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Third order Randić index of phenylenes

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Let PH denote a phenylene, whose third order Randić index is denoted by ${}^{3}\chi(PH)$. The expression of ${}^{3}\chi(PH)$ in terms of their inlet features is found.

KEY WORDS: inlet, phenylene, third order Randić index

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 [5,8,9,11–15].

With the intention of extending the applicability of the connectivity index, Randić, Kier, Hall and co-workers [2,3] 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 $u_1 u_2 \cdots u_{h+1}$ 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, toxicities, etc.) which have appeared in many scientific publications and in two books

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[2,4]. Results related to the mathematical properties of these indices have been reported in the literature [5,6]. Specifically, Rada [10] 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 [7], the second order Randić index of phenylenes has been discussed in [16], so our main concern at present is the third order Randić 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. Their respective molecular graphs are also referred to as phenylenes.

An example of phenylene is shown in figure 1.

Throughout this paper, the notation and terminology are mainly taken from [7,10].

Let PH be a phenylene with n vertices, m edges and h hexagons. If one goes along the perimeter of PH, then a fissure (resp. a bay, cove, fjord, or lagoon) corresponds to a sequence of four (resp. six, eight, ten, or twelve) 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.

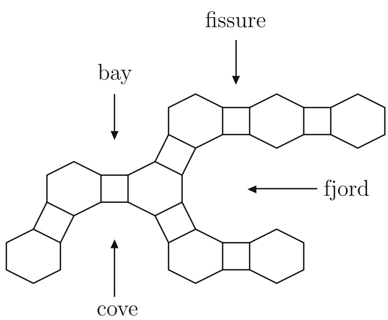

Figure 1. A phenylene (PH).

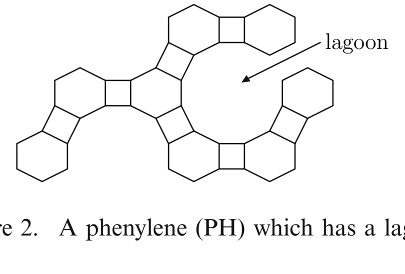

Figure 2. A phenylene (PH) which has a lagoon.

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

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

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

The number of adjacent inlets is denoted by a.

2. Third order Randić index of PH

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

$$
\begin{aligned}
{}^3\chi(\mathrm{PH}) = {} & \frac{1}{4}m_{2222} + \frac{1}{2\sqrt{6}}m_{2223} + \frac{1}{6}(m_{2233} + m_{3223} + m_{2332}) \\
& + \frac{1}{3\sqrt{6}}(m_{2333} + m_{3233}) + \frac{1}{9}m_{3333}, \qquad (1)
\end{aligned}
$$

where m_{ijkl} denotes the number of paths with degree sequence (i, j, k, l). In the following, we will show that the third order Randić index of PH is completely determined by the number of hexagons h, inlets r, fissures f and adjacent inlets a.

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 $m_{3\underbrace{2\ldots2}_{i}3}$ represents the number of paths of degree sequence $(3, \underbrace{2, \ldots, 2}_{i}, 3)$ in PH.

Proof. (1) It is known that

$$m = \sum_{i=0}^{4} (i+1) m_{3\underbrace{2\ldots2}_{i}3},$$

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

$$n_2 = \sum_{i=1}^{4} i \cdot m_{3\underbrace{2\ldots2}_{i}3} = 2h + 4$$

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

$$\begin{aligned}\sum_{i=0}^{4} m_{3\underbrace{2\ldots2}_{i}3} &= \sum_{i=0}^{4} (i+1) \cdot m_{3\underbrace{2\ldots2}_{i}3} - \sum_{i=1}^{4} i \cdot m_{3\underbrace{2\ldots2}_{i}3} \\ &= (8h-2) - (2h+4) \\ &= 6h - 6.\end{aligned}$$

Theorem 1. Let PH be a phenylene with h hexagons, r inlets and a adjacent inlets. Then

$$^{3}\chi(\mathrm{PH}) = \frac{109 + 2\sqrt{6}}{36} h + \frac{14\sqrt{6} - 31}{36} r - \frac{27 - 10\sqrt{6}}{72} a + \frac{5 - 2\sqrt{6}}{18} f - \frac{35 - 2\sqrt{6}}{18}. \tag{2}$$

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

$$m_{3223} = 2r - h - \frac{3}{2}a - 2$$

$$m_{322223} = h - r + \frac{1}{2}a + 2$$

So,

$$m_{2222} = m_{322223} = h - r + \frac{1}{2}a + 2$$

$$m_{2223} = 2m_{322223} = 2h - 2r + a + 4.$$

Furthermore, because the paths of length 3 with degree sequence (2,2,3,3) can be only contain in the paths of length 5 with degree sequence (3,3,2,2,3,3) or (3,3,2,2,2,2,3,3), and $m_{332233} = m_{3223}$, $m_{33222233} = m_{322223}$, we have

$$m_{2233} = 4m_{332233} + 4m_{33222233} = 4m_{3223} + 4m_{322223} = 4(r - a).$$

The vertex of degree 2 on the path of length 3 with degree sequence (3,2,3,3) must be the common vertex of two adjacent inlets, it follows that

$$m_{3233} = 4a.$$

A path of length 3 with degree sequence (2,3,3,2) may be a fissure, or may be in the hexagon with degree sequence (2,3,3,2,3,3) (where the vertices of degree

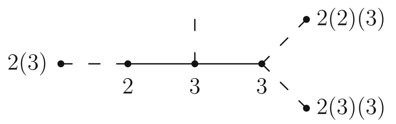

Figure 3.

2 must be the common vertices of two adjacent inlets), or may be in the hexagon with degree sequence (3,2,2,2,2,3). So

$$m_{2332} = f + a + m_{322223} = f + a + h - r + \frac{1}{2}a + 2.$$

To find out m_{2333}, we note that a path of length 2 with degree sequence (2,3,3) may be contained in the path of length 3 with degree sequence (2,2,3,3), or (3,2,3,3), or (2,3,3,2), or (2,3,3,3), as shown in figure 3.

It implies that

$$m_{2233} + m_{3233} + 2m_{2332} + m_{2333} = 3m_{233}$$

and

$$\begin{aligned} m_{2333} &= 12r - (2r + 2f + 2h + 3a + 4) \\ &= 10r - 2f - 2h - 3a - 4. \end{aligned}$$

Similarly, we have

$$m_{2333} + 2m_{3333} = 4m_{333}.$$

Therefore,

$$\begin{aligned} m_{3333} &= \tfrac{1}{2}(50h - 26r + 3a + 2f - 44) \\ &= 25h - 13r + \tfrac{3}{2}a + f - 22. \end{aligned}$$

Now Theorem 2 follows by substituting the values of m_{ijkl} obtained above into equation(1).

Acknowledgments

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