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Topological Properties of Benzenoid Systems. X*. Note on a Graph-Theoretical Polynomial of Knop and Trinajstić

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A new graph-theoretical polynomial $T(G; x)$ was recently introduced by Knop and Trinajstić[1]. $T(G; x)$ differs from the sextet polynomial. The basic mathematical properties of $T(G; x)$ are determined.

In a recent review[1] Knop and Trinajstić have described some of the most important graph-theoretical polynomials which are of interest in the topological theory of conjugated structures. Among them the so called sextet polynomial was also mentioned.

The sextet polynomial is defined as[2-4]

$$P^s(G; x) = \sum_{k=0}^{L} r(G, k)\, x^k \qquad (1)$$

with $r(G, k)$ being the number of ways in which k *mutually resonant* sextets are chosen in a benzenoid system G, *and* $r(G, O) = 1$.

In equation (43) of ref. 1., however, a slightly different definition of the sextet polynomial was given, namely

$$\sum_{k=0}^{L} p(G, k)\, x^k \qquad (2)$$

with $p(G, k)$ being the number of ways in which k disconnected sextets are chosen from G and, in addition, $p(G, O) = 1$. In the following we shall denote the polynomial (2) by $T(G; x)$, since it can be easily verified that the sextet polynomial and $T(G; x)$ differ in general. In other words, the definition of the sextet polynomial proposed by Knop and Trinajstić[1] was not correct.

For example, the sextets 1 and 3 in anthracene, G_1, are disconnected but are not mutually resonant. Therefore, $r(G_1, 2) = 0$ and $p(G_1, 2) = 1$ and consequently, $P^s(G_1; x) = 1 + 3x$ whereas $T(G_1; x) = 1 + 3x + x^2$.

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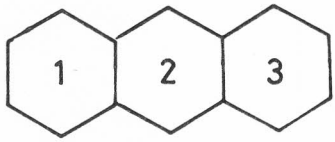
* Parts VIII and IX: I. Gutman, *Z. Naturforsch.* **36a** (1981) 128 and **37a** (1982) 69.



G_1

G_1^*

The above discussion implies that formula (2) (i. e. equation (43) of ref. 1.) can be understood as the definition of a novel graph-theoretical polynomial. Its properties seem to be rather interesting indeed. In the present paper the basic properties of $T(G; x)$ will be determined. We shall follow completely the notation and terminology of ref. 1.

First of all, if two sextets are mutually resonant, then they are necessarily disconnected[2]. (The opposite is not true, as it has already been shown on the example of anthracene.) Therefore, we have the following inequalities.

Proposition 1. — For all benzenoid systems G and for all $k = 1, 2, \ldots,$

$$r(G, k) \leqslant p(G, k)$$

and consequently, for all positive values of the variable x,

$$P^s(G; x) \leqslant T(G; x).$$

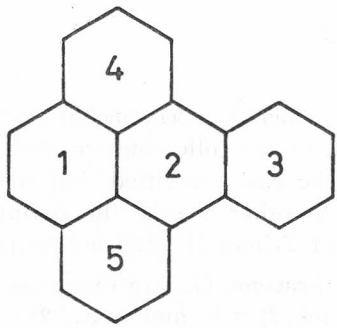
It is not difficult to find the conditions under which the numbers $r(G, k)$ and $p(G, k)$ coincide.

Proposition 2. — The equalities

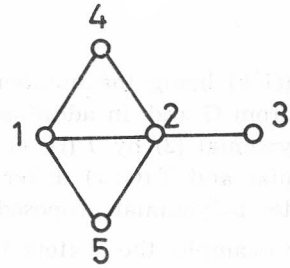
$$r(G, k) = p(G, k)$$

hold for all $k = 1, 2, \ldots$ if and only if an anthracene fragment is not contained in the benzenoid system G. Then, of course, also $P^s(G; x) = T(G; x)$.

According to Proposition 2, the polynomials $T(G; x)$ and $P^s(G; x)$ are different for almost all benzenoid systems.



G_2



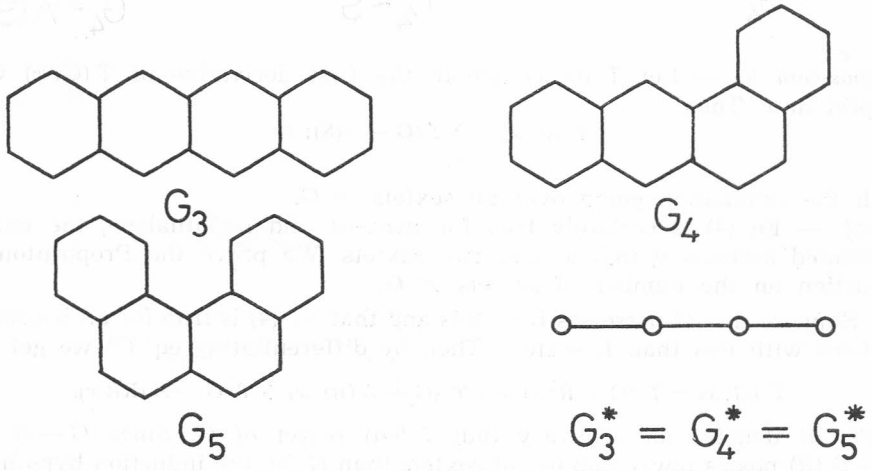
G_2^*

The inner dual G^* of a benzenoid graph G, is a graph whose vertices represent the sextets of G and two vertices of G^* are adjacent if the pertinent sextets are connected[5]. For example, the inner dual G_1^* of the anthracene graph is the path graph of the length two. If the benzenoid system is peri--condensed, then its inner dual is a cyclic graph, as illustrated on the example of the isomer of benzopyrene, formula G_2.

(Note that the inner dual, as defined above, is a graph. Thus, in G^* the angles between the edges play no role. In ref.[5] and elsewhere the so called dualist graph or characteristic graph of a benzenoid system is also considered, in which the angles between the edges are not ignored. In the present paper we are not interested in dualist graphs.) From the definition of the inner dual it follows immediately that $p(G, k)$ is equal to the number of selections of k mutually non-adjacent vertices in G^*. This imples the following

Proposition 3. — If two benzenoid systems have equal inner duals, then they have equal T-polynomials.

For example, G_3, G_4 and G_5 have the same inner dual, namely the path graph of the length three. Consequently, the T-polynomials of G_3, G_4 and G_5 are mutually equal. In fact, $T(G_3; x) = T(G_4; x) = T(G_5; x) = 1 + 4x + 3x^2$. Since G_5 contains no anthracene fragment (contrary to G_3 and G_4), its sextet polynomial is $P^s(G_5; x) = 1 + 4x + 3x^2$. On the other hand, $P^s(G_3; x) = 1 + 4x$ and $P^s(G_4; x) = 1 + 4x + 2x^2$.



Let S be a sextet of the benzenoid system G. Let $A(S)$ be the collection of all sextets of G which are connected with S. By definition also the sextet S belongs to $A(S)$.

There are $p(G - S, k)$ selections of k disconnected sextets in G, such that S has not been chosen. Besides, the number of selections of k disconnected sextets in G, such that S has been chosen is equal to the number of selections of k-1 disconnected sextets in $G - A(S)$. Therefore,

$$p(G, k) = p(G - S, k) + p(G - A(S), k - 1),$$

which substituted back into (2) gives the following recursion relation.

Proposition 4. — Let S be an arbitrary sextet of G. Then

$$T(G; x) = T(G - S; x) + x\,T(G - A(S); x). \tag{3}$$

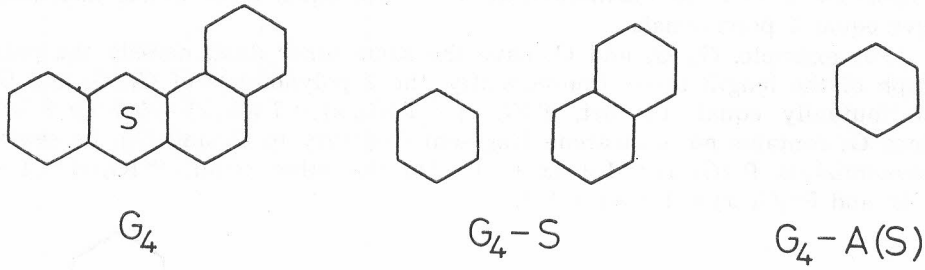
By means of the above Proposition the T-polynomials can be easily calculated also in the case of relatively large (polycyclic) systems. The calculation is further simplified by the following result.

Proposition 5. — If the benzenoid system G is composed of two disconnected parts G_a and G_b, then

$$T(G; x) = T(G_a; x)\,T(G_b; x).$$

For example, the T-polynomial of G_4 is computed as follows.

$$T(G_4; x) = T(G_4 - S; x) + x\,T(G_4 - A(S); x) = (1 + x)(1 + 2x) + x(1 + x) = 1 + 4x + 3x^2.$$



Proposition 6. — Let $T'(G; x)$ denote the first derivative of $T(G; x)$ with respect to x. Then

$$T'(G; x) = \sum_S T(G - A(S); x). \tag{4}$$

with the summation going over all sextets in G.

Proof. — Eq (4) is certainly true for benzene and naphthalene, the unique benzenoid systems with one and two sextets. We prove the Proposiiton by induction on the number of sextets in G.

Suppose that G possesses L sextets and that eq. (4) is true for all benzenoid systems with less than L sextets. Then by differentiating eq. (3) we get

$$T'(G; x) = T'(G - R; x) + x\,T'(G - A(R); x) + T(G - A(R); x),$$

where R denotes an arbitrary (but fixed) sextet of G. Since $G - R$ and $G - A(R)$ posses fewer number of sextets than G, by the induction hypothesis:

$$T'(G; x) = \sum_{S \neq R} T(G - R - A(S); x) + x \sum_{S \neq R} T(G - A(R) - A(S); x) + T(G - A(R); x).$$

By Proposition 4,

$$T(G - R - A(S); x) + x\,T(G - A(R) - A(S); x) = T(G - A(S); x)$$

and therefore we have

$$T'(G; x) = \sum_{S \neq R} T(G - A(S); x) + T(G - A(R); x),$$

which immediately yields eq. (4).

Results analogous to the Proposition 6 exist also for other graph-theoretic polynomials considered in ref. 1. Thus for example, if P^{ac} denotes the acyclic polynomial[6], then the relation

$$P^{ac\prime}(G; x) = \sum_i P^{ac}(G - v_i; x) \tag{5}$$

was obtained in the work[7], whereas the pertinent identity for the characteristc polynomial,

$$P'(G; x) = \sum_i P(G - v_i; x) \tag{6}$$

is known in graph spectral theory[8] and seems to be first explicitely formulated by Clarke[9]. (The matrix-theoretical equivalent of eq. (6) is, however, a commonly known and elementary result.) On the other hand, the authors of ref. 1 were the first to deduce[10] from eq. (6) that »*a collection of subgraphs obtained from G by succesive removal of a single vertex is unique to that graph*« (see p. 508 of ref. 1.) This statement deserves particular attention because of its close relation to Ulam's conjecture[11].

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11. For an exposition of Ulam's hypothesis see for example: F. Harary, *Graph Theory,* Addison-Wesley, Reading 1969, Chapters 2 and 4.

SAŽETAK

Topološka svojstva benzenoidnih sustava. X. Bilješka o jednom grafovskom polinomu Knopa i Trinajstića

I. Gutman

Knop i Trinajstić[1] su nedavno definirali jedan novi graf teorijski polinom $T(G; x)$, koji se u općem slučaju razlikuje od sekstetnog polinoma. Izvedena su temeljna matematička svojstva polinoma $T(G; x)$.