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Recursive formulae for enumeration of LM-conjugated circuits in structurally related benzenoid hydrocarbons *

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The linearly independent and minimal conjugated (LM-conjugated) circuits of benzenoid hydrocarbons play the central role in the conjugated circuit model. For a general case, the enumeration of LM-conjugated circuits may be tedious as it requires construction of all Kekule structures. In our previous work, a recursive method for enumeration of LM-conjugated circuits of benzenoid hydrocarbons was established. In this paper, we further extend the recursive formulae for enumerations of LM-conjugated circuits for both catacondensed benzenoid hydrocarbons and some families of structurally related pericondensed benzenoid hydrocarbons.

KEY WORDS: linearly independent and minimal conjugated circuits, Kekule structures, recursive formulae, benzenoid hydrocarbons

1. Introduction

The conjugated circuit model is a resonance-theoretic model was introduced by Randic [1–3] in 1976 for the study of aromaticity and conjugation in polycyclic conjugated systems. The model was motivated from an empirical point of view elaborating the Clar aromatic sextet theory [4]. The conjugated-circuit model has also a firm quantum-mechanical basis [5–7]. It can be derived regorously from the Pauling–Wheland resonance theory [8,9] via a Simpson–Herndon model Hamiltonian [10,11]. In recent years, many investigations on the conjugated-circuit model have been made [12–24]. The enumeration of LM-conjugated circuits had led to expressions for the resonance energies of polycyclic conjugated hydrocarbons [12]. It is also applied to calculate generalized bond orders of benzenoid hydrocarbons [13]. However, for a general case, the enumeration of LM-conjugated circuits of benzenoid hydrocarbons requires to construct all Kekule

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structures and then to find a set of LM-conjugated circuits for every Kekule structure. When sizes of molecules increase, the numbers of Kekule structures increase fast, hence enumerating LM-conjugate circuits by the method becomes tedious.

It was suggested in [12] that rather than considering individually each single molecule it may be better to review a family of related structures of which the molecule in question is a member. By analyzing a sequence of expressions for the molecular resonance energies, one tries to find some regularity for the coefficients indicating the contributions of the LM-conjugated circuits of different sizes. In this way, the expressions of resonance energies for still larger members of a family of structurally related structures are obtained without explicit construction of Kekule structures.

A useful idea in that approach is a partitioning of resonance energy to the expressions for the individual rings of the structures considered. The contribution of a ring s_j of a benzenoid hydrocarbon B to the summation expression of LM-conjugated circuits of B may be denoted by a sequence of numbers, $(r_1(s_j), r_2(s_j), \ldots, r_n(s_j), \ldots)$, where $r_j(s_j)$ is the number of the LM-conjugated circuits of size $4n + 2$ with respect to the ring s_j, which is called the ring code of s_j. The total sum of ring codes of all rings of B just corresponds to the summation over all LM-conjugated circuits of B.

For some families of structurally related structures, use of ring codes has special advantage. It allows one to perceive regularities for the coefficients from the count of LM-conjugated circuits of different sizes more readily. Figure 1 shows some families of benzenoid hydrocarbons considered in [12]. Their ring codes were given by finding the interrelation of the coefficients of various LM-conjugated circuits or finding the regularities or a recursion of a ring codes to smaller members of the families. However, in general cases, it is usually very difficult to find such regularities among the coefficients of various LM-conjugated circuits and the ring codes between smaller members of a family of related structures.

In a previous work [14], we established a recursive method for enumeration of LM-conjugated circuits of some benzenoid hydrocarbons, by which the summation expression of LM-conjugated circuits (called LM-conjugated circuit polynomial, or simply LMCC-polynomial) of some benzenoid hydrocarbons can be directly obtained from the LMCC-polynomials and the Kekule structure counts of their subgraphs. In order to obtain recursive formulae of LMCC-polynomials of some benzenoid hydrocarbons by the recursive method, further investigations are needed.

In a recent work [15], we also gave another method to obtain ring codes of any benzenoid hydrocarbon from the Kekule structure counts of some subgraphs of the graph. However, for catacondensed benzenoid hydrocarbons and some families of structurally related pericondensed benzenoid hydrocarbons, it is still more convenient to obtain recursive formulae of their LM-conjugated circuit polynomials directly.

In this paper, we extend the recursive formulae for enumeration of LM-conjugated circuits for both catacondensed benzenoid hydrocarbons and some families of structurally related pericondensed benzenoid hydrocarbons.

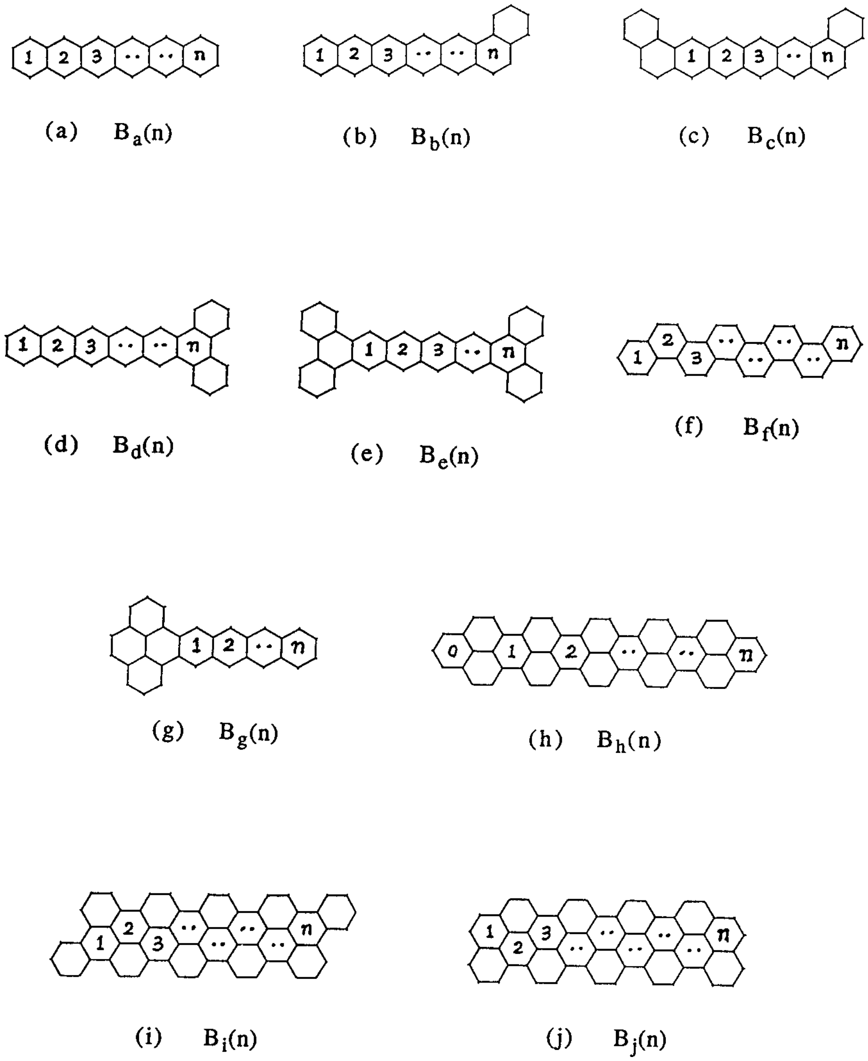


Figure 1. Some families of benzenoid hydrocarbons.

2. Some related definitions and results

Definition 1. A benzenoid hydrocarbon (BH) is a 2-connected plane graph for which every interior face is bounded by a regular hexagon. A connected subgraph of a BH is said to be a BH-fragment (BHF). Let B be a BH. B is said to be normal if B contains no fixed bond (i.e., no bond appearing with the same multiplicity in every Kekule structure); otherwise B is essentially disconnected. A normal component B_i of B is a maximal subgraph of B with no fixed bond (possibly, $B_i = B$, that is, B is normal). All normal components of B are denoted by B^*. The boundary of an interior face of a BH or BH-fragment is called a ring of it.

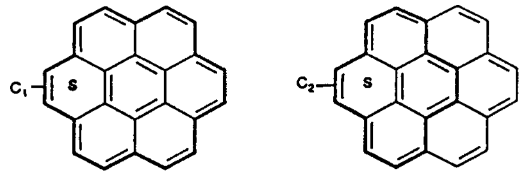


Figure 2. A minimal conjugated circuit C_2 of the ring s in a benzenoid hydrocarbon B (called a crown) (C_1 is not minimal).

Definition 2 [14]. A set S of linearly independent and minimal conjugated circuits of a Kekule structure K_i of a benzenoid hydrocarbon B consists of a maximum number of linearly independent circuits of B in which every circuit is a conjugated circuit of K_i (simply, a K_i-conjugated circuit C, that is, a circuit whose edges alternately present as K_i-double and K_i-single bonds), and has the minimum length.

In fact, a set S of linearly independent and minimal conjugated circuits of a Kekule structure K_i of B is a basis in conjugated circuit space, where "linearly independent" means any circuit in S cannot be obtained by linear combination of other circuits in S.

We denote a circuit of size $4n + 2$ in S by R_n, and the summation expression of S by $R(K_i) = \sum_{R_j \in S} R_j = \sum_{n=1,2,\ldots} r_n(K_i)R_n$, where $r_n(K_i)$ is the number of the circuits of size $4n+2$ in S. The summation over all sets of LM-conjugated circuits of all Kekule structures of B is denoted by $R(B) = R = \sum_{K_i} R(K_i) = \sum_{n=1,2,\ldots} r_n R_n$, where $r_n = \sum_{K_i} r_n(K_i)$. We also say $R(B)$ is the LM-conjugated circuit polynomial of B or simply the LMCC-polynomial of B, which is a polynomial of degree one with multi-variants. $R(B)$ may also be denoted by a sequence of numbers $(r_1, r_2, r_3, \ldots, r_n, \ldots)$, called the LMCC-code of B.

Definition 3 [14]. Let s be a ring of a benzenoid hydrocarbon B, and K_i a Kekule structure of B. A K_i-conjugated circuit C is said to be a minimal conjugated circuit of the ring s if the interior of C contains the interior of s and C has the minimum length. We also say that a K_i-conjugated circuit C of B is minimal if there is a ring s in B such that C is a minimal conjugated circuit of s (see figure 2). The maximal subgraph of B bounded by C is denoted by $B[C]$.

In particular, a circuit C is said to be an minimal conjugated circuit of a ring s if there is a Kekule structure K_i of B such that C is a minimal K_i-conjugated circuit of s. The corollary 2 in [14] shows that a minimal K_i-conjugated circuit C of a ring s of a benzenoid hydrocarbon B corresponds to a unique ring s such that C is a minimal K_i-conjugated circuit C of s in B.

Theorem A [14]. Let K_i be a Kekule structure of a benzenoid hydrocarbon B, and let C be a minimal K_i-conjugated circuit of a ring s of B. Then $B[C]$ is one of the BHs indicated in figure 3, and the K_i-double bonds in $B[C]$ are uniquely determined.

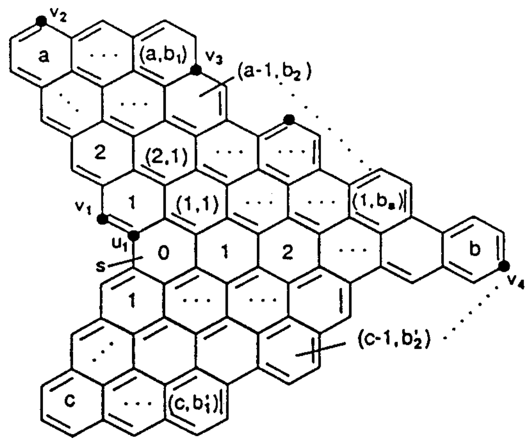


Figure 3. A general configuration of a minimal K_i-conjugated circuit C of a ring s in a benzenoid hydrocarbon B.

Theorem B [14]. Let K_i be a Kekule structure of a benzenoid hydrocarbon B. A set $S = \{C_1, C_2, C_3, \ldots, C_t\}$ of K_i-conjugated circuits of B is a set of LM-conjugated circuits of K_i if and only if for any ring s_j in any normal component of B, there is exactly one circuit C_j in S such that C_j is a minimal K_i-conjugated circuit of s_j.

Theorem B establishes the theoretical basis of the partition of the LMCC-polynomial of B into the LMCC-polynomials of rings of B. The LMCC-polynomial of a ring s in B, denoted by $R_s(B)$, is determined by taking the summation expression of the minimal conjugated circuits of s, one for every Kekule structure of B, and $R(B) = \sum_s^B R_s(B)$. $R_s(B)$ may also be denoted by a sequence of numbers (ring code) $(r_1(s), r_2(s), \ldots, r_n(s), \ldots)$, where $r_n(s)$ is the coefficient of the term R_n in $R_s(B)$.

Theorem C [14]. Let $B_1, B_2, \ldots, B_t$ be either t mutually disjoint BH-fragments with $B = B_1 \cup B_2 \cup \cdots \cup B_t$ or the normal components of an essentially disconnected BH-fragment B. Then $R(B) = \sum_{i=1}^t (K(B)/K(B_i))R(B_i)$.

Definition 4 [14]. For an edge $e = uv$ of a benzenoid hydrocarbon B, let $B_e(B_{\overline{e}})$ denote the labeled graph of B for which the edge e is labeled as double (single) bond, and let $B_e^*(B_{\overline{e}}^*)$ denote the normal components of B–u–v (B–e) (B_e^* and $B_{\overline{e}}^*$ may be thought as the normal components of $B_e(B_{\overline{e}})$, since e is in fact a fixed double (single) bond in $B_e(B_{\overline{e}})$). The subgraph of $B_e(B_{\overline{e}})$ induced by the hexagons in $B_e(B_{\overline{e}})$ which are not in $B_e^*(B_{\overline{e}}^*)$ is denoted by $B_e'(B_{\overline{e}}')$. The contribution of all rings in $B_e^*(B_{\overline{e}}^*)$ to $R(B_e)$ ($R(B_{\overline{e}})$) is denoted by $R^*(B_e)(R^*(B_{\overline{e}}))$, and the contribution of all rings in B_e' ($B_{\overline{e}}'$) to $R(B_e)$ ($R(B_{\overline{e}})$) is denoted by $R'(B_e)$ ($R'(B_{\overline{e}})$).

Theorem D [14]. Let e be an edge on the boundary of a benzenoid hydrocarbon B, and let $S_h(B_e')(S_h(B_{\overline{e}}'))$ be the set of rings in B_e' ($B_{\overline{e}}'$). Let $C_s(B_e)(C_s(B_{\overline{e}}))$ denote the set of

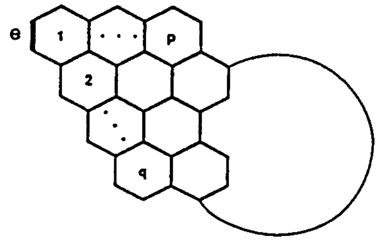


Figure 4. A local structure in a benzenoid hydrocarbon.

minimal conjugated circuits of a ring s in $B_e(B_{\overline{e}})$. Then

$$\begin{aligned} &\text{for } s \in S_h\big(B'_e\big), \quad R_s(B_e) = \sum_{C \in C_s(B_e)} K(B–C)R_{(|C|-2)/4}, \\ &\text{for } s \in S_h\big(B'_{\overline{e}}\big), \quad R_s(B_{\overline{e}}) = \sum_{C \in C_s(B_{\overline{e}})} K(B–C)R_{(|C|-2)/4}, \end{aligned} \tag{1}$$

where $|C|$ denotes the length of C, $K(B–C)$ is the number of Kekule structures of $B–C$;

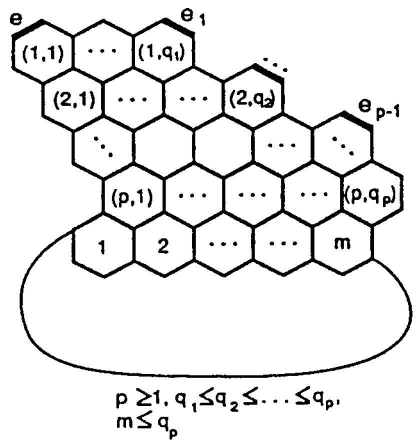
$$R'(B_e) = \sum_{s \in S_h(B'_e)} R_s(B_e) = \sum_{s \in S_h(B'_e)} \sum_{C \in C_s(B_e)} K(B–C)R_{(|C|-2)/4}, \tag{2}$$

$$R'(B_{\overline{e}}) = \sum_{s \in S_h(B'_{\overline{e}})} R_s(B_{\overline{e}}) = \sum_{s \in S_h(B'_{\overline{e}})} \sum_{C \in C_s(B_{\overline{e}})} K(B–C)R_{(|C|-2)/4}.$$

Definition 5 [14]. Let e be an edge on the boundary of a benzenoid hydrocarbon B. If B and e satisfy one of the following conditions: (1) B contains no crown (see the benzenoid hydrocarbon in figure 2) as its subgraph; (2) B contains a local structure as shown in figure 4, and e is the marked edge in figure 4; (3) B contains a local structure as shown in figure 5, and e is the marked edge in figure 5; then e is said to be a recursive edge of B.

Theorem E [14]. Let B be a BH which contains a recursive edge e on the boundary of B. Then

$$\begin{aligned} R(B) &= R^*(B_e) + R^*(B_{\overline{e}}) + R'(B_e) + R'(B_{\overline{e}}) \\ &= R\big(B^*_e\big) + R\big(B^*_{\overline{e}}\big) + \sum_{s \in S_h(B'_e)} \sum_{C \in C_s(B_e)} K(B–C)R_{(|C|-2)/4} \\ &\quad + \sum_{s \in S_h(B'_{\overline{e}})} \sum_{C \in C_s(B_{\overline{e}})} K(B–C)R_{(|C|-2)/4}. \end{aligned}$$



B

Figure 5. A local structure in a benzenoid hydrocarbon.

Definition 6 [14]. Let C be a minimal conjugated circuit of a ring s of a benzenoid hydrocarbon B, and let s' be a hexagon of B for which $C \cap s' \neq \emptyset$ and the interior of s' is contained in the exterior of C. If $C' = C\Delta s'$ (the symmetry difference of edge sets of C and s') is also a minimal conjugated circuit of s, then we say C' is obtained from C by a extension and s' is a extendible hexagon of C. For a ring s in B'_e ($B'_{\overline{e}}$), a minimal conjugated circuit C of s in B_e ($B_{\overline{e}}$) is said to be minimum if C has the smallest length and $B[C]$ contains a smallest number of hexagons.

Theorem F [14]. Let e be a recursive edge of a benzenoid hydrocarbon B, and let s be a ring in B'_e ($B'_{\overline{e}}$). Let C be a minimal conjugated circuit of s in B_e ($B_{\overline{e}}$) which is not minimum. Then C can be obtained from another minimal conjugated circuit of s in B_e ($B_{\overline{e}}$) by an extension.

Procedure 1 [14]. Let e be a recursive edge of a benzenoid hydrocarbon B, and s a ring in $B'_e(B'_{\overline{e}})$. Let C^* be a unique minimum conjugated circuit of s in $B_e(B_{\overline{e}})$.

(1) Set $S_0 = \{C^*\}$, $S_i = S_0$.

(2) For every minimal conjugated circuit C_i in S_i, find all extendible hexagons of C_i, extend C_i to new minimal conjugated circuits, and set them to S_{i+1}.

(3) If $S_{i+1} = 0$, then go to (4). Otherwise set $i + 1 \to i$, go to (2).

(4) Set $C_s(B_e) = \bigcup_{j=1}^{i} S_j$ $(C_s(B_{\overline{e}}) = \bigcup_{j=1}^{i} S_j)$.

An example of application of procedure 1 is shown in figure 6.

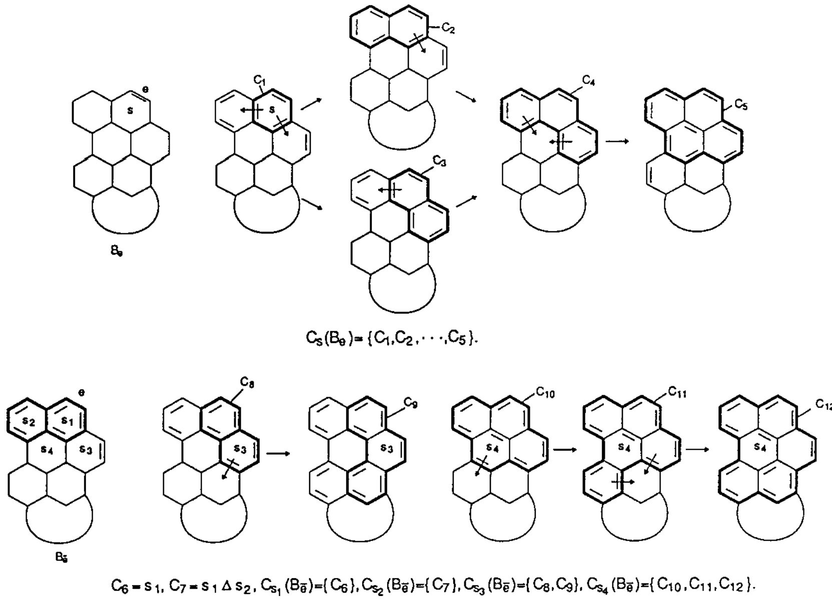


Figure 6. An example for application of procedure 1.

3. LM-conjugated circuits in catacondensed benzenoid hydrocarbons

In general cases, a catacondensed benzenoid hydrocarbon (cata-BH) B has the construction shown in figure 7, where $B_1, B_2, B_3, \ldots, B_{15}$ are subgraphs of B, each of which is a cata-BH. Particularly, if $n_2 = n_3 = 0$, B becomes a straight chain like cata-BH.

Lemma 1. Let $B = B_a(n)$ denote the straight cata-BH with n hexagons (see figure 1(a)). Then

$$R(B) = 2\sum_{i=1}^{n}(n+1-i)R_i. \tag{3}$$

Proof. B_e and $B_{\bar{e}}$ are shown in figure 8. It is easy to verify by theorem E and procedure 1 that

$$R\big(B_e^*\big) = 0, \qquad R\big(B_{\bar{e}}^*\big) = R\big(B_a(n-1)\big), \qquad R'(B_e) = \sum_{i=1}^{n} R_i, \qquad R'(B_{\bar{e}}) = \sum_{i=1}^{n} R_i,$$

and so

$$R\big(B_a(n)\big) = 2\sum_{i=1}^{n} R_i + R\big(B_a(n-1)\big). \tag{4}$$

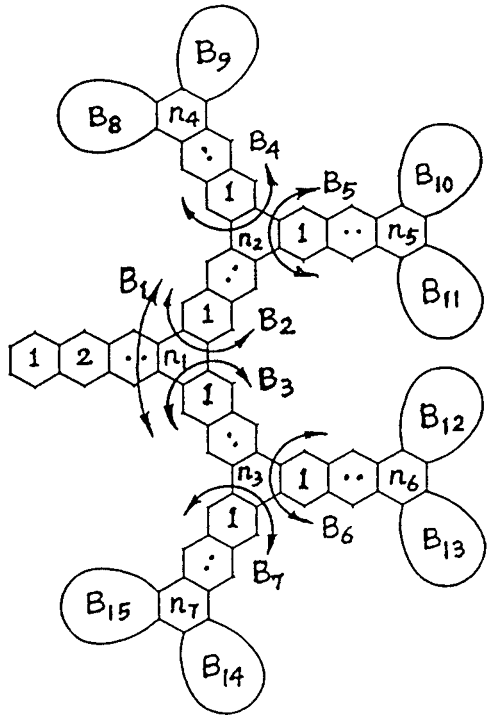


Figure 7. The construction of a catacondensed benzenoid hydrocarbon.

Figure 8. The labeled graphs B_e and $B_{\overline{e}}$ for a straight catacondensed benzenoid hydrocarbon B and an edge e of B.

Repeatedly using equation (4), we have

$$R\big(B_a(n)\big) = 2\sum_{i=1}^{n} R_i + 2\sum_{i=1}^{n-1} R_i + R\big(B_a(n-2)\big) = \cdots = 2\sum_{i=1}^{n}(n+1-i)R_i.$$

Theorem 1. Let B be a cata-BH shown in figure 7. Then

$$R(B) = R(B_1) + (n_1 - 1)\big[K(B_3)R(B_2) + K(B_2)R(B_3)\big] + 2K(B_2)K(B_3)\sum_{i=1}^{n-1}(n-i)R_i$$

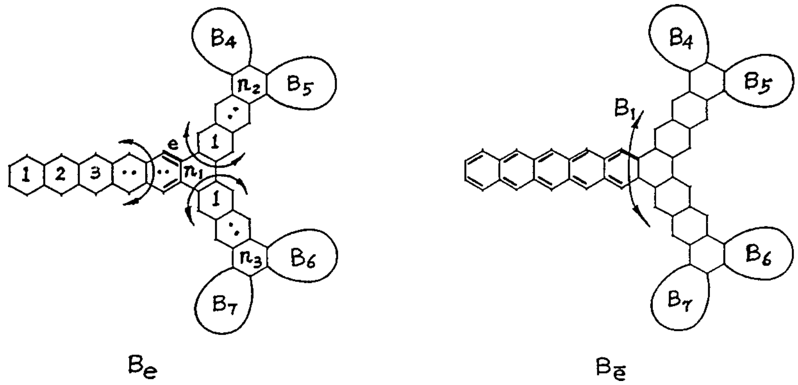


Figure 9. The labeled graphs B_e and $B_{\overline{e}}$ for a catacondensed benzenoid hydrocarbon B and an edge e of B.

$$+\left[\prod_{j=4}^{7} K(B_j)\right]\left[\sum_{i=2}^{n_1}\sum_{j=0}^{n_2-1}\sum_{k=0}^{n_3-1} R_{i+j+k} + \sum_{i=2}^{n_1} R_i\right]$$
$$+\left[\prod_{j=6}^{11} K(B_j)\right]\sum_{i=2}^{n_1}\sum_{k=0}^{n_3-1} R_{i+n_2+k}$$
$$+\left[\prod_{j=4,5,12}^{15} K(B_j)\right]\sum_{i=2}^{n_1}\sum_{j=0}^{n_2-1} R_{i+j+n_3} + \left[\prod_{j=8}^{15} K(B_j)\right]\sum_{i=2}^{n_1} R_{i+n_2+n_3}, \quad (5)$$

where, if $n_2 = 0$ ($n_3 = 0$), then $K(B_j) = 1$ for $j = 2, 4, 5$ ($j = 3, 6, 7$), $K(B_j) = 0$ for $j = 8, 9, 10, 11$ ($j = 12, 13, 14, 15$), and

$$\sum_{i=2}^{n_1}\sum_{j=0}^{n_2-1}\sum_{k=0}^{n_3-1} R_{i+j+k} = \sum_{i=2}^{n_1}\sum_{k=0}^{n_3-1} R_{i+k}\left(\sum_{i=2}^{n_1}\sum_{j=0}^{n_2-1} R_{i+j}\right).$$

Proof. Take a boundary edge e on the hexagon labeled by $n_1 - 1$ as the recursive edge. Then $B_e^* = B_2 \cup B_3 \cup B_a(n_1 - 2)$, $B_{\overline{e}}^* = B_1$ (see figure 9).

By theorems C, E, lemma 1, and procedure 1, we have

$$R\left(B_e^*\right) = 2K(B_2)K(B_3)\sum_{i=1}^{n_1-2}(n_1 - 1 - i)R_i + (n_1 - 1)\left[K(B_2)R(B_3) + K(B_3)R(B_2)\right],$$
$$R'(B_e) = K(B_2)K(B_3)\sum_{i=1}^{n_1-1} R_i + \left[\prod_{j=4}^{7} K(B_j)\right]\left[\sum_{i=2}^{n_1}\sum_{j=0}^{n_2-1}\sum_{k=0}^{n_3-1} R_{i+j+k} + \sum_{i=2}^{n_1} R_i\right]$$
$$+\left[\prod_{j=6}^{11} K(B_j)\right]\sum_{i=2}^{n_1}\sum_{k=0}^{n_3-1} R_{i+n_2+k} + \left[\prod_{j=4,5,12}^{15} K(B_j)\right]\sum_{i=2}^{n_1}\sum_{j=0}^{n_2-1} R_{i+j+n_3}$$

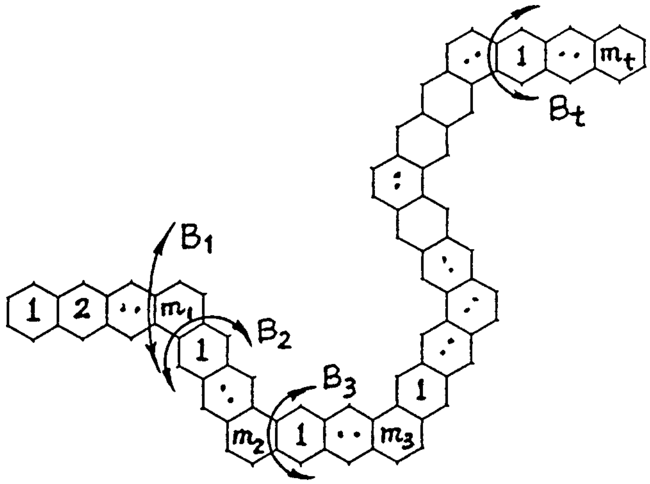


Figure 10. An unbranched catacondensed benzenoid hydrocarbon B.

$$+\left[\sum_{j=8}^{15} K(B_j)\right]\sum_{i=2}^{n_1} R_{i+n_2+n_3},$$

$$R\left(B^*_{\overline{e}}\right)=R(B_1), \qquad R'(B_{\overline{e}})=K(B_2)K(B_3)\sum_{i=1}^{n_1-1} R_i+\left[\prod_{j=4}^{7} K(B_j)\right]\sum_{i=2}^{n_1} R_i,$$

and so (5) holds.

Corollary 1. Let $B=B_{\mathrm{u}}(m_1,m_2,\ldots,m_t)$ denote an unbranched cata-BH as shown in figure 10. Then

$$\begin{aligned} R(B)={}&m_1R(B_2)+R(B_3)+\sum_{i=1}^{m_1-1}\big[2K(B_2)(m_1-i)+K(B_3)\big]R_i+2K(B_3)\sum_{i=1}^{m_2} R_i\\ &+K(B_3)\left[\sum_{i=2}^{m_1}\sum_{j=0}^{m_2-1} R_{i+j}+R_{m_1}-R_1\right]\\ &+K(B_4)\left[\sum_{i=m_2+2}^{m_1+m_2} R_i+2R_{m_2+1}+\sum_{i=m_2+2}^{m_2+m_3} R_i\right]+K(B_5)R_{m_2+m_3+1} \end{aligned}\tag{6}$$

where, if $m_2=0$ ($m_3=0$), then $K(B_j)=1$ for $j=2,3$ ($j=3,4$) and $K(B_j)=0$ for $j\geqslant 4$ ($j\geqslant 5$).

Proof. $B_{\mathrm{u}}(m_1, m_2, \ldots, m_t)$ corresponds to the case in theorem 1 with $n_3 = n_5 = n_9 = 0$, and $n_1 = m_1$, $n_2 = m_2$, $n_4 = m_3$, $n_8 = m_4$. By theorem 1, we have

$$R(B) = R(B_1) + (m_1 - 1)R(B_2) + 2K(B_2)\sum_{i=1}^{m_1-1}(m_1 - 1)R_i + K(B_3)\left[\sum_{i=2}^{m_1}\sum_{j=0}^{m_2-1} R_{i+j} + \sum_{i=2}^{m_1} R_i\right] + K(B_4)\sum_{i=2}^{m_1} R_{i+m_2}. \tag{7}$$

Similarly, we have by theorem E that

$$R(B_1) = R(B_2) + R(B_3) + 2K(B_3)\sum_{i=1}^{m_2} R_i + K(B_4)\Big(2R_{m_2+1} + \sum_{i=m_2+2}^{m_2+m_3} R_i\Big) + K(B_5)R_{m_2+m_3+1}.$$

With the substitution of the expression for $R(B_1)$ into (7), we obtain the expression (6).

Using expressions (5), (6), we can easily obtain the calculation formulae for enumeration of LM-conjugated circuits of the cata-BHs in figure 1 as follows.

Corollary 2. Let $B_{\mathrm{b}}(n)$, $n \geqslant 2$, be the cata-BH shown in figure 1(b). Then

$$R\big(B_{\mathrm{b}}(n)\big) = (6n - 2)R_1 + 4(n - 1)R_2 + \sum_{i=3}^{n}(4n + 3 - 4i)R_i + R_{n+1}.$$

Corollary 3. Let $B_{\mathrm{c}}(n)$, $n \geqslant 1$, be the cata-BH shown in figure 1(c). Then

$$R\big(B_{\mathrm{c}}(n)\big) = 4(4n + 1)R_1 + 8nR_2 + 4\sum_{i=3}^{n}(2n + 3 - 2i)R_i + 6R_{n+1} + 2R_{n+2}.$$

Corollary 4. Let $B_{\mathrm{d}}(n)$, $n \geqslant 2$, be the cata-BH shown in figure 1(d). Then

$$R\big(B_{\mathrm{d}}(n)\big) = 2(8n - 3)R_1 + 2(4n - 5)R_2 + \sum_{i=3}^{n}(8n + 5 - 8i)R_i + 3R_{n+1} + R_{n+2}.$$

Corollary 5. Let $B_{\mathrm{e}}(n)$, $n \geqslant 1$, be the cata-BH shown in figure 1(e). Then

$$R\big(B_{\mathrm{e}}(n)\big) = 96nR_1 + 8R_2 + 8\sum_{i=2}^{n}(4n + 5 - 4i)R_i + 26R_{n+1} + 12R_{n+2} + 2R_{n+3}.$$

Corollary 6. Let $B_{\mathrm{f}}(n)$, $n \geqslant 3$, be the cata-BH shown in figure 1(f). Then

$$R\big(B_{\mathrm{f}}(n)\big) = \sum_{i=0}^{n-1} F_i (2F_{n-i-1} R_1 + 2F_{n-i-2} R_2 + F_{n-i-3} R_3),$$

where $F_i = F_{i-1} + F_{i-2}$ is Fibonacci's number, $F_0 = F_1 = 1$ and $F = 0$ for $i \leqslant -1$.

For more general cases, we give the following examples.

Corollary 7. Let $B_{\mathrm{u}}(m_1, m_2)$ be an unbranched cata-BH (see figure 10). Then

$$R\big(B_{\mathrm{u}}(m_1, m_2)\big) = \sum_{i=1}^{m_1} \big[2(m_2+1)(m_1-i)+1\big] R_i + 2\sum_{i=1}^{m_2} \big[m_1(m_2+1-i)+1\big] R_i + \sum_{i=m_2+2}^{m_1+m_2} R_i + \sum_{i=2}^{m_1} \sum_{j=0}^{m_2-1} R_{i+j} - R_1 + 2R_{m_2+1}.$$

Corollary 8. Let $B_{\mathrm{u}}(m_1, m_2, m_3)$ be an unbranched cata-BH (see figure 10). Then

$$\begin{aligned} R\big(B_{\mathrm{u}}(m_1, m_2, m_3)\big) &= \sum_{i=1}^{m_1-1} \big\{2\big[m_2(m_3+1)+1\big](m_1-i) + (m_3+1)\big\} R_i \\ &\quad + \sum_{i=1}^{m_2} \big[2m_1(m_3+1)(m_2-i) + m_1 + 2m_3 + 2\big] R_i \\ &\quad + 2\sum_{i=1}^{m_3} \big[(m_3+1-i)(m_1m_2+1) + m_1\big] R_i \\ &\quad + (m_3+1) \sum_{i=2}^{m_1} \sum_{j=0}^{m_2-1} R_{i+j} + m_1 \sum_{i=2}^{m_2} \sum_{j=0}^{m_3-1} R_{i+j} + \sum_{i=m_2+2}^{m_1+m_2} R_i + \sum_{i=m_2+2}^{m_2+m_3} R_i \\ &\quad + m_1 \sum_{i=m_3+2}^{m_2+m_3} R_i - (m_1+m_3+1)R_1 + (m_3+1)R_{m_1} + 2R_{m_2+1} + 2m_1 R_{m_3+1} \\ &\quad + R_{m_2+m_3+1}. \end{aligned}$$

Corollary 9. Let $B_{\mathrm{Y}}(n_1, n_2, n_3)$ denote the cata-BH shown in figure 11. Then

$$\begin{aligned} R\big(B_{\mathrm{Y}}(n_1, n_2, n_3)\big) &= \sum_{i=1}^{n_1} \big[2(n_2+1)(n_3+1)(n_1-i)+1\big] R_i + \sum_{i=1}^{n_2} \big[2n_1(n_3+1)(n_2+1-i)+1\big] R_i \end{aligned}$$

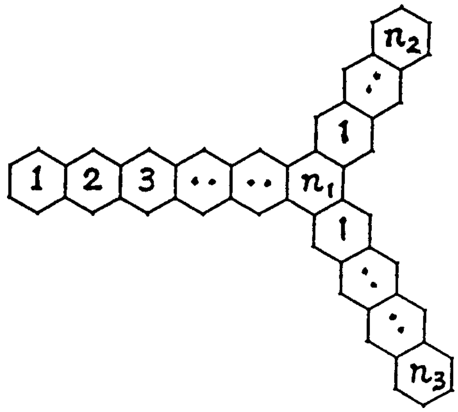


Figure 11. A catacondensed benzenoid hydrocarbon $B_{\mathrm{Y}}(n_1, n_2, n_3)$ consisting of three straight catacondensed benzenoid hydrocarbons.

$$
\begin{aligned}
&+\sum_{i=1}^{n_3} 2\big[n_1(n_2+1)(n_3+1-i)+1\big]R_i+\sum_{i=2}^{n_1}\sum_{j=0}^{n_2-1}\sum_{k=0}^{n_3-1}R_{i+j+k}+\sum_{i=2}^{n_1}\sum_{j=0}^{n_2-1}R_{i+j+n_3}\\
&+\sum_{i=2}^{n_1}\sum_{k=0}^{n_3-1}R_{i+n_2+j}+\sum_{i=2}^{n_2-1}\sum_{j=0}^{n_3-1}R_{i+j}+\sum_{i=n_3+1}^{n_1+n_2+n_3}R_i-2R_1+R_{n_2+1}+R_{n_3+1}.
\end{aligned}
$$

4. LM-conjugated circuits in some families of structurally related pericondensed benzenoid hydrocarbons

For enumerations of LM-conjugated circuits in some families of structurally related pericondensed benzenoid hydrocarbons, we need to use theorem E and procedure 1, and often need to deal with several recursive relations of several families of structurally related subgraphs for a family of structurally related peri-BHs. We will give some results but omit the operation processes.

We first give the recursive formulae for enumeration of LM-conjugated circuits of the peri-BHs in figure 1.

Corollary 10. Let $B_{\mathrm{g}}(n)$ be the BH shown in figure 1(g). Then

$$
\begin{aligned}
R\big(B_{\mathrm{g}}(n)\big)=2\sum_{i=1}^{n}(5n+8-5i)R_i+(10n+6)R_1+4(n+1)R_2+(n+2)R_3+6R_{n+1}\\
+4R_{n+2}+2R_{n+3}.
\end{aligned}
$$

Corollary 11. Let $B_{\mathrm{h}}(n)$ be the BH shown in figure 1(h). Then

$$
\begin{aligned}
R\big(B_{\mathrm{h}}(n)\big) = 2\sum_{i=0}^{n-1} R\big(B_{\mathrm{h}}(i)\big) &+ 2\left[2\sum_{i=-1}^{n-2}(n-1-i)K\big(B_{\mathrm{h}}(i)\big) + K\big(B_{\mathrm{h}}(n-1)\big)\right]R_1 \\
&+ 8\sum_{i=-1}^{n-2} K\big(B_{\mathrm{h}}(i)\big)R_2 + 2\left[3\sum_{i=-1}^{n-3}(n-2-i)K\big(B_{\mathrm{h}}(i)\big) + 2K\big(B_{\mathrm{h}}(n-2)\big)\right]R_3 \\
&+ 8\sum_{i=-1}^{n-3} K\big(B_{\mathrm{h}}(i)\big)R_4 + 4\sum_{i=-1}^{n-4}(n-3-i)K\big(B_{\mathrm{h}}(i)\big)R_5,
\end{aligned}
$$

where

$$
R\big(B_{\mathrm{h}}(0)\big) = 2R_1, \qquad K\big(B_{\mathrm{h}}(n)\big) = 2\textstyle\sum_{i=-1}^{n-1} K\big(B_{\mathrm{h}}(i)\big), \qquad K\big(B_{\mathrm{h}}(0)\big) = 2,
$$

$$
K\big(B_{\mathrm{h}}(-1)\big) = 1, \quad \text{and} \quad K\big(B_{\mathrm{h}}(i)\big) = 0 \quad \text{for } i \leqslant -2.
$$

Corollary 12. Let $B_{\mathrm{i}}(n)$ be the BH shown in figure 1(i). Then, for $n = 2p$,

$$
\begin{aligned}
&R\big(B_{\mathrm{i}}(n)\big) \\
&\quad = 2R\big(B_{\mathrm{i}}(n-1)\big) + \sum_{j=-1}^{(n/2)-2} R\big(B_{\mathrm{i}}(2j+1)\big) \\
&\qquad + 2\left[\sum_{j=-1}^{(n/2)-2}\left(\frac{n}{2}-1-j\right)K\big(B_{\mathrm{i}}(2j+1)\big) + K\big(B_{\mathrm{i}}(n-1)\big)\right]R_1 \\
&\qquad + 2\sum_{j=-1}^{n-2} K\big(B_{\mathrm{i}}(j)\big)R_2 \\
&\qquad + \left\{\sum_{j=-1}^{(n/2)-2}\left(\frac{n}{2}-1-j\right)\big[2K\big(B_{\mathrm{i}}(2j)\big) + K\big(B_{\mathrm{i}}(2j+1)\big)\big] + K\big(B_{\mathrm{i}}(n-2)\big)\right\}R_3 \\
&\qquad + \left\{\sum_{j=-1}^{(n/2)-2}\left[2K\big(B_{\mathrm{i}}(2j)\big) + \left(\frac{n}{2}-2-j\right)K\big(B_{\mathrm{i}}(2j+1)\big)\right] + K\big(B_{\mathrm{i}}(n-3)\big)\right\}R_4;
\end{aligned}
$$

for $n = 2p + 1$,

$$
\begin{aligned}
&R\big(B_{\mathrm{i}}(n)\big) \\
&\quad = 2R\big(B_{\mathrm{i}}(n-1)\big) + \sum_{j=0}^{(n-3)/2} R\big(B_{\mathrm{i}}(2j)\big) \\
&\qquad + 2\left[\sum_{j=-1}^{(n-3)/2}\left(\frac{n-1}{2}-j\right)K\big(B_{\mathrm{i}}(2j)\big) + K\big(B_{\mathrm{i}}(n-1)\big)\right]R_1 + 2\sum_{j=-2}^{n-2} K\big(B_{\mathrm{i}}(j)\big)R_2
\end{aligned}
$$

$$+\left\{\sum_{j=-1}^{(n-3)/2}\left[\left(\frac{n-1}{2}-j\right)K\big(B_{\mathrm{i}}(2j)\big)+2\left(\frac{n-1}{2}-1-j\right)K\big(B_{\mathrm{i}}(2j+1)\big)\right]\right.$$
$$\left.+K\big(B_{\mathrm{i}}(n-2)\big)\right\}R_3$$
$$+\left\{\sum_{j=-1}^{(n-5)/2}\left[\left(\frac{n-1}{2}-1-j\right)K\big(B_{\mathrm{i}}(2j)\big)+2K\big(B_{\mathrm{i}}(2j+1)\big)\right]+K\big(B_{\mathrm{i}}(n-3)\big)\right\}R_4,$$

where

$$R\big(B_{\mathrm{i}}(0)\big)=8R_1,\qquad R\big(B_{\mathrm{i}}(-1)\big)=2R_1,$$
$$K\big(B_{\mathrm{i}}(n)\big)=K\big(B_{\mathrm{i}}(n-1)\big)+\sum_{j=-1}^{(n/2)-1}K\big(B_{\mathrm{i}}(2j+1)\big)\quad\text{for } n=2p,$$
$$K\big(B_{\mathrm{i}}(n)\big)=K\big(B_{\mathrm{i}}(n-1)\big)+\sum_{j=-1}^{(n-1)/2}K\big(B_{\mathrm{i}}(2j)\big)\quad\text{for } n=2p+1,$$
$$K\big(B_{\mathrm{i}}(0)\big)=4,\qquad K\big(B_{\mathrm{i}}(-1)\big)=2,\qquad K\big(B_{\mathrm{i}}(-2)\big)=1\quad\text{and}$$
$$K\big(B_{\mathrm{i}}(j)\big)=0\quad\text{for } j\leqslant 3.$$

Corollary 13. Let $B_{\mathrm{j}}(n)$ be the BH shown in figure 1(j). Then

$$R\big(B_{\mathrm{j}}(n)\big)=R\big(B_{\mathrm{j}}(n-1)\big)+2R\big(B_{\mathrm{j}}(n-2)\big)+\sum_{i=1}^{n-3}R\big(B_{\mathrm{j}}(i)\big)$$
$$+2\left[\sum_{i=-1}^{n-3}(n-1-i)K\big(B_{\mathrm{j}}(i)\big)+2K\big(B_{\mathrm{j}}(n-2)\big)\right]R_1$$
$$+2\left[2\sum_{i=-1}^{n-3}K\big(B_{\mathrm{j}}(i)\big)+K\big(B_{\mathrm{j}}(n-2)\big)\right]R_2$$
$$+\left[\sum_{i=-1}^{n-5}(n-1-i)K\big(B_{\mathrm{j}}(i)\big)+4K\big(B_{\mathrm{j}}(n-3)\big)+4K\big(B_{\mathrm{j}}(n-4)\big)\right]R_3$$
$$+\left[\sum_{i=-1}^{n-5}(n-1-i)K\big(B_{\mathrm{j}}(i)\big)+4K\big(B_{\mathrm{j}}(n-4)\big)\right]R_4,$$

where

$$B_{\mathrm{j}}(n)=0\quad\text{for } j\_0,$$
$$K\big(B_{\mathrm{j}}(n)\big)=K\big(B_{\mathrm{j}}(n-2)\big)+\sum_{i=-1}^{n-1}K\big(B_{\mathrm{j}}(i)\big),$$
$$K\big(B_{\mathrm{j}}(n)\big)=1\quad\text{for } j=0,1,\quad\text{and}\quad K\big(B_{\mathrm{j}}(n)\big)=0\quad\text{for } n\leqslant 3.$$

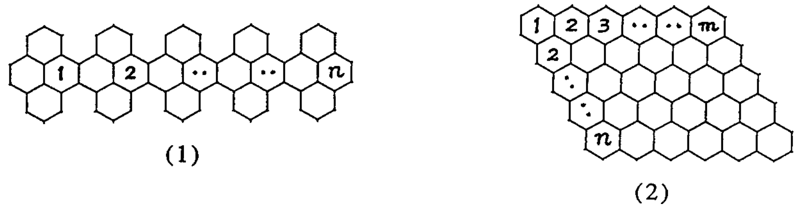


Figure 12. Two families of pericondensed benzenoid hydrocarbons.

Finally, for the two families of peri-BHs shown in figure 12, we give the recursive formulae for enumeration of their LM-conjugated circuits.

Corollary 14. Let $B_{\mathrm{k}}(n)$ be the BH shown in figure 12(1). Then

$$\begin{aligned} R\big(B_{\mathrm{k}}(n)\big) = {} & 5R\big(B_{\mathrm{k}}(n-1)\big) + 4\sum_{i=1}^{n-2} R\big(B_{\mathrm{k}}(i)\big) \\ & + 2\left[4\sum_{i=0}^{n-2}(n-i)K\big(B_{\mathrm{k}}(i)\big) + 5K\big(B_{\mathrm{k}}(n-1)\big) + n\right]R_1 \\ & + 2\left[\sum_{i=0}^{n-2}(8n-7-8i)K\big(B_{\mathrm{k}}(i)\big) + 2K\big(B_{\mathrm{k}}(n-1)\big) + 2n\right]R_2 \\ & + \left[4\sum_{i=0}^{n-2}(n+2-i)K\big(B_{\mathrm{k}}(i)\big) + K\big(B_{\mathrm{k}}(n-1)\big) + n + 2\right]R_3 \\ & + \left[2\sum_{i=0}^{n-3}(2n-3-2i)K\big(B_{\mathrm{k}}(i)\big) + 3K\big(B_{\mathrm{k}}(n-2)\big) + n - 1\right]R_4, \end{aligned}$$

where

$$R\big(B_{\mathrm{k}}(0)\big) = 0, \qquad K\big(B_{\mathrm{k}}(n)\big) = 5K\big(B_{\mathrm{k}}(n-1)\big) + 4\sum_{i=0}^{n-2} K\big(B_{\mathrm{k}}(i)\big) + 1,$$
$$K\big(B_{\mathrm{k}}(0)\big) = 1 \quad \text{and} \quad K\big(B_{\mathrm{k}}(i)\big) = 0 \quad \text{for } i \leqslant -1.$$

Corollary 15. Let $B_{\mathrm{l}}[m,n]$ be the BH shown in figure 12(2). Then

$$\begin{aligned} R\big(B_{\mathrm{l}}[m,n]\big) = {} & R\big(B_{\mathrm{l}}[m-1,n]\big) + R\big(B_{\mathrm{l}}[m,n-1]\big) \\ & + 2\sum_{i=1}^{m}\sum_{j=1}^{n} K\big(B_{\mathrm{l}}[m-i,n-j]\big)K\big(B_{\mathrm{l}}[i-1,j-1]\big)R_{i+j-1}, \end{aligned}$$

where

$$\begin{aligned} K\big(B_{\mathrm{l}}[m,n]\big) = {} & K\big(B_{\mathrm{l}}[m-1,n]\big) + \big(B_{\mathrm{l}}[m,n-1]\big),\ K\big(B_{\mathrm{l}}[m,0]\big) = K\big(B_{\mathrm{l}}[0,n]\big) \\ = {} & K\big(B_{\mathrm{l}}[0,0]\big) = 1. \end{aligned}$$

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References

[1] M. Randic, Chem. Phys. Lett. 38 (1976) 68.
[2] M. Randic, J. Amer. Chem. Soc. 99 (1977) 444.
[3] M. Randic, Tetrahedron 33 (1977) 1905.
[4] E. Clar, *The Aromatic Sextet* (Wiley, London, 1972).
[5] D.J. Klein and N. Trinajstic, Pure Appl. Chem. 61 (1989) 2107.
[6] D.J. Klein, Topics Curr. Chem. 153 (1990) 57.
[7] N. Trinajstic, *Chemical Graph Theory* (CRC Press, 1992).
[8] L. Pauling, J. Chem. Phys. 1 (1933) 280.
[9] L. Pauling and G.W. Wheland, J. Chem. Phys. 1 (1933) 362, 606; 2 (1933) 482.
[10] W.T. Simpson, J. Amer. Chem. Soc. 75 (1953) 593.
[11] W.C. Herndon, J. Amer. Chem. Soc. 95 (1973) 2404; Isr. J. Chem. 20 (1980) 270.
[12] M. Randic, Internat. J. Quant. Chem. 17 (1980) 549.
[13] M. Randic and Xiaofeng Guo, Internat. J. Quant. Chem. 49 (1994) 215.
[14] Xiaofeng Guo and M. Randic, J. Chem. Inf. Comput. Sci. 34 (1994) 339.
[15] Xiaofeng Guo, M. Randic and D. J. Klein, Internat. J. Quant. Chem. 60 (1996) 943.
[16] S. Nikolic, M. Randic, D. J. Klein, D. Plavsic and N. Trinajstic, J. Mol. Struct. 198 (1989) 223.
[17] N. Trinajstic and S. Nikolic, J. Mol. Struct. (Theochem) 229 (1991) 63.
[18] H. Vogler and N. Trinajstic, Theor. Chim. Acta 73 (1988) 437.
[19] S. Nikolic, N. Trinajstic and D.J. Klein, Comput. Chem. 14 (1990) 313.
[20] D. Plavsic, S. Nikolic and N. Trinajstic, Croat. Chem. Acta 63 (1990) 683.
[21] D. Plavsic, S. Nikolic and N. Trinajstic, J. Math. Chem. 8 (1991) 113.
[22] D.J. Klein, W.A. Seitz and T.G. Schmalz, in: *Computational Chemical Graph Theory*, ed. D.H. Rouvray (Nova, New York, 1990) p. 127.
[23] D. Plavsic, N. Trinajstic, M. Randic and C. Venier, Croat. Chem. Acta 62 (1989) 719.
[24] N. Trinajstic, D. Plavsic and D.J. Klein, Croat. Chem. Acta 62 (1989) 711.