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AN APPROACH TO THE CONSTRUCTION OF CERTAIN ISOSPECTRAL AND SUBSPECTRAL GRAPHS

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Abstract. A systematic procedure for the representation of the graph with adjacency matrix that is the square of that of the parent graph is presented.The concepts of T(A) mates and virtual embedding are introduced and utilized in the construction of subspectral, isoabsolutespectral and isospectral conjugated systems.The emphasis is placed on fertile graphs of chemical interest.

1. Introduction

Isospectral, or in mathematical literature cospectral, graphs (1) have long been of current interest in the use of graph theory in chemistry (2-8). The pioneering attempts for constructing the sets of isospectral molecules were

based on either the exhaustive study of secular polynomials (2,9),which would be identical for isospectral graphs, (7) or Heilbronner's partitioning scheme (2-4,8,9). Mowshowitz and Schwenk were the first to realize that many isospectral graphs could be generated from a single graph (fertile graph) of unique qualities (3,4,9,12). It has been established that whole families of isospectral graphs can be derived from a molecular skeleton of vinylbenzene (3) and almost all non-cyclic graphs (tree graphs) have an isospectral mate (2). Also, it has been found that in some instances, a pair of isospectral graphs forms a basis for generation of a family of structurally related isospectral pairs, while in other instances, the production of related systems is not possible (4). Various rules were set forth for the construction of isospectral (3,7) and subspectral (5,6) graphs.

In the chemistry of conjugated systems, the primary interest is focused on graphs in which the degrees of various vertices (valancies) do not exceed three. Within the Hückel molecular orbital (HMO) framework, isospectral molecules (8) and the construction of the corresponding characteristic polynomials have recieved considerable attention , because finding or constructing isospectral graphs have been shown to have both some practical relevance and interest as a graph theoretical problem (13-17) .

In the present study, primarily , systems of interest in chemistry are concerned. A novel type of graph (T(A) graph) is defined which is extensively used to develop some general methods for the construction of certain types of isospectral, isoabsolutespectral and subspectral conjugated systems.

2. Theory

A^2-matrix: The adjacency or topological matrix A (2) of a graph, G(v,e), is identical to the HMO secular matrix for the electronic system isomorphic to the graph (13,14). There exist a vector X and a number , such that,

$$AX = \lambda X \qquad (1)$$

where X is the invariant vector or more commonly, eigenvector and λ an eigenvalue of graph G(v,e). In n-dimensional linear space, it is proved that the eigenvalues of the matrix A^k are equal (with account taken of multiplicities) to the kth power of the eigenvalues of matrix A (18). Hence,

$$A^2X = \lambda^2X \qquad (2)$$

where, the matrix A^2 is symmetric (19) as the adjacency matrix A.

Let R_i and C_j be any row and column vectors of the adjacency matrix A of graph G(v,e). Then, the element b_{ij} of the corresponding matrix A^2 is equal to,

$$b_{ij} = \sum_{k=1}^{v} a_{ik}a_{kj} \qquad (3)$$

where, a_{ik}, a_{kj} etc. are the elements of vectors R_i and C_j respectively. Obviously, only the pairs of elements which are mutually nonzero contribute to the above sum. Hence,

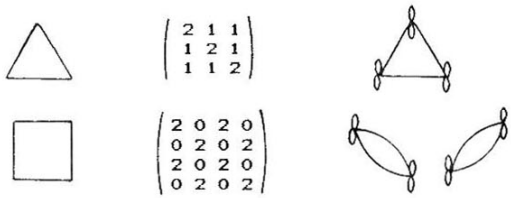
$$b_{ij} = \sum_{\text{all } l} a_{il}a_{lj} \qquad (4)$$

where, l stands for a vertex which is flanked by both vertices i and j . In other words , b_{ij} is the number of all walks of length-2 lying between i and j .

<u>I(A) graphs:</u> By considering the topological meaning of the adjacency matrix A , one can visualize that vertices i and j become source points of the graph obtained from the corresponding Coates graph (20) of G(v,e) by deleting indegrees of i and j . Since, adjacency matrices of conjugated molecules have elements either zero or one, then the off-diagonal elements of A^2- matrices are nothing but zero or one, except for molecules having 4-membered cycles where some off-diagonal elements could be two as well. On the other hand, the diagonal elements of A^2-matrix are equal to degree (d_i) of the respective vertices of graph G(v,e) (13).

In the light of the above considerations, an A^2-matrix can be represented by constructing a graph in which every vertex i is associated with self-loops having weight 1 ,equal to d_i in number , and off-diagonal relations with the

necessary number of edges having weight 1. Henceforth, these types of graphs and their decomposable subgraphs will be called T(A) graphs and T(A) mates, respectively. They are useful graphs to display the degrees of vertices and the nearest nonneighbor (second neighbor) relations simultaneously. As an illustrative purpose, A^2-matrices and the associated T(A) graphs of cylopropenyl and butadiene systems are shown below.



$$\begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$$

$$\begin{pmatrix} 2 & 0 & 2 & 0 \\ 0 & 2 & 0 & 2 \\ 2 & 0 & 2 & 0 \\ 0 & 2 & 0 & 2 \end{pmatrix}$$

<u>Theorem 1:</u> Let G(v,e) be the graph of an alternant conjugated system and A represent its adjacency matrix. Then, the associated T(A) graph has two edge-disjoint subgraphs. Hence, it is decomposable.

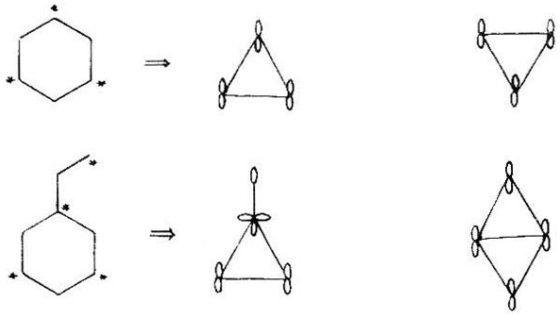
<u>Proof.</u>

Let V^* and V° be disjoint node sets of G(v,e).Since,the off-diagonal elements (b_{ij}) of A^2-matrix are equal to the sum of the number of edges directly joining vertex j to the nearest neighbors of i (eq.4), then all the nonzero b_{ij} elements originate from nodes i and j which are the elements of the same set (V^* or V°). Hence, T(A) graphs of alternant

conjugated systems are decomposable.

Theorem 1 , enables us to construct T(A) graphs of alternant conjugated structures readily by connecting all the nearest nonneighbors of vertex i in G(v,e) and inserting the necessary numbers of self-loops (equal to d_i) of weight 1 and repeating the procedure for all the vertices. Note that, 4-membered rings possess T(A) graphs having two-edged connections. On the other hand, simple odd-membered (nonalternant) monocyclic conjugated systems are characterized by T(A) graphs having the same odd-membered skeletons as the corresponding structures possess.

T(A) graphs of (even, odd, and non-Kekule (21)) alternant conjugated systems are decomposable to two edge-disjoint subgraphs $T(A^*)$ and $T(A^o)$. In the case of an even alternant structure, these subgraphs are sometimes identical or isomorphic and sometimes nonisomorphic.



$T(A^*)$ $T(A^o)$

<u>Theorem 2:</u> $T(A^*)$ and $T(A^\circ)$ graphs of an even alternant conjugated system are isospectral.

<u>Proof.</u> Let the subgraphs of $T(A)$ covering all the starred and unstarred positions of the original graph $G(v,e)$ be $T(A^*)$ and $T(A^\circ)$. Since, $G(v,e)$ is an even alternant system, its eigenvalues are symmetrically distributed about zero (21). On the other hand, the eigenvalues of $T(A^*)$ (or $T(A^\circ)$) are the squares of eigenvalues of $G(v,e)$ (18) . Hence,the set of square roots of the eigenvalues of $T(A^*)$ (or $T(A^\circ)$) which has $v/2$ vertices , covers the whole spectrum of $G(v,e)$. Consequently, $T(A^*)$ and $T(A^\circ)$ have the same eigenvalues.

Note that, evidently, $T(A^\circ)$ graphs of odd alternant and non-Kekule systems are subspectral with the corresponding $T(A^*)$ graphs. If n and m ($n > m$) denote the numbers of starred and unstarred vertices of any of the aforesaid systems, then n-m zeros exist in the spectrum of $G(v,e)$ (21). Hence, the same number of zeros are included in the spectrum of its $T(A^*)$ graph .

<u>Isospectral, subspectral and isoabsolutespectral graphs :</u> Before outlining the practical approach to the construction of certain types of isospectral ,subspectral and isoabsolutespectral conjugated systems, the following corollaries can be drawn in the light of theorem 2 .

<u>Corollary 1 :</u> Let G and G′ be two even (or odd) alternant conjugated systems having v vertices.If they possess at least

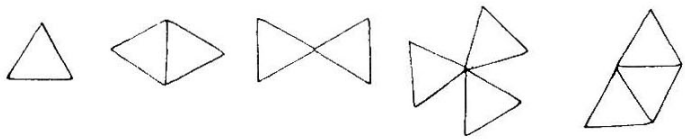
one, identical (or isomorphic) $T(A^*)$ or $T(A^\circ)$ graph, then they are isospectral (Fig. 1).

<u>Corollary 2:</u> Let G and G′ be any two alternant systems having v and v′ (v>v′) vertices. If they have at least one, identical (or isomorphic) $T(A^*)$ or $T(A^\circ)$ graph, then G′ is a subspectral graph of G (Fig.2).

<u>Corollary 3:</u> If an even alternant conjugated system ,G, possesses a T(A) mate ($T(A^*)$or $T(A^\circ)$) identical (or isomorphic) with the T(A) graph of a nonalternant system G′, then G and G′ are isoabsolutespectral graphs that is squares of their eigenvalues are mutually (irrespective of multiplicities) equal.

One should note that, generally, a k-membered nonalternant ring system is isoabsolutespectral with a 2k-membered even alternant ring (Fig. 3).

T(A) graphs of isospectral, subspectral ,and isoabsolutespectral graphs usually have some common elementary subgraphs. Cyclic and acyclic pairs of the abovementioned types of graphs are interrelated through various combinations of 3-membered cyclic subgraphs which are henceforth called "triads". Below, some triad frames obtainable from conjugated systems are shown. Note that, many



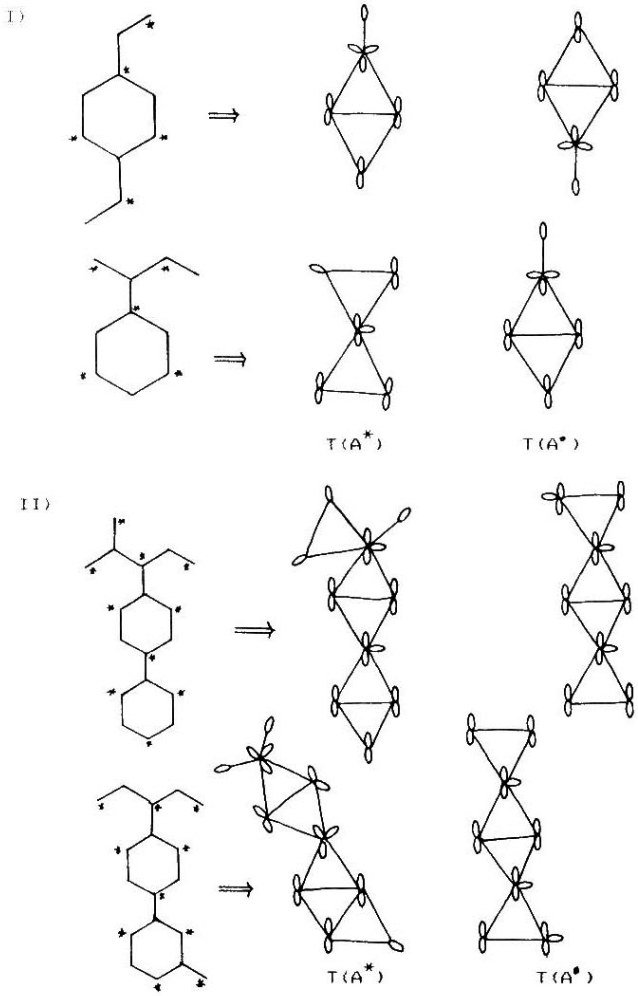


Fig.1 Some isospectral systems and their T(A) mates.

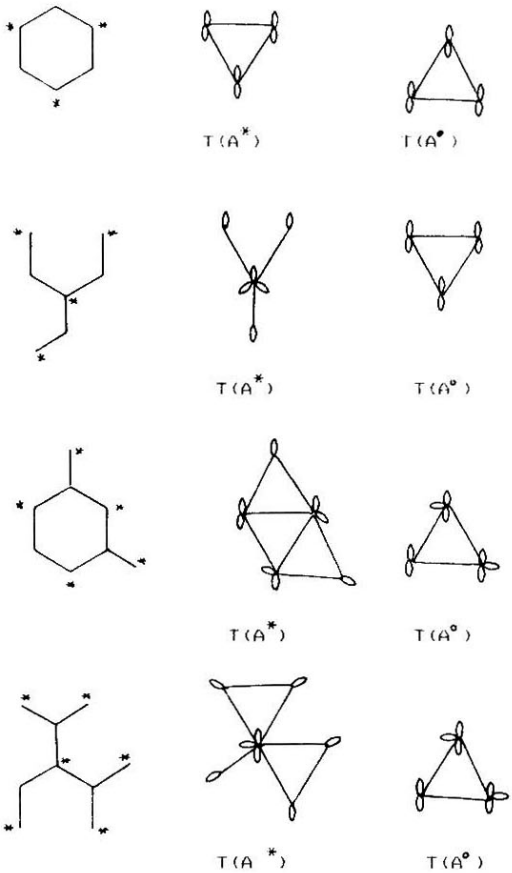


Fig.2 Some subisospectral systems and their T(A) mates.

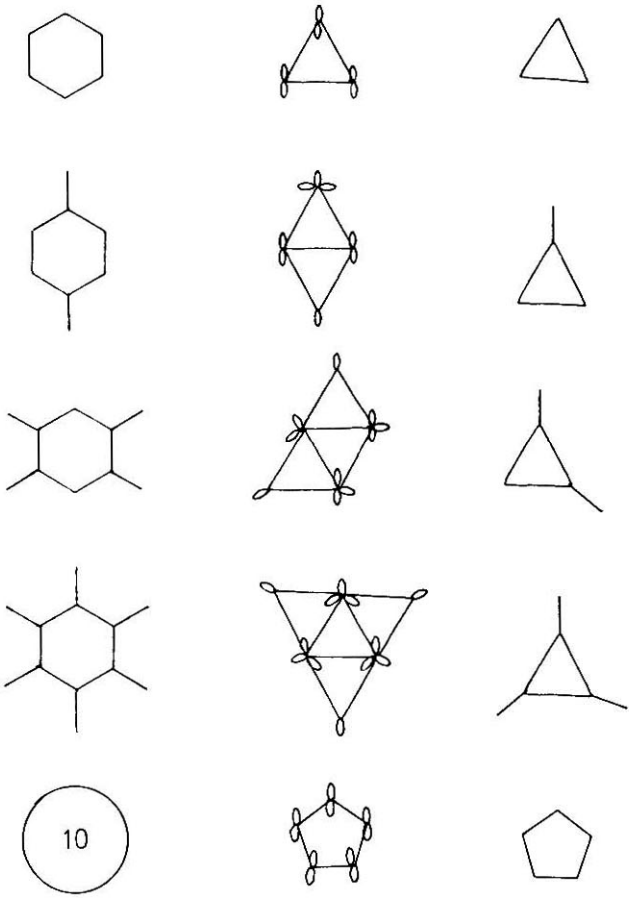
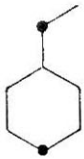
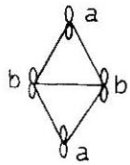


Fig.3 Some isoabsolutespectral pairs and their common T(A) graphs.

molecules have identical or isomorphic T(A) graphs (hence there exist some common triad patterns) such that their spectra are in one way or another interrelated, e.g. cyclopropenyl, benzene, and 3-vinylpentadienyl systems. Consequently, the possibility of matching of T(A) graphs of various structures engenders a special kind of embedding (virtual embedding) concept as distinguished from the embedding of real fragments (23-25). For instance, benzene and 3-vinylpentadienyl system, both contain the virtually embedded cyclopropenyl structure. Thus, the spectrum of cyclopropenyl system is a part of the spectra of the others.

Generation of fertile graphs: In the study of isospectral graphs, certain structures have been noticed such that they lead to one or more families of related isospectral species thus exhibiting " fertility " while the others remain "sterile " (3,4). Vinylbenzene is an example of a fertile graph. By attaching a residual at one of the indicated positions (isospectral points (2,22)) one can generate isospectral pairs (3). Although, these isospectral points are

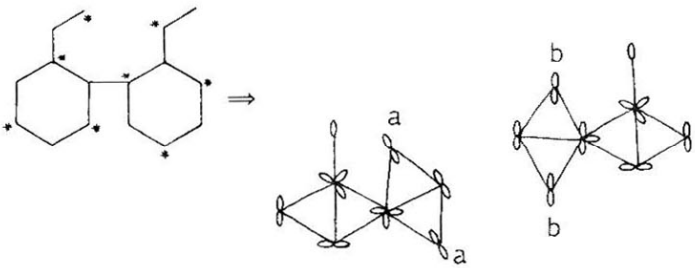




not symmetrically indistinguishable vertices of the corresponding graphs, they are equivalent in terms of the T(A) graph concept developed in the present study. They occupy equivalent positions in one of the T(A) mates where the points labeled with "a" and "b" are the isospectral sites and unrestricted substitution sites (7) respectively. Isospectral points, as seen in the case of vinylbenzene, possess different topological surroundings in the corresponding chemical graph G(v,e) whereas, unrestricted substitution points are topologically equivalent both in G(v,e) and T(A) graphs. Note that the sites of vinylbenzene indicated with "a" (or "b") have molecular orbital coefficients which are equal in absolute value (26). Obviously, the attachment of any residual at any of the sites labelled with "a" ,in the presence or absence of any group(s) at site(s) "b" , always yields superimposable T(A) graphs, thus resulting in isospectral structures. Note that , the interchange of different substituents attached to the isospectral sites of vinylbenzene also yields superimposable T(A) graphs. This fact is simply the underlying reason why vinylbenzene is a fertile system.

As it is pointed out in the above argument, the generation of highly symmetrical T(A) graphs having nonequivalent but isospectral points can be exploited to construct fertile graphs. The whole T(A) graph or a subunit

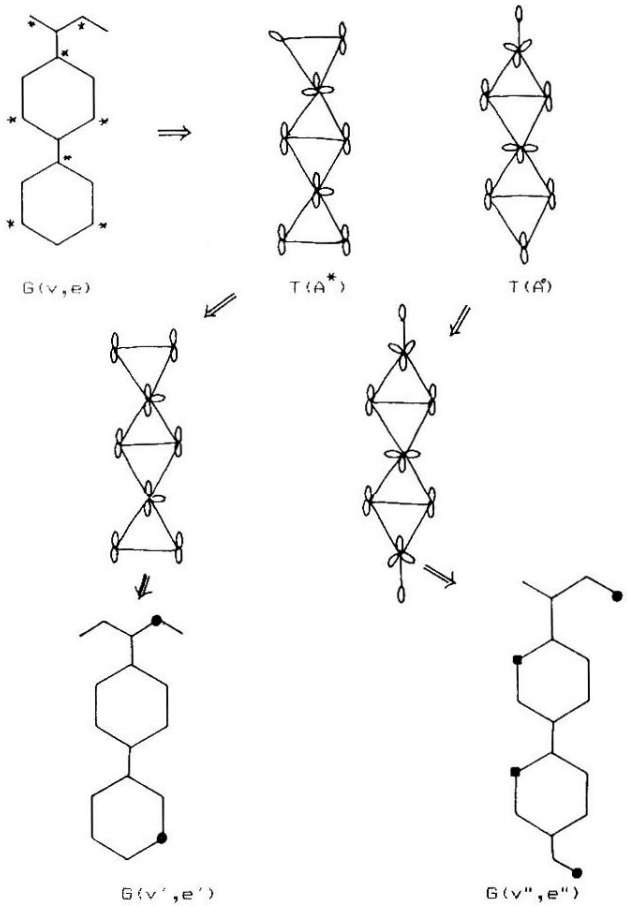
of it may have a symmetry plane through which distinct and nonequivalent isospectral vertices interchange (essential symmetry plane) . In some cases, it may coincide with the internal symmetry plane of a T(A) graph (perfect essential symmetry plane). Each of the following T(A) mates has a subunit which possesses an essential symmetry plane but it is not an internal symmetry plane.



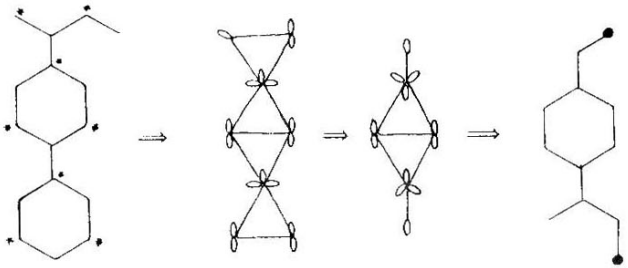
$T(A^*)$ $T(A^o)$

Some novel methods useful for the generation of fertile graphs are presented below. Isospectral vertices of the resultant structures are labeled with black circles, squares etc.

<u>Expansion process:</u> Isospectral points are generated by attaching certain groups to a graph G(v,e) (precursor graph) which leads to a T(A) mate having an essential symmetry plane. The process is schematically presented below.

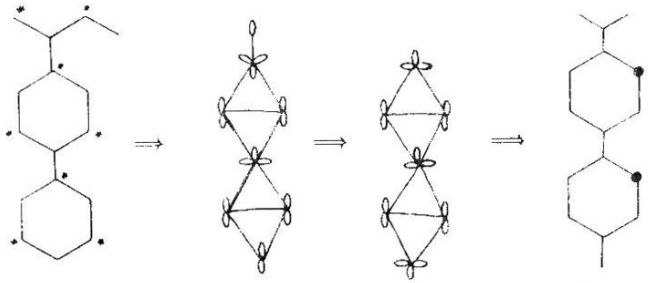


<u>Contraction process:</u> An essential symmetry plane is generated by the elimination of certain groups from the T(A) mates of the precursor graph,e.g.,



G(v,e) T(A*) G(v',e')

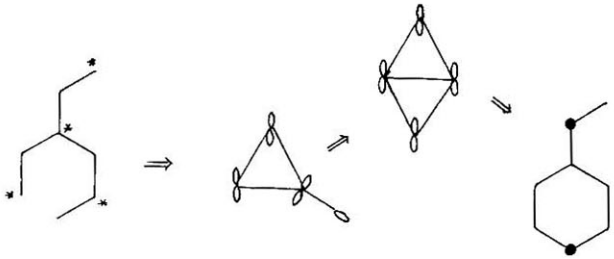
<u>Rearrangement process:</u> A T(A) graph possessing an essential symmetry plane is generated from the T(A) mates of a given precursor graph.e.g.,



G(v,e) T(A°) G'(v ,e)

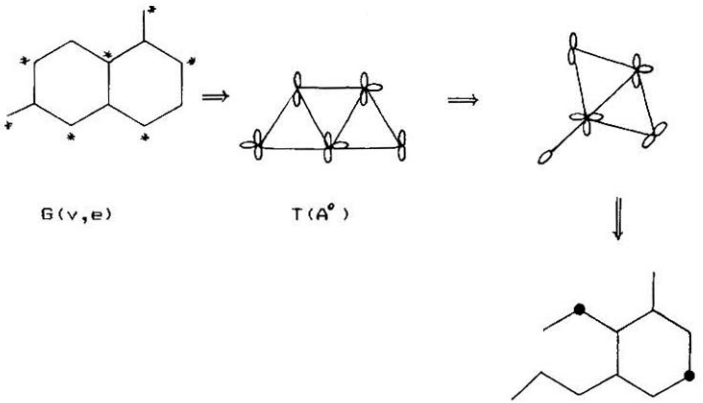
Note that, starting from the same T(A°) mate another fertile graph is obtained by the expansion process.

<u>Cyclization process:</u> A T(A) mate having an essential symmetry plane is generated by the cyclization of the given precursor graph G(v,e), e.g.,



G(v,e) T(A^{o}) G(v,e')

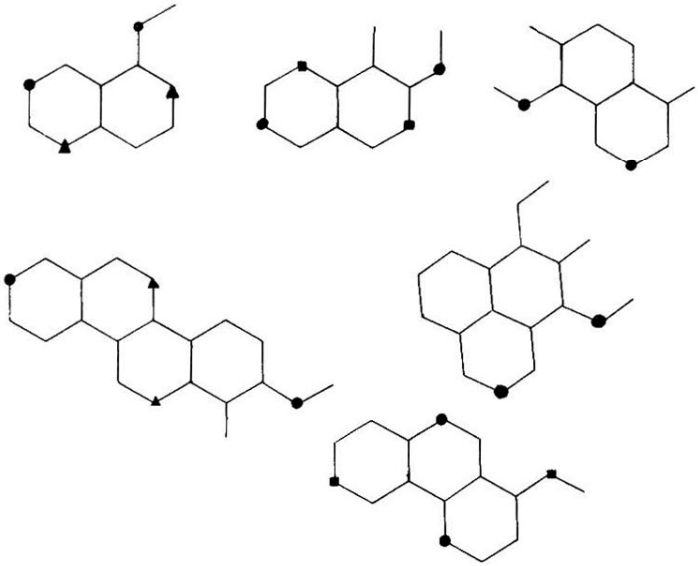
<u>Decyclization process:</u> It is reverse of the cyclization process defined above. An essential symmetry plane forms after the removal of an edge from the given T(A) mate,e.g.,



G(v,e) T(A^{o})

G(v,e')

As it is seen, through all these processes, first the given precursor graph is decomposed into its T(A) mates. Secondly, by reconstructing the suitable mate, one obtains a T(A) graph having fertility which is eventually resolved to the corresponding fertile graph. Below, some condensed fertile graphs are shown. Each set of isospectral points is indicated separately.



3. Concluding remarks:

The methods described in the present study are mostly for the purpose of construction of special types of systems

as based on the matching of T(A) graphs. Although,the concept can be utilized for the purpose of establishing the existing iso-,sub-, and isoabsolutespectral structures between the group of various systems, negative conclusions should not be drawn in the absence of any matching T(A) graphs, because some other furtive topological factors could play role on the spectra of graphs.

Systems containing 4-membered rings possess T(A) mates in which edges having weight greater than 1 exist. These structures constitute a special type of class within themselves ,so that their T(A) graphs hardly ever match with T(A) graphs of any other system having no 4-membered rings. In the case of acyclic structures the matching possibility of the T(A) graphs arises from the mere fact that methylenpropenyl, cyclopropenyl and benzene systems all have the same triad patterns. However, in the family of acyclic structures, methylenpropenyl moiety is the unique subgraph which may lead to a triad pattern. Because of that, T(A) graphs in the acyclic series are less likely to be superimposable with each other as compared to the case in cyclic structures.

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