SOME COMMENTS ON COSPECTRAL GRAPHS

To André Dreiding, on the occasion of his sixtieth birthday, from

Edgar Heilbronner

Physikalisch-chemisches Institut
Universität Basel, Klingelbergstrasse 80
CH-4056 Basel, Switzerland

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ABSTRACT

A method for the construction of simple, connected, bipartite, cospectral graphs is described and illustrated by a few examples.

Using this construction principle, it is shown that the set of simple, connected, bipartite, cospectral graphs with a countably infinite vertex set, but which are locally finite, is uncountably infinite.

1. Preliminary Remarks

The nomenclature used is that of Wilson [1] and of Biggs [2], which in turn derives from the one introduced by Busacker and Saaty [3]. The connex between graph theory and chemistry (if any) is provided through topology conditioned independent electron models [4] by defining an ad hoc pseudo-hamiltonian H, such that its matrix elements

$$H_{uv} = \langle \Phi_u | H | \Phi_v \rangle \tag{1}$$

yield the matrix

$$\mathbf{H} = \beta \mathbf{A} + \alpha \mathbf{E} \tag{2}$$

where ${\bf E}$ is the unit matrix of order n and ${\bf A}=({\bf A}_{\mu\nu})$ the adjacency matrix of the simple graph ${\cal G}$ of order n, the elements ${\bf A}_{\mu\nu}$ of which represent the nearest-neighbour relationship between the two ortho-normal basis orbitals ${\bf \Phi}_{\mu}$ and ${\bf \Phi}_{\nu}$. (For detailed information the reader is referred to the review by Gutman, Graovac and Trinajstić [5]). The vertex set ${\bf V}({\bf G})$, of size n, represents the set of n ortho-normal basis functions $\{{\bf \Phi}_{\mu}\}$, the edge family ${\bf E}({\bf G})$ their interaction matrix elements ${\bf H}_{\mu\nu}$ and the spectrum $\{\lambda_1,\lambda_2,\ldots\lambda_j\ldots\lambda_n\}$ of ${\bf G}$ defines the orbital energies ${\bf E}_{\bf j}=\alpha+\lambda_{\bf j}{\bf B}$.

2. Alternant π -Systems and Bipartite Graphs

In a classical paper Coulson and Rushbrooke showed [6] that π -systems come in two types, alternant and non-alternant ones. Alternant π -systems are characterized, in the sense described in section 1., by a bipartite graph $G(V_{\star}, V_{\odot})$ with vertex sets

of size n* and n° respectively, so that $n=n^*+n^\circ$. By definition the edge family E(G) comprises only edges $e_{\mu\nu}$ between starred (*) and unstarred (0) vertices. Adopting the numbering of vertices specified in (3), the adjacency matrix of the bipartite graph $G(V_*,V_\circ)$ has the form

$$\mathbf{A} = \begin{vmatrix} \mathbf{O}_{+} & \mathbf{a} \\ - & \mathbf{T} \\ \mathbf{a}^{\mathrm{T}} & \mathbf{O}_{0} \end{vmatrix}$$
 (4)

where $\mathbf{0}_{\star}$ and $\mathbf{0}_{\circ}$ are square null-matrices of order n* and n° respectively, where \mathbf{a} is of order n*×n° and \mathbf{a}^{T} its transpose. The matrix \mathbf{A} being symmetric, i.e. $\mathbf{A}^{\mathrm{T}} = \mathbf{A}$, the spectrum

Spec
$$G = \{\lambda_1 - \cdots \lambda_j - \cdots - \lambda_n\}$$
; $\lambda_j = \text{real}$ (5)

of the bipartite graph G consists of n real entries $\lambda_{\mathbf{j}}$.

According to a well known theorem of graph theory, the square of the matrix \mathbf{A} , that is $\mathbf{L} \equiv \mathbf{A}^2$, lists all the walks of length 2 within G. Because of (4), the matrix \mathbf{L} takes the following form

$$\mathbf{L} = \mathbf{A}^2 = \begin{pmatrix} \mathbf{I}_{\star} & \mathbf{O} \\ \mathbf{O}^{\mathrm{T}} & \mathbf{I}_{\mathrm{O}} \end{pmatrix}$$
 (6)

with

$$\mathbf{I}_{\star} = \mathbf{a} \, \mathbf{a}^{\mathrm{T}}; \quad \mathbf{I}_{\mathrm{O}} = \mathbf{a}^{\mathrm{T}} \mathbf{a}. \tag{7}$$

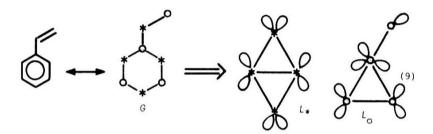
In (7) \mathbf{I}_{\star} and \mathbf{I}_{\circ} are square matrices of order n* and n° respectively, whereas the null-matrix $\mathbf{0}$ is of order n*×n°, and $\mathbf{0}^{\mathrm{T}}$ is its transpose.

If \mathbf{l}_{\star} and $\mathbf{l}_{\scriptscriptstyle O}$ of \mathbf{L} are interpreted as the adjacency matrices of two disconnected graphs l_{\star} and $l_{\scriptscriptstyle O}$, then their vertex sets $\mathrm{V}(l_{\star})$ and $\mathrm{V}(l_{\scriptscriptstyle O})$ satisfy the relationship

$$V(L_{\star}) \equiv V_{\star}(G); V(L_{\Omega}) \equiv V_{\Omega}(G)$$
 (8)

Note that the edge families $\mathrm{E}(L_\star)$ and $\mathrm{E}(L_\mathrm{O})$ comprise loops, so that L_\star and L_O are not simple graphs. Except in the case that G contains circuits of length 4, which we exclude from the present discussion, L_\star and L_O will not exhibit multiple edges.

As an example we use the bipartite graph ${\tt G}$ representing the ${\tt \pi\textsc{-system}}$ of styrene (I):



Short-hand Notation. The number of loops at each vertex v_{μ} of L_{\star} , or v_{ν} of L_{o} equals the degree $\rho(v_{\mu})$ or $\rho(v_{\nu})$ of these vertices in the bipartite graph G. For convenience we shall use in the following sections the convention of replacing the loops at each vertex v_{μ} of L_{\star} , or v_{ν} of L_{o} simply by the number corresponding to the degree of the vertex in the original bipartite graph G, e.g.

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Construction of the L-Graphs from G. To construct L_\star and/or L_O , starting from a given bipartite graph G, proceed as follows: Rewrite the vertices v_μ (v_ν) of the sets $V_\star(G)$ ($V_O(G)$) separately. Link those pairs of vertices v_μ , v_μ , of $V_\star(G)$ (v_ν , v_ν of $V_O(G)$) which are connected in G by a path of length 2, by a single edge $e_{\mu\mu}$, ($e_{\nu\nu}$). (Remember that we are not concerned with those cases where the original bipartite graph G contains circuits of length 4.) Finally add to each vertex v_μ (v_ν) of L_\star (L_O) the degree $\rho(v_\mu)$ ($\rho(v_\nu)$) which it possesses in the original bipartite graph G. This construction procedure is illustrated in (9) and (10).

Symmetry. If $n*\neq n^O$, then L_* and L_O are necessarily different, but even if $n^* = n^O$ (see for example (9) where $n^* = n^O = 4$) L_* will in general not be isomorphic with L_O , except if G exhibits higher symmetry, as for example in the case of the bipartite graph G corresponding to the π -system of naphthalene (II):

However, we shall not discuss the necessary conditions for this to happen.

The matrix L defined in (6) can be considered as the incidence matrix of the union

$$L = L_{\star} \left(\right) L_{0} \tag{12}$$

Because of $L = A^2$ the spectrum

Spec
$$L = \{\Lambda_1, \ldots, \Lambda_j, \ldots, \Lambda_n\}$$
 (13)

consists only of positive eigenvalues $\Lambda_j \geqslant 0$, satisfying the condition $\Lambda_j = \lambda_j^2$ (cf. (5)). Assuming without loss of generality that $n^* \leqslant n^0$, it is easy to show [2][5], starting from a bipartite graph G, that

Spec
$$L = \text{Spec } L_{\star} \bigcup \text{Spec } L_{\circ}$$
 (14)

with

Spec
$$L_{\star} = \{\Lambda_{1} \geqslant \dots \land_{n} \geqslant \dots \land_{n} \star \}$$
 (15)

and

Spec
$$L_o = \{\Lambda_1 \geqslant \dots \land \Lambda_j \geqslant \dots \land \Lambda_{n^*}, \underbrace{0, 0, \dots \ldots 0}_{n^{\circ} - n^* \text{ times}}\}$$
 (16)

It follows that the spectrum of G, see (5), contains at least n^O-n^* zeros and that all other eigenvalues come by pairs $\lambda_j = -\lambda_{n-j+1}$ $j = 1, 2, \ldots, n^*$, a well known result [2][4][5].

3. Cospectral Graphs

As late as 1957 Collatz and Sinogowitz [7] have discovered that, surprisingly, two non isomorphic graphs (necessarily of same order n) can nevertheless possess identical spectra:

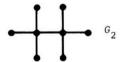
$$G \not \to G'$$
 and Spec $G \equiv Spec G'$ (17)

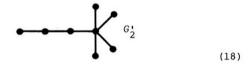
Two such graphs are called <u>cospectral</u> [2] or isospectral [5]. Classical examples are provided by the following pairs [8][9] [10]:



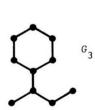


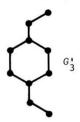
Spec $G_1 = \text{Spec } G_1' = \{2.776, 1.589, 0.276, 0, -1, -1.641, -2\}$





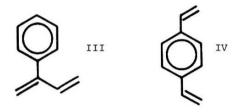
Spec G_2 = Spec G_2 = {±2.303, ±1.303, ±0, ±0}



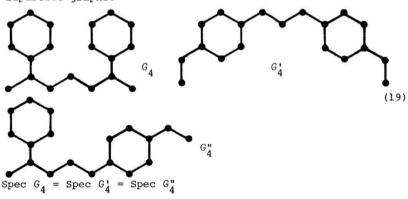


Spec $G_3 = \text{Spec } G_3' = \{\pm 2.214, \pm 1.675, \pm 1, \pm 1, \pm 0.539\}$

Whereas the first pair is "strongly" non-alternant, the other two pairs consist of bipartite graphs, of which the last pair, G_3 , G_3 corresponds, chemically speaking, to the two π -systems of 2-phenylbutadiene (III) and of 1,4-divinylbenzene (IV) respectively.



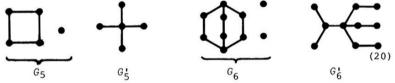
Many other examples have been given by Herndon [9] and by Randic [10], who have used a polynomial method [11] for their derivation. As has already been pointed out by Herndon [9], we note in passing that one is not limited to pairs of cospectral graphs, as exemplified by the following triplet of cospectral, bipartite graphs:



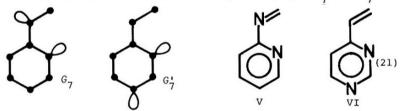
= $\{\pm 2.251, \pm 2.194, \pm 1.795, \pm 1.590, \pm 1.161, \pm 1, \pm 1, \pm 0.811, \pm 0.603, 0\}$

This obviously raises the question, how many non-isomorphic graphs can have the same spectrum, i.e. can be cospectral. The (partial) answer to this problem is that for any positive number K there exists an integer N such that there are at least K non-isomorphic weakly connected digraphs (of order N) or K regular graphs (of order N) which are cospectral [12]. We shall come back to this problem with regard to simple bipartite graphs in section 7.

Before we set out to develop the main theme of this paper, we should perhaps add the following remark: Some of the pairs of cospectral graphs listed in the literature (e.g. [9][10]) are pairs of graphs G, G, of which one or both are disconnected graphs, i.e. they are the union of at least two graphs where in general all but one component are isolated vertices:



Also in some instances, cospectral pairs consist of graphs possessing one or more loops [9], e.g. the graphs G_7 and G_7^* :



In this connection it should be remembered that according to expressions (1) and (2) of section 1. a vertex $\mathbf{v}_{_{11}}$ in a graph \mathcal{G}

representing the topology of a π -system, is interpreted within zeroth order Hückel theory [13] as a 2p basis orbital ϕ_{μ} centered on a carbon atom in position μ . On the other hand a vertex v_{μ} with a single loop $e_{\mu\mu}$ represents a 2p basis orbital ϕ_{μ} of a hetero-atom, in position μ , with higher electro-negativity, e.g. a nitrogen or an oxygen atom. It is in this sense that the "interpretation" of the graphs G_7 and G_7^{\bullet} (shown in (21)) as pertaining to the diaza-aromatic molecules V and VI has to be understood.

In the following section we shall be concerned mainly with "honest" cospectral graphs, by which we mean simple, (connected) graphs without loops and/or multiple edges.

4. Cospectral L-Graphs

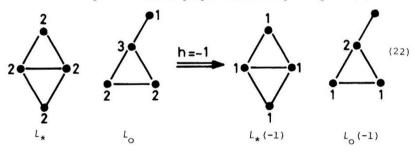
We discuss first a trivial, but potentially useful principle for the construction of pairs of cospectral graphs which follows directly from the contents of section 2.

Given a bipartite graph $G(V_{\star},V_{\scriptscriptstyle O})$ with vertex sets $V_{\star}(G)$ and $V_{\scriptscriptstyle O}(G)$ of same order $n^{\star}=n^{\scriptscriptstyle O}$, we construct the graphs L_{\star} and $L_{\scriptscriptstyle O}$, as shown above. Because of $n^{\star}=n^{\scriptscriptstyle O}$, it follows from (15) and (16) that L_{\star} and $L_{\scriptscriptstyle O}$ are cospectral, even if they are not isomorphic. An example is provided by the pair L_{\star} , $L_{\scriptscriptstyle O}$, which list all the paths of length 2 (between starred or between unstarred vertices) in an arbitrary bipartite graph G with vertex

sets $V_{\star}(G)$, $V_{o}(G)$ of same order, $n^{\star} = n^{o}$, are cospectral.

Note, that for obvious reasons l_{\star} and l_{o} are not "honest" cospectral graphs, because they possess necessarily $\rho(v_{\mu})$ or $\rho(v_{\nu})$ loops at each vertex v_{μ} or v_{ν} , the degrees $\rho(v_{\mu})$ and $\rho(v_{\nu})$ being those of these vertices in the original, bipartite graph G.

Starting with a given cospectral pair L_{\star} , $L_{_{\rm O}}$ we can now construct any number of additional cospectral pairs L_{\star} (h), $L_{_{\rm O}}$ (h) simply by adding (or subtracting) h loops at all the vertices $v_{_{\rm U}}$ of L_{\star} and at all the vertices $v_{_{\rm U}}$ of $L_{_{\rm O}}$. Using the shorthand notation introduced in section 2. (cf. (10)), this is exemplified with respect to the L-graphs shown originally in (9):



The proof is trivial. The spectrum of L_{\star} and of L_{o} is the set of eigenvalues Λ_{j} of I_{\star} or I_{o} (see (6)(14)(15)(16)). Changing the number of loops at all vertices of L_{\star} and of L_{o} by h, yielding L_{\star} (h) and L_{o} (h) is equivalent to changing I_{\star} into I_{\star} + hE and I_{o} into I_{o} + hE (E= unit matrix of order n* = n°). The eigenvalues of I_{\star} + hE and of I_{o} + hE are equal to Λ_{j} + h, i.e. they are simply shifted by h relative to those of I_{\star} and I_{o} . Thus:

Spec $L_{\star}(h) = \{\Lambda_1 + h, \dots, \Lambda_j + h, \dots, \Lambda_{n*} + h\} = \operatorname{Spec} L_o(h)$ (23)

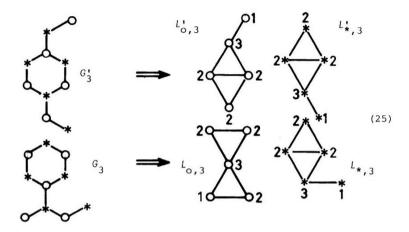
Because of (23) $L_{\star}(h)$ and $L_o(h)$ are cospectral, whatever the value of h. In particular, there is no need that h be an integer.

Of course the result (23) can be generalized for any pair of arbitrary cospectral graphs G, G':

If Spec
$$G$$
 = Spec G' then Spec $G(h)$ = Spec $G'(h)$ (24)

Construction of Cospectral Graphs by the "Wrapping"-Procedure.

Let G and G' be two bipartite graphs of same order, n = n', having vertex sets $V_*(G)$, $V_*(G')$ of same order $n^* = n^*$! (and therefore vertex sets $V_O(G)$, $V_O(G')$ of same order $n^O = n^O$!), but different edge families $E(G) \neq E(G')$. Consequently G and G' are not isomorphic: $G \not\leftarrow G'$. We now construct L_* and L_O from G, and L_* and L_O' from G'. If at least one of the two graphs L_* , L_O of G is isomorphic with at least one of the graphs L_* , L_O' of G' (i.e. $L_* \sim L_Y'$ for at least one of the combinations x,y = **, oo, o*, *o) then G and G' are cospectral. This follows from the results reported in the previous section. An example is provided by the pair G_3 , G_3' shown in (18) of section 3.:

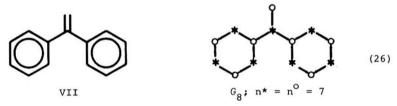


In this particular case we have $L_{\star,3} \sim L_{\star,3}^{*}$ (and also $L_{\star,3} \sim L_{0,3}^{*}$, because of the symmetry of G_{3}^{*}) and therefore G_{3} and G_{3}^{*} are cospectral, as has been shown before by different means (see ref. [5][9] and [10]).

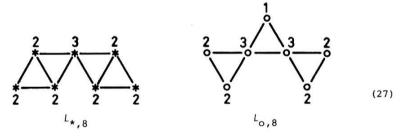
It is obvious that the condition $L_{\mathbf{x}} \sim L_{\mathbf{y}}$ (for at least one of the combinations $\mathbf{x},\mathbf{y} = **,\infty,*\circ,\circ*$) is a sufficent but <u>not</u> a necessary condition for the two bipartite graphs G, G' to be cospectral. An example is provided by the bipartite pair G_2 , G'_2 shown in (18), which incidentally happens to be the cospectral pair of tree-graphs of smallest order. For G_2 we have $n^* = n^0 = 4$ and for G'_2 we have $n^* = 2$, $n^0' = 6$. Therefore G_2 and G'_2 can not yield isomorphic pairs of L-graphs.

This result suggests a rather amusing method for the construction of cospectral, bipartite graphs which we shall name the "wrapping"-procedure (W). Let us assume that a bipartite graph $G(V_{\star},V_{O})$ with edge family E(G) is given. From G we construct L_{\star} (and/or L_{O}) as has been shown above. We now ask the question whether L_{\star} can be "wrapped" by a vertex set V_{O} of same order as $V_{O}(G)$ (and/or L_{O} by a vertex set V_{\star} of same order as $V_{\star}(G)$) using a new edge family $E(G') \neq E(G)$ in such a way, that a new bipartite graph $G' \not\longrightarrow G$ is produced for which $L_{\star}^{!} = L_{\star}$ (and/or $L_{O}^{!} = L_{O}^{!}$) by construction. If this is possible, the G and G' are by necessity cospectral.

Let us demonstrate this "wrapping" procedure for a particular example. We give the bipartite graph G_8 , which corresponds to the π -system of 1,1-diphenylethylene (VII):



From G_8 we construct $L_{\star,8}$ and $L_{o,8}$:



We now add to $L_{\star,8}$ a vertex set $V_{O}(G_8^{\bullet})$ of size $n^{O}=7$ and an edge family $E(G_8^{\bullet})\neq E(G_8)$ (indicated by the dotted lines in the

first diagram of (28)), which "wraps" the graph $L_{\star,8}$ in a valid way, i.e. in such a fashion that $L_{\star,8}$ lists also all the paths of length 2 in the resulting new bipartite graph G_8^{\bullet} . The latter corresponds, within a Hückel model to the π -system of 4-vinylbiphenyl (VIII)

$$L_{\star,8}; \text{ wrapped}$$

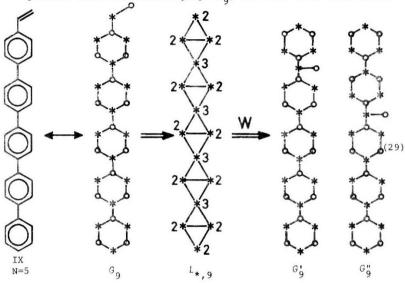
$$VIII$$

Thus, the two graphs G_8 and G_8^{\dagger} ((27) and (28)) are cospectral and consequently 1,1-diphenylethylene (VII) and 4-vinylbiphenyl (VIII) are called "isospectral" molecules, according to the terminology proposed in refs. [5] and [10].

At this stage we shall not further elaborate this procedure for the construction of bipartite, cospectral graphs, but instead illustrate it with some examples chosen at random.

To begin with, we generalize the previous result, starting with the bipartite graph G_9 , which is representative for a paravinyl-substituted polyphenyl containing N benzene moieties. For convenience the case N = 5 is depicted in formula IX and in the graph G_9 of (29). With the starred vertex set $V_*(G_9)$ defined in the diagram of G_9 , the graph $L_{*,9}$ is first obtained as described above. From it we derive by the "wrapping" procedure

(W) two different bipartite graphs G_9^1 and G_9^n which are thus cospectral with the initial graph G_9 , and thus with each other.



The trivial generalization of the particular result presented in (29) is that all the following graphs $G_{10}^{(K)}$, with K = 0,1,2, (N-1)/2, if N = odd, or K = 0,1,2,....N/2 if N = even, are cospectral for a given value of N:

 $K = 0,1,2, \dots (N-1)/2; N \text{ odd}$ $K = 0,1,2, \dots N/2; N \text{ even}$ Here and in the examples below, the subgraph in brackets stands for:

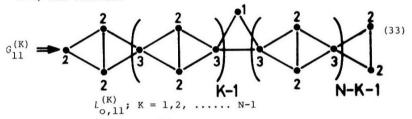
$$\left(\begin{array}{c} \\ \\ \\ \\ \end{array}\right)_{X} \equiv \begin{array}{c} \\ \\ \end{array} \begin{array}{c} \\$$

Note that each graph $G_{10}^{(K)}$ with K > (N-1)/2 for N = odd, or K > N/2 for N = even, is isomorphic by symmetry with one of the previous graphs of the set (30).

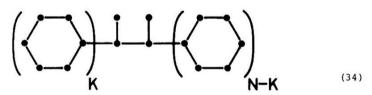
In a similar vein, we can derive a generalization of the pair G_3 , $G_3^{!}$ (cf. (18)) by applying the "wrapping" procedure to the graph $L_{\star,11}^{(K)}$, which yields the sets of cospectral graphs $G_{11}^{(K)}$, each set being characterized by the number N of circuits of length 6:

The two graphs G_3 and G_3^{\dagger} shown in (18) are special cases of (32) with N = 1 and K = 0 and 1.

Whereas the cospectral graphs $G_{11}^{(K)}$ all have the same $L_{\star,11}^{(K)}$ -graph by construction, their $L_{0,11}^{(K)}$ graphs are not isomorphic. Starting with the graphs $G_{11}^{(K)}$ with $K=1, 2, \ldots, N-1$, one obtains:



The graphs $L_{0,11}^{(O)}$ and $L_{0,11}^{(N)}$ derived from $G_{11}^{(O)}$ and $G_{11}^{(N)}$ are unique, in the sense that $L_{0,11}^{(O)}$ does not yield a new cospectral graph other than $G_{11}^{(O)}$ by the "wrapping" procedure, and that $L_{0,11}^{(N)}$ is isomorphic with $L_{\star,11}^{(N)}$ due to the symmetry of $G_{11}^{(N)}$. On the other hand the remaining graphs $L_{0,11}^{(K)}$ presented in (33) can be "wrapped" in such a way that they yield the new set of graphs $G_{12}^{(K)}$, all of which are again cospectral with the graphs $G_{11}^{(K)}$, for a given value of N:



$$G_{12}^{(K)}$$
; $K = 1,2, \dots, (N-1)/2$, $N = \text{odd}$
 $K = 1,2,\dots,N/2$, $N = \text{even}$

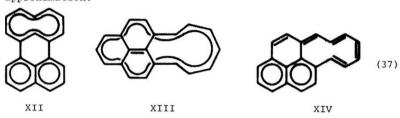
(As before, the set of those graphs with higher K-values is isomorphic with one of the previous graphs). Thus, from a chemical point of view, the following, partially crossconjugated polyphenyls (X,XI) with N>2 benzene moieties form a set of "isospectral" alternant molecules

.....N/2 ; N even

To conclude this section, we domonstrate how the "wrapping" procedure can be used to generate more complicated pairs of cospectral, bipartite graphs, by choosing a self-explanatory example from the work of Herndon [9]:

It has been argued in a previous communication [14] that the fact that two molecules (or their π -systems) are "isospectral" (in the above defined sense) is not relevant for their

chemical and/or physical behaviour. The two π -systems XII and XIII, corresponding to the graphs G_{13} and G_{13}^* respectively are a case in point. Whereas XII consists of a [10]annulene pericondensed to a naphthalene moiety, i.e. two weakly coupled, self-contained π -systems obeying Hückel's rule, the molecule XIII could be looked at as a bridged [18]annulene in a first approximation.



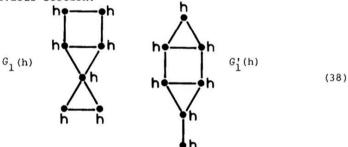
Most probably the latter will undergo second-order bond localization [15], yielding XIV as a lower energy conformer. Obviously the two molecular systems XII and XIII (or XIV) will have very little in common.

6. Construction of Cospectral Graphs from a Set of Simple Cospectral Graphs

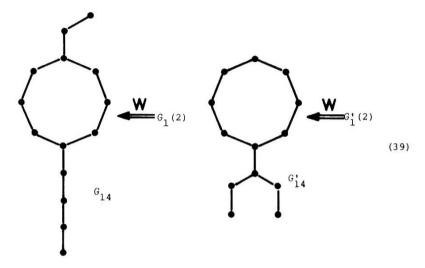
In the previous section we have shown how a bipartite graph G cospectral with a given bipartite graph G can be constructed by applying the "wrapping" procedure to the L_{\star} (or L_{0}) graph of G. We shall now comment briefly on the problem, how a new set of cospectral graphs can be derived from a given set of (simple) cospectral graphs which are not L-graphs, e.g. the pair

of graphs G_1 and G_1^1 shown in (18) of section 3.

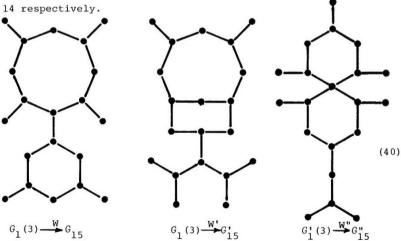
Obviously G_1 and G_1^* , not containing any loops, can not be the graphs listing all paths of length 2 in some bipartite graph. However, according to the rule developed in section 4. and summarised in the formulae (23) and (24), we can transform them into the cospectral pair G_1 (h), G_1^* (h) (e.g. with h = 2 or 3), which are now perfectly good L-type graphs to which the "wrapping" procedure can be applied as in the cases discussed in the previous section.

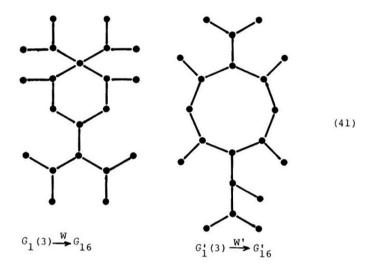


For example, if h is assumed to be 2, so that all the vertices of $G_1(2)$ and $G_1'(2)$ shown in (38) possess two loops, we can add a vertex set V_0 of order $n^0 = 7$ to both $G_1(2)$ and $G_1'(2)$ i.e. of i.e. of same order as the vertex set V_* (with $n^* = 7$) implied by $G_1(2)$ and $G_1'(2)$. Applying the "wrapping" procedure to $G_1(2)$ and then to $G_1'(2)$ yields the following pair of cospectral, bipartite graphs G_{14} and G_{14}' :



On the other hand, if h = 3 is assumed in the two graphs shown in (38), then the triplet of cospectral, bipartite graphs G_{15} , $G_{15}^{"}$, $G_{15}^{"}$ or the pair G_{16} , $G_{16}^{'}$ can be obtained according to the same procedure by adding a vertex set of order n° = 13 or n° =

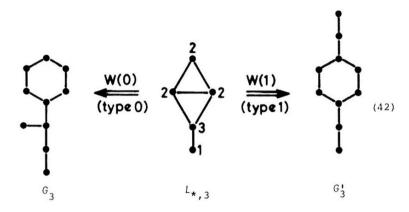




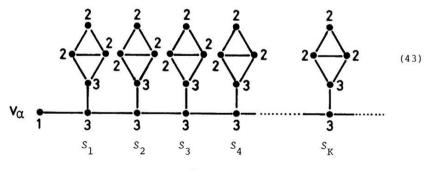
7. A Comment on Infinite Sets of Infinite Cospectral Graphs

To conclude this note, we shall investigate the case of an infinite set of cospectral graphs, by examining one particular case.

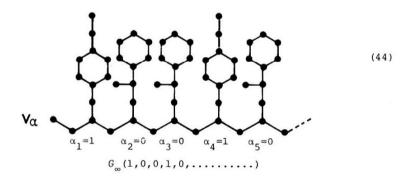
In section 5, formulae (25), it has been shown that the graphs $L_{\star,3} \sim L_{0,3}$ can be "wrapped" to yield either G_3 or $G_3^{!}$, a classical cospectral pair of bipartite graphs. For convenience we name these two different types of "wrapping" W(0) and W(1), i.e. of type 0 and of type 1 respectively:



Consider now the infinite graph L_{∞} shown in (43), which consists of an infinite chain of linked subgraphs S_K with $K=1,2,3,\ldots$. Note that each S_K is identical to $L_{\star,3}$ of (42), except for the fact that the bottom vertex carries now 3 loops instead of a single one in $L_{\star,3}$. The numbering of the subgraphs S_K starts at the left-hand side of L_{∞} , where we have introduced a vertex v_{α} to break the symmetry of the infinite graph L_{∞} .



We now add to each subgraph S_K of L_∞ a vertex set $V_{O,K}$ consisting of $n^O=7$ vertices each. If we now apply the "wrapping" procedure, we can produce a set of infinite bipartite graphs $G_\infty(\alpha_1\alpha_2\alpha_3....\alpha_K....)$ where $\alpha_K=0$ or $\alpha_K=1$ indicates whether the subgraph S_K of L_∞ has been "wrapped" according to W(0) or to W(1). Note that the type of "wrapping" of the subgraph S_K is independent of the type of "wrapping" of the previous subgraphs S_T with I < K. For example:



The vertex set $V(G_{\infty})$ of the infinite, bipartite graph $G_{\infty}=G_{\infty}(\alpha_{1}\alpha_{2}\alpha_{3}.....\alpha_{K}...)$ is countably infinite, independent of the particular type of "wrapping" $W(\alpha_{K})$ of the individual subgraphs S_{K} , i.e. of the α_{K} describing a particular graph G_{∞} . On the other hand it is easy to see that the set of all the infinite graphs $G_{\infty}=G_{\infty}(\alpha_{1}\alpha_{2}\alpha_{4}.....\alpha_{K}...)$ is uncountably infinite.

Indeed, to each of the graphs $G_{\infty} = G_{\infty}(\alpha_1\alpha_2\alpha_3....\alpha_K...)$ corresponds exactly one point $\mathbf{x} = 0.\alpha_1\alpha_2\alpha_3....\alpha_K$ (in binary notation) of the interval $0 < \mathbf{x} < 1$ and not two of these graphs are isomorphic (because of the presence of the vertex \mathbf{v}_{α}). Thus it has been proved, that it is always possible to construct an uncountably infinite set of simple, bipartite and locally finite cospectral graphs on a countably infinite set of vertices.

Acknowledgement

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Addendum: For further reference concerning the spectrum of a graph the reader is referred to the survey by C. Godsil, D.A. Holton and B. McKay [16].

References

- [1] R.J. Wilson, Introduction to Graph Theory, Oliver & Boyd, Edinburgh, 1972.
- [2] N. Biggs, Algebraic Graph Theory, Cambridge University Press, Cambridge, 1974.
- [3] R.G. Busacker and T.L. Saaty, Finite Graphs and Networks, McGraw Hill, New York, 1965.
- [4] H.H. Günthard and H. Primas, Helvetica Chimica Acta 39, 1645 (1956).
- [5] I. Gutman, A. Graovac and N. Trinajstić, Topological Approach to the Chemistry of Conjugated Molecules, Springer Verlag, Berlin, 1977.
- [6] C.A. Coulson and G.S. Rushbrooke, Proc. Cambridge Phil. Soc. <u>36</u>, 193 (1940).
- [7] L. Collatz and U. Sinogowitz, Abh. Math. Sem. Univ. Hamburg, 21, 63 (1957).
- [8] A.T. Balaban and F. Harary, J. Chem. Documentation <u>11</u>, 258 (1971). F. Harary, C. King, A. Mowshowitz and R.C. Read, Bull. London Math. Soc. <u>3</u>, 321 (1971).
- [9] W.C. Herndon, Tetrahedron Lett. 671 (1974), W.C. Herndon and M.L. Ellzey, Tetrahedron 31, 99 (1975).
- [10] T. Zivković, N. Trinajstić and M. Randić, Mol. Physics 30, 517 (1975), M. Randić, N. Trinajstić and T. Zivković, Progress Report 1973 1974, Theoretical Chemistry Department, Oxford University, England; J. Chem. Soc. Faraday Trans. 2, 224 (1976) and references given therein.

- [11] E. Heilbronner, Helvetica Chimica Acta 36, 170 (1953).
- [12] A. Mowshowitz, J. Combinatorial Theory, B <u>12</u>, 177 (1972); R.J. Wilson, in: D.J.A. Welsh and D.R. Woodall, Combinatorics, The Institute of Mathematics and its Applications, Southend-on-Sea, Essex, ().
- [13] A. Streitwieser Jr., Molecular Orbital Theory for Organic Chemists, Wiley & Sons Inc., New York, 1961, E. Heilbronner and H. Bock, The HMO-Model and its Application, Vol. 1 to 3, Wiley-Verlag Chemie, London, 1976.
- [14] E. Heilbronner and T.B. Jones, J. Amer. Chem. Soc. 100, 6506 (1978).
- [15] G. Binsch, E. Heilbronner and J.N. Murrell, Mol. Physics 11, 305 (1966), G. Binsch and E. Heilbronner, Double-Bond Fixation in Linear, Cyclic and Benzenoid π-Electron Systems, in: Structural Chemistry and Molecular Biology, A. Rich and N. Davidson, Edits., W.H. Freeman and Comp., San Francisco, 1968.
- [16] C. Godsil, D.A. Holton and B. McKay, The spectrum of graph, Comb. Math. V, Proc. 5th Aust. Conf., Melbourne 1976, Lect. Notes Math. 622, 91-117 (1977).