A project supported by Scientific Research Fund of Human Provincial Education Department (04B047).

References

[1] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. 97 (1975) 6609–6615.
[2] O. Araujo and J.A. de la Peña, The connectivity index of a weighted graph, Lin. Alg. Appl. 283 (1998) 171–177.
[3] B. Bollobás and P. Erdös, Graphs of extremal weight, Ars Combinatoria, 50 (1998) 225–233.
[4] I. Gutman, O. Araujo and J. Rada, An identity for Randić's connectivity index and its applications, ACH Models Chem. 137 (2000) 572–579.

[5] I. Gutman, O. Araujo and D.A. Morales, Bounds for the Randić connectivity index, J. Chem. Inf. Comput. Sci. 40 (2000) 572–579.
[6] P. Yu, An upper bound on the randic of trees, J. Math. Study (Chinese), 31 (1998) 225–230.
[7] J. Rada, Bounds for the Randić index of catacondensed systems, Utilitas Math. 62 (2002) 155–162.
[8] J. Rada, Hexagonal systems with extremal connectivity index, MATCH Commun. Math. Comput. Chem. 52 (2004) 167–182.
[9] L.H. Clark and J.W. Moon, On the general Randić index for certain families of trees, Ars Comb. 54 (2000) 223–235.
[10] L.B. Kier and L.H. Hall, *Molecular Connectivity in Chemistry and Drug Research* (Academic Press, New York, 1976).
[11] L.B. Kier L.H. Hall, W.J. Murray and M. Randić, Molecular connectivity V. The connectivity concept applied to density, J. Pharm. Sci. 65 (1976) 1226.
[12] L.B. Kier and L.H. Hall, *Molecular Connectivity in Structure-Activity Analysis* (Wiley, New York, 1986).
[13] J. Rada and O. Araujo, Higher order connectivity indices of starlike trees, Discr. Appl. Math. 119(3) (2002) 287–295.
[14] J. Rada, Second-order Randić index of benzenoid systems, Ars Comb. 72 (2004) 77–88.
[15] J. Rada, O. Araujo and I. Gutman, Randić index of benzenoid systems and phenylenes, Croat. Chem. Acta. 74 (2001) 225–235.