Partial Ordering of Properties: The Young Diagram Lattice and Related Chemical Systems

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Abstract

The basic definitions related to the general topic of ordering are reviewed and exemplified including: partial ordering, posets, Hasse diagrams, majorization of structures and comparable / incomparable structures.

Young Diagram lattice (of Ruch) and the ordering scheme of tree graphs (of Gutman and Randić) are described and it is shown, how the two schemes coincide with each other, i.e. generate identical orders.

The role of Young diagrams in the ordering of chemical structures is explained by their relation to alkane hydrocarbons and unbranched catacondensed benzenoid systems.

The Basic Terms: Examples of Posets, The Hasse Diagram

The concept of a partial order appears to be very useful in environmental science when evaluation and comparative study of properties are required. The object to be studied form an object set and the partially order set (≡ poset) depends on the $\leq$, (greater than- or equal to-) relation (Luther et al. (2000). We now introduce some of the popular definitions in an intuitive approach, which avoids the "dryness" of mathematical rigor.

Partially ordered set (poset)

It may be helpful to consider the following graph and analyze some parts of it: (cf. Fig. 1)

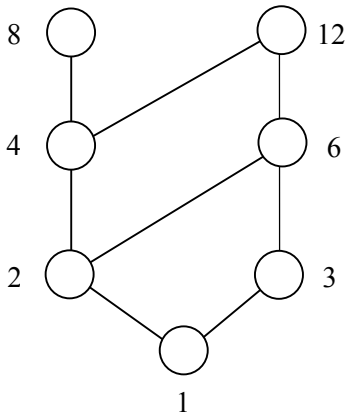


Fig. 1. A labelled graph, which corresponds to a relation on a set of numbers

Obviously, the above graph describes some sort of a relation, R, on the components of the set of integers:

$$S = \{1, 2, 3, 4, 6, 8, 12\} \quad (1)$$

We consider S as ground set (object set), whose elements are labelled vertices of a graph. The relation among the vertices, graphically displayed by lines (called "edges") depends on the questions one has. For example: One observes that numbers, which divide others are connected, those that do not divide each other are not. One, then, says that the above graph represents some sort of ordering relation expressed as.

$$\{(a,b) \mid a \text{ divides } b\} \text{ on } S = \{1, 2, 3, 4, 6, 8, 12\} \quad (2)$$

The relations among integers are described as follows:

a) Because every element of S is related to itself, i. e., $(a, a) \in R$; R is said to be reflexive.
b) While, e.g., 2 divides 4, 4 does not divide 2 and so on. Such a relation is said to be anti-symmetric.

c) The last property may be exemplified on the subset {2, 4, 8}: 2 divides 4; 4 divides 8 hence 2 divides 8, which is true for other components, i. e.: if (a, b) ∈ R and (b, c) ∈ R then (a, b, c) ∈ R.

The above property is called the transitive character of R. A poset may then be defined as a relation R, on a set S if R is reflexive, anti-symmetric and transitive.

The graph, which describes a particular poset, is called a Hasse diagram after the 20th century German mathematician Helmut Hasse (1898-1979) (Rosen 1991). See also chapter by Halfon p. 385.

A word on Hasse diagrams:
Actually the object shown in Fig. 1 is just a graph (not a diagram!): perhaps the word diagram is associated to it from the way it is used to be drawn. In fact all self-evident edges are now removed such as all loops, which describe the reflexive relation and also which result from the transitive character, e.g., edges (2, 8), (3, 12) and (1, all other vertices) are removed. Also arrows that indicate relative positions of components are no longer indicated, yet the "old name": diagram, (instead of graph) remained.

The Hasse diagram can be drawn in different ways maintaining the main information, the order relations. Such Hasse diagrams are isomorphic to each other.

Majorization of Structures: Relative Importance

Sometimes in (partial) ordering problems one may be interested in the relative importance of the components of a set. This situation reminds us with the relation A ≤ B i.e., "A is a descendent of B" or that: "B majorizes A". A popular example is the partial ordering {(A, B) | A ⊆ B} on the power set S = {a, b, c} where A ⊆ B means that A is a subset of B. Whenever this relation exists one says that B majorizes A. The power set S contains $2^3 = 8$ elements, viz., {a}, {b}, {a, b}, {a, c}, {b, c}, {a, b, c} and ∅, where ∅ is the empty set.

For this particular case the Hasse diagram is simply a cube, labelled as shown in Fig. 2.

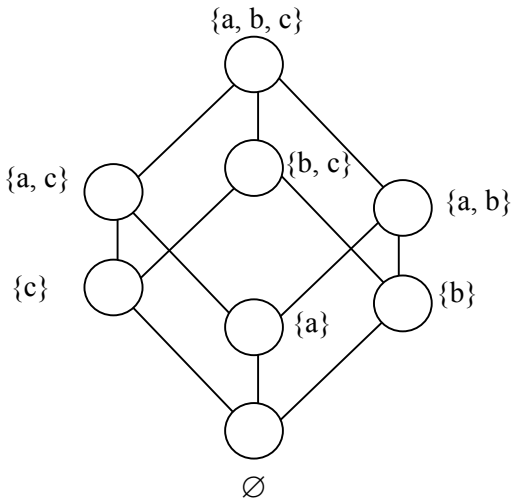


Fig. 2. The Hasse diagram of S = {a, b, c}. Each subset is attached to its direct offspring, so that the descendant (less important components) lies in lower levels

One observes that {a, b}, {a, c} and {b, c} are subsets of {a, b, c} and therefore of lower relative importance and analogously for the single-component subsets {a}, {b}, {c}. The above example represents one of the simplest cases of relative importance ordering problems, which finds chemical applications (section 'Relative importance of Kekulé Structures of Benzenoid Hydrocarbons: Chain ordering').

Comparable and incomparable elements: Chain and Anti-chain

The elements a and b of a poset (S,<) are called comparable if either $a \leq b$ or $b \leq a$. When a and b are elements of S such that neither $a \leq b$ nor $b \leq a$, a and b are called incomparable. For example the subsets {a,c}, {b,c} and {a, b} are incomparable with each other: (they are not directly connected (= adjacent) to each other, cf. Fig. 2). On the other hand, because {a, b, c} majorizes {a, c}, e.g., they are comparable components of S.

Partial ordering may, then, be viewed as first weakening (≡ relaxation) of the usual total ordering which is required for every pair of elements, $a,b \in S$, that it must be $a \leq b$ or $b \leq a$ or $a = b$. Of course the standard total ordering is that of "greater than or equal to" on the set of real members. In Fig. 2, the subset of vertices, labelled {{a, b, c}, {a, c}, {c}, ∅} is called a chain because every two elements of this subset are comparable. On the

other hand the subset {{a, b, c}, {b, c}, {a}, ∅}} is called an anti-chain because every two elements are incomparable.

One can immediately see the advantage of mathematical (graph-theoretical) techniques over quantum-chemical calculations in fields, which requires analysis of structure-property relation (such as environmental sciences). We quote the following paragraph from a paper by Randić et al. (1985).

"Quantum Chemistry appears to be preoccupied with evaluation of the wave function and potential surfaces, a worthy goal- but of limited use when one considers whole families of molecules and when one is concerned with structure-property relationships".

We quote further (Randić et al. 1985):

"Graph Theory is concerned with relations, and, in chemistry, the relationships between molecular structure and molecular properties are of particular interest".

Namely using graph-theoretical techniques, a structure is "replaced", so-to-speak, by a collection of its mathematical properties (≡ graph-invariants) (Randić et al. 1985) and whence allows the generation of various types of posets as we shall see the next section.

Some Posets of Chemical Interest

In this section we show some of the posets produced by researchers in mathematical chemistry over the past quarter of a century:

Relative importance of Kekulé Structures of Benzenoid Hydrocarbons: Chain ordering

Individual formal valence structures of conjugated hydrocarbons are excellent "substrates" for research in chemical graph theory, whereby many of the concepts of discrete mathematics and combinatorics may be applied to chemical problems. The lecture note published by Cyvin and Gutman (Cyvin, Gutman 1988)) outlines the main features of this type of research mostly from enumeration viewpoint. In addition to their combinatorial properties, chemists were also interested in relative importance of Kekulé valence-bond structures of benzenoid hydrocarbons. In fact, as early as 1973, Graovac et al. (1973) published their Kekulé index, which seems to be one of the earliest results on the ordering of Kekulé structures: These authors used ideas from molecular orbital theory to calculate their indices

but the resulting ordering is not partial: it is a chain-type (also called total or linear order).

Graph-theoretical Ordering of Kekulé structures

A few years later, Randić (1977) analyzed a valence-bond Kekulé structure into conjugated circuits of π-electrons: For benzenoid systems R_n implies (4n+2) π-electrons. Randić, then, parameterized his R_n's and ordered them as $R_1 > R_2 > R_3 >$… where he studied both the relative importance of Kekulé structures as well as the stabilities of their benzenoid hydrocarbons (compare Fig. 6, section 'Partial-Ordering of Kekulé Structures').

Partial Ordering of Kekulé Structures

A decade ago El-Basil (1993) generated vertex-transitive graphs (i.e., 2-cube (≡ square), 3-cubes (≡ cube), 4-cube (≡ tesseract), etc.) using terminal R_1 circuits in a (sub)-set of Kekulé structures by defining two Kekulé structures as "adjacent" if one can be obtained from the other by sextet rotation in only one terminal R_1 through 60°. Formally, this is an operation on a power set composed of n terminal R_1 conjugated circuits (≡ terminal sextets). When n=2 one obtains a square (2-cube, because $2^2 = 4$), n=3 generates a cube ($2^3 = 8$) while a tesseract requires 4 terminal circuits ($2^4 = 16$) and so on. The base 2 originates from the fundamental fact that there are only two ways in which the double bonds are arranged in a hexagon, viz., proper, (+1) and improper (-1): (Fig. 3)

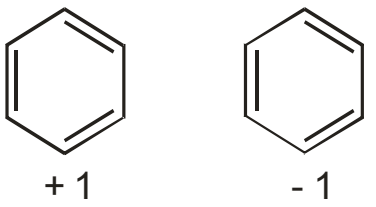


Fig. 3. The two orientations of π-electrons in a hexagon

The sextet rotation operation defines our adjacency relation among the set of Kekulé structures and the vertex-transitive graphs generated are nothing else but posets of Kekulé structures.

Coding Kekulé structures of catacondensed benzenoids

1. Arrange the skeleton of the benzenoid hydrocarbon so that some of its edges are vertical
2. Starting from the top left corner of the benzenoid graph, assign +1 or -1 to terminal rings according to the orientation of their aromatic sextets (Fig. 3).
3. Two Kekulé structures X, Y are defined to be adjacent (El-Basil (1993) if their codes differ in the sign of only one position: A skeleton $X \geq Y$ iff $q_i(X) \geq q_i(Y)$ with q being a sequence of +1 and -1.

An example is shown in Fig. 4

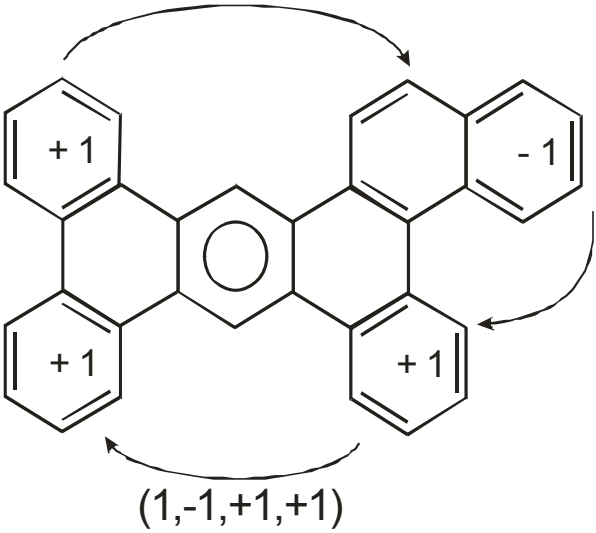


Fig. 4. The code of Kekulé structure of catacondensed benzenoid system containing 4 terminal hexagons. Compare also Fig. 3

In Fig. 5 we show the posets (Hasse diagrams), which correspond to hydrocarbons containing 3, 4 and 5 terminal hexagons.

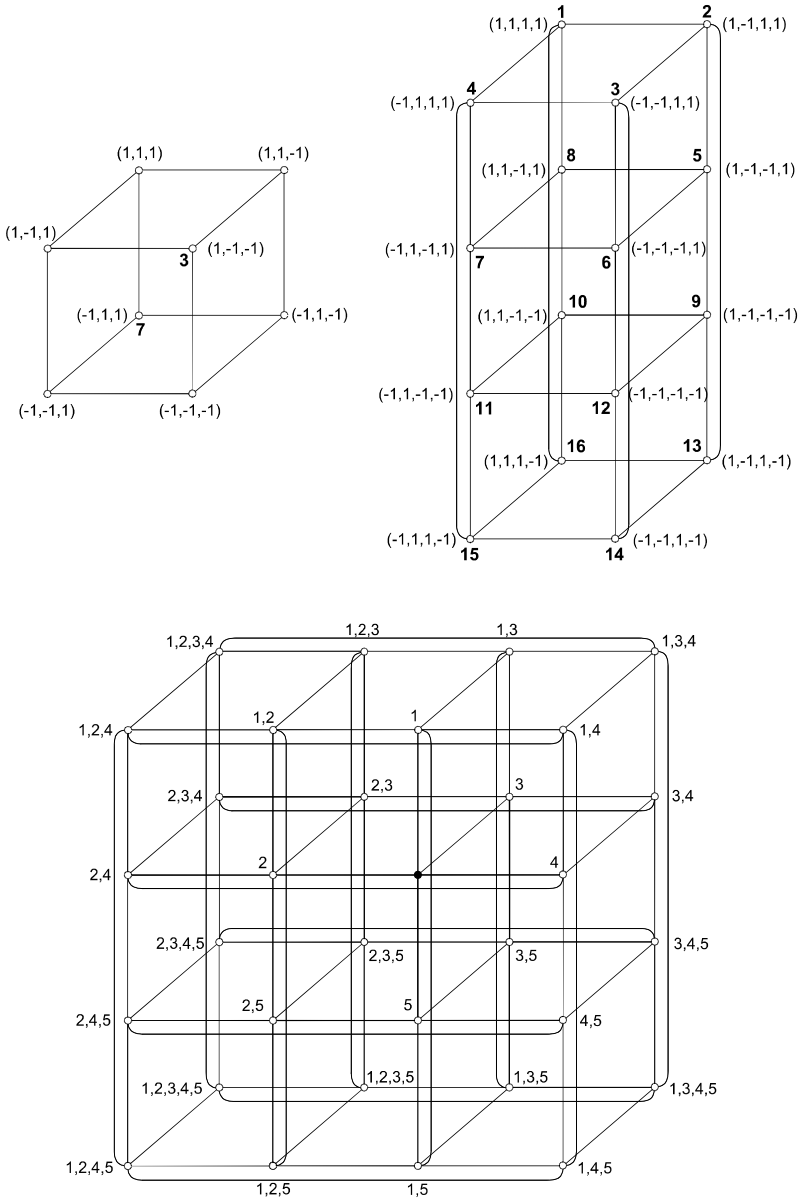


Fig. 5. 3-, 4- and 5-cubes, which represents posets generated from sets of Kekulé structures

Note that in Fig. 5 benzenoid hydrocarbons are shown, having 3, 4 and 5 terminal hexagons. Codes of Kekulé structures are indicated. For the 5-cube only places of negative signs of the code are written

A) The cube poset:
Fig. 6 shows the cube which results when 8 (out of the 9) structures of triphenylene are ordered according to their adjacency relations of their codes (El-Basil (1993).

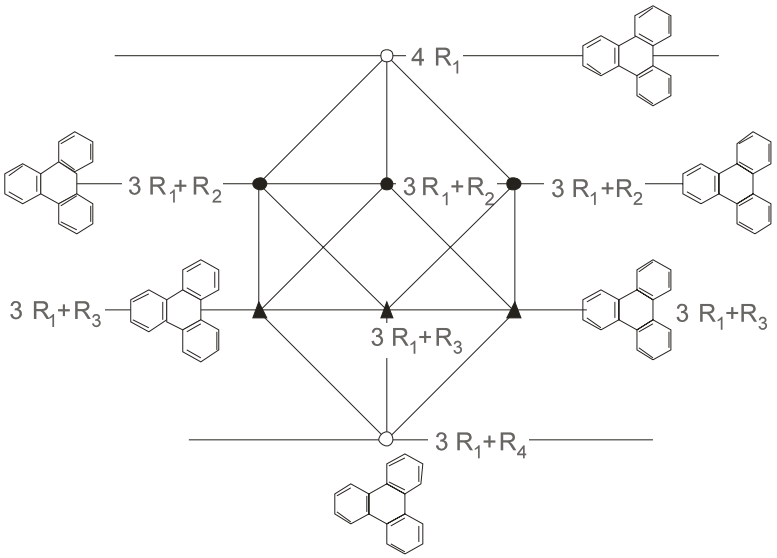


Fig. 6. The Hasse diagram of ordering 8 (out of 9) Kekulé structures of triphenylene

In Fig. 6 incomparable structures are indicated by solid circles and by solid triangles. Dotted lines indicate levels of stability of the Kekulé structures: $4R_1 > 3R_1+R_2 > 3R_1+R_3 > 3R_1+R_4$
Counts of conjugated circuits are shown, from which we see several chain orders, e.g., one of which leads to the following relative stabilities:

$$4R_1 > 3R_1+R_2 > 3\ R_1+R_3 > 3R1+R_4 \qquad (3)$$

All the resulting partial orders are consistent with the conjugated-circuits model of Randić (1977).

Kekulé structures, which correspond to identical circuit counts, e.g. vertices labelled by $(3R_1+R_2)$ and by $(3R_1+R_3)$ in Fig. 6, are incomparable. They represent vertices, which are not connected on the poset. Some Kekulé structures are shown as representative examples along with their conjugated - circuit counts.

B) The tesseract (The 4-dimensional cube)

This 16 (= 2^4) vertex-transitive graph may be generated using a catacondensed benzenoid system with 4 terminal hexagons. Again, the individual Kekulé structures are partially ordered in accord with their conjugated-circuits counts (Randić (1977).

Fig. 7 shows the resulting poset.

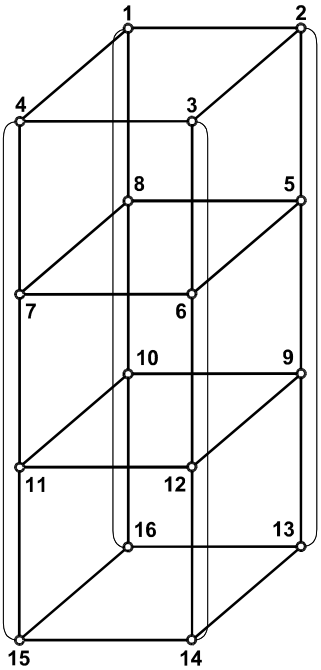


Fig. 7. Four-dimensional cube generated from a benzenoid system containing 4 terminal hexagons

In Fig. 7 the conjugated circuits correspond to Kekulé structure-positions as follows: 1 = ($7R_1$); 2 = ($6R_1 + R_2$); 3 = ($6R_1 + R_3$); 4 = ($6R_1 + R_2$); 5 = ($5R_1 + 2R_2$); 6 = ($5R_1 + R_2 + R_3$); 7 = ($5R_1 + 2R_2$); 8 = ($6R_1 + R_2$); 9 = ($5R_1 + R_2 + R_3$); 10 = ($6R_1 + R_3$); 11 = ($5R_1 + R_2 + R_3$); 12 = ($5R_1 + 2R_3$); 13 = ($5R_1 + 2R_2$); 14 = ($5R_1 + R_2 + R_3$); 15 = ($5R_1 + 2R_2$); 16 = ($6R_1 + R_2$).

The Young-Diagram Lattice, Ordering of Muirhead and generalization of Karamata

Ordering implies a comparison, and instead of actual structures, one normally compares sequences of numbers characterizing a molecular graph of a chemical structure. Frequently the required sequences are derived from an enumeration of selected graph invariants. If the selected invariants lead to integers, then the ordering theory of Muirhead (1903) is most suited for these special cases:

At the beginning of last century Muirhead (1903) introduced a theory of ordering and comparing sequences of integers. Muirhead's method calls for the construction of partial sums derived from integral sequences. If for every entry in two such sequences of partial sums, members of one structure are larger or equal (but not smaller) than the corresponding entries in other sequence, the structures can be ordered with the first structure preceding the second. If these conditions are not satisfied, the structures are not comparable leading to a partial ordering.

$$(a_1 \geq a_2 \geq \ldots \geq a_n > 0) \text{ and } (b_1 \geq b_2 \geq \ldots \geq b_n > 0) \quad (4)$$

Be two sequences of integers. Then, Muirhead's method states that: $(a_1, a_2, \ldots \geq a_n)$ majorizes $(b_1, b_2, \ldots \geq b_n)$, if a series of statement holds: (Table 1):

Table 1. Muirhead's method (Muirhead (1903)

$(a_1,a_2,\ldots,a_n)$	majorizes	$(b_1,b_2,\ldots,b_n)$	if
a_1	$\geq$	b_1	
a_1+a_2	$\geq$	b_1+b_2	
…	$\geq$	…	
$a_1+a_2+\ldots+a_n$	$\geq$	$b_1+b_2+\ldots+b_n$	

Restrictions to integral entries have subsequently been removed and for these more general situations, Karamata (Beckenbach, Bellmann 1961) derived an important theorem, which allows definite conclusions to be drawn from properties of the structures to be studied, if graph invariants are not integral quantities.

More recently Ruch (1975) used ideas of Muirhead in connection with representations of the symmetric group and generated a partial ordering of partitions of integers. For each partition one associates a row of an equal number of dots or boxes so that the rows are arranged in a non-increasing order. For example there are 5 partitions of 4, represented in Fig. 8.

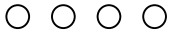
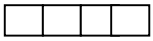
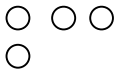
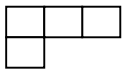
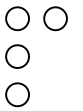
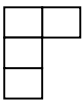
(4)	4		
(3,1)	3+1		
(2^2)	2+2		
($2,1^2$)	2+1+1		
(1^4)	1+1+1+1		

Fig. 8. Partitions of 4 and the corresponding Ferrers graphs and Young diagrams. Both to be read horizontally

Sometimes, the diagrams of dots are referred to as Ferrers graphs (Coleman 1968), after the English mathematician of the latter part of the nineteenth century. However, Young, employed similar devices now known as Young diagrams where he replaces dots with small squares. We let:

$$\Gamma_a = a_1 + a_2 + \ldots + a_n ,$$
$$\Gamma_b = b_1 + b_2 + \ldots + b_n \qquad (5)$$

be two partitions of the same integer (i.e., $a_a + a_2 + \ldots + a_n = b_1 + b_2 + \ldots + b_n$). Then Γ_a is said to dominate or majorize Γ_b if equation (4) is satisfied, otherwise, the two partitions (or the corresponding graphs) are not comparable. As an illustration, we form the partial sums of the partitions of 4:

4 $\rightarrow$ (4, 0, 0, 0) $\rightarrow$ (4, 4, 4, 4)
3+1 $\rightarrow$ (3, 1, 0, 0) $\rightarrow$ (3, 4, 4, 4)
2+2 $\rightarrow$ (2, 2, 0, 0) $\rightarrow$ (2, 4, 4, 4)
2+1+1 $\rightarrow$ (2, 1, 1, 0) $\rightarrow$ (2, 3, 4, 4)

$$1+1+1+1 \rightarrow (1, 1, 1, 1) \rightarrow (1, 2, 3, 4) \quad (6)$$

Muirhead's ordering conditions in the above case are a chain on five vertices because all successive sequences (≡ graphs) are comparable.

For n = 5 there are 7 partitions, the ordering of which also leads to a chain. But starting with n = 6, one observes two pairs of non-comparable graphs (leading to two bifurcations). (This poset is shown in Fig. 10 (section 'The Young-Diagram Lattice, Ordering of Muirhead and generalization of Karamata')).

The first bifurcation is generated at $\Gamma_4 = 4 + 1 + 1$ and $\Gamma_5 = 3 + 3$, which correspond to the partial sums:

$$(4, 5, 6, 6, 6, 6) \quad , \quad (3, 6, 6, 6, 6, 6) \quad (7)$$

We observe that the first component of the first sequence is greater than that of the second sequence, but the reverse order for the second components, i.e. $4 > 3$ but $5 < 6$. Hence the sequences (7) are an incomparable pair. Both Γ_4 and Γ_5 are comparable with $\Gamma_3 = 4 + 2$ whose partial sum is (4, 6, 6, 6, 6, 6) which majorizes both partial sums shown in eqn. (7).

Ordering of Tree graphs

In Gutman and Randić (1977) published their work on the algebraic characterization of skeletal branching of tree graphs (cf. Harary (1972). (A graph is viewed as an abstract representation of a molecule where vertices replace atoms and edges replace chemical bonds. The degree of a vertex equals the valence of the corresponding atom. Often in hydrocarbons a H-suppressed graph is useful, where the hydrogen atoms are neglected.) The steps involved in the scheme of Gutman and Randić are outlined as follows:

a) List the valences of a tree graph in a non-increasing way.
b) Form the partial sums of the above sequence.
c) Order a set of partial sums according to eqn. (4).

Remarkably the poset obtained (by Ruch) for Young diagrams were also obtained (by Gutman and Randić) for the trees! In fact a set of Young diagram containing n vertices is isomorphic with a set of trees containing (n + 2) vertices. As an illustration we show how a set of Young diagrams on 6 boxes and a set of trees on 8 vertices generate the same poset (Fig. 9).

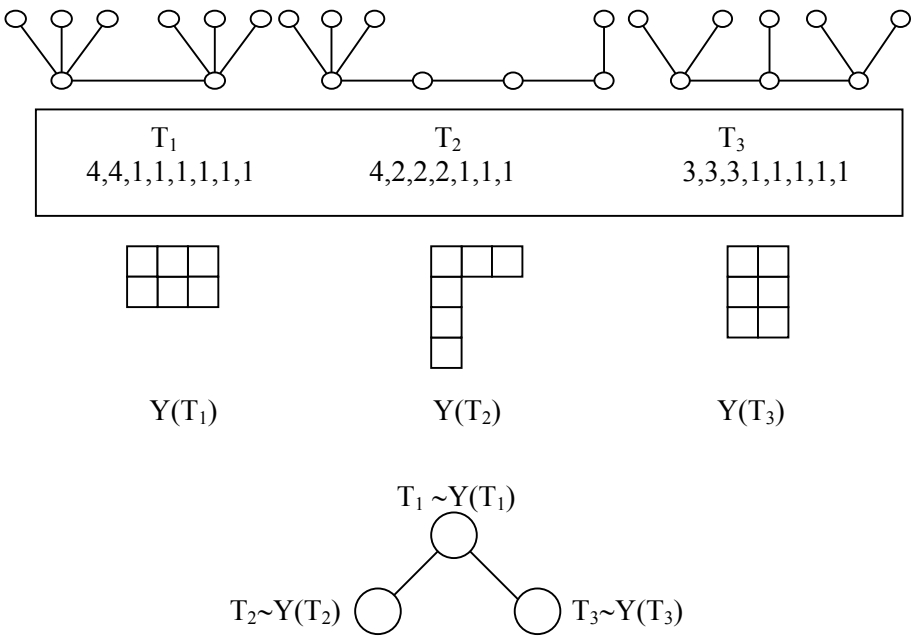


Fig. 9. A set of trees $\{T_1, T_2, T_3\}$ and the corresponding set of Young diagrams $\{Y(T_1), Y(T_2), Y(T_3)\}$, their valence sums and partial sums leading to a poset with one bifurcation which defines a non-comparable pair $\{T_2, T_3\}$, cf. eqn. (5)

The valences of these trees are listed in a non-increasing way together with the corresponding partial sums. When rules of Muirhead (eqn. 4) are applied to these partial sums one obtains the poset shown in Fig. 10. We observe that T_1 majorizes (i.e., more important than ≡ dominates) T_2 and T_3 but T_2 and T_3 cannot be ordered: Muirhead's theory describes T_2 and T_3 (or their corresponding Young diagrams) as being incomparable. Pairs of incomparable objects generate sites of bifurcations.

In Fig. 10 we show the ordering of the set of Young diagrams on 6 boxes according to the rules of Ruch (1975). The corresponding tree graphs are also shown (see also chapter by Seitz p. 367, where a set of Young diagrams with 10 boxes is represented and discussed with respect to complexity measures).

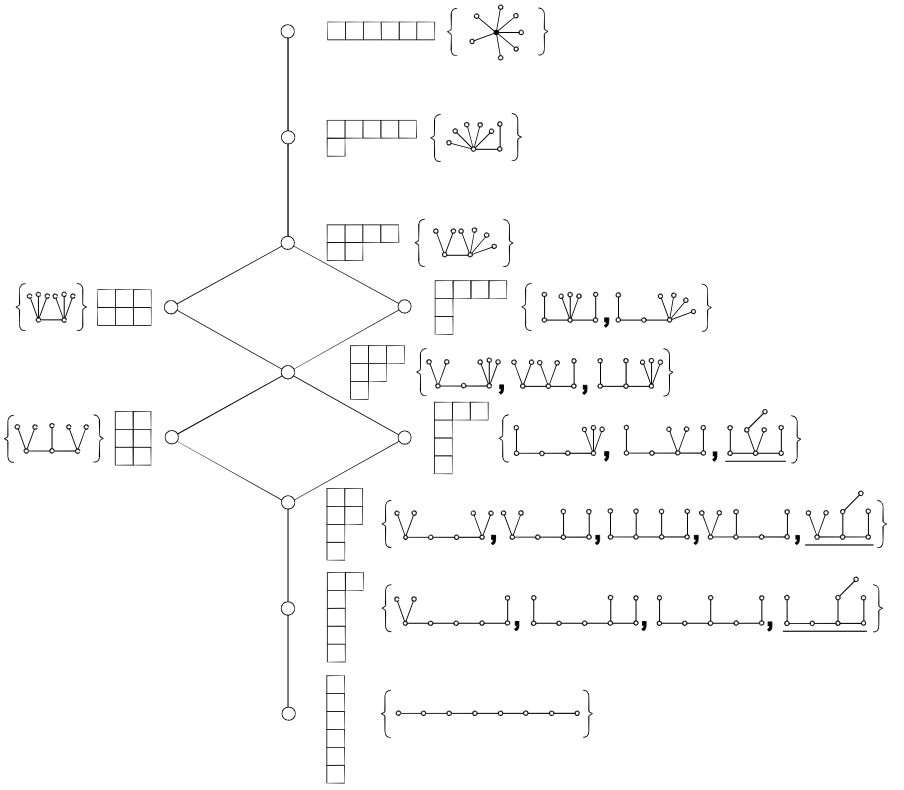


Fig. 10. Ordering of the set of Young diagrams containing 6 boxes. The corresponding tree graphs are shown. Underlined graphs are non-caterpillar trees

The Fig. 10 illustrates how the ordering theory of Ruch (1975) coincides with that of Gutman and Randić (1977) (See also Fig. 12).

The overlap between the ordering schemes of Ruch and that of Gutman & Randić

These two ordering schemes may be made to overlap (i.e., generate the same poset) for a set of trees containing (n = 2) vertices and a set of Young diagrams containing n boxes as follows:

a) Suppress information on terminal vertices (of valence = 1)
b) Reduce valence of each vertex by one
c) The resulting sequence of integers (from left to right) represents rows of boxes from top to bottom.

Example:
T_2 (Fig. 9) generates the following sequence of integers representing valences of vertices arranged in a non-descending order:

4,2,2,2,1,1,1 (8)

We adopt steps a-c:

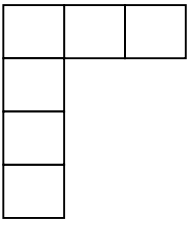
a) Suppressing information of terminal vertices leads to the sequence:

4,2,2,2 (9)

b) Reduction of valence of each vertex by one leads to:

3,1,1,1 (10)

c) The above sequence corresponds to the following Young diagram Fig. 11.



$= Y(T_2)$

Fig. 11. A specific Young diagram, corresponding to the sequence 3,1,1,1

Correlation of Young Diagrams with Alkanes and benzenoid Hydrocarbons

A remarkable type of tree graph is called a Caterpillar El-Basil (1987) (or a caterpillar tree): P_j (m_1, m_2, … , m_j) which is obtained by the addition of m_1 monovalent vertices to the first vertex υ_1 of path P_j , m_2 monovalent vertices to υ_2 of P_j and so on. The three tree graphs shown in Fig. 10 are all caterpillar trees and may be designated respectively as:

$$P_2\,(3,3)\ ;\ P_4\,(3,0,0,1)\ ;\ P_3\,(2,1,2)$$

An example of a non-caterpillar tree is shown in Fig. 12.

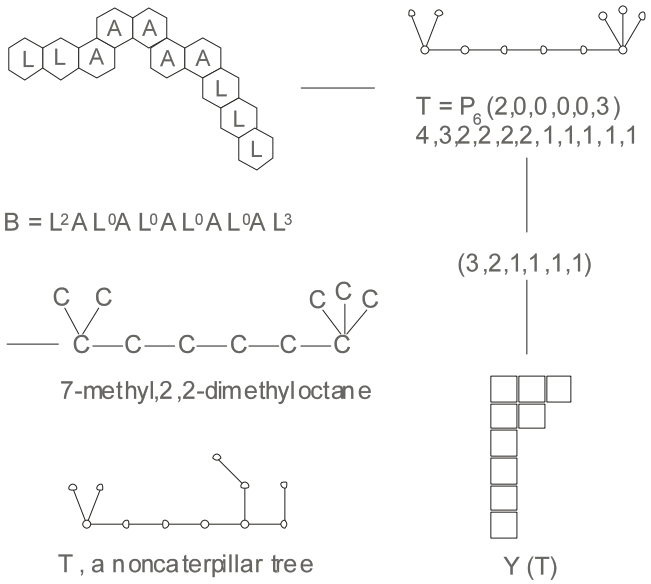


Fig. 12. An unbranched benzenoid hydrocarbon, the corresponding caterpillar tree T, alkane hydrocarbon skeleton and Young diagram. T' is a non-caterpillar tree

Caterpillar trees are related to other combinatorial objects of chemistry and physics (such as rook boards, Clar graphs, and King polyomino graphs) (El-Basil, Randić (1992) but most importantly, caterpillar trees represent in fact unbranched catacondensed benzenoid hydrocarbons (El-Basil 1987), El-Basil, Randić 1992). To envisage this important connection we distinguish two types of annellation of hexagons (Cyvin, Gutman (1988), viz., linear, L, and angular, A, modes (Fig. 13):

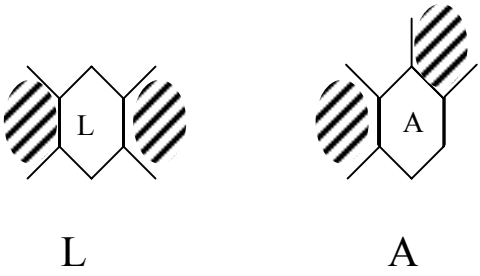


Fig. 13. Linear and angular modes of annelating hexagons

An unbranched benzenoid may thus be "coded" by its LA – sequence written, say, from left to right, as LA – units, viz.

$$L^{m_1} AL^{m_2} A....L^{j}$$

The corresponding caterpillar tree is composed by the addition of m_1 monovalent vertices to υ_1, m_2 monovalent vertices to υ_2 , … , j monovalent vertices to $\underline{j^{th}}$ vertex of path P_j (on j vertices).

In Fig. 12 we illustrate these concepts.

Ordering of Unbranched Benzenoid Hydrocarbons

We have seen in the previous section (cf. Fig. 12) that a caterpillar tree can be made to overlap with an unbranched catacondensed benzenoid hydrocarbon. I.e., the modes of hexagon annellation are, in fact, "stored" so-to-speak in the distribution of the terminal vertices of a caterpillar tree. One is, then, tempted to go back to posets such as the one shown in Fig. 10 and replaces the caterpillar trees by their corresponding benzenoids. In this way a set of benzenoid hydrocarbons has been partially ordered according to the theory of Ruch (1975), using Muirhead's rules (Muirhead (1903) (eqn. 4) or equivalently according to the scheme of Gutman and Randić (1978) using valences of vertices of tree graphs as input for eqn. (4). The question now becomes: does the resulting (purely structural) partial ordering reflect the (chemical) properties of benzenoids? The answer is quite encouraging: In Fig. 12 the corresponding benzenoids are represented as their respective LA-sequences and their stabilities are measured by the set of Herndon's permutation integrals (Herndorn, Ellzey Jr (1974) (γ_1, γ_2, γ_3, γ_4) where γ_i involves permutation of (4i+2) π-electrons. Observing that twice these integrals are numbers of conjugated circuits (cf. Randić (1977),

listed, respectively, as (R_1, R_2, R_3, R_4), we can use this poset to order a set of hydrocarbons according to their stability.

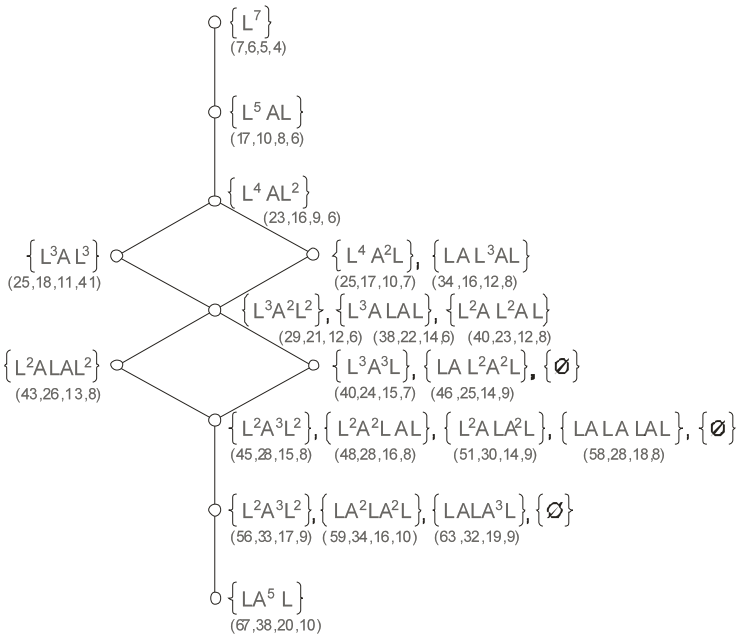


Fig. 14. Partial ordering of the set of unbranched benzenoids containing 7 hexagons. Each benzenoid is coded by its L-A sequence of hexagon annelations

In Figure 14, numbers in parentheses are permutation integrals (Herndorn, Ellzey Jr (1974). The poset is isomorphic with the one shown in Fig. 10. Chemical stability goes up as one goes down along the poset.

In the present case, stability increases as one goes down the edges of the poset. The limits are defined as $\{L^7\}$ and $\{LA^5L\}$ representing a linear acene (heptacene) and a single zigzag chain, all- benzenoid, system. Linear acenes are known to be coloured unstable hydrocarbons while angular annellations of hexagons leads to colourless stable systems (Clar 1972). In Fig. 15 this situation is illustrated with a few examples of unbranched benzenoids for which UV data are available (Clar 1972), which serves to illustrate general features.

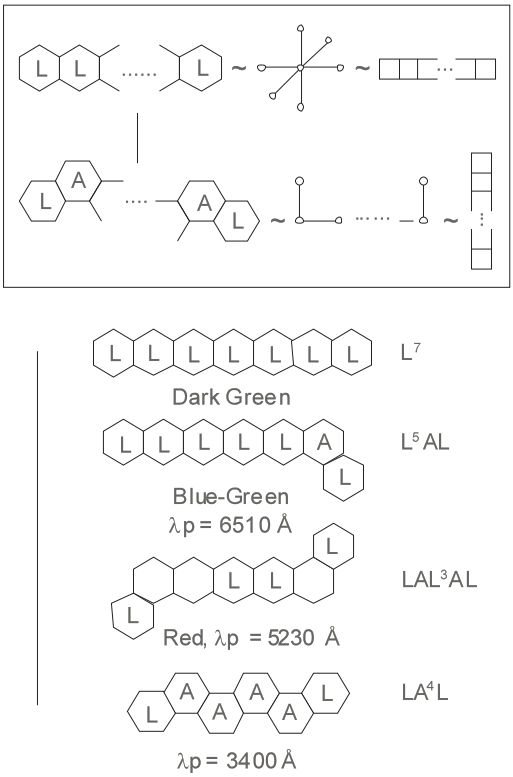


Fig. 15. Limits of stability of a set of catacondensed benzenoids

In Fig. 15 the linear acene represents the most unstable system while the all-kinked acene being the most stable. These limits may be modelled respectively with a star tree (or a row of boxes) and a path (or a column of boxes). The para bands of UV spectra are indicated for some cases for which data are available (Clar (1972). It is interesting to observe that sequences of numbers which represent (γ_1, γ_2, γ_3, γ_4) lead to bifurcations (i.e. incomparable pairs) when the sequences, which correspond to Young diagrams, are also incomparable! For example at the first bifurcation (Fig.'s 10, 12) one finds the following pair of sequences of γ's.

$$(25, 18, 11, 4) , (25, 17, 10, 7), \tag{11}$$

which leads to the following non-comparable partial sums:

$$(25, 43, 54, 58) , (25, 42, 52, 59) \tag{12}$$

i.e., $54 > 52$ while $58 < 59$ leading to a bifurcation!

An observation regarding Young diagrams and tree graphs
While there is a unique Young diagram for every tree graph, the opposite is not true, viz., several trees may occupy the same position characterizing a single Young diagram on a given poset. Namely, several trees lead to the same partition of vertex-valences and whence the same Young diagram. As an illustration one may observe in Fig. 10, that each of position 4, 6, 7, 9, 10 of the poset shown characterizes a single Young diagram but several tree graphs! Take, e.g. the sequence of vertex-degree 3,3,2,2,1,1,1,1, then, the ordering rules of Gutman and Randić (1977) lead to rows of boxes (from top to bottom) of lengths 2,2,1,1 which define a unique Young diagram, but the vertex-degrees in this case generate four caterpillar and one non-caterpillar trees. (position 9 of the poset shown in Fig. 10).

Grid Graphs Based on Molecular Path Codes of Lengths 2 and 3: Relation to Ordering of Young Diagrams

In a series of publications Randić et al. (Randić, Wilkins (1979) generated grid graphs of molecular graphs of classes of compounds based on their path codes of lengths 2 and 3. Such periodic tables are reminiscent of the Hasse diagrams of partial orderings and may be viewed as multiposets, the nodes of which represent the partial ordering of a given property. Several properties were studied, which include enthalpies, heat capacities, critical volumes, index of refraction, entropy changes and several others.

Here, we observe how these grids are related to Young diagrams. As an example we consider in Fig. 14, the diagram that shows positions of the set of octane isomers in the coordinate system (P_2, P_3). We also indicate the corresponding Young diagrams associated with the tree graphs representing the octanes. Interestingly the resulting grid successfully orders subsets of Young diagrams in accord with rules of Ruch (1975) as well as the scheme of Gutman and Randić.

Example (Fig. 16):

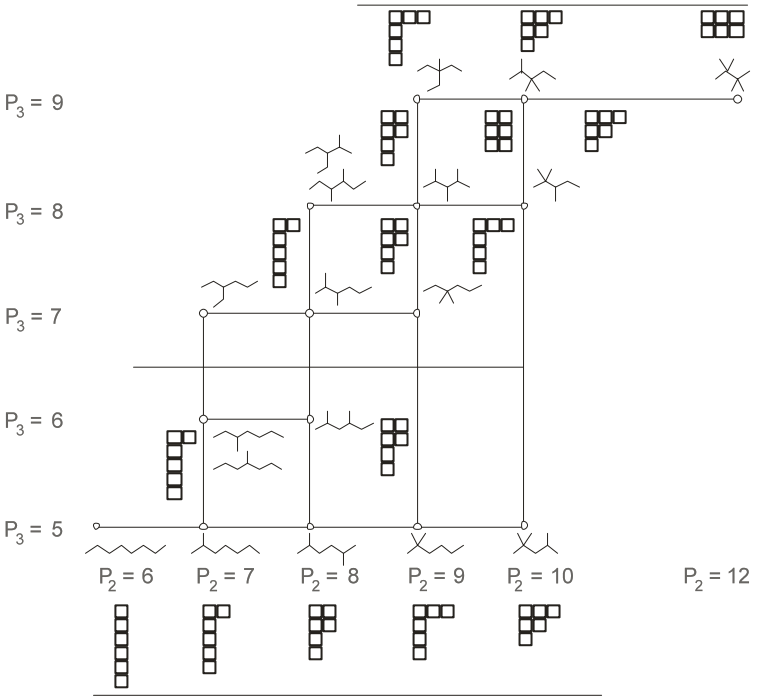


Fig. 16. The diagram showing positions of various octane isomers in the coordinate system (P_2, P_3)

In Fig. 16 the corresponding Young diagrams are correctly ordered in horizontal lines (dashed arrows) in accord with rules of Ruch (1975) as well as Gutman and Randić (1977).

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