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The General Connectivity Indices of Benzenoid Systems and Phenylenes[†]

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Abstract

The general connectivity index $R_\alpha(G)$ of a graph $G = (V, E)$ is defined as $\sum_{uv\in E}(d(u)d(v))^\alpha$, where $d(v)$ denotes the degree of a vertex v and $\alpha \neq 0$ is a real number. In this paper, we give the expressions for computing the general connectivity indices of benzenoid systems and phenylenes, and a relation between the general connectivity indices of a phenylene and its corresponding hexagonal squeeze, and the extremal values of $R_\alpha(G)$ in benzenoid systems with h hexagons for some real numbers α.

1 Introduction

In 1998, Bollobás and Erdős [1] introduced the general connectivity index or the general Randić index of a simple undirected graph $G = (V, E)$:

$$R_\alpha(G) = \sum_{uv\in E}(d(u)d(v))^\alpha$$

where $d(v)$ denotes the degree of a vertex v. It generalized the connectivity index or the Randić index of a molecular structure graph. The latter, invented by the chemist M. Randić [2] in 1975, is the graph-based molecular structure descriptor that is most frequently applied in quantitative structure-property and structure-activity studies [3-5]. Some publications related to the general connectivity index R_α can be found in [6-8] and the references cited therein.

A benzenoid system (or a hexagonal system) ([9]) is a connected geometric figure obtained by arranging congruent regular hexagons in a plane, so that two hexagons are

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either disjoint or have a common edge. This figure divides the plane into one infinite (external) region and a number of finite (internal) regions. All internal regions must be regular hexagons. Benzenoid systems are of considerable importance in theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbons. A vertex of a hexagonal system belongs to, at most, three hexagons. A vertex shared by three hexagons is called an internal vertex. A benzenoid system is said to be catacondensed (or tree-type) if it does not possess internal vertices, otherwise it is said to be pericondensed. The catacondensed benzenoid systems are the graph representations of an important subclass of benzenoid molecules, i.e., catacondensed benzenoids.

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 benzenoid 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 such a PH and its HS are $6h$ and $4h+2$, respectively.

Throughout this paper, the notation and terminology about benzenoid systems, phenylenes and their hexagonal squeezes are mainly taken from [9-11].

Recently, Zheng [12] studied the general connectivity index R_α of a catacondensed benzenoid system and characterized the catacondensed benzenoid systems with the first three extremal general connectivity indices.

In this paper, we will give the the expressions for computing the general connectivity indices of benzenoid systems (not only catacondensed benzenoid systems) and phenylenes, and a relation between the general connectivity indices of a phenylene and its corresponding hexagonal squeeze, and also discuss the extremal values of the general connectivity indices of benzenoid systems with h hexagons.

2 The general connectivity index of benzenoid systems and phenylenes

For a simple graph $G=(V,E)$, n is the number of it vertices, m_{jk} is the number of (j,k)-edges connecting a vertex of degree j with a vertex of degree k. Then, the general

connectivity index of any graph G with n vertices can be denoted by m_{jk}

$$R_\alpha(G) = \sum_{1\le j\le k<n} m_{jk}(jk)^\alpha \tag{1}$$

In the cases of a benzenoid system (S) and a phenylene (PH), which possess only $(2,2)$-, $(2,3)$-, and $(3,3)$-edges, the equation (1) reduces to

$$R_\alpha(G) = m_{22}4^\alpha + m_{23}6^\alpha + m_{33}9^\alpha \tag{2}$$

In a benzenoid system, fissures, bays, coves and fjords are structural characteristics of the perimeter of the benzenoid systems playing some role in their theory [10]. If one goes along the perimeter of a benzenoid system, then a fissure is a structural feature formed by a 2-vertex, followed by a 3-vertex, followed by a 2-vertex. A simple bay is formed by a 2-vertex, followed by two 3-vertices, followed by a 2-vertex. A cove and a fjord are features formed, respectively, by three and four consecutive 3-vertices, lying between 2-vertices. In addition, the lagoon is a feature of the perimeter, formed by a 2-vertex, followed by five 3-vertices, followed by a 2-vertex. Lagoons cannot occur in (geometrically planar) benzenoids, but only in helicenic systems.

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

In the case of phenylenes, a fissure, bay, cove, fjord, and lagoon are defined in full analogy to the benzenoid systems. An illustrative example is depicted in Figure 1.

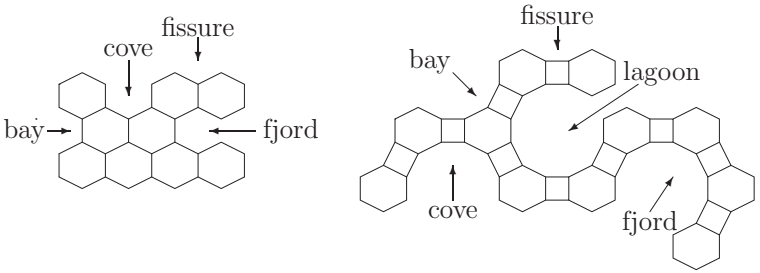


Figure 1. Types of inlets occurring on the perimeter of a benzenoid system and a phenylene.

Lemma 1([9]). (i) Let S be a benzenoid system with n vertices, h hexagons and r inlets. Then $m_{22} = n - 2h - r + 2$, $m_{23} = 2r$, $m_{33} = 3h - r - 3$;

(ii) Let PH be a phenylene with h hexagons and r inlets. Then $m_{22} = 2h - r + 4$, $m_{23} = 2r$, $m_{33} = 6h - r - 6$.

Now, we can express the general connectivity index of S and PH in terms of the numbers of vertices and inlets.

Theorem 2. (i) Let S be a benzenoid system with n vertices, h hexagons and r inlets. Then

$$R_\alpha(S) = (n - 2h - r + 2) \cdot 4^\alpha + 2r \cdot 6^\alpha + (3h - r - 3) \cdot 9^\alpha \tag{3}$$

(ii) Let PH be a phenylene with h hexagons and r inlets. Then

$$R_\alpha(PH) = (2h - r + 4) \cdot 4^\alpha + 2r \cdot 6^\alpha + (6h - r - 6) \cdot 9^\alpha \tag{4}$$

If n_i is the number of internal vertices of S_0, then $n = 4h + 2 - n_i$ and so

$$R_\alpha(S) = (2h - r - n_i + 4) \cdot 4^\alpha + 2r \cdot 6^\alpha + (3h - r - 3) \cdot 9^\alpha.$$

Note that the connectivity index of a benzenoid system is obtained by substituting $\alpha = -\frac{1}{2}$ to (3), and also $n = 4h + 2$ for a catacondensed benzenoid system with n vertices and h hexagons. So, we have

Corollary 3. (i)([10]) If G is a benzenoid system or a phenylene with n vertices and r inlets, then the connectivity index of G is

$$R_{-\frac{1}{2}}(S) = \frac{n}{2} - \frac{5 - 2\sqrt{6}}{6};$$

(ii)([12]) If S is a catacondensed hexagonal system (i.e., $n_i = 0$) with h hexagons and r inlets, then the general connectivity index of S is

$$R_\alpha(S) = (2h - r + 4) \cdot 4^\alpha + 2r \cdot 6^\alpha + (3h - r - 3) \cdot 9^\alpha. \tag{5}$$

From the equations (3)-(5) above, we can see that (i) the general connectivity index of a benzenoid system is completely determined by the numbers of vertices, hexagons and inlets; (ii) the general connectivity indices of a catacondensed benzenoid system and a phenylene are completely determined only by the numbers of hexagons and inlets, and (iii) among all catacondensed benzenoid systems and all phenylenes with an equal number of hexagons (or vertices, since $n = 4h + 2$ for a catacondensed benzenoid system with n vertices and h hexagons, and $n = 6h$ for a phenylene with n vertices and h hexagons), the general connectivity indices are monotone decreasing over the number of inlets, since the coefficient of r in (4) and (5) is $-(4^\alpha - 2 \cdot 6^\alpha + 9^\alpha) = -(2^\alpha - 3^\alpha)^2 < 0$ for $\alpha \neq 0$.

Corollary 4. (i)([12]) Let S_1 and S_2 be two catacondensed benzenoid systems with an equal number of hexagons (or vertices), and r_1 and r_2 inlets, respectively. Then $R_\alpha(S_1) < R_\alpha(S_2)$ if and only if $r_1 > r_2$ for $\alpha \neq 0$;

(ii)Let PH_1 and PH_2 be two phenylenes with an equal number of hexagons (or vertices), and r_1 and r_2 inlets, respectively. Then $R_\alpha(PH_1) < R_\alpha(PH_2)$ if and only if $r_1 > r_2$ for $\alpha \neq 0$.

3 A relation between the general connectivity indices of a phenylene and its hexagonal squeeze

Several properties of a phenylene (PH) are found to be closely related to the analogous properties of the corresponding hexagonal squeeze (HS). For instance, the algebraic structure count of PH is equal to the Kekulé structure count of HS [13]; A relation between the Wiener indices of PH and HS was discovered [14]; A relation between the connectivity indices of PH and HS was established [10]; A relation between the second order Randić indices of PH and HS was also established [15]. Here, we also give a relation between the general connectivity indices of PH and HS.

From Theorem 2(ii) and Corollary 3(ii), we obtain a relation between the general connectivity indices of a phenylene and its corresponding hexagonal squeeze.

Theorem 5. Let PH be a phenylene with h hexagons and r inlets, HS its hexagonal squeeze. The general connectivity indices of PH and HS are related as

$$R_\alpha(PH) = R_\alpha(HS) + 3(h-1) \cdot 9^\alpha.$$

By substituting $\alpha = -\frac{1}{2}$ to the equation above, it was obtained in [10] that $R_{-\frac{1}{2}}(PH) = R_{-\frac{1}{2}}(HS) + (h-1)$.

From Theorem 5, we know that

(i) If PH_1 and PH_2 are two phenylenes with an equal number of hexagons (or vertices), HS_1 and HS_2 are their hexagonal squeezes, respectively. Then $R_\alpha(PH_1) < R_\alpha(PH_2)$ if and only if $R_\alpha(HS_1) < R_\alpha(HS_2)$;

(ii) If PH has the smallest (or largest) general connectivity index among all phenylenes with h hexagons if and only if its hexagonal squeeze HS has the smallest (or largest) general connectivity index among all catacondensed benzenoid systems with h hexagons;

(iii) It is known in [12] that a catacondensed hexagonal system has the smallest (or largest, respectively) general connectivity index among all catacondensed benzenoid systems with h hexagons if and only if it is the linear hexagonal chain L_h (or it has $\lfloor \frac{h}{2} \rfloor - 1$ branched hexagons and $\lceil \frac{h}{2} - \lfloor \frac{h}{2} \rfloor \rceil$ kinks, respectively). So, we have

Corollary 6. Among all phenylenes with h hexagons, a phenylene has the smallest (or largest, respectively) general connectivity index if and only if its hexagonal squeeze is the linear hexagonal chain L_h (or has $\lfloor \frac{h}{2} \rfloor - 1$ branched hexagons and $\lceil \frac{h}{2} - \lfloor \frac{h}{2} \rfloor \rceil$ kinks, respectively).

4 The extremal values of R_α in benzenoid systems with h hexagons

In this section, we approach the extremal values of R_α in benzenoid systems with h hexagons.

4.1 The smallest general connectivity index in benzenoid systems with h hexagons

Let n, n_i, B, C, F be the numbers of vertices, internal vertices, bays, coves and fjords of a benzenoid system S with h hexagons, respectively. Then $b = B + 2C + 3F$ is the number of bay regions. It is deduced in [9,11] that

$$r = n - 2h - 4 - b, \qquad n = 4h + 2 - n_i$$

and so by the equation (3) in Theorem 2,

$$R_\alpha(S) = 3^\alpha(2^{\alpha+1} - 3^\alpha)n + (2^\alpha - 3^\alpha)^2 b + 6 \times 4^\alpha - (4h+8) \times 6^\alpha + (5h+1) \times 9^\alpha \quad (6)$$

$$R_\alpha(S) = -3^\alpha(2^{\alpha+1} - 3^\alpha)n_i + (2^\alpha - 3^\alpha)^2 b + 6 \times 4^\alpha + (h-1)(4 \times 6^\alpha + 9^\alpha). \quad (7)$$

If $2^{\alpha+1} - 3^\alpha < 0$, approximately, $\alpha \in (1.70951, +\infty)$, then, from (7), we know that in benzenoid systems with h hexagons, the smaller n_i and b are, the smaller R_α is. Moreover, $n_i \geq 0$ and $b \geq 0$. So, we have

Theorem 7. For any real number α with $2^{\alpha+1} - 3^\alpha < 0$, a benzenoid system S_0 has the smallest general connectivity index in the benzenoid systems with h hexagons if and only if $n_i(S_0) = b(S_0) = 0$, i.e., $S_0 = L_h$.

If $2^{\alpha+1} - 3^\alpha > 0$, approximately, $\alpha \in (-\infty, 1.70951)$, then, from (6), we know that in benzenoid systems with h hexagons, the smaller (or larger, respectively) n and b are, the smaller (or larger, respectively) R_α is. This will rely on a result of Harary and Harborth [16]:

For every benzenoid system with h hexagons,

$$2h + 1 + u \leq n \leq 4h + 2 \quad (8)$$

where $u = \lceil \sqrt{12h-3} \rceil$ and $\lceil x \rceil$ denotes the smallest integer greater or equal to x. Moreover, the lower bound is reached in the spiral hexagon system T_h, the upper bound is reached in the benzenoid system E_h (see Figure 2) and the hexagonal chains.

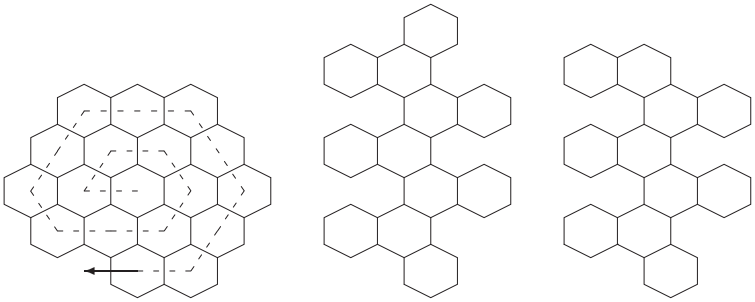


Figure 2. Benzenoid systems T_h and E_h

By (6) and (8), we have

Theorem 8. Let α be a real number with $2^{\alpha+1} - 3^\alpha \geq 0$. If S_0 is a benzenoid system with h hexagons such that

$$\begin{cases} n(S_0) = 2h + 1 + u \\ b(S_0) = 0, \end{cases} \tag{9}$$

then S_0 has the smallest general connectivity index in the benzenoid systems with h hexagons, and $R_\alpha(S_0) = 6 \times 4^\alpha + (2u-6) \times 6^\alpha + (3h-u) \times 9^\alpha$.

It is showed in [11] that the set of relations in (9) is equivalent to the following system of equations having a solution $(q, r, s, t) \in N^* \times N \times N^* \times N$

$$\begin{cases} rq + \frac{1}{2}(r-1)r + (s+t)(q+r) - \frac{1}{2}t(t+1) = h \\ 2q + 3r + 2s + t - 1 = u \end{cases} \tag{10}$$

where $N = \{0, 1, 2, 3, \cdots\}$ is the set of natural numbers and $N^* = N - \{0\}$.

A precise description of benzenoid systems with h hexagons such that $b = 0$ and an effective algorithm for finding all solutions of (10) can be found in [11]. Given a positive integer h, it can be constructed a benzenoid system with the smallest general connectivity index in the benzenoid systems from a solution of (10).

Problem 1. If α is a real number such that $2^{\alpha+1} - 3^\alpha \geq 0$, and h is a positive integer such that the system of equations (10) has no solution, what is the smallest general connectivity index R_α in the benzenoid systems with h hexagons?

When $\alpha = -\frac{1}{2}$, Rada [11] showed that the spiral T_h has the smallest connectivity index $R_{-\frac{1}{2}}$ in the benzenoid systems with h hexagons. Here, we will show that the spiral T_h also has the smallest general connectivity index R_α in the benzenoid systems with h hexagons for any real number α such that

$$\begin{cases} 2^{\alpha+1} - 3^\alpha \geq 0 \\ 4 \times 6^\alpha - 4^\alpha - 2 \times 9^\alpha > 0 \end{cases} \tag{11}$$

approximately, $\alpha \in (-3, 1.318)$.

Theorem 9. If α is a real number satisfying (11), and h is a positive integer such that the system of equations (10) has no solution, then the spiral T_h has the smallest general connectivity index in the benzenoid systems with h hexagons. In this case, $R_\alpha(T_h) = 7 \times 4^\alpha + (2u-8) \times 6^\alpha + (3h+1-u) \times 9^\alpha$.

Proof. Note that $b(T_h) = 0$ or 1. If the system of equations (10) has no solution, then $b(T_h) = 1$ since $n(T_h) = 2h + 1 + u$. By the equation (6),

$$R_\alpha(S) - R_\alpha(T_h) = 3^\alpha(2^{\alpha+1} - 3^\alpha)(n(S) - (2h+1+u)) + (2^\alpha - 3^\alpha)^2(b(S) - 1)$$

If $b(S) = 0$, then $n(S) - (2h+1+u) \geq 1$ and

$$R_\alpha(S) - R_\alpha(T_h) \geq 3^\alpha(2^{\alpha+1} - 3^\alpha) - (2^\alpha - 3^\alpha)^2 > 0;$$

if $b(S) \geq 1$, then $R_\alpha(S) - R_\alpha(T_h) \geq (2^\alpha - 3^\alpha)^2(b(S) - 1) \geq 0$, since the real number α satisfies (11). Hence, $R_\alpha(S) \geq R_\alpha(T_h)$.

4.2 The largest general connectivity index in benzenoid systems with h hexagons

In the following, we will discuss the largest general connectivity index in the benzenoid systems with h hexagons.

Rada [11] showed that the benzenoid system E_h has the largest general connectivity index among all catacondensed benzenoid systems with h hexagons. We will show that E_h also has the largest general connectivity index in the benzenoid systems with h hexagons for any real number α satisfying $2^{\alpha+1} - 3^\alpha > 0$.

Theorem 10. If α is a real number such that $2^{\alpha+1} - 3^\alpha > 0$, and S is a benzenoid system with h hexagons, then

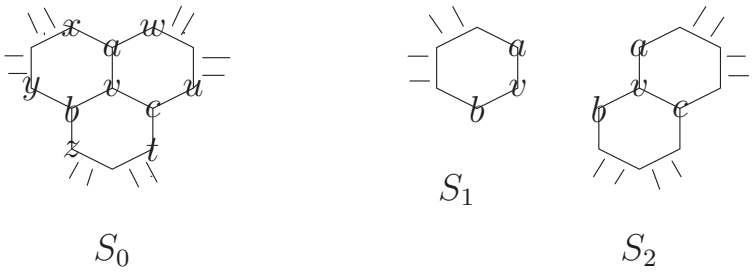
$$\begin{aligned} R_\alpha(S) \leq\ & R_\alpha(E_h) \\ =\ & 9^\alpha \left(h - 1 + \lfloor \tfrac{3h-6}{2} \rfloor\right) + 6^\alpha \left(4h - 2\lfloor \tfrac{3h-6}{2} \rfloor - 4\right) + 4^\alpha \left(\lfloor \tfrac{3h-6}{2} \rfloor + 6\right) \end{aligned}$$

with equality if and only if S is a catacondensed benzenoid system with $\lfloor\frac{h}{2}\rfloor-1$ branched hexagons and $\lceil\frac{h}{2}-\lfloor\frac{h}{2}\rfloor\rceil$ kinks.

Proof. We use induction on the number of internal vertices $n_i(S)$.

If $n_i(S)=0$, then S is a catacondensed benzenoid system and the result follows from [12]. Assume as inductive hypothesis, the result is true for $n_i(S)\leq k$, $k\geq 0$. Let S_0 be a benzenoid system with h hexagons and $n_i(S_0)=k+1$. We choose an internal vertex v such that v is as far to the center of S_0 as possible. Then not all adjacent vertices of v are internal. We consider the following cases:

Case I. All the three adjacent vertices a,b,c of v are external vertices (see Figure 3). At least one of t,u,w,x,y,z has degree 2 since v is as far to the center of S_0 as possible. Without loss of generality, we assume that the $d(z)=2$.



S_0 S_1 S_2

Figure 3.

S_0 can be split into two benzenoid systems S_1 and S_2 with h_1 and h_2 hexagons, respectively, and $h_1+h_2=h$.

$$\begin{aligned}
& R_\alpha(S_0)\\
= \;& R_\alpha(S_1)+R_\alpha(S_2)-((2d(x))^\alpha+2\times 4^\alpha+(2d(y))^\alpha)\\
& -((2d(w))^\alpha+2\times 6^\alpha+(2d(z))^\alpha)+(3d(x))^\alpha+(3d(y))^\alpha\\
& +(3d(w))^\alpha+(3d(z))^\alpha+2\times 9^\alpha\\
= \;& R_\alpha(S_1)+R_\alpha(S_2)+(3^\alpha-2^\alpha)(d^\alpha(x)+d^\alpha(y)+d^\alpha(z)+d^\alpha(w))\\
& +2(9^\alpha-6^\alpha-4^\alpha)\\
\leq \;& 9^\alpha(h_1-1+\lfloor\tfrac{3h_1-6}{2}\rfloor)+6^\alpha(4h_1-2\lfloor\tfrac{3h_1-6}{2}\rfloor-4)+4^\alpha(\lfloor\tfrac{3h_1-6}{2}\rfloor+6)\\
& +9^\alpha(h_2-1+\lfloor\tfrac{3h_2-6}{2}\rfloor)+6^\alpha(4h_2-2\lfloor\tfrac{3h_2-6}{2}\rfloor-4)+4^\alpha(\lfloor\tfrac{3h_2-6}{2}\rfloor+6)\\
& +(3^\alpha-2^\alpha)(d^\alpha(x)+d^\alpha(y)+d^\alpha(z)+d^\alpha(w))+2(9^\alpha-6^\alpha-4^\alpha)\\
& (\text{by the inductive hypothesis}).
\end{aligned}$$

If h_1 and h_2 are even, then

$$\begin{aligned} R_\alpha(S_0) &\leq 9^\alpha(h-1+\lfloor\tfrac{3h-6}{2}\rfloor)+6^\alpha(4h-2\lfloor\tfrac{3h-6}{2}\rfloor-4)+4^\alpha(\lfloor\tfrac{3h-6}{2}\rfloor+6) \\ &\quad +(3^\alpha-2^\alpha)(d^\alpha(x)+d^\alpha(y)+d^\alpha(z)+d^\alpha(w))-2\times 9^\alpha+4^\alpha \\ &= R_\alpha(E_h)+(3^\alpha-2^\alpha)(d^\alpha(x)+d^\alpha(y)+d^\alpha(z)+d^\alpha(w)) \\ &\quad -2\times 9^\alpha+4^\alpha. \end{aligned}$$

Note that

$$\min\{4\times 2^\alpha, 3\times 3^\alpha+2^\alpha\}\leq d^\alpha(x)+d^\alpha(y)+d^\alpha(z)+d^\alpha(w)\leq \max\{4\times 2^\alpha, 3\times 3^\alpha+2^\alpha\},$$

and

$$(3^\alpha-2^\alpha)\times 4\times 2^\alpha-2\times 9^\alpha+4^\alpha=-2(2^\alpha-3^\alpha)^2-4^\alpha<0,$$

$$(3^\alpha-2^\alpha)(3\times 3^\alpha+2^\alpha)-2\times 9^\alpha+4^\alpha=3(3^\alpha-2^{\alpha+1})<0$$

since $2^{\alpha+1}-3^\alpha>0$. So, $R_\alpha(S_0)<R_\alpha(E_h)$.

If h_1 and h_2 are odd, then

$$\begin{aligned} R_\alpha(S_0) &\leq R_\alpha(E_h)+(3^\alpha-2^\alpha)(d^\alpha(x)+d^\alpha(y)+d^\alpha(z)+d^\alpha(w)) \\ &\quad -3\times 9^\alpha+2\times 6^\alpha \\ &\leq R_\alpha(E_h)+(3^\alpha-2^\alpha)(d^\alpha(x)+d^\alpha(y)+d^\alpha(z)+d^\alpha(w)) \\ &\quad -2\times 9^\alpha+4^\alpha-(3^\alpha-2^\alpha)^2 \\ &< R_\alpha(E_h). \end{aligned}$$

If h_1 and h_2 have opposite parity, then

$$\begin{aligned} R_\alpha(S_0) &\leq R_\alpha(E_h)+(3^\alpha-2^\alpha)(d^\alpha(x)+d^\alpha(y)+d^\alpha(z)+d^\alpha(w)) \\ &\quad -2\times 9^\alpha+4^\alpha \\ &< R_\alpha(E_h). \end{aligned}$$

Case II. v has two adjacent external vertices a and c (see Figure 4).

S_0 can be split into two benzenoid systems S_1 and S_2 with h_1 and h_2 hexagons, respectively, and $h_1+h_2=h$.

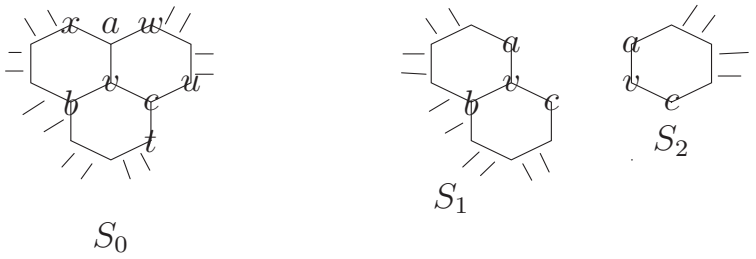


Figure 4.

$$
\begin{aligned}
& R_\alpha(S_0) \\
= \; & R_\alpha(S_1) + R_\alpha(S_2) - ((2d(x))^\alpha + 2\times 4^\alpha + (2d(y))^\alpha) \\
& -((2d(w))^\alpha + 2\times 6^\alpha + (2d(z))^\alpha) + (3d(x))^\alpha + (3d(y))^\alpha \\
& +(3d(w))^\alpha + (3d(z))^\alpha + 2\times 9^\alpha \\
= \; & R_\alpha(S_1) + R_\alpha(S_2) + (3^\alpha - 2^\alpha)(d^\alpha(x) + d^\alpha(y) + d^\alpha(z) + d^\alpha(w)) \\
& +2(9^\alpha - 6^\alpha - 4^\alpha).
\end{aligned}
$$

An analogous argumaent as in Case I can show that $R_\alpha(S_0) < R_\alpha(E_h)$.

Case III. If S_0 does not have internal vertices satisfying Cases I or II, then S_0 has an internal vertex with adjacent vertex a as shown in Figure 5.

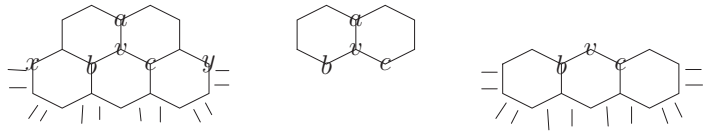
In this case,

$$
\begin{aligned}
R_\alpha(S_0) \; = \; & R_\alpha(S_1) - ((2d(x))^\alpha + 4\times 6^\alpha + (2d(y))^\alpha) \\
& +(3d(x))^\alpha + 4\times 9^\alpha + (3d(y))^\alpha) + 4\times 6^\alpha + 2\times 4^\alpha + 9^\alpha \\
= \; & R_\alpha(S_1) + (3^\alpha - 2^\alpha)(d^\alpha(x) + d^\alpha(y)) \\
& +5\times 9^\alpha + 2\times 4^\alpha \\
\leq \; & R_\alpha(E_{h-2}) + (3^\alpha - 2^\alpha)(d^\alpha(x) + d^\alpha(y)) \\
& +5\times 9^\alpha + 2\times 4^\alpha \qquad \text{(by the inductive hypothesis)} \\
= \; & 9^\alpha(h-3+\lfloor\tfrac{3h-12}{2}\rfloor) + 6^\alpha(4h - 2\lfloor\tfrac{3h-12}{2}\rfloor - 12) + 4^\alpha(\lfloor\tfrac{3h-12}{2}\rfloor + 6) \\
& +(3^\alpha - 2^\alpha)(d^\alpha(x) + d^\alpha(y)) + 5\times 9^\alpha + 2\times 4^\alpha \\
= \; & 9^\alpha(h-1+\lfloor\tfrac{3h-6}{2}\rfloor) + 6^\alpha(4h - 2\lfloor\tfrac{3h-6}{2}\rfloor - 4) + 4^\alpha(\lfloor\tfrac{3h-6}{2}\rfloor + 6) \\
& +(3^\alpha - 2^\alpha)(d^\alpha(x) + d^\alpha(y)) - 2\times 6^\alpha - 4^\alpha \\
= \; & R_\alpha(E_h) + (3^\alpha - 2^\alpha)(d^\alpha(x) + d^\alpha(y)) - 2\times 6^\alpha - 4^\alpha \\
< \; & R_\alpha(E_h)
\end{aligned}
$$

since $\min\{2\times 2^\alpha, 2\times 3^\alpha\} \leq d^\alpha(x) + d^\alpha(y) \leq \max\{2\times 2^\alpha, 2\times 3^\alpha\}$.

Therefore, the result is true by the induction and the proof is completed.

Problem 2. If α is a real number such that $2^{\alpha+1} - 3^\alpha \leq 0$, what is the largest general connectivity index R_α in the benzenoid systems with h hexagons?



S_0 Figure 5. S_1

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