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RECURSIVE AND EXPLICIT FORMULAE FOR THE DEGREE OF FREEDOM OF CATA-CONDENSED BENZENOID HYDROCARBONS

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Abstract

It is shown that the degree of freedom of a Kekulé structure K of a cata-condensed benzenoid hydrocarbon H is equal to the number of maximum disjoint hexagons containing three double bonds. From this property, a recursive relation for the degree of freedom of H is derived. By using the powerful generating function method, closed form formulae for the degree of freedom of three infinite classes of cata-condensed benzenoid hydrocarbons are obtained.

Key words: Kekulé structure, degree of freedom, benzenoid, cata-condensed, generating function.

1 Introduction

A new graph invariant, the "degree of freedom" of a graph was recently defined and studied [1-3]. This concept captures the intuitive idea that knowledge of how many elements (of a type to be defined) must be fixed in a graph for uniquely determining the structure (again to be defined) of the graph tells much about this graph. The *degree of freedom* of a Kekulé structure K of a graph G is the minimal number of double bonds of K which belong simultaneously to no other Kekulé structure of G. The *degree of freedom* of G, denoted by $f(G)$, is the sum of the degrees of freedom over all Kekulé structures of G. The potential usage of the degree of freedom of a graph in chemistry is also discussed in the cited papers. The degree of freedom of a Kekulé structure is the same as the *forcing number* of a perfect matching proposed by Harary *et al.* [3]. The concept of degree of freedom or forcing number can be naturally extended to different structures in chemical graph theory or in general graph theory. For example, the degree of freedom or the forcing number of a Clar formula C ([4]; [5], page 96) can be defined as the minimum number of benzenes in C which belong simultaneously to no other Clar formula. The degree of freedom or forcing number of a spanning tree T of G can be defined as the minimum number of edges of T which belong simultaneously to no other spanning tree of G, etc.

A transfer matrix method [6] to compute the degree of freedom of a zigzag chain was described in [2]. To compute the degree of freedom of a graph in general appears to be

hard, except if one uses an enumeration method, which may be quite time consuming. In this paper, we confine our discussion to cata-condensed benzenoid systems. We give in Section 3 a recursive method to compute the degree of freedom for graphs in this class. In Section 4, we apply this recursion to several subclasses of cata-condensed benzenoid systems and derive by the powerful generating function method explicit formulae for the degrees of freedom of all graphs in these subclasses. In particular, we give an explicit formula for the degree of freedom of a zigzag chain, also studied in [2].

2 Computing the degree of freedom of a Kekulé structure

We first specify some definitions and notation. A *Kekulé structure* (or perfect matching) of a graph G is a set of independent edges which cover all vertices of G. A *dominating set* of a Kekulé structure (or perfect matching) M of G is a set of bonds of M which belong simultaneously to no other Kekulé structure of G. Thus the degree of freedom of M is equal to the cardinality of a minimum dominating set of M.

A *benzenoid system* is a planar graph with no cut vertices and in which each interior face is a regular hexagon. The skeleton of a benzenoid hydrocarbon B is usually represented by a benzenoid system H [7]. The carbon atoms of B correspond to the vertices of H.

A benzenoid system is *cata-condensed* if it has no interior vertices.

Let H be a benzenoid system and M a Kekulé structure. A hexagon of H is *M-resonant* if it contains three double bonds of M. An *M-resonant set* of M is a set of disjoint M-resonant hexagons. A *maximum resonant set* of M is an M-resonant set of M which has the maximum cardinality.

All benzenoid systems considered below are assumed to be cata-condensed unless otherwise specified. In the following lemma and theorem we study the relationship between the degree of freedom and maximum resonant sets.

Lemma 1 *Let M be a Kekulé structure of H. If s is an M-resonant hexagon of H which has at most one neighboring M-resonant hexagon, then s belongs to a maximum resonant set of M.*

Proof. Let S be a maximum resonant set of M. If s does not belong to S, then the neighboring M-resonant hexagon s' of s belongs to S. Thus $S - \{s'\} + \{s\}$ is a maximum resonant set of M which contains s. □

Theorem 1 *Let H be a cata-condensed benzenoid system and M be a Kekulé structure. The degree of freedom of M is equal to the cardinality of a maximum resonant set of M.*

Proof. Let D be a minimum dominating set and S be a maximum resonant set of M. Note that each member of S contains at least one double bond in D and all hexagons in S are disjoint. Hence $|D| \geq |S|$ (where $|*|$ is the cardinality of $*$). We next show that $|D| \leq |S|$.

Let H' be the subgraph consisting of all M-resonant hexagons of H. Then H' may have several connected components and each of them is a cata-condensed benzenoid system. So

there is an M-resonant hexagon s which has at most one neighboring M-resonant hexagon. By Lemma 1, we can assume that s belongs to S. If s is an isolated hexagon of H', select a double bond e in s in an arbitrary way. Otherwise select the common double bond of s and its neighboring hexagon in H'. Replace H' by the subgraph consisting of M-resonant hexagons of H which do not contain e and also denote it by H'. Note that all hexagons of H' are disjoint from s, and that $S - s$ is contained in H'. Repeat the above procedure until H' becomes empty. Let D' be the set of double bonds selected. Clearly, $|D'| = |S|$. Also each M-resonant hexagon contains a double bond of D'. We assert that D' is a dominating set. Otherwise, D' will be contained in another Kekulé structure M'. Then consider the symmetric difference Q of M' and M (i.e. the set of double bonds belonging to M or M' but not to both). Since each vertex of Q is incident with two bonds, there is a circuit C contained in Q. Let $C(H)$ be the cata-condensed benzenoid system which has C as its boundary. Then $M \cap C(H)$ is a Kekulé structure of $C(H)$. By Lemma 3 of [8], $C(H)$ has a hexagon which contains three double bonds of $M \cap C(H)$ and this hexagon does not contains any double bond of D'. This is a contradiction. Therefore $|D'| = |S| \geq |D|$. The proof is completed. □

The above proof actually provides a method to compute a maximum resonant set of a given Kekulé structure M as well as its degree of freedom. We write down this procedure formally as follows:

FREEDOM: Select an M-resonant hexagon of M which has at most one neighboring M-resonant hexagon; delete this hexagon together with the bonds incident to it from H; repeat the foregoing steps until an empty graph is obtained. The selected hexagons form a maximum resonant set of M.

3 The degree of freedom of cata-condensed benzenoid hydrocarbons

Let H be a cata-condensed benzenoid system and s a hexagon which has only one neighboring hexagon. Let $H(s)$ be the longest hexagon chain of H with s as one of its end hexagons such that all hexagons in $H(s)$ are in a row. Let s' be the other end hexagon of $H(s)$. Let H_s be the graph consisting of the hexagons of H not in $H(s)$. Let $H * s$ be the graph obtained from H_s by deleting the bonds of s' together with their end vertices, consecutively deleting the pendant bonds with their vertices and finally deleting the bonds which do not belong to any remaining hexagon but not their vertices. Note that each connected component of H_s or $H * s$ is a cata-condensed benzenoid system. Also H_s and $H * s$ may be empty. Figure 1 gives an illustration of H_s and $H * s$. Let r be the number of hexagons of $H(s)$. Let $k(G)$ denote the number of Kekulé structures of a graph G. When G is empty, by convention, let $f(G) = 0$ and $k(G) = 1$. Then we have the following result:

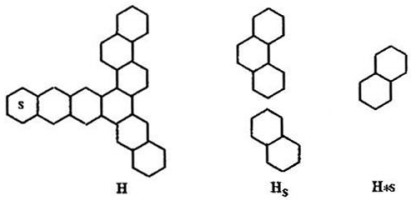


Figure 1: The illustration of H, H_s and H*s.

Theorem 2 *Let H be a cata-condensed benzenoid system and s be a hexagon having only one neighboring hexagon. Then*

$$\begin{aligned} k(H) &= rk(H_s) + k(H * s), \\ f(H) &= k(H) + rf(H_s) + f(H * s). \end{aligned}$$

Proof. Without loss of generality, let H be embedded in the plane in such a way that $H(s)$ is horizontal (i.e. the centers of all hexagons of $H(s)$ are on the same horizontal line). Let $e_0, e_1, ..., e_r$ be the vertical bonds of $H(s)$ such that e_0 and e_r are the leftmost and the rightmost of them respectively. We partition the Kekulé structures of H into $r+1$ sets $A_0, A_1, ..., A_r$ such that all Kekulé structures in A_i contains e_i. First we show this is indeed a partition of the Kekulé structures of H. Note that H is a bipartite graph. We color the vertices of H in black and white such that no two adjacent vertices have the same color. Let H_1 and H_2 be the two connected subgraphs obtained from H by deleting $e_0, ..., e_r$ but not their end vertices. Through a simple calculation, we have that the difference between the number of white vertices and the number of black vertices of H_j $(j = 1, 2)$ is 1 or -1. This means any Kekulé structure of H contains one and only one of $e_0, e_1, ..., e_r$ and therefore $A_0, A_1, .., A_r$ are a partition of all Kekulé structures of H.

Next we calculate the sum of the degrees of freedom of Kekulé structures in each A_i. We do this for A_0 and A_r. The calculation for the otherA_i can be done in a similar way. Let M be a Kekulé structure in A_0. Then s is resonant in M. Note that all double bonds of M which belong to $H(s)$ are uniquely determined by e_0. Thus each Kekulé structure of H_s can be uniquely extended to a Kekulé structure in A_0 and the restriction of each Kekulé structure in A_0 to H_s is a Kekulé structure of H_s. Thus $|A_0| = k(H_s)$. By Lemma 1, s belongs to a maximum resonant set S of M. One can check easily that $S - s$ is contained in H_s which is also a maximum resonant set of $M \cap H_s$. Recall that the degree of freedom of a Kekulé structure M is equal to the cardinality of a maximum resonant set of M. Thus the sum of the degrees of freedom of Kekulé structures in A_0 is $|A_0| + f(H_s) = k(H_s) + f(H_s)$. Similarly, we can show that the sum of the degrees of freedom of Kekulé structures in A_i is $k(H_s) + f(H_s)$ for $(i = 1, 2, ..., r-1)$. Note that the number of black vertices is equal to the number of white vertices in each connected component of H_s. All Kekulé structures in A_r have s' as a resonant hexagon (where s' is the end hexagon of $H(s)$ containing e_r). Also s' is not adjacent to any other resonant hexagon. Thus s' belongs to a maximum resonant

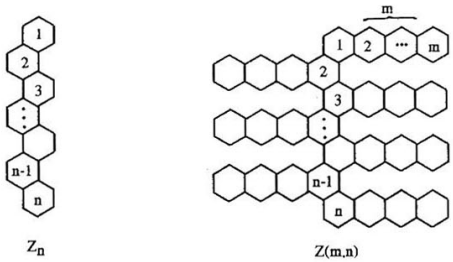


Figure 2: Illustration of Z_n and Z(m,n).

set of each Kekulé structure in A_r. We can show that there is no other resonant hexagon of a Kekulé structure in A_r which is contained in $H(s)$. Each Kekulé structure of $H * s$ can be extended to a Kekulé structure in A_r in a unique way and the restriction of each Kekulé structure in A_r to $H * s$ is a Kekulé structure of $H * s$. Thus the sum of the degrees of freedom of Kekulé structures in A_r is equal to $|A_r| + f(H * s) = k(H * s) + f(H * s)$. Therefore $f(H) = rk(H_s) + k(H * s) + rf(H_s) + f(H * s) = \sum_{i=0}^{r} |A_i| + rf(H_s) + f(H * s) = k(H) + rf(H_s) + f(H * s)$. The proof is completed. □

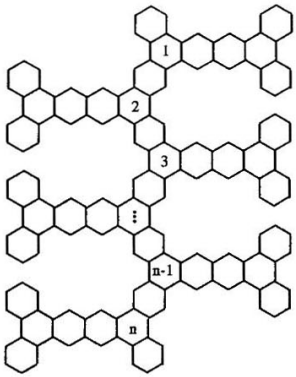
4 Degree of freedom of cata-condensed benzenoid systems in three special classes

In this section, we derive an explicit formula for the degree of freedom of benzenoid systems contained in three special subclasses which are described below.

A *zigzag chain* Z_n is a cata-condensed benzenoid system with n hexagons as shown in Figure 2. Let f_n and k_n denote the degree of freedom and the number of Kekulé structures of Z_n respectively. More generally, a (m, n) – *zigzag chain* $Z(m, n)$ is a cata-condensed benzenoid system with mn hexagons as shown also in Figure 2. Clearly a Z_n is a (1,n)-zigzag chain. Let $f_m(n)$ and $E_m(n)$ denote the degree of freedom and the number of Kekulé structures of $Z(m, n)$ respectively.

A *R(n)* is a cata-condensed benzenoid system with $6n$ hexagons as shown in Figure 3. Let r_n and q_n denote the degree of freedom and the number of Kekulé structures of $R(n)$ respectively.

We first derive a recursive relation for f_n by Theorem 2 and then calculate the generating function of f_n and give a formula for f_n in terms of k_n. Finally we present an explicit formula for f_n. We give details about our derivation in the next subsection. In the other two subsections, we only give the formulae obtained. We first mention a result of [2] which is used in the derivation of the explicit formulas for the degree of freedom of $Z(m, n)$ and $R(n)$: let $G = A \cup B$ and $A \cap B = \emptyset$ (where A and B are two graphs); then $f(G) =$



R(n)

Figure 3: Illustration of R(n).

$k(A)f(B) + k(B)f(A)$.

4.1 The degree of freedom of Z_n

The generating function of a sequence of integers $g_0, g_1, ...g_n, ...$ is defined as $g(x) = \sum_{i=0}^{\infty} g_i x^i$. One of the most frequent uses of generating functions is the solution of recursive relations. The question is as follows: given a sequence $g_0, g_1, ..., g_n, ...$ which satisfies a given recurrence, to find a closed form for g_n. Use of the generating function method for solving this problem consists of the following four steps (see also [9]):

1. Write down a single equation that expresses g_n in terms of other elements of the sequence.

2. Multiple both sides of the equation by x^n and sum over all $n \geq 0$. The left side of the sum gives $g(x)$ and the right side gives (after manipulations) an expression involving $g(x)$.

3. Solving the resulting equation, a closed form of $g(x)$ is obtained.

4. Expand $g(x)$ into a power series. Then the coefficient of x^n gives a closed form expression of g_n.

We demonstrate the above for f_n and k_n. Let $k(x)$ and $f(x)$ be the generating functions of k_n and f_n respectively. Note that $k_0 = 1, k_1 = 2, f_0 = 0, f_1 = 2$, and $f_2 = 3$.

By Theorem 2, we have

Corollary 1

$$\begin{aligned} k_n &= k_{n-1} + k_{n-2} \qquad for\ n \geq 2, \\ f_n &= k_n + 2f_{n-2} + f_{n-3} \qquad for\ n \geq 3. \end{aligned}$$

□

By the above corollary, we have

$$\begin{aligned} k(x) &= \sum_{i\geq 0} k_i x^i = 1 + 2x + \sum_{i\geq 2} k_i x^i \\ &= 1 + 2x + \sum_{i\geq 2}(k_{i-1} + k_{i-2})x^i \\ &= 1 + 2x + x\sum_{i\geq 1} k_i x^i + x^2 \sum_{i\geq 0} k_i x^i \\ &= 1 + x + xk(x) + x^2 k(x), \\ k(x) &= \frac{1+x}{1-x-x^2}. \end{aligned}$$

Similarly, we can obtain an explicit formula for $f(x)$ as follows:

$$\begin{aligned} f(x) &= \sum_{i\geq 0} f_i x^i = 2x + 3x^2 + \sum_{i\geq 3} f_i x^i \\ &= 2x + 3x^2 + \sum_{i\geq 3} k_i x^i + \sum_{i\geq 3}(2f_{i-2} + f_{i-3})x^i \\ &= -1 + k(x) + (2x^2 + x^3)f(x), \\ f(x) &= \frac{1 + x - (1 - x - x^2)}{(1-x-x^2)(1-2x^2-x^3)}. \end{aligned}$$

By further simplifications, we obtain

$$f(x) = \frac{1 + x - (1 - x - x^2)}{(1-x-x^2)^2(1+x)} = \frac{1}{(1-x-x^2)^2} - \frac{1}{(1+x)} - \frac{x}{(1-x-x^2)}.$$

In order to derive a formula for f_n, we need the generating functions for the following two sequences: one is the Fibonacci numbers which are defined as $F_0 = 0, F_1 = 1, F_2 = k_0, F_3 = k_1, F_4 = k_2, ..., F_n = k_{n-2}, ...$ and the other one is defined as $b_0 = 1, b_1 = k_0, b_2 = k_1, ..., b_n = k_{n-1}, ...$ Let their generating functions be $F(x)$ and $b(x)$ respectively. In the same way as when deriving $k(x)$, we obtain $F(x) = \dfrac{x}{1-x-x^2}$ and $b(x) = \dfrac{1}{1-x-x^2}$.

Let $\phi = \dfrac{1+\sqrt{5}}{2}$ and $\hat{\phi} = \dfrac{1-\sqrt{5}}{2}$. Then

$$1 - x - x^2 = (1 - \phi x)(1 - \hat{\phi} x),$$

and

$$\begin{aligned} \frac{1}{(1-x-x^2)^2} &= \left(\frac{1}{2\sqrt{5}}\left(\frac{1+\sqrt{5}}{1-\phi x} - \frac{1-\sqrt{5}}{1-\hat{\phi} x}\right)\right)^2 \\ &= \frac{1}{20}\left(\frac{6+2\sqrt{5}}{(1-\phi x)^2} + \frac{8}{(1-\phi x)(1-\hat{\phi} x)} + \frac{6-2\sqrt{5}}{(1-\hat{\phi} x)^2}\right) \\ &= \frac{1}{20}((6+2\sqrt{5})\sum_{n\geq 0}(n+1)\phi^n x^n + 8\sum_{n\geq 0} b_n x^n + \\ &\quad (6-2\sqrt{5})\sum_{n\geq 0}(n+1)\hat{\phi}^n x^n). \end{aligned}$$

Also

$$\frac{1}{(1+x)} + \frac{x}{(1-x-x^2)} = \sum_{n\geq 0}(F_n + (-1)^n)x^n.$$

Thus we have

$$f_n = \frac{1}{20}(6(n+1)(\phi^n + \hat{\phi}^n) + 2\sqrt{5}(n+1)(\phi^n - \hat{\phi}^n) + 8b_n) - (F_n + (-1)^n).$$

Recalling that $\phi + \hat{\phi} = 1$, we have that $\phi^n + \hat{\phi}^n$ is equal to the nth coefficient of

$$\begin{aligned} \frac{1}{1-\phi x} + \frac{1}{1-\hat{\phi} x} &= \frac{2-(\phi+\hat{\phi})x}{(1-\phi x)(1-\hat{\phi} x)} \\ &= \frac{2-x}{1-x-x^2} \\ &= 2\sum_{n\geq 0} b_n x^n - \sum_{n\geq 0} F_n x^n. \end{aligned}$$

Therefore $\phi^n + \hat{\phi}^n = 2b_n - F_n$.

Similarly, $\phi^n - \hat{\phi}^n$ is equal to the nth coefficient of

$$\begin{aligned} \frac{1}{1-\phi x} - \frac{1}{1-\hat{\phi} x} &= \frac{\sqrt{5}x}{(1-\phi x)(1-\hat{\phi} x)} \\ &= \frac{\sqrt{5}x}{1-x-x^2} \\ &= \sqrt{5}\sum_{n\geq 0} F_n x^n. \end{aligned}$$

Thus

$$\begin{aligned} f_n &= \frac{1}{20}(6(n+1)(2b_n - F_n) + 10(n+1)F_n + 8b_n) - (F_n + (-1)^n) \qquad (1) \\ &= \frac{1}{20}((12(n+1)+8)k_{n-1} + 4(n+1)k_{n-2}) - (k_{n-2} + (-1)^n) \end{aligned}$$

for $n \geq 2$.

One more step, using the relation $k_n = k_{n-1} + k_{n-2}$, leads to

$$f_n = \frac{n-4}{5}k_n + \frac{2n+9}{5}k_{n-1} - (-1)^n, \quad n \geq 2.$$

Summarizing all the above, we have

Theorem 3

$$f_n = \frac{n-4}{5}k_n + \frac{2n+9}{5}k_{n-1} - (-1)^n \quad n \geq 2$$

and

$$k_n = \frac{1}{\sqrt{5}}(\phi^{n+2} - \hat{\phi}^{n+2}).$$

Proof. The second formula comes from the fact that k_n is the $(n+2)^{th}$ Fibonacci number (see also [7], page 41). □

In TABLE 1, we present values of k_n and f_n for n up to 21.

n	k_n	f_n	n	k_n	f_n
0	1	0	11	233	1220
1	2	2	12	377	2140
2	3	3	13	610	3738
3	5	9	14	987	6487
4	8	16	15	1597	11213
5	13	34	16	2584	19296
6	21	62	17	4181	33094
7	34	118	18	6765	56570
8	55	213	19	10946	96430
9	89	387	20	17711	163945
10	144	688	21	28567	278087

TABLE 1. The number of Kekulé structures and the degree of freedom of Z_n.

Values in TABLE 1 coincide with those computed by Klein and Randić (up to $n = 14$) [2].

4.2 The degree of freedom of $Z(m,n)(m \geq 2)$

Note that $E_m(0) = 1, E_m(1) = m+1, f_m(0) = 0$ and $f_m(1) = m+1$. By Theorem 2, we have the following corollary:

Corollary 2

$$\begin{aligned} f_m(n) &= m(E_m(n-1) + E_m(n-2)) + \\ &\quad m(f_m(n-1) + f_m(n-2) + E_m(n-2)), \\ E_m(n) &= m(E_m(n-1) + E_m(n-2)) \end{aligned}$$

for $m \geq 2$, $n \geq 2$. □

From this result and computations similar to above, it follows that:

Theorem 4

$$\begin{aligned} \sum_{n\geq 0} E_m(n)x^n &= \frac{1+x}{1-mx-mx^2}. \\ \sum_{n\geq 0} f_m(n)x^n &= \frac{(1+x)(1+mx^2)}{(1-mx-mx^2)^2} - \frac{1}{1-mx-mx^2} \\ &= \frac{(1+x+mx+mx^2)}{(1-mx-mx^2)^2} - \frac{1}{1-mx-mx^2}. \end{aligned}$$

□

Let $\delta = \frac{m+\sqrt{m^2+4m}}{2}$, $\hat{\delta} = \frac{m-\sqrt{m^2+4m}}{2}$. $A = \frac{-\hat{\delta}}{\delta-\hat{\delta}}$, $B = \frac{\hat{\delta}}{\delta-\hat{\delta}}$, $F(i) = A^2(i+1)\delta^i + B^2(i+1)\hat{\delta}^i + 2AB(A\delta^i + B\hat{\delta}^i)$. Then we have

$$\frac{1}{1-mx-mx^2} = \frac{1}{(1-\delta x)(1-\hat{\delta}x)} = \frac{A}{1-\delta x} + \frac{B}{1-\hat{\delta}x}.$$

$$\frac{1}{(1-mx-mx^2)^2} = \frac{A^2}{(1-\delta x)^2} + \frac{B^2}{(1-\hat{\delta}x)^2} + \frac{2AB}{(1-\delta x)(1-\hat{\delta}x)}.$$

Note that $F(i)$ is the ith coefficient of $\frac{1}{(1-mx-mx^2)^2}$. Further easy computations lead to:

Theorem 5

$$f_m(n) = F(n) + F(n-1) + mF(n-2) + mF(n-3) - (A\delta^n + B\hat{\delta}^n).$$

□

In TABLE 2, we present the values of $E_m(n)$ and $f_m(n)$ for $m = 2$ and n up to 15.

n	$E_2(n)$	$f_2(n)$	n	$E_2(n)$	$f_2(n)$
0	1	0	8	3344	26752
1	3	3	9	9136	82224
2	8	16	10	24960	249600
3	22	66	11	68192	750112
4	60	240	12	186304	2235648
5	164	820	13	508992	6616896
6	448	2688	14	1390592	19468288
7	1224	8568	15	3799168	56987520

TABLE 2. The number of Kekulé structures and the degree of freedom of Z(2,n).

4.3 The degree of freedom of R(n)

By convention, let $r_0 = q_0 = 2$. Also by simple calculation, $q_1 = 40$ and $r_1 = 176$. Computations similar to those of the previous subsections lead to the following recursive relations for r_n and q_n.

Corollary 3

$$\begin{aligned} r_n &= 4q_n - 4q_{n-1} + 64q_{n-2} + 18r_{n-1} + 36r_{n-2}, \\ q_n &= 18q_{n-1} + 36q_{n-2}, \end{aligned}$$

for $n \geq 2$. □

If we let $r(x)$ and $q(x)$ denote the generating functions of r_n and q_n respectively, then we obtain

Theorem 6

$$\begin{aligned} q(x) &= \frac{2+4x}{1-18x-36x^2}, \\ r(x) &= \frac{-12x-6+(4-4x+64x^2)q(x)}{1-18x-36x^2} \\ &= \frac{-12x-6}{1-18x-36x^2} + \frac{8+8x+112x^2+256x^3}{(1-18x-36x^2)^2}. \end{aligned}$$

□

Further notations are needed. Let

$$\begin{aligned} \gamma &= 9+3\sqrt{13}, \\ \hat{\gamma} &= 9-3\sqrt{13}, \\ a &= \frac{-\gamma}{\hat{\gamma}-\gamma}, \\ b &= \frac{\hat{\gamma}}{\hat{\gamma}-\gamma}, \\ G(n) &= a^2(n+1)\gamma^n + b^2(n+1)\hat{\gamma}^n + 2ab(a\gamma^n + b\hat{\gamma}^n). \end{aligned}$$

With these notations and computations similar to those leading to Theorem 5, we obtain:

Theorem 7

$$\begin{aligned} r_0 &= 2, r_1 = 176, \\ r_n &= -6(a\gamma^n + b\hat{\gamma}^n) + 18(a\gamma^{n-1} + b\hat{\gamma}^{n-1}) + 8G(n) \\ &\quad +8G(n-1) + 112G(n-2) + 256G(n-3). \end{aligned}$$

In TABLE 3, we present the values of q_n and r_n for n up to 5.

n	q_n	r_n
0	2	2
1	40	176
2	792	6376
3	15696	183280
4	311040	4760640
5	6163776	116705088

TABLE 3. The number of Kekulé structures and the degree of freedom of R(n).

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