Fourth order Randić index of phenylenes *

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Abstract

The higher order connectivity index is a graph invariant defined as ${}^{h}\chi(G) = \sum_{u_1u_2\cdots u_{h+1}} \frac{1}{\sqrt{d_{u_1}d_{u_2}\cdots d_{u_{h+1}}}}$, where the summation is taken over all possible paths of length h , and d_{u_i} denotes the degree of the vertex u_i of graph G. In this paper, an exact expression for the fourth order connectivity index of Phenylenes is given.

Keywords: connectivity index, Phenylenes, hexagonal squeeze

1 Introduction

A topological index of molecules is a numeric quantity. It is structure invariant. The first reported use of a topological index in chemistry was by Wiener(see, [1])in the study of paraffin boiling points. Since then, in order to model various molecular properties, many topological index have been designed (see, [2]).

In 1975 M. Randić(see, [3]) introduced Randić index(also called connectivity index) defined as:

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

where d_u denotes the degree of the vertex u and $E(G)$ the set of edges of graph G. Connectivity index is one of the most important topological indices in Chemical Graph Theory. There is a good correlation between it and several physicochemical properties of alkanes: boiling pointssurface areasenergy levels, etc. Connectivity index has bee widely investigated and

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applied in mathematics and chemistry. Afterward, in [4] Randić, Kier, Hall considered the higher order connectivity indices of a general graph G as:

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

where the summation is taken over all possible paths of length h of graph G and approved that higher order connectivity indices have widely practice meaning in physics and chemistry

For Benzenoid systems and Phenylenes, J.Rada, O.Araujo, I.Gutman have worked out a computational formula of the fist connectivity indices and established the relation between a phenylene and the corresponding hexagonal squeeze (see [5]); Afterward, J.Rada has worked out a computational formula of the second connectivity indices of Benzenoid systems(see [6]). In [7,8], Deng and Zhang investigate the second order and third order connectivity indices of hexagonal systems and get their computational formula. In this paper, we go on the investigation and consider the fourth order connectivity index of phenylenes , and get a computational formula.

2 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. Clearly, a PH with h hexagons possesses $h-1$ squares. The number of vertices of PH are $6h$; The number of edges of PH are $8h-2$.

For PHs, some results related to the mathematical properties of Wiener index, Randić index and the second-order Randić index have been reported in the literature [4-9].

If along the boundary of a hexagonal benzene appear a path with degree sequence $(2,3,3,2)$, $(2,3,3,3,3,2)$, $(2,3,3,3,3,3,3,2)$, $(2,3,3,3,3,3,3,3,3,2)$ or $(2,3,3,3,3,3,3,3,3,3,3,2)$, then call a fissure, a bay, a cove, a fjord or a lagoon, respectively.

Let PH be a hexagonal benzene with n vertices, m edges and h hexagons. We use various bay to characterize the border feature of hexagonal benzenes. See figure 1

In a molecular graph, let the number of various boundary characteristics: fissures, bays, coves fjords and lagoons be f, B, C, F and L, respectively. Fissures, bays, fjords and lagoons collectively referred to as entrance. Let the sum of various entrances on boundary of PH be r, namely $r = f + B + C + F + L$. In PH, two entrances are called adjacent if and only if they have a common 2 degree point. Let the number of adjacent entrances (i.e., the pairs of entrances that have a common 2 degree point) be a, the number of adjacent fissures (i.e., the fissures in these pairs) be f_a.

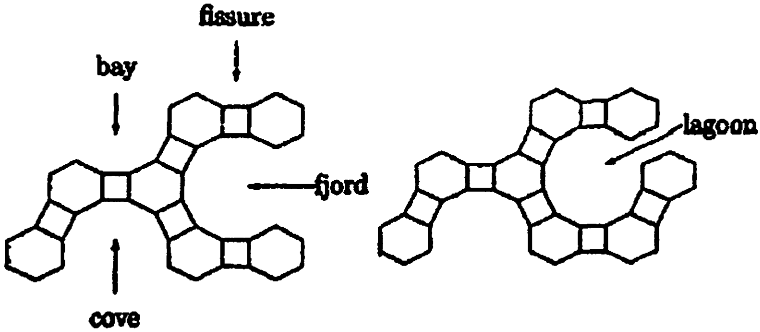

Figure 1 A phenylene (PH).

3 The fourth order Randić index of phenylenes

Since all vertices in a phenylene have degrees equal to 2 or 3, the path of length 4 have degrees sequence $(2,2,2,2,3)$, $(2,2,2,3,3)$, $(2,2,3,3,3)$, $(2,3,3,3,3)$, $(3,3,3,3,3)$, $(2,2,3,3,2)$, $(3,3,2,2,3)$, $(2,3,3,3,2)$, $(2,3,3,2,3)$, $(3,2,3,3,3)$, and $(3,3,2,3,3)$. It follows that

$$\begin{aligned} {}^4\chi(PH) &= \tfrac{1}{6\sqrt{3}}(m_{22333}+m_{33223}+m_{23332}+m_{23323}) \\ &\quad +\tfrac{1}{6\sqrt{2}}(m_{22233}+m_{22332})+\tfrac{1}{4\sqrt{3}}m_{22223} \\ &\quad \tfrac{1}{9\sqrt{2}}(m_{23333}+m_{32333}+m_{33233})+\tfrac{1}{9\sqrt{3}}m_{33333} \end{aligned} \tag{1}$$

where m_{abcde} denotes the number of paths with degrees sequence (a,b,c,d,e).

Let PH be a phenylene with n vertices, m edges and h hexagons, then $n=6h$ and $m=8h-2$. If let n_j denote the number of vertices with degree j, then $n_2+n_3=n, 2n_2+3n_3=2m$. Therefore $n_2=2h+4, n_3=4h-4$.

Lemma 3.1 (see,[8]) *Let PH be a phenylene with n vertices, m edges and h hexagons($h \geq 2$), then*

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

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

Theorem 3.2 *Let PH be a phenylene with h hexagons, r entrances, a adjacent entrances and f_a adjacent fissures, then*

$$
\begin{aligned}
{}^4\chi(PH) \;=\; & \tfrac{16\sqrt{2}+5\sqrt{3}}{18}h + 33\tfrac{\sqrt{2}-13\sqrt{3}}{54}r + \tfrac{\sqrt{3}-\sqrt{2}}{18}f + \tfrac{15\sqrt{2}+17\sqrt{3}}{108}a \\
& + \tfrac{28\sqrt{2}-39\sqrt{3}}{108}f_a + \tfrac{26\sqrt{2}-\sqrt{3}}{9}.
\end{aligned}
$$

Proof: Firstly, since $m_{23} = 2r, m_{23} + 2m_{33} = 3n_3$ and $n_3 = 4h - 4$, then

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

By the definition of adjacent entrance, we easily see $m_{323} = a$. From Lemma 3.1 and m_{33}, m_{323}, we can get

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

Clearly, there are not paths with degrees sequence $(2, 2, 2, 2, 2, 3)$ and with degrees sequence $(2, 3, 2)$ in PH, then

$$m_{22223} = 2m_{322223} = 2h - 2r + a + 4$$

and

$$m_{33223} = m_{3223} = 2r - \frac{3}{2}a - h - 2.$$

Since in PH, paths with degrees sequence $(2, 2, 2, 3, 3)$ only can be in paths with degrees sequence $(3, 3, 2, 2, 2, 2, 3, 3)$ or hexagon with degrees sequence $(3, 2, 2, 2, 2, 3)$, then

$$m_{22233} = 2m_{322223} + 2m_{33222233} = 4m_{322223} = 4h - 4r + 2a + 8.$$

Taking notice of the facts that the vertex of degree 2 of paths with degrees sequence $(3, 3, 2, 3, 3)$ must lie on two adjacency entrances and there are not degree sequence $(2, 3, 2)$, then $m_{33233} = 4a$.

Since a path with degrees sequence $(3, 2, 3, 3, 2)$ must include paths with degree $(3, 2, 3)$ or $(2, 3, 3, 2)$, which implies that every adjacent fissure contain a path with degree sequence $(3, 2, 3, 3, 2)$. Then $m_{32332} = f_a$.

In PH, a fissure only adjacent with one other entrance corresponds to two paths with degrees sequence $(2, 3, 3, 3, 2)$. So $m_{23332} = 2f_a$.

A paths of length 3 with degrees sequence $(3, 2, 3, 3)$ must be included in paths of length 4 with degrees sequence $(3, 3, 2, 3, 3), (3, 2, 3, 3, 3), (3, 2, 3, 3, 3)$ or $(3, 2, 3, 3, 2)$ as following figure 2

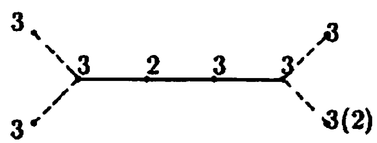

Figure 2

So $4m_{3233} = 2m_{33233} + m_{32333} + m_{32332}$. From [8], $m_{3233} = 4a$. Therefore

$$\begin{aligned} m_{32333} &= 4m_{3233} - 2m_{33233} - m_{32332} \\ &= 16a - 8a - f_a = 8a - f_a. \end{aligned}$$

Similarly, we have

$$3m_{2333} = m_{23333} + 2m_{23332} + m_{32333} + m_{22333}.$$

Obviously, a path with degree $(2,2,3,3,3)$ must lie in paths with degree $(2,2,2,3,3,3)$ or $(3,2,2,3,3,3)$. Then $m_{22333} = 6(h - r + \frac{1}{2}a + 2) + 8(2r - h - 2a - 2) - 2(f - f_a) - f_a = 10r - 2h + 3a - 2f + f_a - 14$, and $m_{2333} = 10r - 2f - 2h - 3a - 4$, by [8]. Therefore

$$\begin{aligned} m_{23333} &= 3m_{2333} - m_{32333} - 2m_{23332} - m_{22333} \\ &= 3(10r - 2f - 2h - 3a - 4) - (8a - f_a) - 4f_a \\ &\quad -(10r - 2h + 3a - 2f + f_a - 14) \\ &= 20r - 4f - 4h - 7a - 4f_a - 2. \end{aligned}$$

From [8], we can see $m_{2332} = f + h - r + \frac{3}{2}a + 2$. On the other hand, a path of length 3 with degrees sequence $(2,3,3,2)$ must be included in paths of length 4 with degrees sequence $(2,2,3,3,2), (2,3,3,2,3)$ as following figure 3

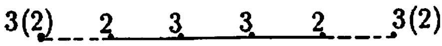

Figure 3

So

$$2m_{2332} = m_{32332} + m_{23322}$$

Therefore

$$m_{22332} = 2f + 2h - 2r + 3a + 4 - f_a.$$

Similarly, we can get $4m_{3333} = m_{23333} + 2m_{33333}$. From [8], we get $m_{3333} = 25h - 13r + \frac{3}{2}a + f - 22$. Therefore

$$m_{33333} = 2m_{3333} - \frac{1}{2}m_{23333} = 27h - 23r + 3f + 5a + 2f_a - 21.$$

Substituting the values of m_{abcde} in equation (1), we obtain:

$$
\begin{aligned}
{}^4\chi(PH) &= \frac{1}{6\sqrt{2}}(6h - 6r + 2f + 5a - f_a + 12) \\
&\quad + \frac{1}{6\sqrt{3}}(14r - 2a - 5h - f + 4f_a + 4) \\
&\quad + \frac{1}{4\sqrt{3}}(2h - 2r + a + 4) \\
&\quad + \frac{1}{9\sqrt{2}}(20r - 4h - 4f - 5a - 5f_a - 2) \\
&\quad + \frac{1}{9\sqrt{3}}(27h - 23r + 3f + 5a + 2f_a - 21) \\
&= \frac{16\sqrt{2}+5\sqrt{3}}{18}h + 33\frac{\sqrt{2}-13\sqrt{3}}{54}r + \frac{\sqrt{3}-\sqrt{2}}{18}f + \frac{15\sqrt{2}+17\sqrt{3}}{108}a \\
&\quad + \frac{28\sqrt{2}-39\sqrt{3}}{108}f_a + \frac{26\sqrt{2}-\sqrt{3}}{9}.
\end{aligned}
$$

Therefore, our result holds.

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