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# Sextet and Cell Polynomials of Hexagonal Systems

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**Abstract.** Mathematical properties of the sextet and cell polynomials of a hexagonal system are developed including recursive expressions for their calculation and expressions for their derivatives.

## 1. Introduction.

Let B be a plane bipartite graph and has a perfect matching such that the boundaries of its interior faces are cycles. Let C be a non-empty set of interior faces of B. We call C a resonant set of B if the interior faces of C are pair-wise disjoint and there exists a perfect matching of B that contains a perfect matching of each face in C (Abeledo and Atkinson [2000]) or equivalently if the interior faces of B are pair-wise disjoint and B-(C) has a perfect matching or is empty (B-(C) denotes the subgraph of B obtained by deleting from B all the vertices of the faces in C together with their incident edges) (Gutman [1983]). It is convenient here to consider the empty set as a resonant set.

We denote by r(B, k) the number of resonant sets of the graph B with cardinality k. By definition r(B, 0)= 1. The sextet polynomial (Hosoya and Yamaguchi [1975]) of the graph B is defined as $\sigma(B)=\sigma(B, x)= r(B, 0)+ r(B, 1) x^1+ \ldots + r(B, m) x^m$, where m is the cardinality of a maximum resonant set, called the Clar number (Hansen and Zheng [1992]). The sextet polynomial of a graph is the product of the sextet polynomials of its connected components (Gutman et al. [1977]).

Let $R_1, R_2, \ldots, R_h$ be the interior faces of the graph B. Associate a variable $x_i$ to the interior face $R_i$, i= 1, 2, …, h. Let C= {$R\_i_1$, $R\_i_2$, …, $R\_i_k$} be a resonant set of B. Then to this resonant set, we associate a so-called "resonant ring (sextet) monomial" E(C)= $x\_i_1$ $x\_i_2$… $x\_i_k$. By definition E(Φ)= 1. The cell polynomial of B (Gutman [1981]) is defined as

$\rho$ (B)= $\rho(B, x_1, x_2, \ldots, x_h)= \sum_C E(C)$, where the summation goes over all the resonant sets of B (including the empty set). The cell polynomial is a direct generalization of the sextet polynomial (Gutman [1981]) since $\rho(B, x_1= x, x_2= x, \ldots, x_h= x)= \sigma(B, x)$.

A hexagonal system is a connected subgraph of the hexagonal lattice without non- hexagonal interior faces or cut edges. The vertices of a hexagonal system H are divided into external and internal. A vertex of H lying on the boundary of the exterior face of H is called an external vertex; otherwise it is called an internal vertex. A hexagon of H such that none of its vertices is external is called an internal hexagon; otherwise it is an external hexagon. If a hexagonal system has no internal vertices, it said to be catacondensed; otherwise, it is pericondensed. A pericondensed hexagonal system is fat if it has an internal hexagon, or equivalently if it has coronene (see Fig. 1) as a subgraph, otherwise, it is thin. A hexagonal system is to be placed on the plane so that a pair of edges of each hexagon lies in parallel with the vertical axis. A hexagon of a hexagonal system has twelve modes (Gutman and Cyvin [1989]) with respect to the number of its adjacent hexagons and their mutual positions. A perfect matching of a hexagon is called a sextet (Ohkami et al. [1981]). It is proper if the right vertical edge of the hexagon is in the perfect matching; otherwise, it is improper.

A catacondensed hexagonal system has the property that its sextet polynomial evaluated at x=1 is equal to number of its perfect matchings (Gutman et al. [1977]). A pericondensed hexagonal system H has this property if and only if for any coronene which is a subgraph of H, the subgraph of H obtained by deleting from H all the vertices of the coronene (together with their incident edges) has no perfect matching (Zhang and Chen [1986]).

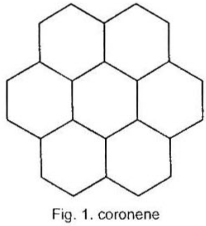

Fig. 1. coronene

An edge of a graph H that has a perfect matching is a fixed single (fixed double) edge if it belongs to none (all) the perfect matchings of H. An edge is fixed if it is either a fixed single edge or a fixed double edge. The unfixed subgraph U(H) of a graph H is obtained by deleting from H all its fixed double edges together with their end vertices and all its fixed single edges without their end vertices.

A hexagonal system is normal if it has a perfect matching and no fixed edges (Hansen and Zheng [1993]) or equivalently (Zhang and Chen [1991]) if each hexagon is resonant. A catacondensed hexagonal system is normal (Gutman et al. [1977]). A pericondensed hexagonal system is normal if and only if the boundary of its exterior face is an alternating cycle (Zhang and Chen [1991]).

Let H be a hexagonal system. Let R be a hexagon of H. By H-R, we denote the subgraph of H obtained by deleting from H the vertices and the edges that belong only to R. By H-(R), we denote the subgraph of H obtained by deleting from H all the vertices of R (together with their incident edges).

## 2. Results

**Proposition 1.** Let H be a hexagonal system that has a perfect matching. Let R be a hexagon of H with $L_1$ mode. Then C is a resonant set of H that does not contain R if and only if C is a resonant set of H-R. Hence, the sum of the resonant sextet monomials of H that define the resonant sets of H that do not contain R is ρ(H-R).

**Proof.** *If part:*

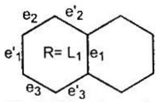

Fig. 2. R has $L_1$ mode

Let C be a resonant set of H-R. Let M be a perfect matching of H-R that contains a sextet of each hexagon in C. $M \cup \{e_2, e_3\}$ is a perfect matching of H that contains a sextet of each hexagon in C. Hence, C is a resonant set of H that does not contain R.

*Only if part:*

Let C be a resonant set of H that does not contain R. Let M be a perfect matching of H that contains a sextet of each hexagon in C.

*Case: $e'_1 \notin M$*

Then $e_2, e_3 \in M$ and $e'_2, e'_3 \notin M$. Hence, $M \setminus \{e_2, e_3\}$ is a perfect matching of H-R that contains a sextet of each hexagon in C. Hence, C is a resonant set of H-R.

*Case: $e'_1 \in M$*

Then $e_2, e_3 \notin M$ and $e'_2, e'_3 \in M$. Thus, M contains an improper sextet of R. Rotate R into a proper sextet and obtain another perfect matching of H that also contains a sextet of each hexagon in C (recall that R does not belong to C and also note that the hexagon adjacent to R does not belong to C either since $e'_2 \in M$). Subtracting $\{e_2, e_3\}$ from this latter perfect matching of H (that contains a proper sextet of R), we obtain a perfect matching of H-R that contains a sextet of each hexagon in C. Hence, C is a resonant set of H-R.

**Q.E.D.**

**Proposition 2.** Let H be a catacondensed hexagonal system. Let R be a hexagon of H with $A_2$ or $A_3$ mode. Then C is a resonant set of H that does not contain R if and only if C is a resonant set of H-R. Hence, the sum of the resonant sextet monomials of H that define the resonant sets of H that do not contain R is $\rho(H\text{-}R)$.

**Proof.** Case: R is $A_2$

*If part:*

Let C be a resonant set of H-R. Let M be a perfect matching of H-R that contains a sextet of each hexagon in C. $M \cup \{e'_3\}$ is a perfect matching of H that contains a sextet of each hexagon in C. See Fig. 3. Hence, C is a resonant set of H that does not contain R.

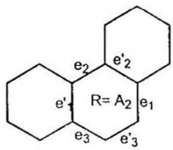

Fig. 3. R has $A_2$ mode

*Only if part:*

Let C be a resonant set of H that does not contain R. Let M be a perfect matching of H that contains a sextet of each hexagon in C.

*Case: $e'_3 \in M$*

Then $e_1, e_3 \notin M$. $e_2 \notin M$ since a catacondensed (sub) system has an even number of vertices. $M \setminus \{e'_3\}$ is a perfect matching of H-R that contains a sextet of each hexagon in C. Hence, C is a resonant set of H-R.

*Case: $e'_3 \notin M$*

Then $e_1, e_3 \in M$. $e_2 \in M$ since a catacondensed (sub) system has an even number of vertices. Hence, M contains a proper sextet of R. Rotate R into an improper sextet and obtain another perfect matching of H that contains a sextet of each hexagon in C (recall that R does not belong to C and note that none of the two hexagons that are adjacent to R belongs to C since $e_2 \in M$). Subtracting $\{e'_3\}$ from this latter perfect matching of H (that contains an improper sextet of R), we obtain a perfect matching of H-R that contains a sextet of each hexagon in C. Thus, C is a resonant set of H-R.

*Case: R is $A_3$*

*If part:*

Let C be a resonant set of H-R. Let M be a perfect matching of H-R that contains a sextet of each hexagon in C. Then M is a perfect matching of H that contains a sextet of each hexagon in C. See Fig. 4. Thus, C is a resonant set of H that does not contain R.

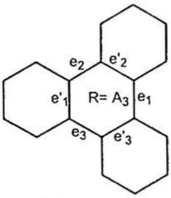


Fig. 4. R has $A_3$ mode

*Only if part:*

Let C be a resonant set of H that does not contain R. Let M be a perfect matching of H that contains a sextet of each hexagon in C. Consider the number of edges among $e_1$, $e_2$ and $e_3$ that belong to M. This number cannot be one or two since a catacondensed (sub) system has an even number of vertices.

*Case: $e_1, e_2, e_3 \notin M$*

M is a perfect matching of H-R that contains a sextet of each hexagon in C. Thus, C is a resonant set of H-R.

*Case: $e_1, e_2, e_3 \in M$*

M contains a proper sextet of R. Rotate R into an improper sextet and obtain another perfect matching of H that contains a sextet of each hexagon in C (recall that R does not belong to C and note that none of the three hexagons that are adjacent to R belongs to C since $e_1, e_2 \in M$). This latter perfect matching of H (that contains an improper sextet of R) is a perfect matching of H-R and contains a sextet of each hexagon in C. Thus, C is a resonant set of
H-R.

**Q.E.D.**

**Remark.** Proposition 2 cannot be extended to pericondensed hexagonal systems. Counter examples are in Fig. 5.

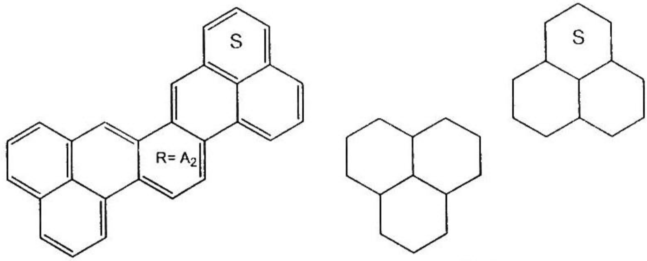


Fig. 5-a. {S} is a resonant set of H, but not a resonant set of H-R

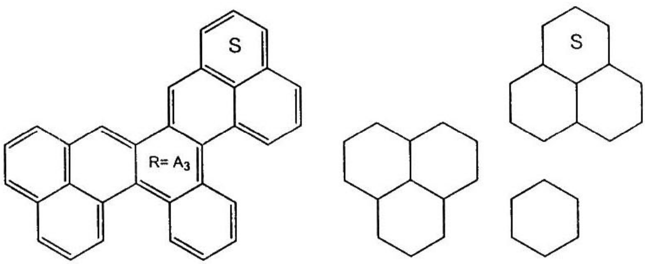


Fig. 5-b. {S} is a resonant set of H, but not a resonant set of H-R

**Remark.** Proposition 1 and proposition 2 are not valid if R has any mode other than $L_1$, $A_2$ or $A_3$. Counterexamples are given in Fig. 6. The examples given for $L_2$ are for catacondensed and pericondensed hexagonal systems.

**Proposition 3.** Let H be a hexagonal system with a perfect matching such that for any coronene which is a subgraph of H, the subgraph of H obtained by deleting from H all the vertices of the coronene (together with their incident edges) has no perfect matching. Let R be a resonant hexagon of H. Then C is a resonant set of H that contains R if and only if C\ {R} is a resonant set of H- (R). Hence the sum of the resonant sextet monomials of H that define the resonant sets of H that contain R is xρ(H- (R)), where x the variable that corresponds to R.

**Proof.** *Only if part:*

Let C be a resonant set of H that contains R.

*Case: C\ {R} is empty*

Then, by definition, C\ {R} is a resonant set of H- (R).

*Case: C\ {R} is not empty*

Then, it is composed of hexagons (interior faces) of H- (R). It is clear that these hexagons are pair-wise disjoint. Let M be a perfect matching of H that contains a sextet of each hexagon in C. Subtracting the sextet of R from M, we obtain a perfect matching of H- (R) that contains a sextet of each hexagon in C\ {R}. Hence, C\ {R} is a resonant set of H-(R).

*If part:*

Let C be a resonant set of H- (R).

*Case: C is empty*

C∪{R} = {R} is a resonant set of H by assumption.

*Case: C is not empty*

*Subcase: R is an external hexagon of H*

C is composed of hexagons of H and so is C∪{R}.

*Subcase: R is an internal hexagon of H, i.e. $L_6$ mode*

C is composed of hexagons of H since the boundary of the coronene whose central hexagon is R cannot belong to C. Hence, C∪{R} is composed of hexagons of H.

In either subcase, it is clear that the hexagons of C∪{R} are pair-wise disjoint. Let M be a perfect matching of H- (R) that contains a sextet of each hexagon in C. Adding to M, a sextet of R, we obtain a perfect matching of H that contains a sextet of each hexagon in C∪{R}. Hence, C∪{R} is a resonant set of H.

**Q.E.D.**

**Remark.** Proposition 3 is not valid for any (general) hexagonal system with a perfect matching. See Fig. 7.

**Corollary 4** (Gutman [1981], Salem and Gutman [2003]) Let H be a catacondensed hexagonal system and let $R_i$ be a terminal hexagon. Then the following recursion relation holds:

$\rho(H)= \rho(H\text{-}R)+ x_i\, \rho(H\text{-}(R_i))$

**Proof.** This follows from proposition 1 and proposition 3.

**Q.E.D**

**Corollary 5** (Gutman et al. [1977], Salem and Gutman [2003]) Let H be a catacondensed hexagonal system and let $R_i$ be a terminal hexagon. Then the following recursion relation holds:

$\sigma(H) = \sigma(H\text{-}R_i) + x\ \sigma(H\text{-}(R_i))$

**Proof.** This follows from corollary 4.

**Q.E.D.**

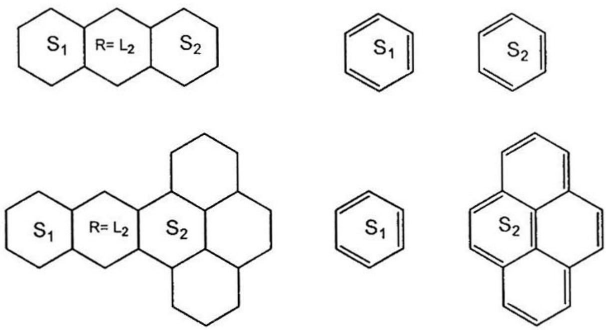


Fig. 6-1. {$S_1$, $S_2$} is a resonant set of H-R, but not a resonant set of H

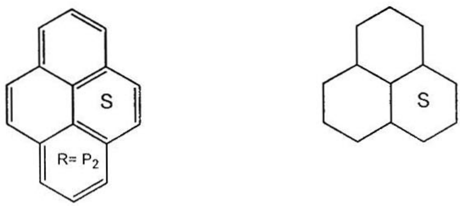


Fig. 6-2. {S} is a resonant set of H, but not a resonant set of H-R

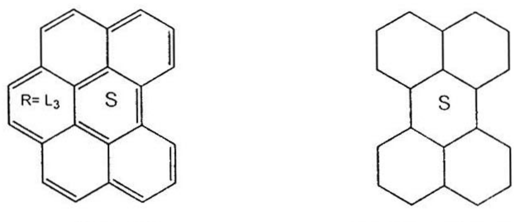


Fig. 6-3. {S} is a resonant set of H, but not a resonant set of H-R

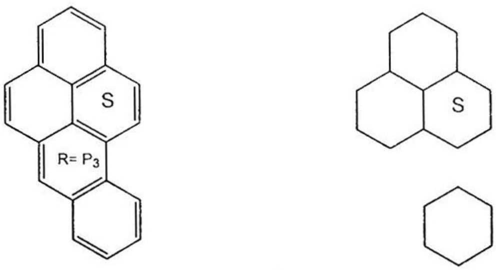


Fig. 6-4. {S} is a resonant set of H, but not a resonant set of H-R

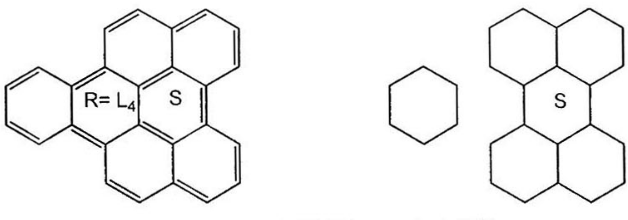


Fig. 6-5. {S} is a resonant set of H, but not a resonant set of H-R

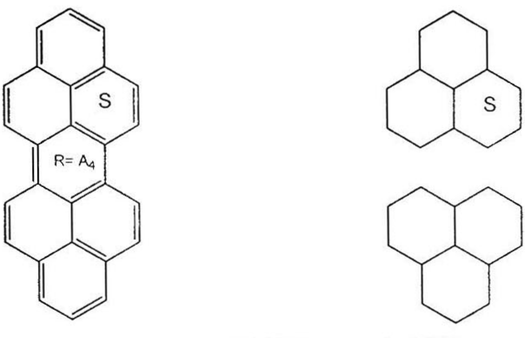


Fig. 6-6. {S} is a resonant set of H, but not a resonant set of H-R

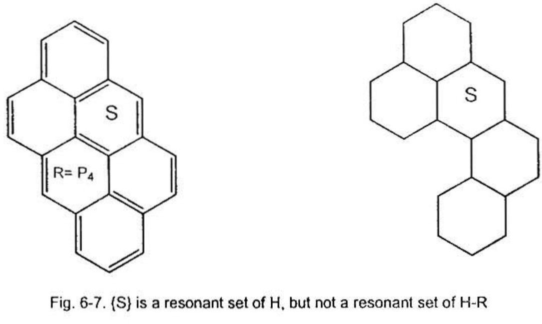


Fig. 6-7. {S} is a resonant set of H, but not a resonant set of H-R

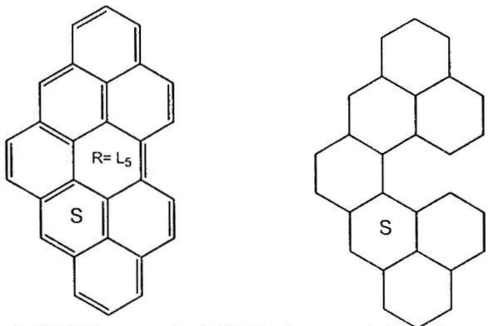


Fig. 6-8. {S} is a resonant set of H, but not a resonant set of H-R

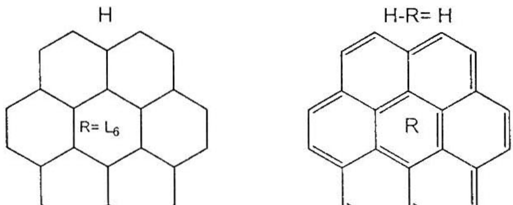


Fig. 6-9. {R} is a resonant set of H-R (=H), but not a resonant set of H that does not contain R

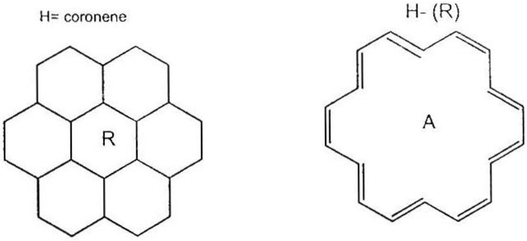


Fig. 7. {A} is a resonant set of H- (R), but {A}+{R} is not a resonant set of H

**Proposition 6.** Let H be a hexagonal system with a perfect matching such that for any coronene which is a subgraph of H, the subgraph of H obtained by deleting from H all the vertices of the coronene (together with their incident edges) has no perfect matching. Then

$(d/dx)\ \sigma(H) = \sigma(H\text{-}(R\_i_1)) + \ldots + \sigma(H\text{-}(R\_i_m))$, where,

R's are the resonant hexagons of H.

**Proof.** Let the hexagons of H be $R_1, R_2, \ldots, R_h$. Consider $\rho(H, x_1, \ldots, x_h)$. Put $x_i = x$, $i = 1, 2, \ldots, h$. Then

$(d/dx)\ \sigma(H) = (\partial/\partial x_1)\ \rho(H, x_1, \ldots, x_h) + \ldots + (\partial/\partial x_h)\ \rho(H, x_1, \ldots, x_h) \mid x_r = x,\ r = 1, 2, \ldots, h.$

Consider the term $(\partial/\partial x_i)\ \rho(H, x_1, \ldots, x_h)$.

*Case: $R_i$ is not a resonant hexagon of H*

$(\partial/\partial x_i)\ \rho(H) = 0.$

*Case: $R_i$ is a resonant hexagon of H*

By proposition 3, the sum of the resonant sextet monomials of H that define the resonant sets of H that contain $R_i$ is $x_i\ \rho(H\text{-}(Ri))$. Hence, $(\partial/\partial x_i)\ \rho(H) = \rho(H\text{-}(R_i))$.

**Q.E.D.**

**Corollary 7.** Let H be a normal hexagonal system with a perfect matching such that for any coronene which is a subgraph of H, the subgraph of H obtained by deleting from H all the vertices of the coronene (together with their incident edges) has no perfect matching. Then

$(d/dx)\ \sigma(H) = \sigma(H\text{-}(R_1)) + \ldots + \sigma(H\text{-}(R_h))$, where,

R's are the hexagons of H.

**Corollary 8** (Gutman [1981], Salem and Gutman [2003]) Let H be a catacondensed hexagonal system. Then (d/dx) σ(H) = σ(H- ($R_1$)) + … + σ(H- ($R_h$)), where, R's are the hexagons of H.

**Lemma 9.** (Salem) Let H be a connected subgraph of the hexagonal lattice without non- hexagonal interior faces and has a perfect matching. Then each connected component of the unfixed subgraph of H is a normal hexagonal system.

**Proposition 10.** Let H be a hexagonal system that has a perfect matching such that for any coronene which is a subgraph of H, we have,

(i) the subgraph of H obtained by deleting from H all the vertices of the coronene has no perfect matching, and

(ii) the subgraph of H obtained by deleting from H all the vertices of the central hexagon of the coronene has no perfect matching. In other words, the central hexagon of the coronene is not a resonant hexagon of H.

Then, (d/dx) σ(H)|x=1 = K(H-(R_$i_1$)) + … + K(H-(R_$i_m$)), where
R's the resonant hexagons of H. K(G) denotes the number of perfect matchings of G.

**Proof.** By proposition 6,
(d/dx) σ(H) = σ(H-(R_$i_1$)) + … + σ(H-(R_$i_m$)), where,
R's are the resonant hexagons of H.

Let R be a resonant hexagon of H. R is not an internal hexagon because of condition (ii). Hence, R is an external hexagon. H-(R) is a subgraph of the hexagonal lattice without non- hexagonal interior faces and has a perfect matching. Let U be the unfixed graph of H-(R). Each connected component of U is a normal hexagonal system (lemma 9). Furthermore, each connected component of U satisfies condition (i) since H satisfies condition (i). Therefore, for each connected component of U, the sextet polynomial evaluated at x=1 is equal to the number of perfect matchings. Thus, σ(U, x=1) = K(U).

Now, we show that the resonant sets of H-(R) are those of U. Let L be a resonant set of U. Then, there exists a perfect matching of U that contains a sextet of each hexagon in L. Adding to this perfect matching, the fixed double edges of H-(R), we obtain a perfect matching of H-(R) that contains a sextet of each hexagon in L. Hence, L is a resonant set of H-(R). Conversely, let L be a resonant set of H-(R). The edges of each hexagon in L belongs to U. Otherwise, an edge of some hexagon in L does not belong to U. Hence, that edge is either a fixed single edge of H-(R), a fixed double edge of H-(R) or is adjacent to a fixed double edge of H-(R). In any case, it is a fixed edge of H-(R) that belongs to a resonant hexagon of H-(R), a contradiction. Therefore, L is a non- empty set of hexagons of U. There exists a perfect matching of H-(R) that contains a sextet of each hexagon in L. Removing from this perfect matching the fixed double edges of H-(R), we obtain a perfect matching of U that contains a sextet of each hexagon in L. Hence, L is a resonant set of U. Therefore, $\rho(U) = \rho(H\text{-}(R))$.

Since, $\sigma(U, x=1) = K(U)$, $\sigma(U) = \sigma(H\text{-}(R))$ and $K(U) = K(H\text{-}(R))$, we obtain $\sigma(H\text{-}(R), x=1) = K(H\text{-}(R))$ and the proposition follows. **Q.E.D.**

**Corollary 11** (Salem and Gutman [2003]) Let H be a catacondensed hexagonal system. Then, $(d/dx)\, \sigma(H)|x=1 = K(H\text{-}(R_1)) + \ldots + K(H\text{-}(R_h))$, where R's the hexagons of H. K(G) denotes the number of perfect matchings of G.

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