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An Easy Combinatorial Algorithm for the Construction of Sextet Polynomials of Cata-Condensed Benzenoid Hydrocarbons*

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Two types of pruning techniques for certain trees are described and utilized into an easy combinatorial algorithm for the systematic construction of sextet polynomials of catacondensed benzenoid hydrocarbons of large sizes.
The algorithm offers an alternative to existing methods for the enumeration of Kekulé structures which is not restricted to non-branched systems.

1. INTRODUCTION

A few years ago Hosoya and Yamaguchi[1] introduced the sextet polynomial, $B_G(X)$ of benzenoid hydrocarbons defined as:

$$B_G(X) = \sum_{k=0}^{m} r(G,k)\ X^k \qquad (1)$$

where $r(G, k)$ is the number of ways in which k disconnected but mutually resonant sextets are chosen from molecular graph G and is called the resonant sextet number; $r(G, O)$ is defined as unity. The parameter m is the maximal possible value of k in G. This polynomial, has so far attracted the attention of organic chemists as well as of graph theorists. Its importance in organic chemistry led Aihara[2] to define a resonance polynomial, $A_G(X)$, given by

$$A_G(X) = \sum_{k=0}^{m} (-1)^k\, r(G,k)\ X^{2m-2k} \qquad (2)$$

The roots of $A_G(X)$ were found to correlate well with known resonance energies[2]. In graph theory two important developments took place, viz.,

1) Gutman demonstrated[3] that the coefficients of $B_G(X)$ were identical to the coefficients of the characteristic polynomials of certain trees, T, Thus

$$r(G,k) = p(T,k) \qquad (3)$$

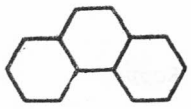
where $p(T, k)$ is the number of ways in which k nonincident edges can be selected from T. In a related recent development Gutman[4] constructed

* Dedicated to Professor Dr. Ivan Gutman for his elegant work on the subject (refs. 3,4).

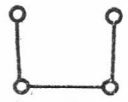
new graphs, called C graphs from the corresponding molecular graphs of benzenoid hydrocarbons, BH's, such that the vertices v_r and v_s of the C graph are adjacent if and only if the hexagons of BH are mutually not resonant. Gutman, then, elegantly showed[4] that such C graphs are actually the line graphs[5] of the trees, T's, whose coefficients enter into eqn. (3), thus

$$C = \alpha(T); \qquad (4)$$
$$T = \alpha^{-1}(C)$$

As an illustration we consider the molecular graph of phenanthrene, its C graph and the corresponding $T = \alpha^{-1}(C)$. Details are found in ref. 4.



C

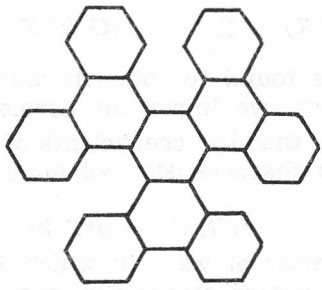


$\mathcal{L}^{-1}(C) = T$

ii) Quite recently, the author[6] partitioned the factor graphs[7] (previously called submolecule graphs) corresponding to the Kekulé structures of BH according to numbers of bivalent vertices: thus if m is the maximal number of bivalent vertices possessed by a factor graph of some BH, a_m is the population (number) of factor graphs possessing m bivalent vertices, then for non-branched catacondensed all-benzenoid hydrocarbons, one has:

$$a_m = r(G, 0)$$
$$a_{m-1} = r(G, 1)$$
$$a_{m-j} = r(G, j) \qquad (5)$$

Other relations were also discovered[8] for various types of topologies.
The above brief history of the sextet polynomial indicates its importance in chemistry. So far, however, the literature seems to be devoid of a general and systematic method of constructing such polynomials for large (or even small) size BH's without resorting to the tendious task of drawing and closely inspecting all Kekulé structures of the BH as originally suggested by Hosoya and Yamaguchi[1]. For example the BH whose molecular graph is shown below



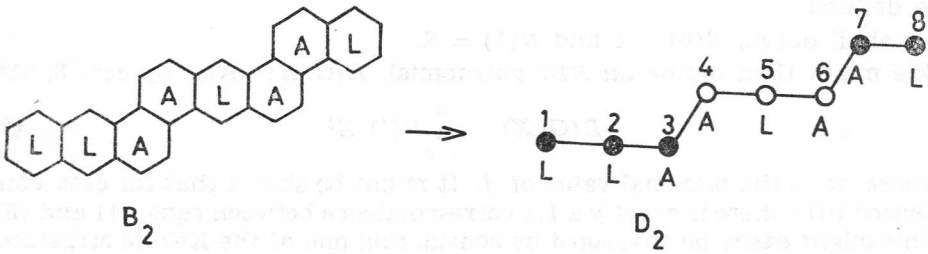
B_1

has 189 Kekulé structures and obviously to construct its sextet polynomial by drawing and examining all such Kekulé structures would be both very cumbersome and error prone. In this paper we introduce a very simple combinatorial method for systematically counting the resonant numbers without drawing any Kekulé structures. It must be emphasized, however, that our objective is not to count K (number of Kekulé structures) since elegant methods already exist for doing so[9]. Our algorithm, nevertheless, besides computing coefficients of sextet polynomials of BH's provides an interesting alternative to finding K which is not limited to nonbranched systems.

2. DEFINITIONS

Dualist[10], D

When the hexagons of the molecular graph of a BH are replaced by vertices and then the vertices that correspond to hexagons having a common edge are connected a dualist *D*, results, E.g.



We observe that each kink in D corresponds to an angularly annelated hexagon[3] (See B_2, where L = linear and A = angular annelation).

Dualist Subgraphs, $< S >$

The dualist of the molecular graph might be partitioned into a number of induced[11] subgraphs. For our purpose we distinguish two types of dualist-induced subgraphs, viz.,

$$<S_1> = L^{s_1}A; \qquad s_1 = 1, 2, 3, \ldots\ldots \tag{6}$$

where $L^{s_1}A$ and $AL^{s_2}A$ are sequences of the L—A symbols[3] indicating

$$<S_2> = AL^{s_2}A; \qquad s_2 = 0, 1, 2, \ldots\ldots \tag{7}$$

modes of ring annelations in a particular subset of dualist vertices as described in details in ref. 3. As an illustration we consider all $<S_1>$'s and $<S_2>$'s present in D_2. There are two $<S_1>$'s, viz., $\{1, 2, 3\} = L^2A$ $(s = 2)$ and $\{8, 7\} = LA$ $(s_1 = 1)$, where the numbers in brackets correspond to numbers assigned to dualist vertices. There are three $<S_2>$'s in D_2: these are:

$$\begin{aligned} \{3, 4\} &= A^2 = AL^0A \ \text{(i.e. } s_2 = 0) \\ \{4, 5, 6\} &= ALA \quad (s_2 = 1) \\ \{6, 7\} &= A^2 \quad (s_2 = 0) \end{aligned}$$

One observes that both $<S_1>$ and $<S_2>$ define subsets of dualist vertices linked in straight lines i.e. devoid of any kinks.

(This might cause some confusion since the symbol A is taken to mean an angular annelation i.e. a kink. However such a kink is formed only when we consider the dualist as a whole. E.g., in D_2, $<S_1> = L^2A$ i.e. the solid circles, however, when this part is excised from the dualist it becomes simply an L^3, which has no kinks. Such induced subgraphs were called--erroneously by this author-linear subgraphs[12].

Restricted Disjoint Interactions (6), RDI's

An element of an RDI, $(v_i, v_j, v_k, \ldots)$ is defined as a subset of dualist vertices $v_i, v_j, v_k, \ldots$ such that:

(a) No two vertices are adjacent, and (b) No two vertices belong to the same $<S>$. Thus one defines pairs of *RDI*'s, $N(2)$'s, as the sum of all possible pairs of dualist vertices complying with (a) and (b). E.g. D_2 has the following elements of:

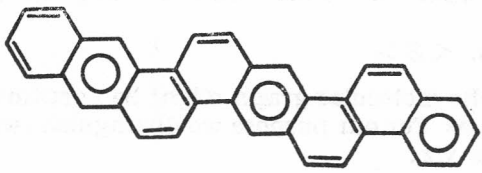
$N(2)$: (14), (15), (16), (17), (18); (24), (25), (26), (27), (28); (35), (36), (37), (38); (47), (48); (57), (58); (68). Thus $N(2)_{D_2} = 19$. Similarly $N(3)$, $N(4), \ldots, N(j)$; $j<v$ (v = number of vertices in D) might analogously be defined.

We shall define $N(0) = 1$ and $N(1) = R$.

One might then define an *RDI* polynomial, $R(G, X)$ given by eqn. 8, viz.,

$$R(G, X) = \sum_{j=0}^{m} N(j)\, X^j \tag{8}$$

where m is the maximal value of j. It might be shown that for cata-condensed BH's there is exactly a 1:1 correspondence between eqns. (1) and (8). This might easily be envisaged by considering one of the Kekulé structures of B_2 drawn using Clar's notation[13]



We observe that there is only one resonant sextet per each $<S>$ as defined in (6) and (7).

Thus counting resonant sextet numbers boils down to counting doublets of RDI's, which is the subject of this work. We shall do so graphically by employing two types of pruning operators applied to dualist graphs.

3. PRUNING OPERATORS

(A) Non-Branched BH's

(i) P(I)

The operator $P(I)$ successively prunes terminal vertices, one by one, (arbitrarily to the left of the tree). Thus the successive operation by $P(I)$ on L_2 generates the following trees.

An Illustration of P(I) *on* D_2

$$L^2A^2LA^2L \xrightarrow{P(I)} LA^2LA^2L \xrightarrow{P(I)} LALA^2L \; D_2 \xrightarrow{P(I)} L^2A^2L \xrightarrow{P(I)} LA^2L \xrightarrow{P(I)}$$

$$\xrightarrow{P(I)} LAL \xrightarrow{P(I)} L^2 \xrightarrow{P(I)} L \xrightarrow{P(I)} \Phi \text{ (empty set)} \qquad (9)$$

We observe that when a terminal L us adjacent to an A is operated by $P(I)$ two operations occur: (a) The terminal L is removed, and (b) the A is replaced by an L.

(ii) P(II)

This operator carries out two operations on D: (a) It removes an $<S_1>$, and (b) it changes the terminal A from the left (if any) into an L. Thus when D_2 is subjected to $P(II)$ the following trees are generated

$$L^2A^2LA^2L \xrightarrow{P(II)} L^2A^2L \xrightarrow{P(II)} L^2 \xrightarrow{P(II)} \Phi. \qquad (10)$$

$P(II)$ prunes L^s, $(s = 1, 2, \ldots..)$.

A terminal tree, $T(t)$, in the sequence of trees generated by $P(I)$ operator on a dualist, is defined to be the graph containing the smallest number of vertices with at least one kink and which when subjected to the action of P(II) becomes the dualist of a linear acene (i.e. becomes devoid of any kinks). In the sequence defined by (9), the graph LAL is $T(t)$ $(LAL \xrightarrow{P(II)} L)$.

4. GRAPHICAL SYNTHESIS OF SEXTET POLYNOMIAL

(a) The dualist tree, D, is subjected to the successive operations of $P(I)$ until D is pruned down to a tree containing the smallest number of vertices which vhen subjected to $P(II)$ leads to an L^s $(s = 1, 2, \ldots)$. The trees generated from $P(I)$, called $P(I)$-trees, $T(P(I))$ define a graph, $G(P(I))$, containing as many components as the number of $P(I)$ trees. A tree is identified by a subscript indicating the number of times $P(I)$ is applied to it and a superscript indicating the number of vertices in it. Also the graph $G(P(I))$ is identified by a subscript indicating the number of pruning cycles which led to it. A pruning cycle starts at $T(P(I)_0{}^v)$ and ends at $T(t)$. (See later).

(b) Each $T(P(I)_i{}^j)$ is operated by $P(II)$, the last tree being $T(t)$. The graph resulting from $P(II)$ operations is called $G(P(II))_1$. (The subscript 1 indicates one pruning cycle). The order of $G(P(II))_1$, i.e. number of its vertices, $|P(II)|_1$ is equal to $N(2)$.

(c) The $T(P(II)_i^j)$ trees are used to feed a second $P(I)$ cycle, i.e. every $T(P(II)_i^j)$ is equated to a $T(P(I)_0^j)$. Again the resulting $T(P(I)_i^j)$'s are operated by $P(II)$, the resulting disconnected graph, $G(P(II))_2$ is used to calculate $N(3)$:

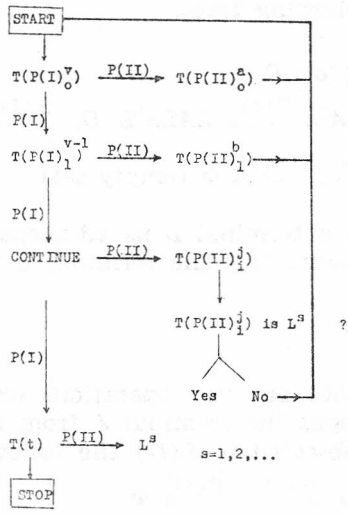


Figure 1. Algorithm describing pruning cycles of trees. $P(I)$, $P(II)$ and $T(t)$ are explained in the text. At the end of the jth cycle the order of the total graph composed of all pruned trees is $N(j+1) = r(G, j+1)$.

$$|P(II)|_2 = N(3)$$

(d) Again the cycle is repeated by starting with $T(P(II)_i^j)$'s and a $G(P(II))_3$ is generated.
In general one has

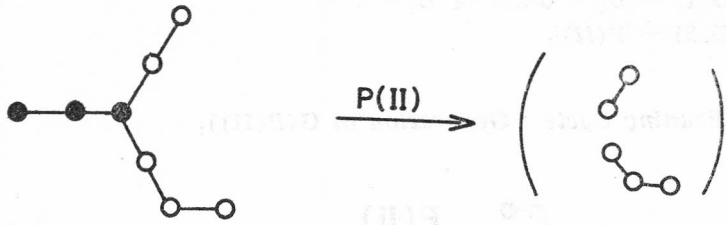
$$|P(II)|_j = N(j+1) = r(G, j+1) \tag{11}$$

(e) The pruning cycles are terminated when all the resulting $T(P(II)_i^j)$'s are linear acenes-dualists i.e. L^s, $s = 1, 2, \ldots$.

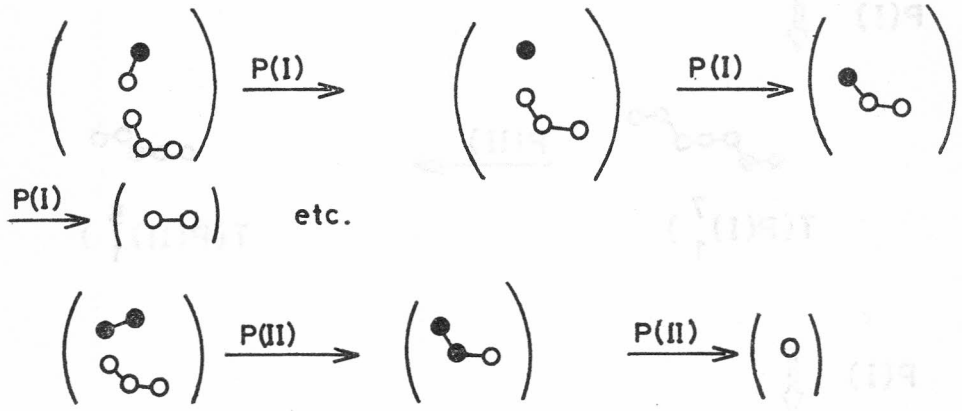
Steps (a—e) are worked out in detail for both a branched and a non-branched system. In the rseults Figure 1 outlines the pruning algorithm.

B. Branched HB's

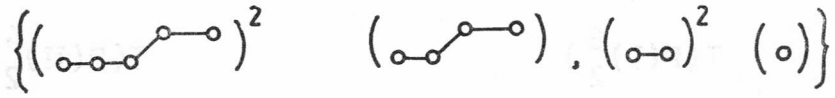
The application of either $P(I)$ *or* $P(II)$ to a non-branched cata-condensed BH-dualist leads to a connected graph. When $P(II)$, however, operates on a branched dualist, sometimes a disconnected graph results; e.g.



The application of either $P(I)$ or $P(II)$ to the resulting multicomponent graph follows the cited operations of the operators, e.g.



It is convenient to define the graph $G(P(II)_j)$ the components of which result in the jth pruning cycle. Thus for D_2, $G(P(II)_1)$ is given by (see results) where the supprescripts indicate multiplicities of the components.



Thus $|P(II)|_1 = 2 \times 5 + 4 + 2 \times 2 + 1 = 19 = N(2)$.
$G(P(II)_j)$ graphs are shown for D_1, a branched system, in the results.

5. RESULTS

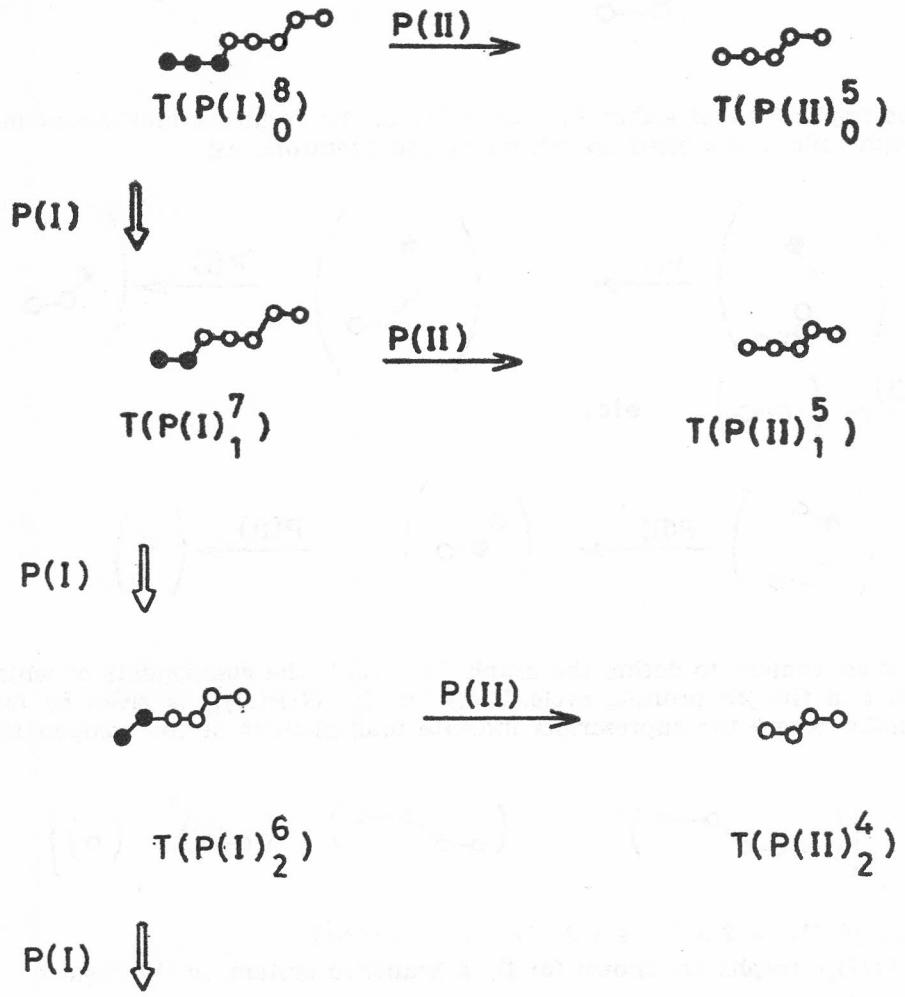
Throughout the following charts, the solid circles indicate $<S_1>$

I. Construction of Sextet Polynomial of D_2

$N(0) = r(G, 0) = 1$

$N(1) = r(G, 1) = |D_2|$ = order of $D_2 = 8$
$N(2) = r(G, 2) = |P(II)|_1$

The First Pruning Cycle : Generation of $G(P(II))_1$



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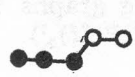


$T(P(I)^5_3)$ $T(P(II)^2_3)$

P(I) ⇓

$T(P(I)^4_4)$ $T(P(II)^2_4)$

P(I) ⇓

o

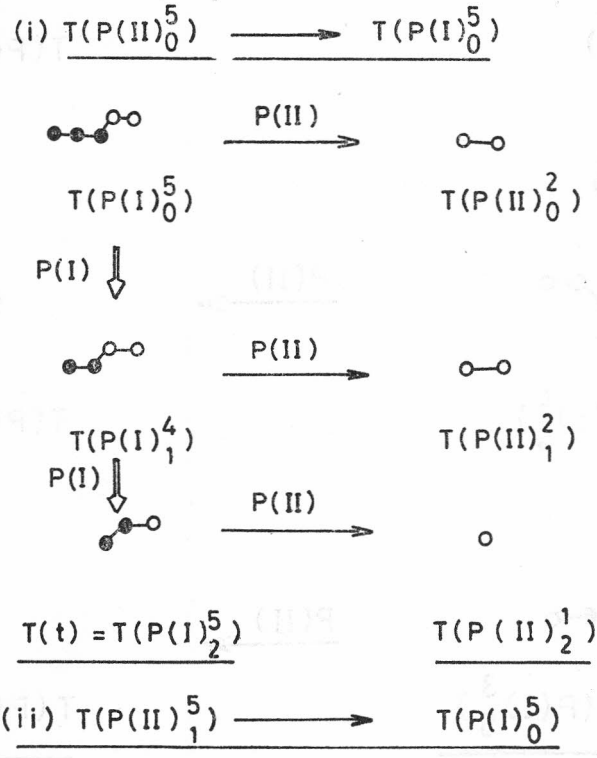
$$T(t) = \frac{T(P(I)^3_5)}{T(P(I)^j_i)_1 \cdot s} \qquad \frac{T(P(II)^1_5)}{T(P(II)^j_i)_1 \cdot s}$$

$$\Sigma T(P(II)^j_i)_1 \subset G(P(II))_1 =$$

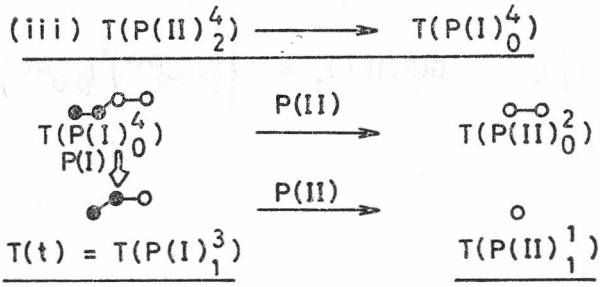
$|P(II)|_1 = 2 \times 5 + 4 + 2 \times 2 + 1 = 19 = N(2) = r(G, 2).$

The second Pruning Cycle: Generation of $G(P(II))_2$

We have only three trees that yield non-vanishing graphs when subjected to $P(II)$, viz, $T(P(II)_0{}^5)$, $T(P(II)_1{}^5)$ and $(T(P(II)_2{}^4)$.



We obtain an identical graph as in (i), viz., $(o—o)^2$, (o)



$$\sum T(P(II)_i^j)_2 \subset G(P(II))_2 = \left\{(o\text{-}o)^5, (o)^3\right\}$$

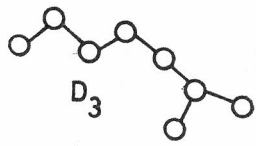
$$|P(II)|_2 = 5 \times 2 + 3 \times 1 = 13 = N(3) = r(G, 3).$$

Since all $P(II)$-trees in the second pruning cycle are either K_2 or K_1, $N(4) = r(G, 4) = 0$ and $m = 3$.

The Sextet polynomial of B_2 is thus $1+8X+19X^2+13X^3$ and $K = 1+8+ +19+13 = 41$.

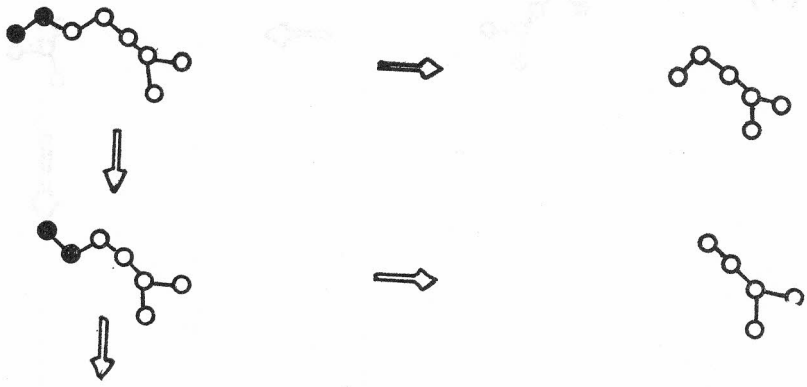
II. Sextet Polynomial of a Branched BH

We consider a BH whose dualist is B_3, viz,



We shall omitt tree symbols. Horizontal arrows are $P(II)$'s while vertical ones are $P(I)$'s.

First pruning cycle $\longrightarrow G(P(II))_1 \longrightarrow |P(II)|_1 = N(2)$



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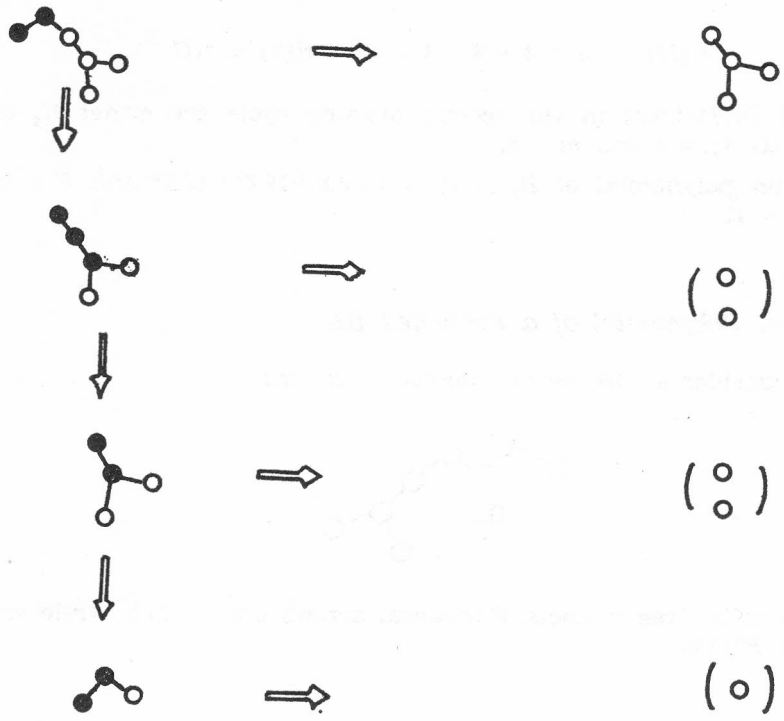

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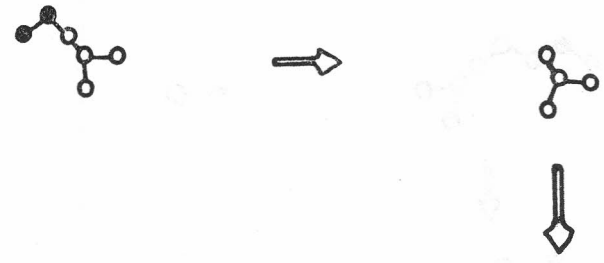
Second pruning cycle $\longrightarrow G(P(II))_2 \longrightarrow |P(II)|_2 = N(3)$

(i)



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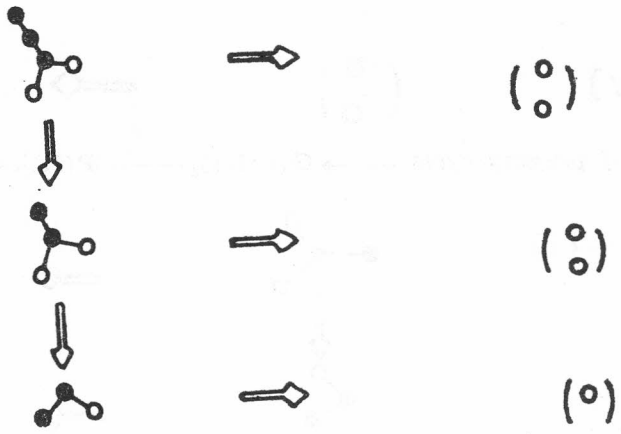
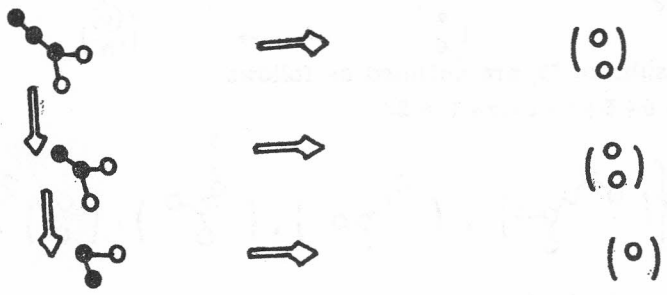
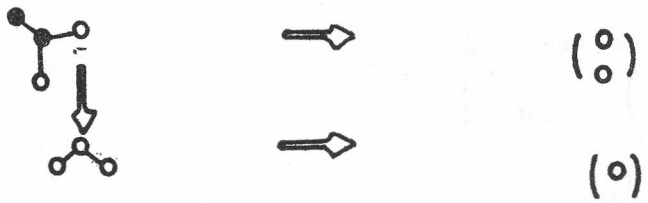
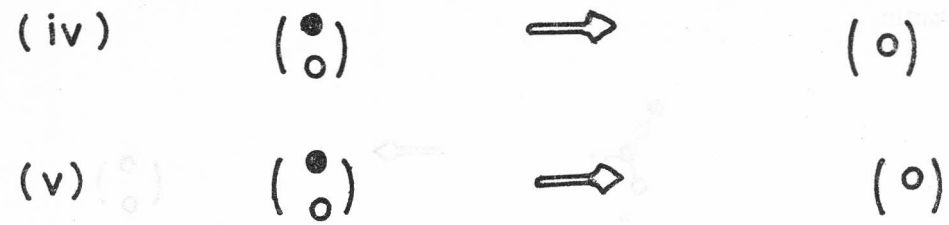


(ii)

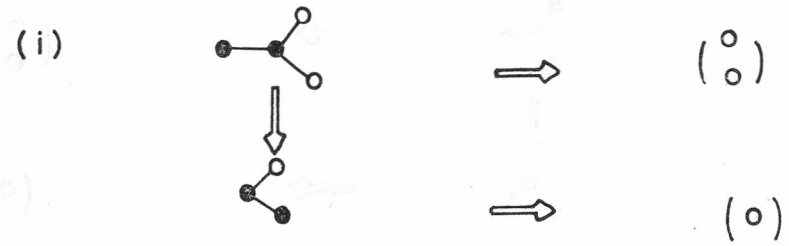


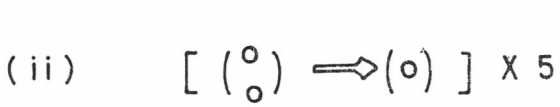
(iii)





Third pruning cycle $\longrightarrow G(P(II))_3 \longrightarrow |P(II)|_3 = N(4)$

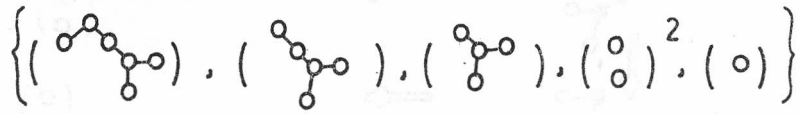




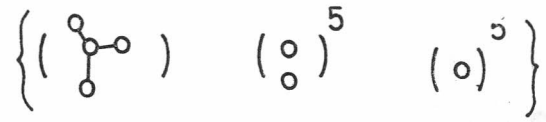
Fourth pruning cycle $\longrightarrow G(P(II))_4 \longrightarrow |P(II)|_4 = N(5)$

The results of D_3 are outlined as follows:

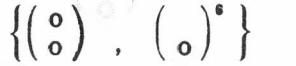
$N(2) = 6+5+4+2\times2+1 = 20$



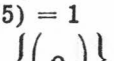
$N(3) = 4+2\times5+5\times1 = 19$



$N(4) = 2\times1+6\times1 = 8$



$N(5) = 1$



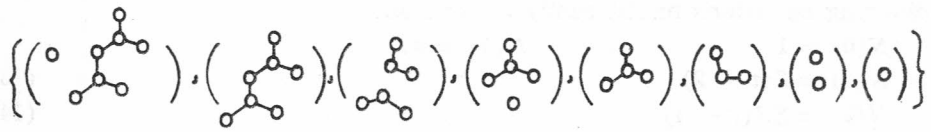
$$B(G_3, X) = 1+8X+20X^2+19X^3+8X^4+X^5$$

$$K = 1+8+20+19+8+1 = 57$$

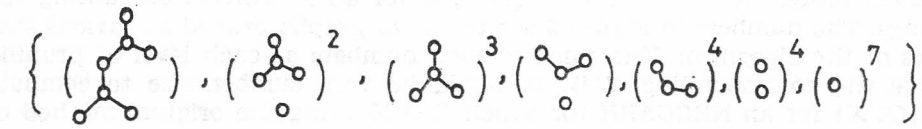
III — Pruned Graphs of D_1

$N(1) = 10$

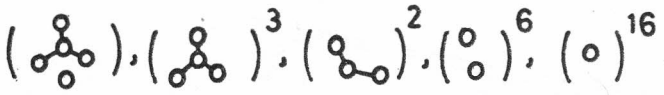
$N(2) = 36$



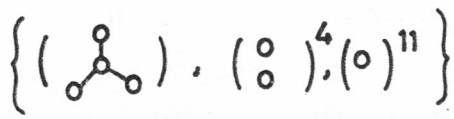
$N(3) = 60$



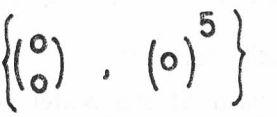
$N(4) = 51$



$N(5) = 23$



$N(6) = 7$



$N(7) = 1$

$\{(o)\}$

$B(G_1, X) = 1+10X+36X^2+60X^3+51X^4+23X^5+7X^6+X^7;$

$K = 189.$

6. SOME SPECIAL TOPOLOGIES

I. Non-branched Cata-condensed All-benzenoid Hydrocarbons, NBCCABH's

Calculation of $N(j)$'s $(= r(G, j)$'s) of this class of BH's obey a relatively simple arithmetic.
First we define the following quantities:

$$S(j) = j + (j-1) + (j-2) + \ldots + 1; \tag{12a}$$

$$\Sigma S(j) = S(j) + S(j-1) + S(j-2) + \ldots + S(1), \tag{12b}$$

$$S(1) = 1 \tag{12c}$$

Let v be the number of vertices of the dualist graph of an NBCCABH : The following equations might easily be written:

$$N(0) = 1 \quad ; \quad N(1) = v$$

$$N(2) = S(v-2) \tag{13}$$

$$N(3) = \Sigma S(v-4) \tag{14}$$

$$N(4) = \Sigma S(v-6) + \Sigma S(v-7) + \ldots + S(1) \tag{15}$$

Expressions for higher interactions are more involved. Figure 2 is a graphical representation of these equations for an NBCCABH containing ten rings. The numbers in Figure 2 are orders of graphs pruned at various stages of the algorithm. The sums of such numbers at each level of pruning give the corresponding $N(j)$. It would be very cumbersome to compute $B(G; X)$ for an NBCCABH for which $R = 10$ using the original method of

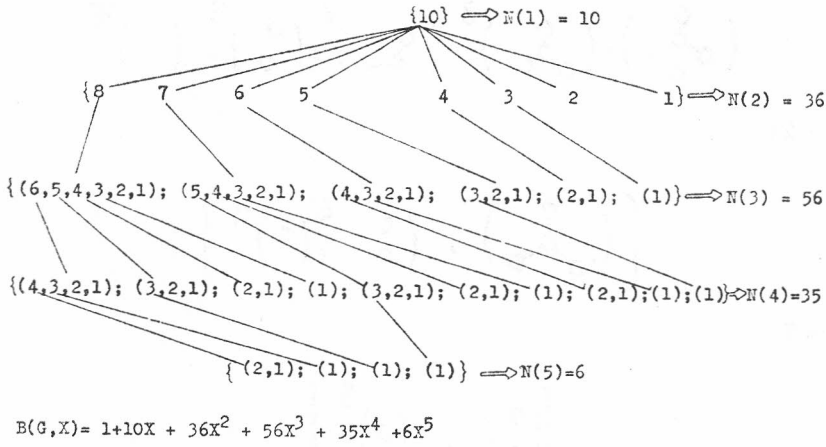
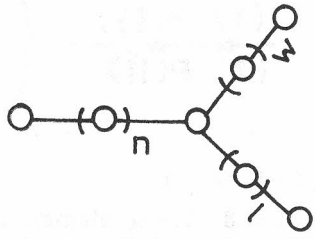


Figure 2. Graphical construction of the sextet polynomial of an NBCCABH containing 10 hexagons. The lines indicate successive P(II) operations.

Hosoya and Yamaguchi[1] or using Gutman's[3] method or the author's[6] method depending on the partitioning of the corresponding Kekulé-factor--graphs.

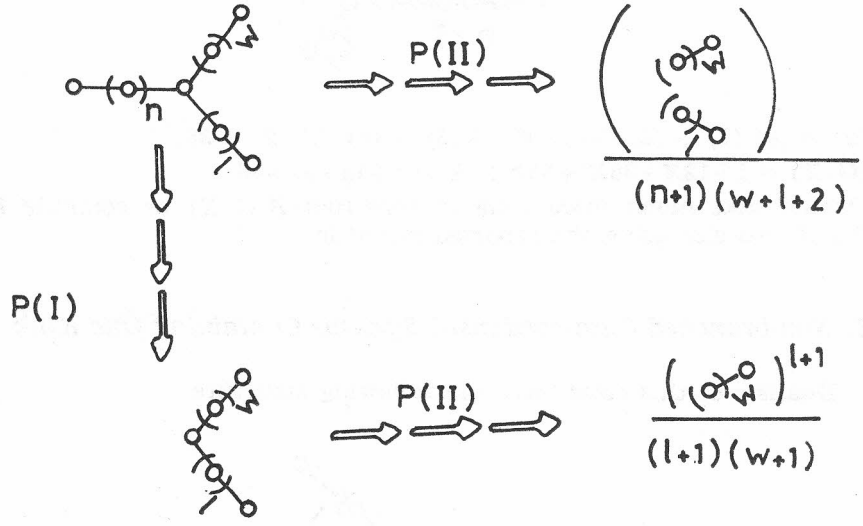
II. Branched Cata-condensed Systems Containing One Branched Ring

The dualists of such BH's have one trivalent vertex. A general representation of such systems is shown below:



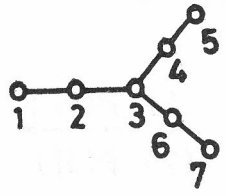
Pruning cycles are illustrated in a compact form as follows

N(2) Graphs



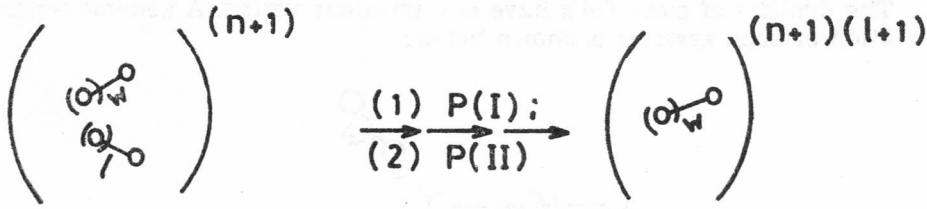
Therefore $N(2) = (n+1)\,(w+l+2) + (l+1)\,(w+1)$ (16)

Suppose, e.g., $n = m = l = 1$; we will have



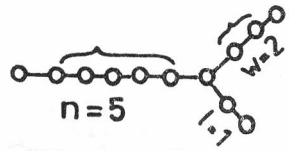
$N(2) = (1+1)\,(1+1+2) + (1+1)\,(1+1) = 12$. These elements are: (1), (15), (16), (17), (24), (25), (26), (27), (57), (56), (46), (47).

N(3) Graphs



Therefore $N(3) = (w+1)\ (n+1)\ (l+1)$ (17)

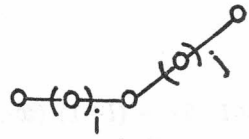
Again if $w = n = l = 1$ $N(3) = 8$. These elements are (146), (147), (156), (157), (246), (247), (256), (257). Eqns. (16) and (17) become essential when dealing with large sizes, e.g.



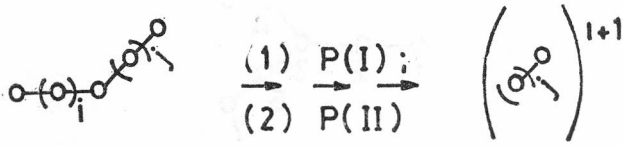
$N(2) = (6)\ (5) + (2)\ (3) = 36$; $N(3) = (6)\ (3)\ (2) = 36$;
$B(G, X) = 1+12X+36X^2+36X^3$; $K = 1+12+36+36$.
It would take much more time to construct $B(G, X)$ or compute K for BH's of this size using the reported methods.

III. Non-branched Cata-condensed Systems Containing One Kink

Dualists of this class have the following structure



There is only one pruning cycle i.e. $m = 2$ and $N(3) = 0$:



Therefore $N(2) = (i+1)\ (j+1)$. (18)
Analogous formulae are easily derived for other topologies.

Topological Origin of the Method

The outlined algorithm rests on an important topological character of Kekulé structures of BH's: there is only one resonant sextet in each subset of benzene rings corresponding to dualist vertices defining $<S_1>$ and/or $<S_2>$ (c.f. eqns. 6; 7). This fact leads in cata-condensed BH's to a 1:1 correspondence between the sextet polynomial, eqn. 1, and the RDI polynomial, eqn. 8 i.e.

$$r(G, j) = N(j)$$

where $j = 0, 1, \ldots, m$, m being the maximum number of disconnected but mutually resonant sextets or the maximum number of dualist vertices defining a subset in which: (i) no two vertices are adjacent, and (ii) no two vertices belong to the same $<S>$. We can now understand the operations of $P(I)$ and $P(II)$ operators. Suppose we wish to calculate the number of vertices in D_2 which are allowed to form pairs of RDI's with v_1. To do this we remove $<S_1> = \{1, 2, 3\}$; the resulting tree contains the required number of vertices. This is the operation of $P(II)$. When this operation is repeated with the rest of the vertices and the order of the resulting disconnected graph is computed (i.e. the total number of its vertices) $N(2)$ results. The operation of $P(I)$ is to avoid counting an interaction more than once, while $P(II)$ removes all vertices adjacent to or belonging to the same $<S_2>$ relative to a particular vertex in the dualist. $N(3)$ is simply the sum of $N(2)$ values corresponding to all trees generated in the first pruning cycle, $N(4)$ is the sum of $N(2)$ values of all trees generated in the second cycle and so on until all trees become terminal. The operation of $P(II)$ on a particular vertex is thus a graphical representation of $N(2)$ of that vertex.

7. SOME REMARKS ABOUT PRUNING METHODS

(i) Ulam's conjecture[14] is one of the early useful pruning methods in graph theory.

(ii) The computation of matching polynomials of graphs[15] using Heilbronner's formula[16] uses a special pruning method.

(iii) Recently, Balaban[17] deviced a topological index by adopting a special pruning of graphs.

(iv) Quite recently, Balasubramanian[18] developed a method for obtaining spectra of chemical trees adopting a pruning technique. He[19] has also used a similar method for isomer enumeration.

In this work we introduced two pruning methods which lead to the systematic synthesis of sextet polynomials of BH's of relatively large size.

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   The concept was first introduced by: H. Joela, *Theoret. Chim. Acta (Berlin)*, **39** (1975) 241 and was adopted under the name *Submolecule Graph* to study MO-VB characters of Kekulé structures by: S. El-Basil, *Internat. J. Quantum Chem.* **21** (1982), 771; 779, 793. The name *Factor Graph* was suggested to the author by Professor M. Randić (private communication) by analogy with line graphs[5] and the fact that double bonds are known as 1-factors.
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SAŽETAK

Jednostavan kombinatorni algoritam za konstrukciju sekstetnog polinoma kata-kondenziranih benzenoidnih ugljikovodika

Sherif El-Basil

Opisana su dva tipa obrezivanja za određena stabla i iskorištena u jednostavnomu kombinatornom algoritmu za sustavnu konstrukciju sekstetnih polinoma kata-kondenziranih benzenoidnih ugljikovodika velikih dimenzija.

Algoritam nudi alternativu postojećim metodama za prebrojavanje Kekuléovih struktura koja nije ograničena na sisteme bez grananja.