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ORIGINAL PAPER

The general connectivity indices of catacondensed hexagonal systems

Jie Zheng

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Abstract The general connectivity index $R_\alpha(G)$ of a graph G is defined as $\sum_{(uv)}(d_u d_v)^\alpha$, where uv is an edge of G, $\alpha \in \mathbb{R}$ and $\alpha \neq 0$. In this paper, a formula is given for computing the general connectivity indices R_α of catacondensed hexagonal systems. We show that the general connectivity index R_α is monotone decreasing over the number of inlets in the system. The catacondensed hexagonal systems with the first up to the third extremal general connectivity indices are completely characterized.

Keywords The general connectivity index · Catacondensed hexagonal system · Inlet

1 Introduction and notations

The *connectivity index* (now also called the *branching index* or the *Randić index*), invented by the chemist M. Randić [20] in 1975, is the graph-based molecular structure descriptor that is most frequently applied in quantitative structure-property and structure-activity studies [5,6,13,14]. For a simple undirected graph $G = (V, E)$, its connectivity index $R(G)$ is defined as the sum over all edges of the graph of the terms $1/\sqrt{d_u d_v}$. That is,

$$R(G) = \sum_{(u,v)\in E} \frac{1}{\sqrt{d_u d_v}}, \tag{1}$$

J. Zheng (✉)
Department of Applied Mathematics, Donghua University, 201620 Shanghai,
People's Republic of China
e-mail: jzheng@dhu.edu.cn

where u and v are the vertices incident with the respective edge $(u, v) \in E$ and d_u and d_v are the degrees of the vertices u and v, respectively.

Later, in 1998 Bollobás and Erdös [2] generalized this index by replacing $-\frac{1}{2}$ with any real number α, which is called the *general connectivity index* or the *general Randić index*.

Definition 1.1 For a simple undirected graph $G = (V, E)$, the general connectivity index $R_\alpha(G)$ of G is the sum of $(d_u d_v)^\alpha$ over all edges (u, v) of G, i.e.,

$$R_\alpha(G) = \sum_{(u,v)\in E} (d_u d_v)^\alpha, \tag{2}$$

where d_u and d_v denote the degrees of the vertices u and v, respectively, and α is an arbitrary real number not equal to 0.

There are many contributions on the general connectivity index R_α. See [1–3,11, 12,15–18]. Obviously, $R_{-\frac{1}{2}}(G) = R(G)$.

Throughout this paper, the following notations and terminology will be used. A *hexagonal system* is a finite connected plane graph without cut vertices, in which every interior face is bounded by a regular hexagon of side of length one. A hexagonal system with n hexagons is called an *n-hexagonal system* for short. Hexagonal systems are of great importance for theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbons. A considerable amount of research in mathematical chemistry has been devoted to hexagonal systems [7,9,10].

Suppose H is a hexagonal system. Denote by $H(C)$ the graph whose vertex set is the set of hexagons in H, and two vertices of which are adjacent in $H(C)$ if the corresponding hexagons have a common edge in H. The graph $H(C)$ is called the *centroid-induced graph* [21] or the *dualist graph* [4] of H. A hexagonal system without internal vertex is called a *catacondensed hexagonal system*. Clearly the centroid-induced graph of a catacondensed hexagonal system is a tree. A hexagonal system is called a *hexagonal chain*, if its centroid-induced graph is a path. A vertex in H is called a *j-vertex* if it has degree j in H. For a catacondensed hexagonal system H, a hexagon A of H is called a *kink* [4] if A has exactly two consecutive 2-vertices in H, and A is called a *branched hexagon* [4] if A has no 2-vertex, i.e., the hexagon A corresponds to a 3-vertex in $H(C)$. An n-hexagonal chain with no kink is called a *linear hexagonal chain* and is denoted by L_n. For the definitions, see Fig. 1.

The following definitions were introduced in [19]. If one goes along the perimeter of a hexagonal 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. See Fig. 2.

The fissures, bays, coves, and fjords are called various types of *inlets*. The number of inlets is defined as the sum of the numbers of the fissures, bays, coves, and fjords.

The extremal hexagonal systems with respect to some useful topological indices in chemical applications have been extensively studied, and many results concerning this topic can be found in [4,8,19,21–24].

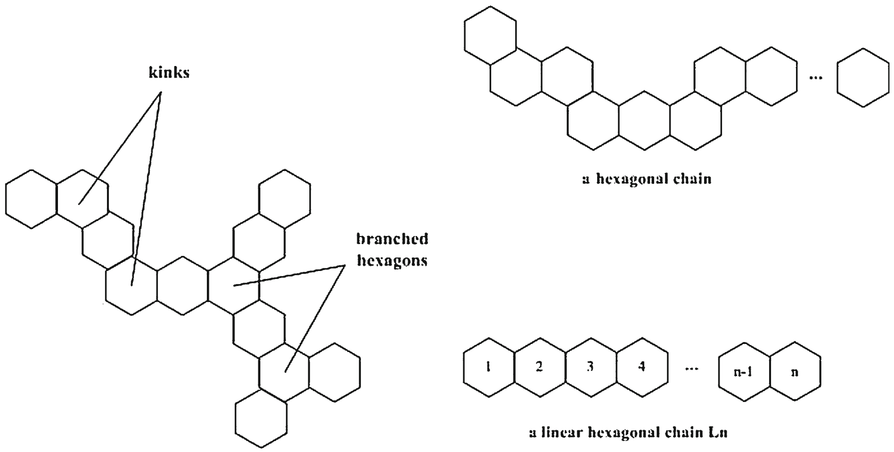

Fig. 1 Kinks, branched hexagons, a hexagonal chain and a linear hexagonal chain

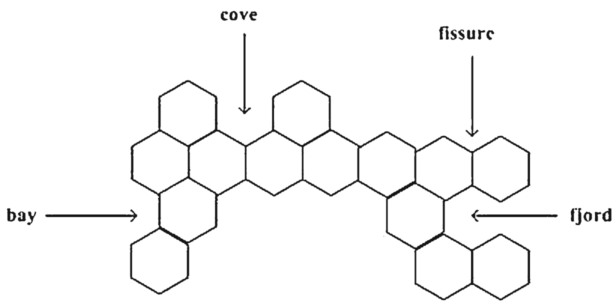

Fig. 2 Bay, cove, fissure and fjord in a hexagonal system

In this paper, we are interested in the general connectivity index of catacondensed hexagonal systems. A formula ((3) in Theorem 2.1) is obtained for computing the general connectivity index of a catacondensed hexagonal system. Using this formula, we find the extremal catacondensed hexagonal systems with the first three largest or smallest general connectivity index. In fact, we can order all n-catacondensed hexagonal systems according to their general connectivity indices.

2 A formula for computing R_α

Our main result in this section is the following theorem.

Theorem 2.1 *For an n-catacondensed hexagonal system H with l inlets, its general connectivity index $R_\alpha(H)$ is equal to*

$$R_\alpha(H) = (3n - l - 3) \times 9^\alpha + 2l \times 6^\alpha + (2n - l + 4) \times 4^\alpha. \tag{3}$$

Lemma 2.2 *Let H be an n-catacondensed hexagonal system with k kinks, b branched hexagons and l inlets. Then $l + 3b + k = 2(n - 1)$.*

Proof If one goes along the perimeter of H, then we can obtain a degree sequence S of the vertices in H beginning with four 2s. For example, $S = 2222323233232323233332\cdots$. The sequence S is of length $4n + 2$ and the number of 3 in S is $2(n - 1)$. The edges one goes along are called outer edges. Every subsequence in S without number 2 is called a block. There are four types of blocks: 3, 33, 333 and 3333. They correspond to fissures, bays, coves and fjords in H, respectively. Obviously, the number of blocks is the number of inlets l. If the block is of type 33, then it corresponds to a kink or an outer edge of a branched hexagon. If the block is of type 333, then there are three cases: (1) it corresponds to two kinks; (2) it corresponds to a kink and an outer edge of a branched hexagon; (3) it corresponds to two outer edges of two branched hexagons. If the block is of type 3333, then there are four cases: (1) it corresponds to three kinks; (2) it corresponds to two kinks and an outer edge of a branched hexagon; (3) it corresponds to one kink and two outer edges of two branched hexagons. (4) it corresponds to three outer edges of three branched hexagons. We can replace every block in S in the following way. The first 3 in the block is replaced by an inlet, the other 3 in the block are replaced by the corresponding kinks or outer edges of branched hexagons. Because every branched hexagon has exactly three outer edges, we can count the numbers of 3 in S by the numbers of inlets, kinks and branched hexagons as $l + 3b + k$. The proof is completed. □

Proof for Theorem 2.1 Let H be an n-catacondensed hexagonal system with l inlets, k kinks and b branched hexagons. By Lemma 2.2, to prove (3), it is enough to prove

$$R_\alpha(H) = (n + 3b + k - 1) \times 9^\alpha + (4n - 6b - 2k - 4) \times 6^\alpha + (3b + k + 6) \times 4^\alpha. \tag{4}$$

We will prove (4) by an induction on n.

If $n = 1$, then $k = b = 0$. The 1-hexagonal system H has its general connectivity index $R_\alpha(H) = 6 \times 4^\alpha = (1+0+0-1) \times 9^\alpha + (4-0-0-4) \times 6^\alpha + (0+0+6) \times 4^\alpha$.

Suppose for $n = j$, we can use (4) to compute the general connectivity index of any j-catacondensed hexagonal system. For $n = j + 1$, let H be a $(j + 1)$-catacondensed hexagonal system with k kinks and b branched hexagons. Choose a hexagon A that corresponds to a 1-vertex in the centroid-induced graph $H(C)$. Suppose B is the unique hexagon that has a common edge with A in H. Delete A from H. Then we get a j-catacondensed hexagonal system $H - A$.

1. If B is a kink in H. Then the j-catacondensed hexagonal system $H - A$ has $k - 1$ kinks and b branched hexagons. By induction hypothesis,

$$R_\alpha(H - A) = (j + 3b + k - 2) \times 9^\alpha + (4j - 6b - 2k - 2) \times 6^\alpha + (3b + k + 5) \times 4^\alpha.$$

Then

$$\begin{aligned} R_\alpha(H) &= R_\alpha(H-A) - 2\times 4^\alpha - 6^\alpha + 2\times 9^\alpha + 3\times 6^\alpha + 3\times 4^\alpha \\ &= ((j+1)+3b+k-1)\times 9^\alpha + (4(j+1)-6b-2k-4)\times 6^\alpha \\ &\quad + (3b+k+6)\times 4^\alpha, \end{aligned}$$

which satisfies (4).

2. If B is a branched hexagon in H. Then the j-catacondensed hexagonal system $H-A$ has $k+1$ kinks and $b-1$ branched hexagons. By induction hypothesis,

$$R_\alpha(H-A) = (j+3b+k-3)\times 9^\alpha + (4j-6b-2k)\times 6^\alpha + (3b+k+4)\times 4^\alpha.$$

Then

$$\begin{aligned} R_\alpha(H) &= R_\alpha(H-A) - 2\times 6^\alpha - 4^\alpha + 3\times 9^\alpha + 2\times 6^\alpha + 3\times 4^\alpha \\ &= ((j+1)+3b+k-1)\times 9^\alpha + (4(j+1)-6b-2k-4)\times 6^\alpha \\ &\quad + (3b+k+6)\times 4^\alpha, \end{aligned}$$

which satisfies (4).

3. If B is neither a kink nor a branched hexagon. Then the j-catacondensed hexagonal system $H-A$ has k kinks and b branched hexagons. By induction hypothesis,

$$\begin{aligned} R_\alpha(H-A) &= (j+3b+k-1)\times 9^\alpha + (4j-6b-2k-4)\times 6^\alpha \\ &\quad + (3b+k+6)\times 4^\alpha. \end{aligned}$$

Then

$$\begin{aligned} R_\alpha(H) &= R_\alpha(H-A) - 3\times 4^\alpha + 9^\alpha + 4\times 6^\alpha + 3\times 4^\alpha \\ &= ((j+1)+3b+k-1)\times 9^\alpha + (4(j+1)-6b-2k-4)\times 6^\alpha \\ &\quad + (3b+k+6)\times 4^\alpha, \end{aligned}$$

which satisfies (4).

Therefore, the result is true by the induction and the proof for Theorem 2.1 is completed. □

J. Rada [19] gave the following formula for computing the connectivity index of hexagonal systems.

Theorem 2.3 (Theorem 2 in [19]) *Let H be a hexagonal system (not necessarily be catacondensed) with m vertices and l inlets. Then*

$$R(H) = \frac{m}{2} - \frac{5-2\sqrt{6}}{6}l. \quad (5)$$

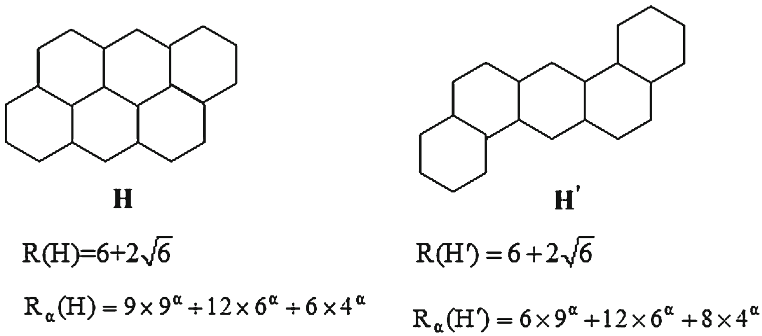

Fig. 3 The connectivity index R and the general connectivity index R_α

By substituting $\alpha = -\frac{1}{2}$ to (3), we have

$$R_{-\frac{1}{2}}(H) = R(H) = \frac{3n-l-3}{3} + \frac{2l}{\sqrt{6}} + \frac{2n-l+4}{2} = \frac{4n+2}{2} - \frac{5-2\sqrt{6}}{6}l,$$

which obviously satisfies (5) because an n-catacondensed hexagonal system H has $4n+2$ vertices.

Theorem 2 in [19] shows that the numbers of vertices and inlets in a hexagonal system completely determine its connectivity index. But in general, it is not true for the general connectivity index. For example, each of the hexagonal systems in Fig. 3 has 22 vertices and 6 inlets. They have the same connectivity index R, but quite different general connectivity index R_α.

3 Extremal problem

Lemma 3.1 *Suppose H and H' are two n-catacondensed hexagonal systems with l and l' inlets, respectively. Then $R_\alpha(H) < R_\alpha(H')$ for any real number $\alpha \neq 0$ if and only if $l > l'$.*

Proof For (3), we have

$$\begin{aligned} R_\alpha(H) &= (3n-l-3) \times 9^\alpha + 2l \times 6^\alpha + (2n-l+4) \times 4^\alpha \\ &= (3n-3) \times 9^\alpha + (2n+4) \times 4^\alpha - l(3^\alpha - 2^\alpha)^2. \end{aligned}$$

So for any $\alpha \neq 0$, $R_\alpha(H)$ is strictly decreasing on the variable l. Thus $R_\alpha(H) < R_\alpha(H')$ if and only if $l > l'$. □

If fact, Lemma 3.1 can help us sort all n-catacondensed hexagonal systems according to their general connectivity index R_α.

Theorem 3.2 *For an n-catacondensed hexagonal system $H(n \geq 3)$, we have*

1. *$R_\alpha(H) \geq (n-1) \times 9^\alpha + (4n-4) \times 6^\alpha + 6 \times 4^\alpha$, with equality if and only if $H = L_n$;*

2. *$R_\alpha(H) \le (n-1+\lceil\frac{3n-7}{2}\rceil)\times 9^\alpha + (4n-2\lceil\frac{3n-7}{2}\rceil-4)\times 6^\alpha + (\lceil\frac{3n-7}{2}\rceil+6)\times 4^\alpha$, with equality if and only if H has $\lfloor\frac{n-2}{2}\rfloor$ branched hexagons and $\lceil\frac{n}{2}-\lfloor\frac{n}{2}\rfloor\rceil$ kinks.*

Proof 1. By Lemma 2.2, for an n-catacondensed hexagonal system H, its inlets number $l \le 2(n-1)$ and with equality if and only if H has no kink nor branched hexagon. That is, H is the linear hexagonal chain L_n. Then by Lemma 3.1, we have

$$\begin{aligned} R_\alpha(H) &\ge (3n-2(n-1)-3)\times 9^\alpha + 2\times 2(n-1)\times 6^\alpha \\ &\quad + (2n-2(n-1)+4)\times 4^\alpha \\ &= (n-1)\times 9^\alpha + (4n-4)\times 6^\alpha + 6\times 4^\alpha. \end{aligned}$$

with equality if and only if $H = L_n$.

2. It is sufficient to prove

$$R_\alpha(H) \le \begin{cases} \frac{5n-8}{2}\times 9^\alpha + (n+2)\times 6^\alpha + \frac{3n+6}{2}\times 4^\alpha, & \text{if } n \text{ is an even;} \\ \frac{5n-9}{2}\times 9^\alpha + (n+3)\times 6^\alpha + \frac{3n+5}{2}\times 4^\alpha, & \text{if } n \text{ is an odd.} \end{cases}$$

and with equality if and only if H has $\frac{n-2}{2}$ branched hexagons and 0 kink (if n is an even) or H has $\frac{n-3}{2}$ branched hexagons and 1 kink (if n is an odd).
Suppose n is an even and H is an n-catacondensed hexagonal system with l inlets, b branched hexagons and k kinks. $H(C)$ is the centroid-induced graph of H. Obviously, a branched hexagon and a kink in H correspond to a 3-vertex and a 2-vertex in $H(C)$, respectively. Suppose there are u 2-vertices in $H(C)$ that do not correspond to kinks in H. Then there are $n-b-k-u$ 1-vertices in $H(C)$. Since $H(C)$ is a tree with n vertices, we have

$$(n-b-k-u)+2(u+k)+3b = 2(n-1), \tag{6}$$

which implies

$$b \le \frac{n-2}{2},$$

with equality if and only if $k=0$ and $u=0$. Submit $3b+k+l=2(n-1)$ (Lemma 2.2) to (6), we also have

$$l = n+u-b \ge n-\frac{n-2}{2} = \frac{n+2}{2}, \tag{7}$$

with equality if and only if $u=0$ and $b=\frac{n-2}{2}$.
Lemma 3.1, (3) and (7) imply

$$\begin{aligned} R_\alpha(H) &\le (3n-\frac{n+2}{2}-3)\times 9^\alpha + 2\times\frac{n+2}{2}\times 6^\alpha + (2n-\frac{n+2}{2}+4)\times 4^\alpha \\ &= \frac{5n-8}{2}\times 9^\alpha + (n+2)\times 6^\alpha + \frac{3n+6}{2}\times 4^\alpha, \end{aligned}$$

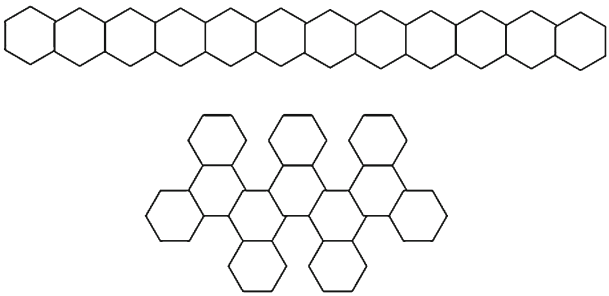

Fig. 4 The extremal hexagonal systems with the smallest R_α and the largest R_α

with equality if and only if $b = \frac{n-2}{2}$ and $k = 0$.($u = 0$ can be obtained from these two conditions.) That means H has $\frac{n-2}{2}$ branched hexagons and 0 kink.

If n is an odd, the theorem can be proved similarly. □

Example 3.3 Among all 12-catacondensed hexagonal systems, the two systems in Fig. 4 have the smallest and the largest general connectivity index $R_\alpha(\alpha \neq 0)$, respectively.

Analogously, the following results can be obtained. We omit their proof and leave it for the reader.

Theorem 3.4 *Among all n-catacondensed hexagonal systems, H has the second smallest general connectivity index if and only if H has* 1 *kink and* 0 *branched hexagon; H has the third smallest general connectivity index if and only if H has* 2 *kinks and* 0 *branched hexagon.*

Theorem 3.5 *Among all n-catacondensed hexagonal systems($n \geq 5$), if n is even, H has the second largest general connectivity index if and only if H has* $\frac{n-4}{2}$ *branched hexagons and* 2 *kinks; if n is odd, H has the second largest general connectivity index if and only if H has* $\frac{n-3}{2}$ *branched hexagons and* 0 *kink or H has* $\frac{n-5}{2}$ *branched hexagons and* 3 *kinks.*

Theorem 3.6 *Among all n-catacondensed hexagonal systems($n \geq 5$), if n is even, H has the 3rd largest general connectivity index if and only if H has* $\frac{n-4}{2}$ *branched hexagons and* 1 *kink; if n is odd, H has the 3rd largest general connectivity index if and only if H has* $\frac{n-5}{2}$ *branched hexagons and* 2 *kinks.*

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