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"Crowns", and Aromatic Sextets in Primitive Coronoid Hydrocarbons

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Summary. A type of graphs derived from a cycle and associated with primitive coronoids are referred to as "crowns". The characteristic polynomials and matching polynomials of crowns are studied. These notions are used to calculate the sextet polynomial for primitive coronoids. Patterns of aromatic sextets are treated in some detail.

Keywords. "Crown"; Coronoid; Aromatic sextet.

"Crowns" und aromatische Sextette in einfachen coronoiden Kohlenwasserstoffen

Zusammenfassung. Eine Graphentype, die von einem Cyclus abgeleitet ist und mit einfachen Coronoiden verknüpft ist, wird als "Crown" bezeichnet. Die charakteristischen Polynome und die „matching" Polynome der Crowns werden untersucht. In diesem Rahmen werden die Sextett-Polynome für einfache Coronoide berechnet. Die Muster der aromatischen Sextette werden im Detail behandelt.

Introduction

A coronoid [1–3] is a geometrically planar system consisting of congruent regular hexagons like a benzenoid, but having a hole of a size equal to at least two hexagons. The class of primitive coronoids [1] has been studied in particular [3–10]. These systems consist of a single chain of hexagons in a circular arrangement. They have chemical counterparts in the interesting class of conjugated polycyclic hydrocarbons called cycloarenes [11–15].

In the present work we define "crowns" as graphs associated with primitive coronoids. The characteristic polynomials and matching polynomials of crowns are studied. The latter class of polynomials appears to be related to the sextet polynomials of primitive coronoids.

Results and Discussion

Characteristic Polynomial

The characteristic polynomial is a fundamental concept in graph theory found in current textbooks on this topic. It has found important chemical applications [16–19]. The characteristic polynomial of a graph G with n vertices is defined by

$$\varphi(\mathrm{G}\,|\,x) = |x\mathbf{I} - \mathbf{A}(\mathrm{G})| = (-1)^n |\mathbf{A}(\mathrm{G}) - x\mathbf{I}|$$

where $\mathbf{A}(\mathrm{G})$ is the adjacency matrix of G, and $\mathbf{I}$ is the identity matrix.

The graph spectral theory is closely related to the familiar Hückel theory of conjugated hydrocarbons, which is treated in many textbooks of organic and physical chemistry. The Hückel determinant is actually

$$|\mathbf{A}(G) + x\mathbf{I}| = (-1)^n \varphi(G| -x) \tag{2}$$

Cycle

Let a cycle with n vertices (and n edges) be identified by the symbol C_n. The coefficients of its characteristic polynominal, viz.

$$\varphi(C_n | x) = x^n \sum_{i=1}^{n} a_i x^{n-i} \tag{3}$$

are known. They are given by [18].

$$a_i = \begin{cases} 0; & i \text{ odd and } i < n \\ -2; & i \text{ odd and } i = n \\ (-1)^p \frac{n}{p}\binom{n-p-1}{p-1}; & i = 2p \text{ and } i < n \\ 2[(-1)^p - 1]; & i = 2p \text{ and } i = n \end{cases} \tag{4}$$

In a more compressed form this polynomial reads [20]

$$\varphi(C_n | x) = x^n - 2 + \sum_{j=1}^{[n/2]} (-1)^j \frac{n}{j}\binom{n-j-1}{j-1} x^{n-2j} \tag{5}$$

Explicit formulas for $\varphi(C_n | x)$ exist in different pictures, e.g.

$$\varphi(C_n | x) = \left[\frac{x + \sqrt{x^2 - 4}}{2}\right]^n + \left[\frac{x - \sqrt{x^2 - 4}}{2}\right]^n - 2 \tag{6}$$

which has an accompanying recurrence relation:

$$\varphi(C_{n+3} | x) = (x + 1)[\varphi(C_{n+2} | x) - \varphi(C_{n+1} | x)] + \varphi(C_n | x) \tag{7}$$

Table 1 shows the characteristic polynomials for cycles with $n \leqslant 8$. Degenerate cycles with $n = 0$, 1 and 2 are included. The appropriate polynomials for these systems are defined according to eqn. (6).

Crown

A crown, denoted by $C_{n,k}$, is obtained from the cycle C_n in the following way:
(1) to each vertex X_i of C_n a set V_i of k new vertices is added;
(2) X_i is joined by an edge to each of the k vertices of V_i ($i = 1, 2, \ldots, n$).

This definition is illustrated by the example of $C_{6,2}$; see Fig. 1.

When we define $C_{n,0} \equiv C_n$ the cycle becomes a special case of crowns.

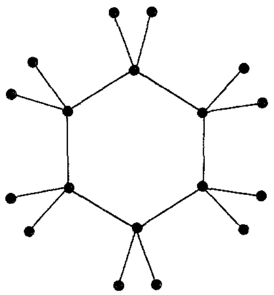


Fig. 1. The crown $C_{6,\,2}$

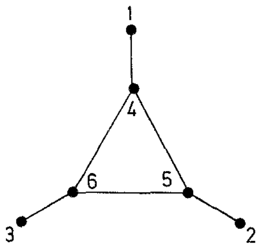


Fig. 2. The crown $C_{3,\,1}$ with numbered vertices

Table 1. Characteristic polynomials for some cycles

n	$\varphi\,(C_n\,\vert\,x)$
0	0
1	$x - 2$
2	$x^2 - 4$
3	$x^3 - 3x - 2$
4	$x^4 - 4x^2$
5	$x^5 - 5x^3 + 5x - 2$
6	$x^6 - 6x^4 + 9x^2 - 4$
7	$x^7 - 7x^5 + 14x^3 - 7x - 2$
8	$x^8 - 8x^6 + 20x^4 - 16x^2$
9	$x^9 - 9x^7 + 27x^5 - 30x^3 + 9x - 2$
10	$x^{10} - 10x^8 + 35x^6 - 50x^4 + 25x^2 - 4$

By means of a useful theorem [18] we find the characteristic polynomial of a crown $C_{n,\,k}$ as

$$\varphi\,(C \quad |\,x) = x^{nk}\,\varphi \;\; C \;|\,x - \frac{k}{\;}$$

A generalization of the recurrence relation (7) reads

$$\varphi\,(C_{n+3,k}\,|\,x) = \left(x + 1 - \frac{k}{x}\right)[x^k\,\varphi\,(C_{n+1,k}\,|\,x) - x^{2k}\,\varphi\,(C_{n+1,k}\,|\,x)] + x^{3k}\,\varphi\,(C_{n,k}\,|\,x) \qquad (9)$$

Table 2. Characteristic polynomials for some crowns

n	$\varphi(C_{n,k} \mid x)$
0	0
1	$x^{k-1}(x^2 - 2x - k)$
2	$x^{2(k-1)}[x^4 - 2(k+2)x^2 + k^2]$
3	$x^{3(k-1)}[x^6 - 3(k+1)x^4 - 2x^3 + 3k(k+1)x^2 - k^3]$
4	$x^{4(k-1)}[x^8 - 4(k+1)x^6 + 2k(3k+4)x^4 - 4k^2(k+1)x^2 + k^4]$
5	$x^{5(k-1)}[x^{10} - 5(k+1)x^8 + 5(2k^2+3k-1)x^6 - 2x^5 - 5k(2k^2+3k-1)x^4 + 5k^3(k+1)x^2 - k^5]$
6	$x^{6(k-1)}[x^{12} - 6(k+1x^{10} + 3(k+1)(5k+3)x^8 - 2(10k^3+18k^2+9k+2)x^6 + 3k^2$ $(k+1)(5k+3)x^4 - 6k^4(k+1)x^2 + k^6]$

For the sake of exemplification we apply eqn. (8) to the crown $C_{3,1}$, which is depicted in Fig. 2. By means of Table 1 it is readily obtained

$$\varphi(C_{3,1} \mid x) = x^3\left[\left(x - \frac{1}{x}\right)^3 - 3\left(x - \frac{1}{x}\right) - 2\right] = x^6 - 6x^4 - 2x^3 + 6x^2 - 1 \quad (10)$$

The same result was obtained by a direct expansion of the determinant (1). With the numbering of vertices as chosen in Fig. 2 it reads

$$\varphi(C_{3,1} \mid x) = \begin{vmatrix} -x & 0 & 0 & 1 & 0 & 0 \\ 0 & -x & 0 & 0 & 1 & 0 \\ 0 & 0 & -x & 0 & 0 & 1 \\ 1 & 0 & 0 & -x & 1 & 1 \\ 0 & 1 & 0 & 1 & -x & 1 \\ 0 & 0 & 1 & 1 & 1 & -x \end{vmatrix} \quad (11)$$

In Table 2 the characteristic polynomials for some crowns are collected.

Matching Polynomial

The matching polynomial [21–25] has been invented in the chemical context several times and under different names; see Godsil and Gutman [24] for a historical survey. The matching polynomial for a graph G is defined by

$$\alpha(G \mid x) = \sum_{j=0}^{m} (-1)^j p(G,j)\, x^{N-2j} \quad (12)$$

where $p(G, j)$ is the number of distinct selections of j independent edges in G. Some authors define the matching polynomial as

$$\bar{\alpha}(G \mid x) = \sum_{j=0}^{m} p(G,j)\, x^{N-2j} \quad (13)$$

It is clear that if we know $\alpha(G \mid x)$ we can easily obtain $\bar{\alpha}(G \mid x)$.

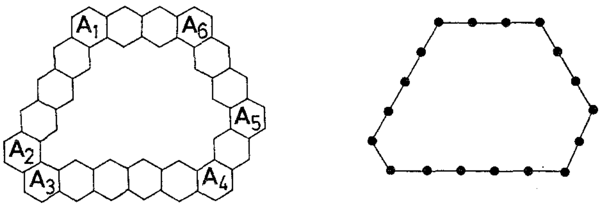


Fig. 3. A primitive coronoid (left) and its dualist (right)

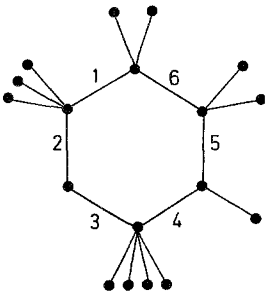


Fig. 4. The generalized crown associated with the primitive coronoid of Fig. 3

For a crown, including the cycle as its special case, the matching polynomial is determined by

$$\alpha(C_{n,k}\,|\,x) = \varphi(C_{n,k}\,|\,x) + 2\,x^{nk} = x^{nk}\left[\varphi\left(C_n\,|\,x - \frac{k}{x}\right) + 2\right] \tag{14}$$

since $C_{n,k}$ has only one cycle.

The importance of matching polynomials for crowns lies in the fact that they give a clue to the computation of sextet polynomials for primitive coronoids. In the next paragraph we establish the link between a primitive coronoid and a generalization of crowns.

Generalized Crown

Assume a primitive coronoid as exemplified in Fig. 3. The chosen example may be designated in terms of the lengths of segments [3, 9] as /5,2,6,3,4,4/ or /5,2,6,3,4^2/. The six angularly annelated hexagons (A) are numbered.

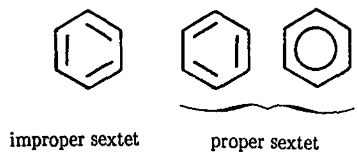
A generalized crown associated with the primitive coronoid in question is constructed in the following way (cf. Fig. 4). A cycle C_6 corresponds to the six A hexagons. For the sake of clarity its edges are numbered in consistence with the A_i ($i = 1, 2, \ldots, 6$) of Fig. 3. Assume that the segment $A_i - A_j$ holds l linearly annelated hexagons (where l may be zero). Add l vertices and connect each with the vertex being common to the edges i and j of the cycle.

This is a generalization of crowns which are defined above. The special case emerges when all l are equal. These graphs (crowns) are associated with primitive coronoids of equidistant segments. Here we shall refer to such primitive coronoids as regular.

A generalized crown is analogous to the graphs [26] associated with single unbranched chains of hexagons and called caterpillars [27–29] or Gutman trees [29, 30].

Sextet Polynomial

Consider a Kekuléan benzenoid or coronoid system with the corresponding graph G. The sextet polynomial [32] is defined via the number of (resonant) sextets, say j, in a Kekulé structure of G, represented by a generalized Clar formula. Let $r(\mathrm{G},j)$ be the number of distinct generalized Clar formulas with j sextets, where $j = 1, 2, \ldots, s$. Only proper sextets are counted and indicated by inscribed circles:



An example of a Kekulé structure and the corresponding generalized Clar formula is shown in Fig. 5. Now the sextet polynomial of G is defined by

$$\sigma(\mathrm{G}\,|\,x) = \sum_{j=0}^{s} r(\mathrm{G},j)\,x^j \tag{15}$$

The total number of Kekulé structures of G is obviously

$$K(\mathrm{G}) = \sum_{j=0}^{s} r(\mathrm{G},j) = \sigma(\mathrm{G}\,|\,1) \tag{16}$$

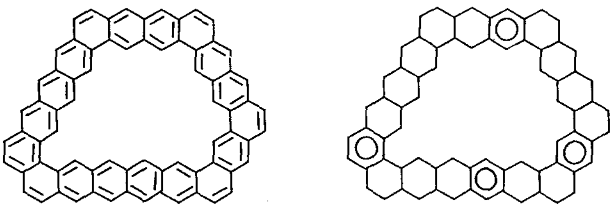


Fig. 5. A Kekulé structure for the primitive coronoid of Fig. 3 (left) and the corresponding generalized Clar formula (right)

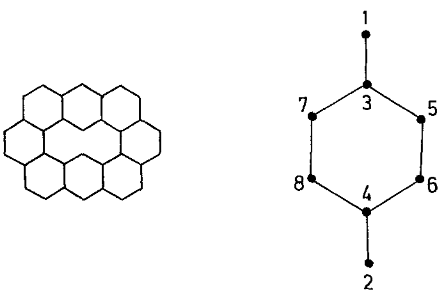


Fig. 6. The smallest coronoid, viz. $/2^2,3/^2$ (left) and the generalized crown associated with it (right)

For general treatments of Kekulé structures the reader is again referred to current textbooks in chemistry. Especially for their enumerations (computations of K), see a recent monograph [31].

Aromatic Sextets in Primitive Coronoids: General Treatment and the Smallest Coronoid

Gutman trees or caterpillars [26–30] are useful in calculations of sextet polynomials of unbranched catacondensed benzenoids (single chains of hexagons) [33]. In an analogous way there is a close connection between the sextet polynomial of a primitive coronoid and the matching polynomial of the corresponding generalized crown. This polynomial, say $\bar{\alpha}$ (gen. crown | x), in fact contains the coefficients of a sextet polynomial which we shall designate by $\bar{\sigma}$ (prim. coronoid | x). Specifically, if

$$\bar{\alpha}(\text{gen. crown} \mid x) = \sum_{j=0}^{m} p(\text{gen. crown} \mid j)\, x^{N-2j} \tag{17}$$

in consistence with eqn. (13), then

$$\bar{\sigma}(\text{prim. coronoid} \mid x) = \sum_{j=0}^{m} p(\text{gen. crown} \mid j)\, x^{j} \tag{18}$$

Here $\bar{\sigma}$ symbolizes the "uncorrected" sextet polynomial. We shall in the following explain the necessary corrections which lead from $\bar{\sigma}$ to σ.

As a first example consider the smallest coronoid (with eight hexagons), which is shown in Fig. 6 along with its generalized crown. Using the indicated numbering, the characteristic polynomial of the generalized crown, say c, was obtained by direct expansion of the appropriate determinant with the result

$$\varphi(\mathrm{c} \mid x) = \begin{vmatrix} -x & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -x & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & -x & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -x & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & -x & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & -x & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -x & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & -x \end{vmatrix}$$

$$= (x^2-1)^4 - 4x^2(x^2-1)^2 + 4x^2(x^2-1) \tag{19}$$
$$= x^8 - 8x^6 + 18x^4 - 12x^2 + 1$$

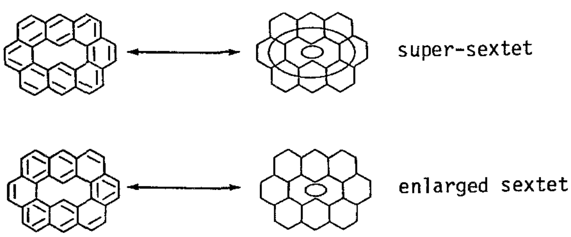


Fig. 7. The Kekulé structures of the smallest coronoid corresponding to the super-sextet and enlarged sextet

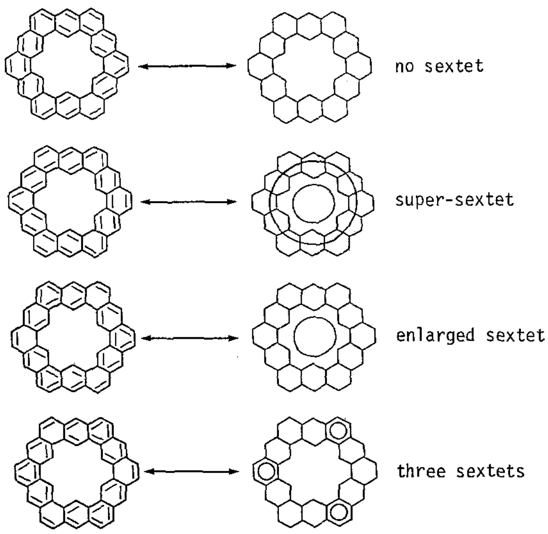


Fig. 8. The four annulenoid Kekulé structures in kekulene, $/3/^6$, and the corresponding generalized Clar formulas

The matching polynomial according to the definition (12) is

$$\alpha(\mathrm{c}\,|\,x) = \varphi(\mathrm{c}\,|\,x) + 2x^2 = x^8 - 8x^6 + 18x^4 - 10x^2 + 1 \tag{20}$$

and in the version of eqn. (13):

$$\bar{\alpha}(\mathrm{c}\,|\,x) = x^8 + 8x^6 + 18x^4 + 10x^2 + 1 \tag{21}$$

Finally we arrive at the uncorrected sextet polynomial for the smallest coronoid (Fig. 6) as:

$$\bar{\sigma}(/2^2,3/^2\,|\,x) = 1 + 8x + 18x^2 + 10x^3 + x^4 \tag{22}$$

Ohkami et al. [34], during their studies of sextet polynomials, reported a detailed mapping of the aromatic sextet patterns in the smallest coronoid. In order to establish a one-to-one correspondence between the generalized Clar formulas and Kekulé structures they had to add two units to $r(/2^2,3/^2,1)$, viz. the number of formulas with one sextet. These special sextets were referred to as a super-sextet and an enlarged sextet (cf. Fig. 7). With the pertinent correction the sextet polynomial reads

$$\sigma(/2^2,3/^2\,|\,x) = 1 + 10x + 18x^2 + 10x^3 + x^4 \tag{23}$$

The sextet polynomial (23) now obeys the property (16);

$$K(/2^2,3/^2\,|\,1) = \sigma(/2^2,3/^2\,|\,1) = 40 \tag{24}$$

in consistence with the known K number for the coronoid in question [1].

The situation with a super-sextet and an enlarged sextet is quite general for primitive coronoids. For the sake of clarity, let us show another example by considering $/3/^6$, which corresponds to the cycloarene called kekulene [11]. The complete set of sextet patterns for this system are treated in the next paragraph.

In an annulenoid Kekulé structure of a primitive coronoid the two perimeters (boundaries) are conjugated circuits, while all the internal (radial) edges are associated with single bonds. There are exactly four annulenoid Kekulé structures in a primitive coronoid, as is illustrated for kekulene in Fig. 8. The corresponding sextet patterns are indicated through the generalized Clar formulas which are depicted.

Aromatic Sextets in Regular Primitive Coronoids

The above treatment of crowns and their matching polynomials enables us to calculate straightforwardly the sextet polynomial for regular primitive coronoids.

As an example, consider the crown associated with kekulene, viz. $C_{6,1}$. From Table 2 (with $k = 1$) we obtain the characteristic polynomial

$$\varphi(C_{6,1}|x) = x^{12} - 12x^{10} + 48x^8 - 78x^6 + 48x^4 - 12x^2 + 1 \quad (25)$$

Furthermore, according to eqn. (14):

$$\alpha(C_{6,1}|x) = \varphi(C_{6,1}|x) + 2x^6 \quad (26)$$

which leads to

$$\bar{\alpha}(C_{6,1}|x) = x^{12} + 12x^{10} + 48x^8 + 76x^6 + 48x^4 + 12x^2 + 1 \quad (27)$$

This gives the uncorrected sextet polynomial for kekulene as

$$\bar{\sigma}(/3/^6|x) = 1 + 12x + 48x^2 + 76x^3 + 48x^4 + 12x^5 + x^6 \quad (28)$$

The equation is identical with the result of Gutman and El-Basil [35]. After the correction for the super-sextet and the enlarged sextet we attain at

$$\sigma(/3/^6|x) = 1 + 14x + 48x^2 + 76x^3 + 48x^4 + 12x^5 + x^6 \quad (29)$$

in consistence with Ohkami et al. [34]. Now the known number of Kekulé structures for kekulene [1, 36] is reproduced by

$$K(/3/^6) = \sigma(/3/^6|1) = 200 \quad (30)$$

In Fig. 9 a complete mapping of the generalized Clar formulas of kekulene is given.

As the next example consider the coronoid $/3/^{10}$, which is shown in Fig. 10 together with the crown associated with it. In order to compute its sextet polynomial we first need the characteristic polynomial of the crown $C_{10,1}$ (see Fig. 10). The polynomials $\varphi(C_{n,1}|x)$ are found for $n \leqslant 6$ on inserting $k = 1$ in the expressions of Table 2. They are entered into Table 3, which then was extended up to $n = 10$ by means of the recurrence relation (9). Following the procedure outlined above it was arrived at the corrected sextet polynomial

$$\sigma(/3/^{10}|x) = 1 + 22x + 160x^2 + 660x^3 + 1\,520x^4 + 2\,004x^5 + 1\,520x^6 + 660x^7 + 160x^8 + 20x^9 + x^{10} \quad (31)$$

This equation reproduces correctly the K number of the coronoid in question [7] as

$$K(/3/^{10}) = \sigma(/3/^{10}|1) = 6\,728 \quad (32)$$

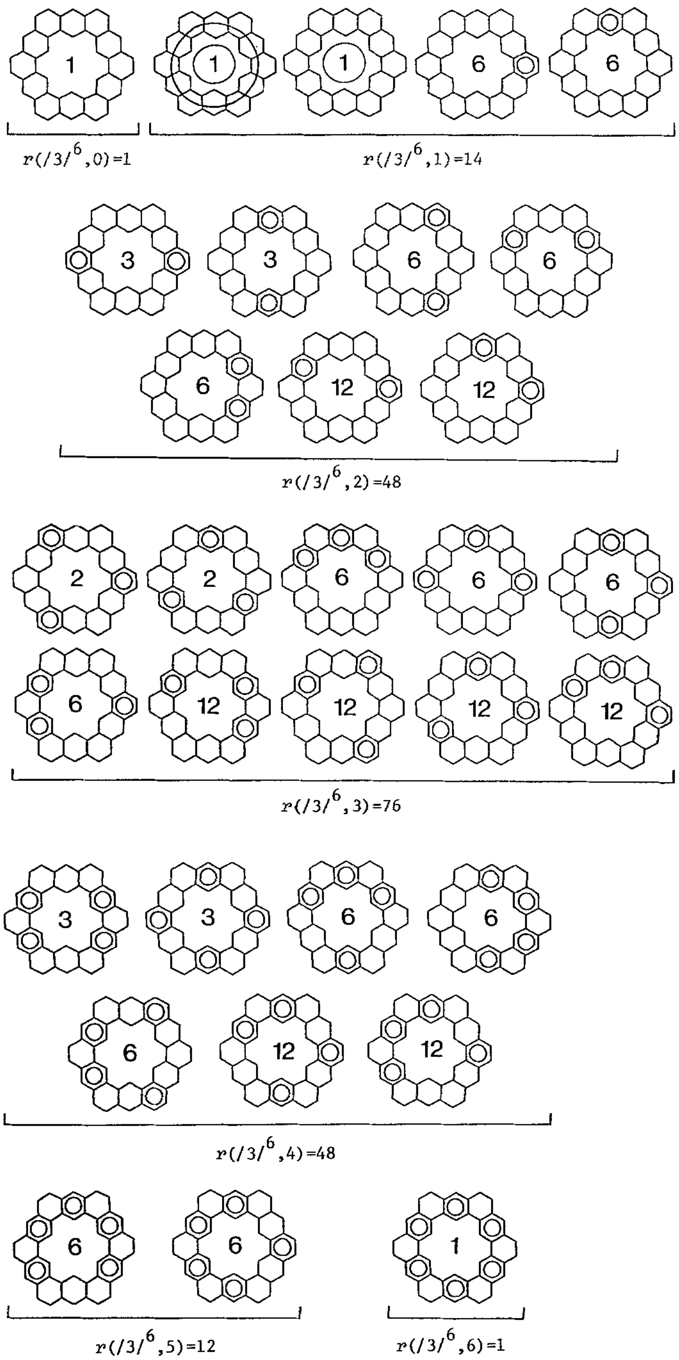


Fig. 9. The sextet patterns of kekulene. The inscribed numbers are multiplicities indicating the number of symmetrically equivalent generalized Clar formulas

As a final example we shall derive a combinatorial formula for the sextet polynomial of a class or regular primitive coronoids, of which eqn. (29) is a special case. Consider the kekulene homologs $/k + 2/^6$. This system is associated with the crown $C_{6,k}$, of which the characteristic polynomial is found at the bottom of Table 2.

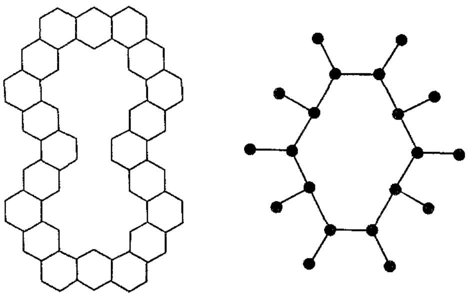


Fig. 10. The primitive coronoid $/3/^{10}$ (left) and the crown $C_{10,1}$ (right), which is associated with the coronoid

Table 3. Characteristic polynomials for some crowns ($k = 1$)

n	$\varphi(C_{n,1}\mid x)$
0	0
1	$x^2 - 2x - 1$
2	$x^4 - 6x^2 + 1$
3	$x^6 - 6x^4 - 2x^3 + 6x^2 - 1$
4	$x^8 - 8x^6 + 14x^4 - 8x^2 + 1$
5	$x^{10} - 10x^8 + 30x^6 - 2x^5 - 30x^4 + 10x^2 - 1$
6	$x^{12} - 12x^{10} + 48x^8 - 78x^6 + 48x^4 - 12x^2 + 1$
7	$x^{14} - 14x^{12} + 70x^{10} - 154x^8 - 2x^7 + 154x^6 - 70x^4 + 14x^2 - 1$
8	$x^{16} - 16x^{14} + 96x^{12} - 272x^{10} + 382x^8 - 272x^6 + 96x^4 - 16x^2 + 1$
9	$x^{18} - 18x^{16} + 126x^{14} - 438x^{12} + 810x^{10} - 2x^9 - 810x^8 + 438x^6 - 126x^4 + 18x^2 - 1$
10	$x^{20} - 20x^{18} + 160x^{16} - 660x^{14} + 1\,520x^{12} - 2006x^{10} + 1\,520x^8 - 660x^6 + 160x^4 - 20x^2 + 1$

With the aid of this expression we have arrived at the final result:

$$\begin{aligned}\sigma(/k + 2/^6\mid x) = {} & 1 + (6k + 8)x + (15k^2 + 24k + 9)x^2 \\ & + (20k^3 + 36k^2 + 18k + 2)x^3 \\ & + (15k^4 + 24k^3 + 9k^2)x^4 + (6k^5 + 6k^4)x^5 + k^6x^6 \end{aligned} \quad (33)$$

It is noted that the K number obtained as

$$\begin{aligned} K(/k + 2/^6) & = \sigma(/k + 2/^6\mid 1) \\ & = k^6 + 6k^5 + 21k^4 + 44k^3 + 60k^2 + 48k + 20 \\ & = (k^2 + 2k + 2)^2(k^2 + 2k + 5) \end{aligned} \quad (34)$$

is consistent with the previously determined combinatorial formula for this quantity [4–6]; see also especially Cyvin et al. [2].

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