

ON THE ORDERING OF KEKULÉ STRUCTURES ,

Spectral moments of factor graphs of
benzenoid hydrocarbons

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Abstract

Spectral moments of factor graphs (Refs. 6-9) of all benzenoid hydrocarbons containing up to four rings are computed up to eighth power. Comparability conditions (of Muirhead) are applied to the resulting codes. The resulting hierarchical diagrams successfully predict actual orders of several graph-theoretical and MO characters of the factor graphs and their corresponding Kekulé structures. Several mathematical properties of the spectral moment codes of the $F(k)$'s are given. They are used to construct hierarchical diagrams of the corresponding benzenoid hydrocarbons which predict the actual ordering of their heats of atomizations, electron-affinities , polarographic reduction potentials and resonance energies.

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The fact that Kekulé structures are permutations of double bonds has been explicitly stated only recently¹. It turns out that such various permutations lead to "conjugation contents"² of varying degrees in the individual hypothetical "localised" mathematical states. This phenomenon was qualitatively generalised by Fries³, many years ago, and was recently computed in terms of a VB-MO index, called Kekule index⁴, $K(L)$, given by eqn. 1 for an alternant system containing $2N$ pi-electrons :

$$K(L) = \frac{1}{2N} \sum_{(i,j) \in L} (2 + 2 p_{ij})^{\frac{1}{2}} \quad (1)$$

Where p_{ij} is bond order between atoms i and j and the summation is made over all double bonds of the particular Kekulé structure. When a Kekulé structure is transformed into the subspace of its double bonds a factor graph⁵, $F(K)$, results. As a result we consider the following Kekulé structure, k_1 , and its factor graph, $F(k_1)$:



Several graph theoretical properties of the $F(k)$'s have been studied by one of the authors⁶⁻¹⁷. Thus connectivity indices¹⁸ of cata-condensed⁶, peri-condensed⁷ and non-benzenoid hydrocarbons⁸ of some one hundred $F(k)$'s were correlated with the corresponding $K(L)$ values of the VB structures. Similarly non-adjacent numbers¹⁹ of Hosoya (i.e. sets of K_2 subgraphs) were computed⁹ for $F(k)$ graphs and again were correlated with the relevant Kekulé indices.

The mathematical properties of the $F(k)$'s were recently investigated^{10,12}. An important theorem¹³⁻¹⁶ in relation to sextet polynomial (of Hosoya and Yamaguchi²⁰) was discovered. Quite recently spectral moments of cyclobutadiene derivatives and their factor graphs were computed¹⁷.

This paper extends our graph-theoretical study to include computation of spectral moments of factor graphs of benzenoid hydrocarbons. The details of the graph theoretical method and comparability criterion may be found in Ref. 17. In addition, an Appendix of definitions is included at the end of this paper which helps the follow up of this paper.

RESULTS

Table 1 lists spectral moment codes, $\{s_1, s_2, \dots, s_8\}$, truncated after eighth power, of all factor graphs studied in this work. (fig 1). We list the following mathematical properties of the $F(k)$ moments.

1^o. s_i ($i \neq 1$) is always an even number.

2^o. Let the number of three membered cycles in an $F(k)$ be n_3^C , the following relation exists :

$$s_3 [F(k)] = (n_3^C / R) s_2 [F(k)] . \quad (1)$$

where R = total number of rings in $F(k)$.

Thus , e.g. $s_3 [\text{graph}] = (1/2) s_2 [\text{graph}] = 6$;

$$s_3 [\text{graph}] = \left(\frac{2}{3}\right) s_2 [\text{graph}] = \left(\frac{2}{3}\right)(18) = 12$$

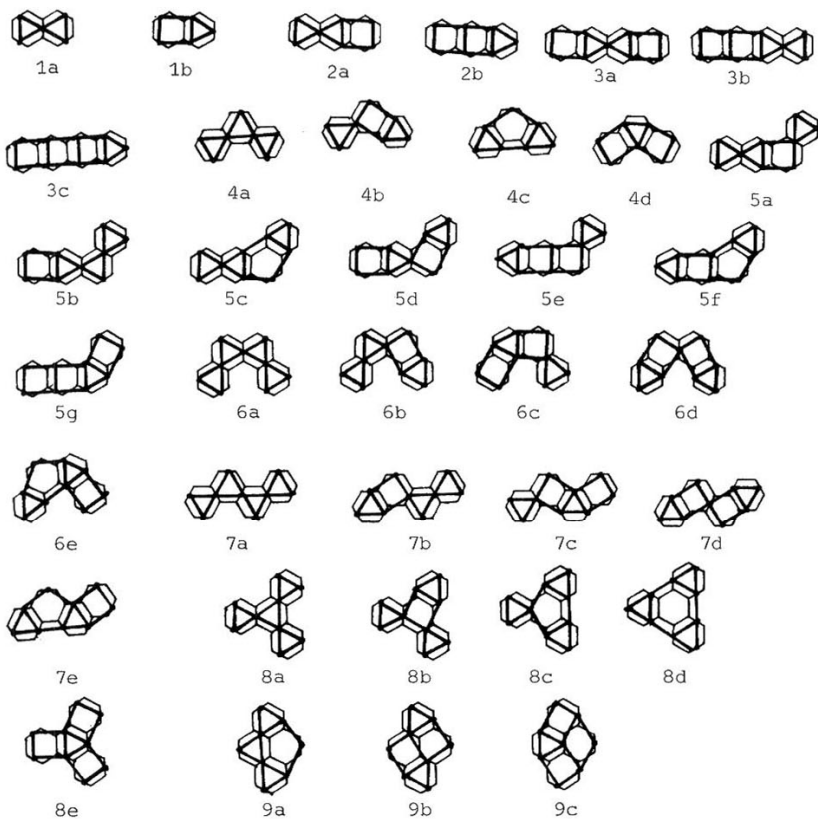


Fig. 1

Factor graphs, $F(k)$'s, studied in this work. They are heavily outlined into their corresponding polyhex graphs

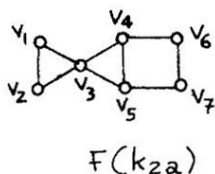
An interesting corollary is that $s_3 = s_2$ for $F(k)$'s which are composed of three-membered cycles only. Since such cycles are double bond transformates of aromatic sextets, we have the following topological property of all-benzenoid hydrocarbons²¹: Kekulé structures of benzenoid hydrocarbons which have full sextets in all of its rings are characterised by having $s_2 = s_3$.

The above property might be understood by realising that :

$$s_2 = \sum_{i=3}^{5,6} n_i C_i \quad ; \quad (2)$$

$$s_3 = n_3 C_3 \quad (3)$$

where in general $n_j C_j$ is the number of C_j rings in $F(k)$. The summation in Eqn(2) is over C_3, C_4, C_5 for nonbranched cata-condensed hydrocarbons and C_3, C_4, C_5, C_6 for branched systems (C.F. Ref. 10 for the mathematical properties of the factor graphs). From Eqns (2), (3) when all cycles are C_3 's , $s_2 = s_3$. We illustrate this property by considering all w_2 and w_3 (i.e. self-returning walks of lengths two and three respectively) in $F(k_{2a})$, (C.f. Fig 1) :

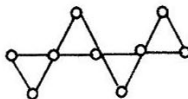


We have the following walks (self-returning):

	v_1	v_2	v_3	v_4	v_5	v_6	v_7	
w_2	2	2	4	3	3	2	2	$\sum w_2 = s_2 = 18$
w_3	2	2	4	2	2	0	0	$\sum w_3 = s_3 = 12$

E.g. v_1 is associated with two w_a 's : (v_1, v_3, v_1) ,
 (v_1, v_2, v_1) , and two w_3 's : (v_1, v_3, v_2, v_1) ,
 (v_1, v_2, v_3, v_1) . One observes that both v_6 and v_7 are
 not associated with w_3 .

A natural result of the above property is the following
 important topological result : " All-benzenoid hydrocarbons
 generate factor graphs for which $s_2 = s_3$ ". E.g. chrysene, an
 all-benzenoid hydrocarbon has five non-symmetry equivalent
 $F(k)$'s , (7a - 7e) , Fig 1, of which the one of highest
 Kekulé index⁴, and highest χ^{-1} ¹⁸ (see appendix) is composed
 of four C_3 's :



$$s_2 = s_3 = 24$$

Such a situation does not occur with non-all-benzenoids
 such as benz [a] anthracene. This result might be of
 importance in the problem of graph recognition²²: An $F(k)$
 for which $s_2 = s_3$ signals an all-benzenoid hydrocarbon
 topology.

3^o. Values of s_5 of factor graphs derived from polyhex graphs²³
 (cata-condensed and peri-condensed) are always integral
 multiple of ten.

4^o. Let Δs_6 be the difference between two s_6 values of two
 $F(k)$'s belonging to a cata-condensed benzenoid hydrocarbon.

The set of $F(k)$'s group themselves into subsets for each of which Δs_6 is an integral multiple of 12. Some illustrations serve to understand this property : (See Fig 1 and Table 1).

(a) Tetracene

S_6 values increase regularly by factors of 24
(= 12 x 2), thus

$$\Delta s_6 \{ \text{[Diagram 1]}; \text{[Diagram 2]} \} = 864 - 840 = 12 \times 2$$

$$\Delta s_6 \{ \text{[Diagram 3]}; \text{[Diagram 4]} \} = 840 - 816 = 12 \times 2.$$

(b) Phenanthrene

There are two groups , viz., { [Diagram 5]; [Diagram 6]; [Diagram 7] }

and { [Diagram 8] } , we have

$$\Delta s_6 \{ \text{[Diagram 5]}; \text{[Diagram 6]} \} = 12 ;$$

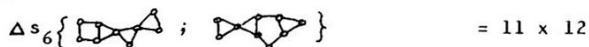
$$\Delta s_6 \{ \text{[Diagram 6]}; \text{[Diagram 7]} \} = 10 \times 12.$$

The "single" member , { [Diagram 8] } , has five conjugated circuits while all other members contains four such circuits each. Such "single" graphs have been mentioned in connection with a recently published suggested definition of parity of Kekulé structures of benzenoid hydrocarbons.^{11,24} (See also relation to Clar's sextet theory²⁵ at the end of the text).

(c) Benz [a] anthracene

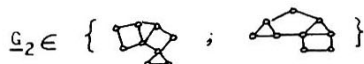
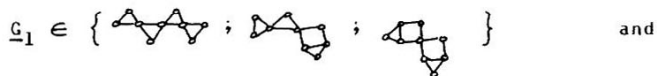
$\Delta s_6 = 12n$ (n benign integer) for all pairs of its $F(k)$'s.

Examples :



(d) Chrysene

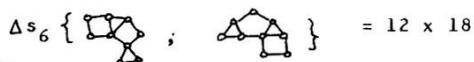
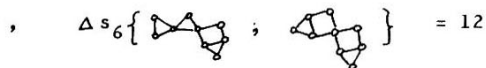
Two groups are distinguished, viz.,



For each group Δs_6 is an integral multiple of 12.

It is illuminating to note that members of G_1 contains 4 conjugated circuits each while members of G_2 contains 5 such circuits.²⁶

Illustration :




However,

$$\Delta^s_6 \left\{ \begin{array}{c} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \quad \diagup \quad \diagdown \\ \text{---} \text{---} \text{---} \end{array} ; \begin{array}{c} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \quad \diagup \quad \diagdown \\ \text{---} \text{---} \text{---} \end{array} \right\} = 76 \neq 12n$$


(n is an integer).

5⁰. According to the definitions of strict order and total strict order given in appendix we state the following observations :

(a) None of the F(k)'s of polyhex graphs²³ generate a set of $\{s_i\}$, $i = 1, 2, 3, \dots$ values defining a total strict order. However, a numeration²⁷ might be selected so as to define a set satisfying the conditions of a total strict order. Generally the set $\{s_3, s_4, \dots, s_8\}$ define such numerations , for the most important Kekulé structures (i.e. those structures having highest Kekulé indices).

(b) In general the F(k)'s corresponding to the least important Kekulé structures (i.e. those possessing lowest K(L)) have more inflection points²⁸ than their more important ones. E.g. the F(k) of tetracene corresponding to Kekulé structure of lowest K(L) , viz.,  has three inflection points defined by three subsets:

$(s_2, \underline{s_3}, s_4)$; $(s_4, \underline{s_5}, s_6)$; $(s_6, \underline{s_7}, s_8)$. In contrast , the F(k) corresponding to highest K(L), viz.,

 , has only one inflection point defined by $(s_2, \underline{s_3}, s_4)$.

Ordering and Comparability of the Factor Graphs²⁹

We use criteria of comparability presented in the Appendix to compare and order the factor graphs. Table 1 lists individual spectral moments up to eighth power, and their partial sums (generated from left to right).

Hierarchical diagrams of F(k)'s , (Fig. 2)

The function $\{v_1^a, v_2^a, \dots, v_k^a\}$ defined in Appendix

Fig. 2

Hierarchical diagrams of $F(k)$'s based on imposing comparability conditions (Eqns A-4, A-5) on their spectral moment codes, (truncated after s_8). The figures correspond to the $F(k)$'s of the following hydrocarbons :

- Fig. 2-a : naphthalene
- 2-b : nathracene
- 2-c : tetracene
- 2-d : phenanthrene
- 2-e : benzanthracene
- 2-f : benzo [c] phenanthrene
- 2-g : triphenylene
- 2h : pyrene

The numbers to the right of the $F(k)$'s are : conjugated circuits, Kekulé index , $K(L)$, and reciprocal of connectivity index, χ^{-1} , respectively.

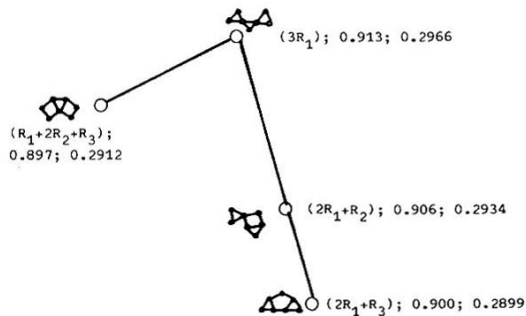
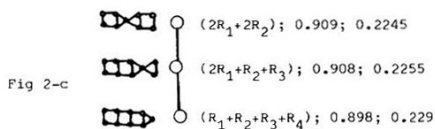
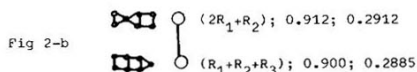
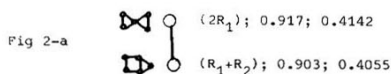


Fig 2d

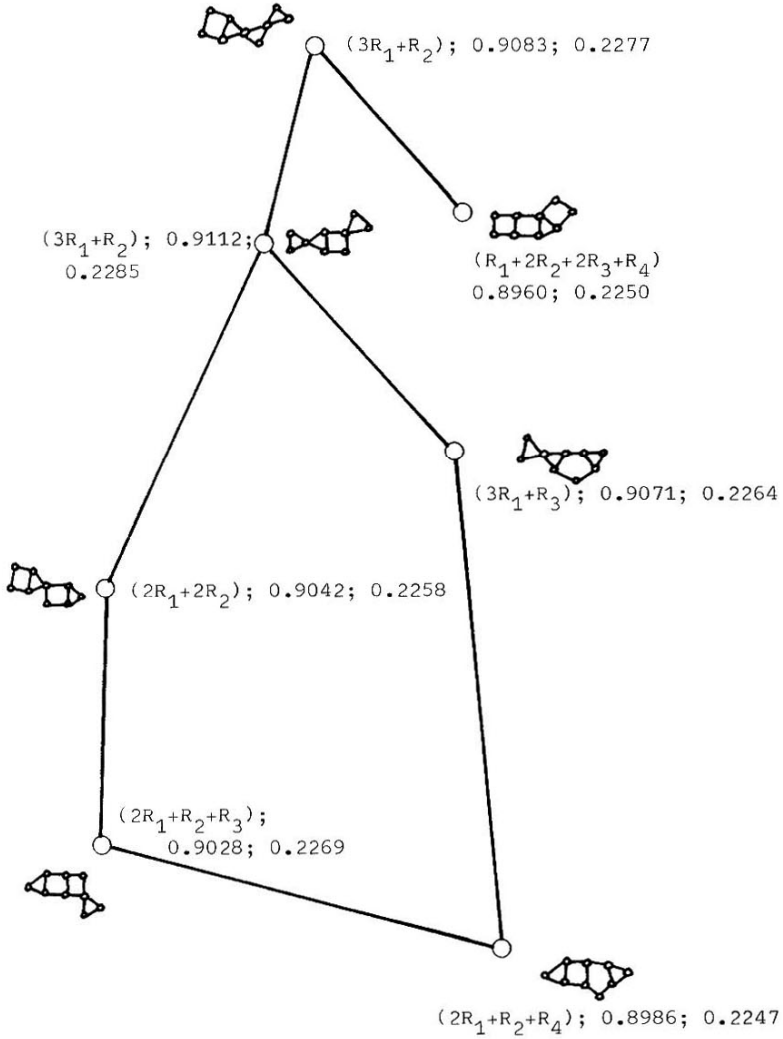


Fig 2e

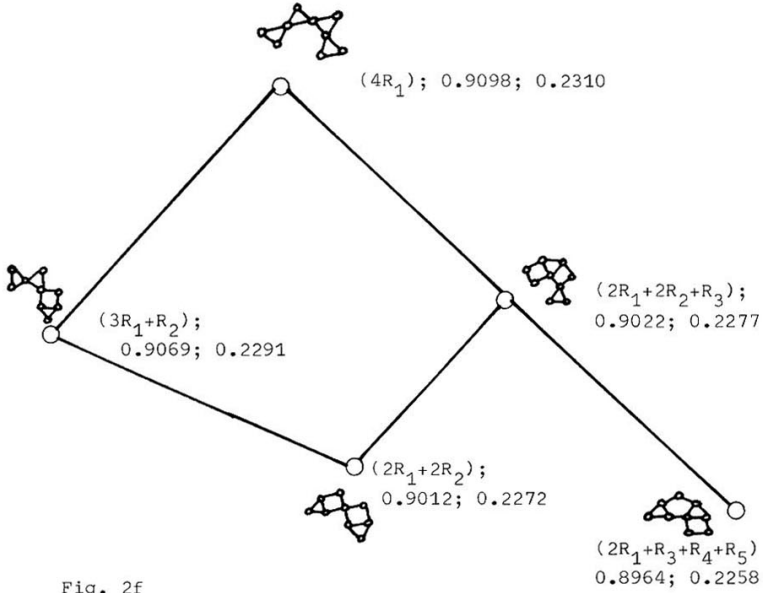


Fig. 2f

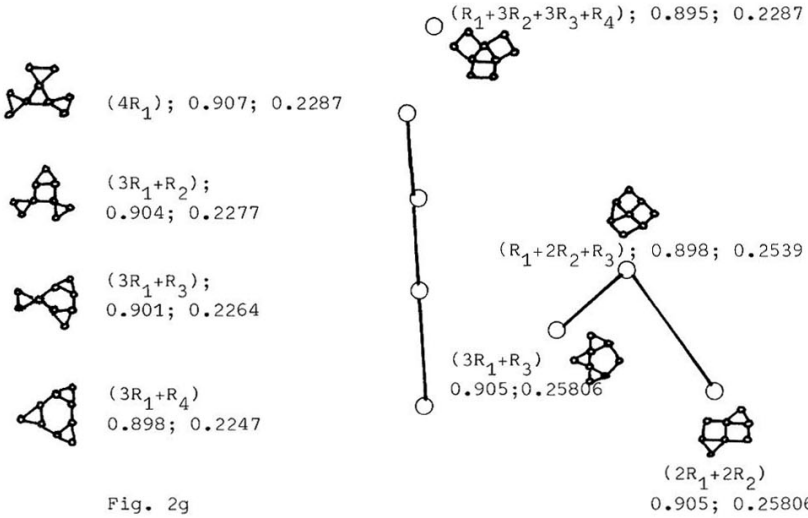



Fig. 2g

Fig. 2h

is identified by equating the v's (i.e. the variables) to spectral moments, while the a's are their populations. Thus, e.g. for  our function would be expressed as follows

$$\{ s_1^0 \quad s_2^{12} \quad s_3^{12} \quad s_4^{52} \quad s_5^{100} \quad s_6^{300} \quad s_7^{700} \quad s_8^{1892} \}$$

The code, therefore would be

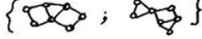

$$\{ 0, 12, 12, 52, 100, 300, 700, 1892 \} .$$

The first partial sum is

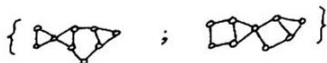
$$\{ 0, 12, 24, 76, 476, 1176, 3068 \} \quad ;$$

where the first entry is a_1 , the second is $(a_1 + a_2)$, the third is $(a_1 + a_2 + a_3)$ and so on. These partial sums form the basis of our ordering-comparability scheme as defined in Appendix. When comparable adjacent points (representing $F(k)$'s) are connected a hierarchical diagram is produced. These diagrams are shown in Figs 2(a-h). Two graph-theoretical properties, viz. conjugated circuits² and the reciprocal of connectivity index¹⁸, χ^{-1} ; and an MO-VB character, the Kekulé index⁴, $K(L)$, are correlated with the order computed from the spectral moments. In most cases an excellent correspondence occurs (The levels of the points of hierarchical diagrams are meant to be roughly proportional

$$t_0 \sum_{i=1}^8 s_i \quad). \quad \text{Some observations are worthy of mention:}$$

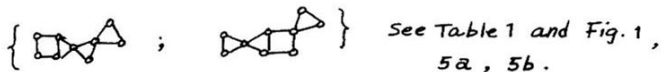
- 1) When two $F(k)$'s are non-comparable from their spectral moments, their conjugated circuits also generate codes whose partial sums are non-comparable also ! Thus, e.g. phenanthrene (Fig 2d) generates four non-symmetry equivalent $F(k)$'s, of which the last one (corresponding to Kekule structure of lowest $K(L)$) is only comparable with the most important $F(k)$. Thus  and  are two pairs of non-comparable graphs from the point of view of their first

eight spectral moments. The first pair generate the following two conjugated circuits codes³⁰ : (1,2,1);(2,1,0) whose partial sums are $\{1,3,4\}$; $\{2,3,3\}$ for which $a'_1 > a_1$ but $a'_3 < a_3$ and thus are non-comparable. Another example that is probably more illuminating is the case of benz [a] anthracene , Fig 2-e. A pair of F(k)'s whose spectral moment codes are not comparable is



The circuit codes of this pair are (3,0,1) and (2,2,0) respectively ; and their partial sums being $\{3,3,4\}$ and $\{2,4,4\}$. Agin , they are non-comparable !

- 2) When two F(k)'s correspond to Kekulé structures possessing identical conjugated circuits , the ordering based on their $K(L)$ and α^{-1} values are opposite to the spectral moment ordering.³¹ As an illustration we consider the pair



belonging to benz [a] anthracene.

- 3) The least important Kekulé structure of triphenylene (Fig. 2g) generates an F(k) which is non-comparable with any of the rest of the members. In fact this member ,



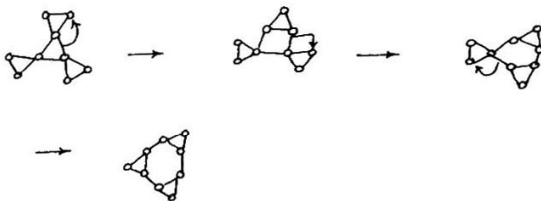
is anomalous in many respects:

- a) It is the only member whose Kekulé structure has only one sextet, and contains eight conjugated circuits.

- b) The $K(L)$ index of its Kekulé structure ($= 0.895$) predicts this graph to be the least important while its χ^{-1} is as high as that of the most important graph, viz.,



- c) All non-symmetry equivalent $F(k)$'s of triphenylene are related to one another by a degenerate transformation³² but this graph :



$F(k_{8e})$, Fig 1, is not related to any of the above $F(k)$'s.

The Ordering of Molecular Properties of the Corresponding Benzenoid Hydrocarbons:

The spectral moment codes of the factor graphs can be made to order the molecular properties by the following procedure³³: Let some benzenoid hydrocarbon possessing K Kekulé structures, and thus K factor graphs, $F(k_1), F(k_2), \dots, F(k_K)$, and let their spectral moments be defined as follows:

$$\begin{aligned}
 F(k_1) &\rightarrow s_{11}, s_{12}, \dots, s_{18} \\
 F(k_2) &\rightarrow s_{21}, s_{22}, \dots, s_{28} \\
 &\vdots \\
 F(k_K) &\rightarrow s_{K1}, s_{K2}, \dots, s_{K8}
 \end{aligned}$$

where the first subscript indicate the particular $F(k)$ and the second subscript corresponds to the power of the corresponding adjacency matrix (in our case the highest power is 8). Thus a code might be associated with the benzenoid hydrocarbon given by :

$$\left(\sum_{i=1}^K S_{i1} , \sum_{i=1}^K S_{i2} , \dots , \sum_{i=1}^K S_{i8} \right)$$

A partial sum might be constructed from the above code. These codes and their partial sums are listed in Table 2. Figs 3 represent hierarchical diagrams resulting when comparability conditions explained in Appendix are applied to such partial sums. It is clear that the linear segments (indicated by arrows in Figs 3) define orders consistent with orders of molecular properties including heats of atomizations³⁴, electron affinities³⁴, resonance energies, RE's, (of Randić, of Herndon³⁵, and of Dewar and deLlano)³⁶, and polarographic half-wave reduction potentials.³⁴ Excellent agreement of computed with actual orders are observed in most cases.

Relation to Clar's Sextet Theory^{23,25}

In their graph-theoretical analysis of Clar's aromatic sextet theory, Hosoya et.al. and Gutman²³ defined two types of sextets, viz., proper and improper as shown below :

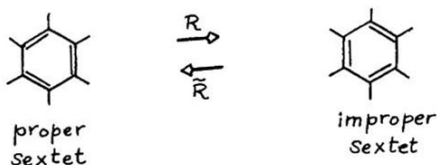


Fig. 3

Ordering of molecular properties of benzenoid hydrocarbons using codes derived by summing the individual moments of all $F(k)$'s of the hydrocarbon (Table 2). The figures correspond to the following properties :

- Fig. 3a : Heats of atomization (eV) of the hydrocarbons and their radical anions (in parentheses).
- 3b : Electron affinities (eV)
- 3c : Polarographic half-wave reduction potentials (V).
- 3d : Resonance energies (of Randić) , eV.

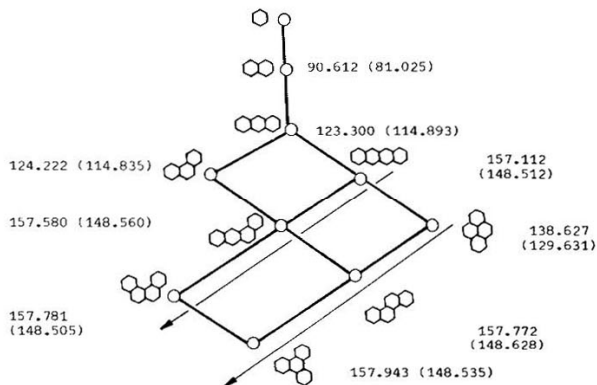


Fig 3(a)

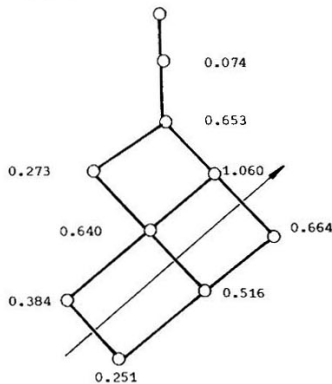


Fig. 3(b)

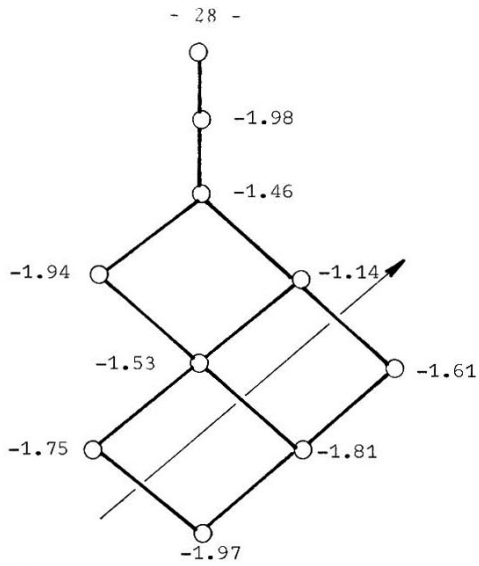


Fig. 3(c)

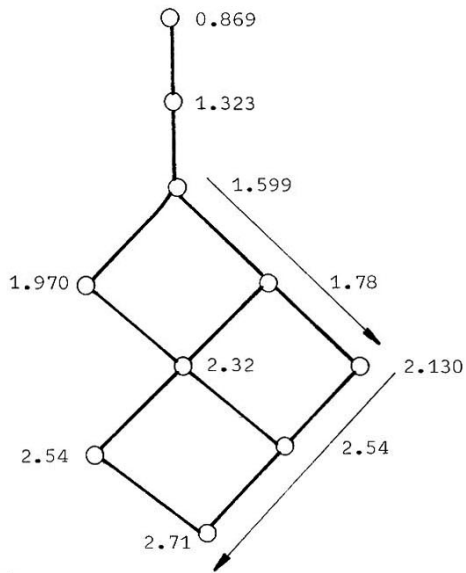


Fig. 3(d)

Furthermore they related the two sextets by a transformation³⁷ R , thus : letting k_i and k_j be two Kekulé structures of a benzenoid hydrocarbon which differ in only one of their sextets , then :

$$R(k_i) = k_j \quad ; \quad \tilde{R}(k_j) = k_i$$

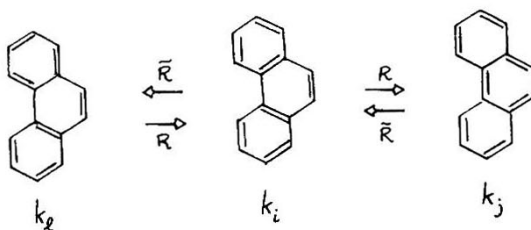
Then we might write for the corresponding $F(k)$'s a similar transformation , viz.,

$$T(F(k_i)) = F(k_j) \quad ; \quad \tilde{T}(F(k_j)) = F(k_i)$$

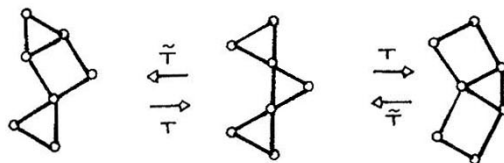
where T (\tilde{T}) is an operator which :

- transforms $F(k_i)$ into k_i and then,
- transforms k_i into k_j via R (\tilde{R}) transformation

E.g.



The corresponding $F(k)$'s are being related as follows :



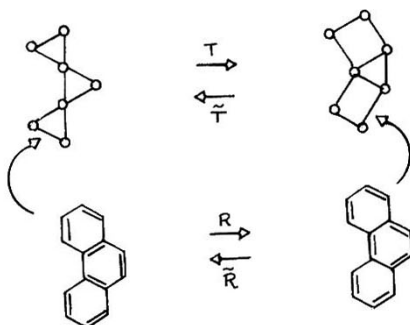
We can now state the following conjecture :

" Two $F(k)$'s which are directly related by a T (or \tilde{T}) transformation will have adjacent spectral moment partial sums".

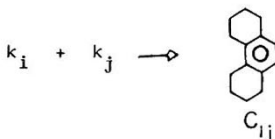
Illustrations :

1) Phenanthrene (Fig 2d)

The $F(k)$ possessing least $K(L)$ is adjacent to the one having highest value of $K(L)$ in the hierarchical diagram generated from their spectral moment codes. This is not consistent with overall order of $K(L)$ values or values of conjugated circuits of the rest of the $F(k)$'s of this hydrocarbon. However this "discrepancy" would be expected if one realises that the most and least important graphs of phenanthrene are directly connected by a T (\tilde{T}) transformation thus :



When their corresponding Kekulé structures are superposed followed by transforming double bonds into single bonds a Clar's formula, C , results containing one circle :



We may generalize :

Kekulé structures whose F(k)'s have adjacent spectral moment codes yield Clar's structures containing one circle when superposed ;

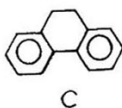
Kekulé structures whose F(k)'s have spectral moment codes that are separated by one code in the hierarchy generate Clar's structures containing two circles when superposed. E.g.



in phenanthrene hierarchy. They correspond to



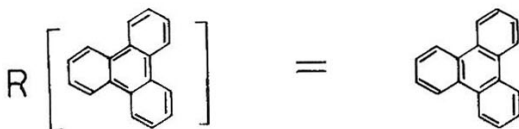
which when superposed yield :



Therefore the number of circles in the resulting Clar's formula gives an indication about the relative positions of the corresponding F(k)'s in their spectral moment hierarchy

ii) Triphenylene hierarchy (Fig. 2g)

Again the most and least important Kekulé structures are related by the transformation :



We should, therefore, no longer be disappointed to find their $F(k)$'s to have adjacent positions in their spectral moment hierarchy albeit corresponding values based on conjugated circuits or $K(L)$ values which are not consistent among overall order of the $F(k)$'s of triphenylene. Therefore such sextet rotations might be taken as a tool to forecast discrepancies in graph-theoretical characters of $F(k)$'s (viz., conjugated circuits, and connectivity) as well as MO-VB character, the Kekulé index when ordered according to their spectral moments.

APPENDIX OF DEFINITIONS

Kekulé Index⁴, $K(L)$

An MO-VB index which relates a given set of molecular properties to orbitals localised on pairs of adjacent carbons. It is given by :

$$K(L) = \frac{1}{2N} \sum_{(\mu, \nu) \in L} (\varphi_{\mu} + \varphi_{\nu} + 2p_{\mu\nu})^{\frac{1}{2}} \quad A-1$$

where $2N$ is number of pi-electrons, while φ and p are charge density and bond orders respectively. For alternant hydrocarbons Eqn. A-1 reduces to Eqn. 1.

Connectivity Index¹⁸, χ

It is defined according to eqn. A-2 :

$$\chi = \sum_{i,j} (m_i m_j)^{-\frac{1}{2}} \quad A-2$$

where m_i is degree of i th vertex (i.e. number of its nearest neighbors). The summation is being taken over all (i,j) -edge types. In the present work, the reciprocal of χ is computed for factor graphs i.e.

$$X^{-1} = \left[\sum_{(i,j) \in F(k)} (m_{i,j})^{-1/2} \right]^{-1} \quad A-3$$

Comparability of Graphs²⁹

Comparability conditions of graphs were rigorously defined by Muirhead²⁹ by attaching a sequence of integers to each graph and comparing the partial sums of the integers. Thus, e.g. for two factor graphs one associates two functions, $F_1 = F_1(v_1, v_2, \dots, v_k)$ and $F_2 = F_2(v_1, v_2, \dots, v_k)$ which are said to be comparable if there is an inequality between them (either $F_1 \geq F_2$ or $F_1 \leq F_2$) valid for all values of the variables v_i from a given interval. A special class of such functions of many variables is :

$$\{ v_1^{a_1} \quad v_2^{a_2} \quad \dots \quad v_k^{a_k} \}$$

where a_i 's are non-negative integers (The a 's are viewed as populations of the variable v 's). In our work the v 's are spectral moments derived from topological (adjacency) matrices of various powers and the a 's being their numbers, i.e. populations. The two structures are said to be comparable if for every entry in their two partial sums-sequences members of one structure are larger or equal (but not smaller) than the corresponding entries in the other sequence. This is expressed by A-4 and A-5, viz.,

$$\left. \begin{aligned} a_1' &\geq a_1 \\ a_1' + a_2' &\geq a_1 + a_2 \\ a_1' + a_2' + a_i' &\geq a_1 + a_2 + \dots + a_i \end{aligned} \right\} A-4$$

$$a_1' + a_2' + \dots + a_k' = a_1 + a_2 + \dots + a_k \quad A-5$$

where k is the number of variables and $1 < i < k$.
eqn. A-5 is viewed as optional by some authors as it is the case here.

Spectral moment³⁸ s_k

These quantities are defined as the trace, tr, of connection (adjacency) matrices, A, raised to various powers, i.e

$$s_k = \text{tr } \underline{A}^k \quad \text{A-6}$$

A diagonal element a_{ii} in \underline{A}^k is self-returning walks from vertex i to itself and whose length is k

In the present work k is varied from 1 to 8. i.e. s_1, s_2, \dots, s_8 are computed.

Strict order²⁷

When one orders spectral moments characterizing a graph in order of increasing powers of their corresponding \underline{A}^k matrices, one obtains a string $B_i^m = \{s_{i1}, s_{i2}, s_{i3} \dots s_{im}\}$ where i is a subscript of a particular sequence and the number next to it is the power to which A of graph is raised ($m = 8$ in this work). Let the relation $<$ be identified in the set of s_i values defining B_i^m . A strict order relation in set B_i^m possesses the following properties :

a) $s_{ir} < s_{ir}$ does not hold for any $s_{ir} \in B_i^m$

where $i \leq r \leq m$.

b) If $s_{ia} < s_{ib}$ and $s_{ib} < s_{ic}$ then

$$s_{ia} < s_{ic} \quad ; \quad 1 \leq a, b, c \leq m.$$

c) If $s_{ia} < s_{ib}$ holds, then $s_{ib} < s_{ia}$ is impossible.
property (c) is a natural result of (a) and (b).

Point of inflection²⁸

Let $\{s_{ia}, s_{ib}, s_{ic}\}$ be three successive (i.e. adjacent) values of spectral moments belonging to some graph (i.e. $c > b > a$).

A point of inflection is identified when

$$\begin{aligned} s_{ia} &> s_{ib} \quad ; \\ s_{ib} &< s_{ic} \end{aligned}$$

given that a, b and c are adjacent members, s_{ib} will be termed a point of inflection in the code.

Total strict order²⁷

A strict order relation, $<$, is called a total strict order if for every pair s_{ia} and s_{ib} of the set B_i^m , either $s_{ia} < s_{ib}$ or $s_{ib} < s_{ia}$ holds. This condition, then, demands no two spectral moments to have identical values in the same set.

Table 1:
Spectral moments and their partial sums of factor graphs,
 $F(k)$'s shown in Fig. 1.

<u>$F(k)$</u>	<u>Code (s_1, s_2, \dots, s_8) and its partial sum</u>
1a	0, 12, 12, 52, 100, 300, 700, 1892 0, 12, 24, 76, 176, 476, 1176, 3068
1b	0, 12, 6, 56, 60, 300, 448, 1696 0, 12, 18, 74, 134, 434, 882, 2578
2a	0, 18, 12, 90, 130, 558, 1134, 3874 0, 18, 30, 120, 250, 380, 938, 2072, 5946
2b	0, 18, 6, 94, 60, 582, 518, 3814 0, 18, 24, 118, 178, 760, 1278, 5092
3a	0, 24, 12, 128, 160, 816, 1568, 5888 0, 24, 36, 164, 324, 1140, 2708, 8596
3b	0, 24, 12, 128, 130, 840, 1204, 6020 0, 24, 36, 164, 294, 1134, 2338, 8358
3c	0, 24, 6, 132, 60, 864, 518, 6028 0, 24, 30, 162, 222, 1086, 1604, 7632
4a	0, 18, 18, 86, 170, 558, 1386, 4102 0, 18, 36, 122, 292, 850, 2236, 6338
4b	0, 18, 12, 90, 110, 546, 896, 3602 0, 18, 30, 120, 230, 776, 1672, 5274
4c	0, 18, 12, 78, 100, 426, 840, 2630 0, 18, 30, 108, 208, 634, 1474, 4104
4d	0, 18, 6, 98, 90, 624, 910, 4282 0, 18, 24, 122, 212, 836, 1746, 6028

Table 1 (cont.)

<u>F(k)</u>	<u>Code (s₁, s₂, ... , s₈) and its partial sum</u>
5a	0,24, 18, 124, 180, 804, 1582, 5812 0,24, 42, 166, 346, 1150, 2732, 8544
5b	0, 24, 18, 124, 200, 816, 1820, 6116 0, 24, 42, 166, 366, 1182, 3002, 9118
5c	0, 24, 18, 112, 180, 684, 1498, 4580 0, 24, 42, 154, 334, 1018, 2516, 7096
5d	0, 24, 12, 128, 140, 804, 1302, 5536 0, 24, 36, 164, 304, 1108, 2410, 7946
5e	0, 24, 12, 128, 110, 828, 910, 5736 0, 24, 36, 164, 274, 1102, 2012, 7748
5f	0, 24, 12, 116, 120, 684, 994, 4404 0, 24, 36, 152, 272, 956, 1950, 6354
5g	0, 24, 6, 136, 90, 912, 980, 6608 0, 24, 30, 166, 256, 1168, 2148, 8756
6a	0, 24, 24, 120, 240, 816, 2072, 6344 0, 24, 48, 168, 408, 1224, 3296, 9640
6b	0, 24, 18, 124, 180, 804, 1554, 5758 0, 24, 42, 166, 346, 1150, 2704, 8462
6c	0, 24, 12, 132, 140, 880, 1372, 6476 0, 24, 36, 168, 308, 1188, 2560, 9036
6d	0, 24, 12, 128, 120, 816, 1008, 5576 0, 24, 36, 164, 284, 1100, 2108, 7684
6e	0, 24, 12, 120, 140, 664, 1308, 5168 0, 24, 36, 156, 296, 960, 2268, 7436

Table (cont.)

<u>F(k)</u>	<u>Code (s_1, s_2, \dots, s_8) and its partial sum</u>
7a	0, 24, 24, 120, 240, 816, 2072, 6344 0, 24, 48, 168, 408, 1224, 3296, 9640
7b	0, 24, 18, 124, 180, 804, 1554, 5764 0, 24, 42, 166, 346, 1150, 2704, 8468
7c	0, 24, 12, 132, 140, 870, 1358, 6258 0, 24, 36, 168, 308, 1178, 2536, 8804
7d	0, 24, 12, 128, 120, 816, 1008, 5576 0, 24, 36, 164, 284, 1100, 2108, 7684
7e	0, 24, 12, 120, 140, 738, 1274, 5064 0, 24, 36, 156, 296, 1036, 2308, 7372
8a	0, 24, 24, 120, 240, 840, 2184, 6888 0, 24, 48, 168, 408, 1248, 3432, 10320
8b	0, 24, 18, 124, 160, 816, 1400, 5988 0, 24, 42, 166, 326, 1142, 2542, 8530
8c	0, 24, 18, 112, 160, 660, 1302, 4456 0, 24, 42, 154, 314, 974, 2276, 6732
8d	0, 24, 18, 108, 150, 594, 1134, 3732 0, 24, 42, 150, 300, 894, 2028, 5760
8e	0, 24, 6, 144, 120, 1038, 1512, 8160 0, 24, 30, 174, 294, 1332, 2844, 11004
9a	0, 22, 18, 110, 200, 754, 1862, 5990 0, 22, 40, 150, 350, 1104, 2966, 8956
9b	0, 22, 12, 126, 140, 892, 1400, 6878 0, 22, 34, 160, 300, 1192, 2592, 9470
9c	0, 22, 6, 130, 90, 928, 1036, 7098 0, 22, 28, 158, 248, 1176, 2212, 9310

Table 2 :

Spectral moment codes and their partial sums
derived by summing moments of the individual
F(k)'s of the hydrocarbons.

Naphthalene	0, 36, 24, 164, 220, 900, 1596, 5284 0, 36, 60, 224, 444, 1344, 2940, 8224
Anthracene	0, 72, 36, 368, 380, 2280, 3304, 15376 0, 72, 108, 476, 856, 3136, 6440, 21816
Phenanthrene	0, 108, 72, 520, 680, 3127, 5768, 20848 0, 108, 180, 700, 1380, 4507, 10275, 31123
Tetracene	0, 120, 48, 648, 540, 4224, 5012, 29984 0, 120, 168, 816, 1356, 5580, 10592, 40576
Benzanthracene	0, 168, 96, 868, 1020, 5528, 9086, 38792 0, 168, 264, 1132, 2152, 7680, 16766, 55558
Chrysene	0, 192, 120, 1000, 1280, 6328, 11578, 46724 0, 192, 312, 1312, 2592, 8920, 20498, 67222
Benzo [c] phenanthrene	0, 192, 120, 1000, 1280, 6456, 11452, 46112 0, 192, 312, 1312, 2592, 9048, 20500, 66612
Triphenylene	0, 216, 156, 1080, 1470, 6900, 12936, 50112 0, 216, 372, 1452, 2922, 9822, 22758, 72870
Pyrene	0, 132, 72, 732, 860, 5148, 8596, 39932 0, 132, 204, 936, 1796, 6944, 15540, 55472

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