

ON THE EXISTENCE OF A HERMITIAN MATRIX WHOSE CHARACTERISTIC
POLYNOMIAL IS THE MATCHING POLYNOMIAL OF A MOLECULAR GRAPH

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(Received: May 5, 1982)

Abstract

Necessary and sufficient conditions are determined under which a Hermitian matrix (with certain special properties) exists, such that its characteristic polynomial is equal to the matching polynomial of a molecular graph. The four theorems proved in the present study generalize a number of previously obtained results [8,9,11].

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INTRODUCTION

In all theoretical schemes for calculating the resonance energy, this quantity is defined as

$$RE = E - E^R$$

where E is the energy (or pi-electron energy) of the corresponding conjugated molecule, whereas E^R is the energy of a suitably chosen reference structure. Various resonance energies which are proposed in the literature, differ essentially in the nature of the reference structure. In the topological resonance energy (TRE) model [1,2], E^R is computed without the knowledge of the actual reference structure. Although the reference energy in the TRE model is precisely and unambiguously defined, the "lack" of the reference structure caused some confusion among the potential users of this method [3].

Herndon et al. [4] were the first to introduce the notion of a kind of reference structure in the TRE model. Namely, they discovered that for certain molecular graphs G a closely related graph G^R with weighted edges can be constructed, such that the characteristic polynomial of G^R coincides with the matching polynomial [5] of G . Then, naturally, G^R could be interpreted as the molecular graph of the reference structure. Unfortunately, the reference graph G^R can be constructed only for a limited number of molecular graphs and, in particular, Herndon's idea is fully inapplicable to condensed polycyclic conjugated systems.

Aihara [8] proposed a completely different approach to the "reference structure problem". To a given graph G he associated a Hermitian matrix $H(G)$, (with complex matrix elements), such that the characteristic polynomial of $H(G)$ is equal to the matching polynomial of G . Since the eigenvalues of a Hermitian matrix are real, Aihara's method provided an elegant demonstration of the reality of the zeros of the matching polynomial. The same approach was also proposed in [9]. In both papers [8] and [9], the consideration was restricted to monocyclic conjugated hydrocarbons (or at most, to non-condensed polycyclic systems, see later). In [10] the method was extended to monocyclic heteroconjugated systems, while in [11] one of the authors constructed the H -matrix for a symmetrical condensed bicyclic molecule as illustrated on the example of naphthalene.

In the present paper we shall examine the construction of $H(G)$ matrices in more detail, with a particular emphasis to the case of condensed polycyclic molecules. We shall demonstrate that the H -matrices exist only under some very specific conditions. A full solution of this problem will be given for the bicyclic case.

The main conclusion of our work is that Hermitian matrices with the desired properties do not exist for the majority of molecular graphs and therefore the approach proposed and elaborated in [8-11] is of limited value as a basis for determining the zeros of the matching polynomial via matrix diagonalization.

The other motivation for the search for H-matrices was to offer a proof of the reality of the zeros of the matching polynomial in a more pictorial manner as compared to the solution [12] reached by using completely different mathematical techniques. Recently it was discovered [13] that the matching polynomial of every graph is contained as a factor in the characteristic polynomial of a certain acyclic graph; the relevance of this result for the theory of TRE is discussed elsewhere [14].

PRELIMINARIES

Let G be the graph representation of the conjugated system under consideration. We shall assume that G is a simple graph, i.e. that G possesses no loops and multiple edges; the weight of every edge of G is equal to unity. The edges of G are not directed, but can be always replaced by a pair of oppositely oriented arcs.

G possesses n vertices which will be labelled by v_1, v_2, \dots, v_n . The edge connecting the vertices v_j and v_k will be labelled by e_{jk} .

The matching polynomial [5] of G is defined as

$$\alpha(G) = \alpha(G, x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k p(G, k) x^{n-2k}$$

with $p(G, k)$ denoting the number of ways in which k independent edges can be selected in G , $k=1, 2, \dots, \lfloor n/2 \rfloor$. In addition, $p(G, 0) = 1$. For more details on the matching polynomial the reader should consult the reviews [6, 15].

The adjacency matrix $A = A(G)$ of the graph G is an $n \times n$ matrix, whose matrix elements are defined as

$$A_{jk} = A_{kj} = 1 \quad \text{if the edge } e_{jk} \text{ exists in } G, \text{ and}$$

$$A_{jk} = 0 \quad \text{otherwise.}$$

Then the characteristic polynomial of the adjacency matrix,

$$\phi(G) = \phi(G, x) = \det(x I - A(G))$$

is called the characteristic polynomial of the graph G .

Let Z_a , $a=1, \dots, r$ be the cycles contained in the graph G .

The matching and the characteristic polynomials are then related as follows [6,16].

$$\begin{aligned} \phi(G) = \alpha(G) - 2 \sum_a \alpha(G-Z_a) + 4 \sum_{a<b} \alpha(G-Z_a-Z_b) - & \quad (1) \\ - 8 \sum_{a<b<c} \alpha(G-Z_a-Z_b-Z_c) + \dots \end{aligned}$$

The size of the cycle Z_a is denoted by $|Z_a|$. Note that the second, third, etc. summations on the right-hand side of eq. (1) go over pairwise disjoint cycles [16].

The technique used in the papers [8-11] is to construct a matrix $H = H(G)$ whose matrix elements are given as

$$H_{jk} = W_{jk} = \exp(i\theta_{jk}) \quad \text{if the edge } e_{jk} \text{ exists in } G, \text{ and} \quad (2a)$$

$$H_{jk} = 0 \quad \text{otherwise,} \quad (2b)$$

In addition, it is assumed that

$$\theta_{jk} = -\theta_{kj} \quad (3)$$

which then implies that H is Hermitian and that

$$W_{jk}W_{kj} = 1 \quad (4)$$

whenever the edge e_{jk} is in the graph G . Of course, θ_{jk} is assumed to be real.

The idea of [8-11] was then to adjust the parameters θ_{jk} so that the characteristic polynomial of the matrix $H(G)$,

$$\phi(H) = \phi(H, x) = \det (xI-H)$$

coincides with the matching polynomial of the graph G ,

$$\phi(H) = \alpha(G). \quad (5)$$

The matrix $H=H(G)$ can be represented by a weighted digraph G^* . In order to construct G^* we have to replace the edges of G by pairs of oppositely directed arcs. A weight W_{jk} is associated with the arc starting at the vertex v_j and ending at the vertex v_k .

Because of (4),

$$\alpha(G^*) = \alpha(G) \quad (6)$$

and if V is any subset of the vertex set of G (or G^*),

$$\alpha(G^*-V) = \alpha(G-V) \quad (7)$$

The matrix which satisfies the conditions (2), (3) and (5) will be called the H -matrix of the graph G . The existence of the H -matrix for monocyclic graphs was demonstrated in [8,9].

In Ref. [9] a failure to construct H-matrix for naphthalene, as an example of condensed polycyclic system, was reported. The solution for this particular question was offered in Ref. [11] by treating θ_{jk} 's as generally variable parameters which idea is also used in the present paper.

GENERAL CONDITIONS FOR THE EXISTENCE OF H(G)

In this section we assume that G is a given molecular graph and that $H = H(G)$ is a matrix satisfying the conditions (2) and (3). We will examine here under which conditions $H(G)$ satisfies also the equation (5).

Let Z be a cycle of the molecular graph G. For reasons of simplicity we shall assume that the vertices v_1 and $v_{|Z|}$ and also v_j and v_{j+1} , $j = 1, \dots, |Z|-1$ are connected in Z. Then we define the function t as

$$t = [W_{12} W_{23} \dots W_{|Z|-1, |Z|} W_{|Z|, 1} + \\ + W_{1, |Z|} W_{|Z|, |Z|-1} \dots W_{32} W_{21}]^{1/2}.$$

From (2) and (3) it follows immediately that

$$t = \cos(\theta_{12} + \theta_{23} + \dots + \theta_{|Z|-1, |Z|} + \theta_{|Z|, 1}). \quad (8)$$

Applying the Sachs theorem [18] to the characteristic polynomial of the digraph G^* and taking into account the relations (6) and (7), it can be shown that

$$\begin{aligned} \emptyset(H) = & \alpha(G) - 2 \sum_a t_a \alpha(G-Z_a) + 4 \sum_{a<b} t_a t_b \alpha(G-Z_a-Z_b) - \\ & (9) \\ & - 8 \sum_{a<b<c} t_a t_b t_c \alpha(G-Z_a-Z_b-Z_c) + \dots \end{aligned}$$

which is fully analogous to eq. (1). Here and later t_a symbolizes the t -function corresponding to the cycle Z_a . Using the terminology of [17], we recognize that the right-hand side of eq. (9) is just the μ -polynomial of the graph G , the weight t_a of the cycles Z_a , $a = 1, 2, \dots, r$ being given by formulas of the form (8). These weights, however, are not independent quantities (as in [17]), but are functions of the parameters \emptyset_{jk} . (The actual independent variables in our problem are the parameters \emptyset_{jk} . They still remain to be determined.)

From eq. (9) we immediately reach the following result.

Theorem 1. The H-matrix exists if and only if there is a choice of the variables \emptyset_{jk} , such that the polynomial $T(X)$,

$$\begin{aligned} T(x) = & \sum_a t_a \alpha(G-Z_a) - 2 \sum_{a<b} t_a t_b \alpha(G-Z_a-Z_b) + \\ & (10) \\ & + 4 \sum_{a<b<c} t_a t_b t_c \alpha(G-Z_a-Z_b-Z_c) - \dots \end{aligned}$$

is identically equal to zero.

Identifying every coefficient of $T(X)$ with zero we obtain a system of (non-linear) homogenous equations in the unknowns t_a , $a = 1, 2, \dots, r$. This system has always solutions, but the obtained t_a 's, $a = 1, 2, \dots, r$ need not always have solutions in \emptyset_{jk} 's, provided, of course, that \emptyset_{jk} 's are real.

One solution of the identity

$$T(x) \equiv 0 \quad (11)$$

can be immediately found, namely

$$t_a = 0 \quad \text{for all } a = 1, 2, \dots, r \quad (12)$$

We will call the system of solutions (12) the trivial solution of the identity (11). In Theorem 2 will be established that in the case of the molecular graphs of condensed polycyclic systems, the trivial solution is incompatible with any choice of the parameters θ_{jk} .

COROLLARY 1.1. In the case of a monocyclic system G , infinitely many $H(G)$ matrices exist.

Proof. For monocyclic systems ($r=1$), eq. (9) has the simple form

$$\phi(H) = \alpha(G) - 2t \alpha(G-Z)$$

and consequently,

$$T(x) = t \alpha(G-Z).$$

Of course, the latter polynomial is identically equal to zero if and only if $t = 0$. Then from (8) we see that any choice of the parameters θ_{jk} , such that

$$\theta_{12} + \theta_{23} + \dots + \theta_{|Z|-1, |Z|} + \theta_{|Z|, 1} = \frac{J}{2} + J\pi$$

($J = \text{integer}$)

results in a H -matrix with the required property (5).

COROLLARY 1.2. If G is polycyclic, but no two cycles of G are condensed, then there exist infinitely many $H(G)$ matrices.

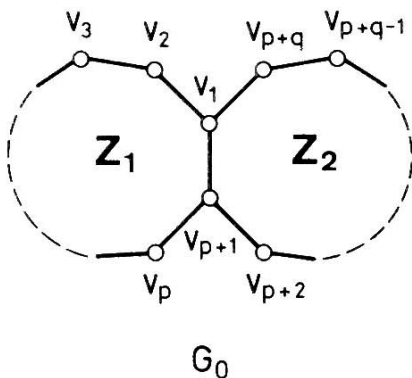
Proof. The assumption that no two cycles of G are condensed means that no edge of G belongs to two or more cycles. Then no two t -functions depend on the same variable θ_{jk} . Hence the trivial solution (12) represents a set of r independent equations, each of which can be solved in the manner described in the Corollary 1.1.

We prove now that Corollary 1.2. can not be extended to arbitrary polycyclic graphs.

THEOREM 2. H -matrices based on the *trivial solution* of (11) exist only for graphs, no two cycles of which are condensed.

Proof. Having in mind Corollary 1.2., we need only to demonstrate that for graphs with condensed cycles, the trivial solution leads to contradictions.

Let us consider first a graph G_0 containing only two condensed cycles Z_1 and Z_2 . Let Z_3 be the cycle obtained as the sum of Z_1 and Z_2 . We shall label the vertices of G_0 as follows.



Hence $|Z_1| = p + 1$, $|Z_2| = q + 1$ and $|Z_3| = p + q$.

The vertices v_1 and v_{p+1} are assumed to be first neighbours, since this is the only chemically relevant case. This assumption has no importance for the following discussion. Arbitrary acyclic side groups can be attached to (some of) the vertices $v_2, v_3, \dots, v_{p-1}, v_p, v_{p+2}, \dots, v_{p+q-1}$ and v_{p+q} .

Let us introduce the notation

$$\alpha = \theta_{12} + \theta_{23} + \dots + \theta_{p-1,p},$$

$$\beta = \theta_{p,p+1} + \dots + \theta_{p+q-1,p+q} + \theta_{p+q,1},$$

$$\gamma = \theta_{p+1,1}.$$

Then the trivial solution $t_1 = t_2 = t_3 = 0$ results in the equations

$$\cos(\alpha + \gamma) = 0, \quad (13a)$$

$$\cos(\beta - \gamma) = 0, \quad (13b)$$

$$\cos(\alpha + \beta) = 0. \quad (13c)$$

From (13a) and (13b) follows

$$\alpha + \beta = \frac{\pi}{2} + I\pi,$$

$$\beta - \gamma = \frac{\pi}{2} + J\pi,$$

where I and J are integers. Therefore

$$\alpha + \beta = (I + J + 1)\pi$$

which is evidently incompatible with (13c). Hence Theorem 2 is verified for the case of two condensed cycles.

Graphs possessing more than two condensed cycles necessarily have a subgraph of the type G_0 . Then the above analysis applies to a part of the trivial solution and shows that even a part of this solution leads to contradictions.

This proves Theorem 2.

THE BICYCLIC CASE

In this section we shall examine in more detail the existence of an H-matrix for the molecular graph of the type G_0 given in the previous section.

Let us for brevity denote

$$G_0 - Z_1 = G_1, \quad G_0 - Z_2 = G_2, \quad G_0 - Z_3 = G_3.$$

Then according to (10),

$$T(x) = t_1\alpha(G_1) + t_2\alpha(G_2) + t_3\alpha(G_3), \quad (14)$$

because the cycles Z_1 , Z_2 and Z_3 have common vertices and therefore [17],

$$\alpha(G_0 - Z_1 - Z_2) = \alpha(G_0 - Z_1 - Z_3) = \alpha(G_0 - Z_2 - Z_3) = \alpha(G_0 - Z_1 - Z_2 - Z_3) = 0.$$

Because of Theorem 2 we will not be interested in the trivial solution $t_1 = t_2 = t_3 = 0$.

We say that the cycles Z_1 and Z_2 are equivalent in the graph G_0 if the subgraphs $G_1 = G_0 - Z_1$ and $G_2 = G_0 - Z_2$ are isomorphic.

THEOREM 3. If the cycles Z_1 and Z_2 are equivalent, then $H(G_0)$ exists.

Proof. If G_1 and G_2 are isomorphic, then $\alpha(G_1) = \alpha(G_2)$ and by identifying (14) with zero we get the system of equations

$$t_1 + t_2 = 0$$

$$t_3 = 0$$

i.e.

$$\cos(\alpha + \gamma) + \cos(\beta - \gamma) = 0 \quad (15a)$$

$$\cos(\alpha + \beta) = 0.$$

It is now easy to verify that the system (15) has (infinitely many) solutions in the variables α, β, γ .

The H-matrix of naphthalene [11] is an example of application of Theorem 3. The actual form of the matrix follows directly from the solutions of the equations (15).

COROLLARY 3.1. If $\alpha(G_1) = \alpha(G_2)$, respective whether G_1 and G_2 are isomorphic or not, $H(G_0)$ exists.

In the case when the cycles Z_1 and Z_2 are non-equivalent, we will distinguish between three possibilities:

- Z_1 and Z_2 are of different size;
- Z_1 and Z_2 are of equal, odd size;
- Z_1 and Z_2 are of equal, even, size.

THEOREM 4a. If $\alpha(G_1) \neq \alpha(G_2)$ and $|Z_1| \neq |Z_2|$, then the H-matrix of G_0 does not exist.

Proof. Using the previously adopted notation, $|Z_1| = p+1$, $|Z_2| = q+1$ and $|Z_3| = p+q$. Without losing the generality of our proof, we can assume that $|Z_1| < |Z_2|$, that is, $p < q$. Note that it is also $|Z_2| < |Z_3|$.

Now, the degree of the polynomials $\alpha(G_1)$, $\alpha(G_2)$ and $\alpha(G_3)$ is $n-p-1$, $n-q-1$ and $n-p-q$, respectively. Then also $T(x)$ in eq. (14) is a polynomial of degree $n-p-1$. Identifying the x^{n-p-1} -coefficient of $T(x)$ with zero, we obtain $t_1 = 0$. Then $T(x)$ becomes $t_2\alpha(G_2) + t_3\alpha(G_3)$, a polynomial of degree $n-q-1$. Identifying the x^{n-q-1} -coefficient with zero, we obtain $t_2 = 0$. Applying this argument once again we can also deduce that $t_3 = 0$. But by Theorem 2 the system $t_1 = t_2 = t_3 = 0$ is not solvable. Therefore the construction of $H(G_0)$ is not possible.

THEOREM 4b. If $\alpha(G_1) \neq \alpha(G_2)$ and $|Z_1| = |Z_2| = \text{odd}$, then the H-matrix of G_0 does not exist.

Proof. Note first that if $|z_1|$ and $|z_2|$ are odd then $|z_3|$ is even. Then directly from the definition of the matching polynomial follows that if $\alpha(G_1)$ is a polynomial of odd powers of x , then $\alpha(G_3)$ is a polynomial of even powers of x , or vice versa. In addition, $2|z_1| > |z_3|$.

Therefore, x^{n-p-q} -coefficient of $T(x)$, eq. (14), must be equal to zero. Hence we obtain $t_3 = 0$. Then $T(x) \equiv 0$ gives the set of equations

$$t_1 p(G_1, k) + t_2 p(G_2, k) = 0$$

for $k = 0, 1, \dots$. Setting $k = 0$ we deduce $t_1 + t_2 = 0$ (because of $p(G_1, 0) = p(G_2, 0) = 1$), which implies

$$t_1 [p(G_1, k) - p(G_2, k)] = 0$$

for $k = 1, 2, \dots$. Now if we set $t_1 = 0$, then also $t_2 = t_3 = 0$ which is impossible. If, however, we set $t_1 \neq 0$, then it must be $p(G_1, k) = p(G_2, k)$ for all k , i.e. $\alpha(G_1) = \alpha(G_2)$, contrary to what was initially assumed.

Therefore no H-matrix exists.

THEOREM 4c. If $\alpha(G_1) \neq \alpha(G_2)$ and $|z_1| = |z_2| = \text{even}$, then the H-matrix of G_0 exists if and only if the following identities are simultaneously fulfilled:

$$p(G_1, k) = p(G_2, k) \text{ for } 0 \leq k < K \tag{16a}$$

and

$$p(G_1, k) = p(G_2, k) + p(G_3, k-K) [p(G_1, K) - p(G_2, K)] \quad (16b)$$

for $k \geq K$,

where $K = |z_1|/2 - 1 = |z_2|/2 - 1$.

Proof. The identity $T(x) \equiv 0$ is equivalent to the system of equations

$$t_1 p(G_1, k) + t_2 p(G_2, k) = 0, \quad k = 0, 1, \dots, K-1$$

$$t_1 p(G_1, k) + t_2 p(G_2, k) + t_3 p(G_3, k-K) = 0, \quad k = K, K+1, \dots$$

First, it can not be $t_1 = t_2 = 0$, because then for $k = K$ we would have $t_3 p(G_3, 0) = 0$, i.e. $t_3 = 0$. Second, for $k = 0$ we have $p(G_1, k) = p(G_2, k) = 1$ and therefore $t_1 + t_2 = 0$. Therefore $t_2 = -t_1 \neq 0$.

Dividing the above equations by $t_1 \neq 0$, we get

$$p(G_1, k) - p(G_2, k) = 0, \quad 0 \leq k < K$$

$$p(G_1, k) - p(G_2, k) + (t_3/t_1) p(G_3, k-K) = 0, \quad k \geq K.$$

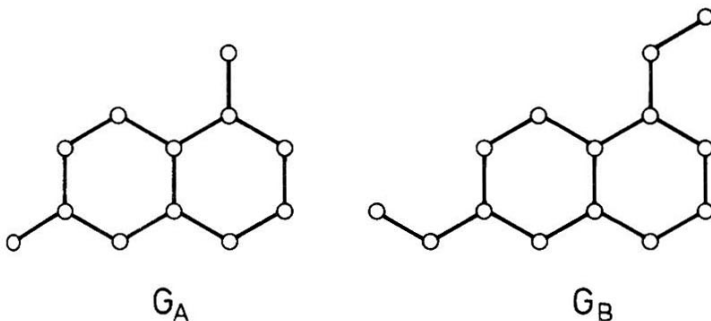
Finally, for $k = K$, $p(G_3, k-K) = p(G_3, 0) = 1$ and thus

$(t_3/t_1) = -[p(G_1, K) - p(G_2, K)]$. The equations (16) follow now straightforwardly.

COROLLARY 4.1. The graphs considered in Theorem 4c have no H-matrix if for at least one k , $0 < k < K$, $p(G_1, k) \neq p(G_2, k)$.

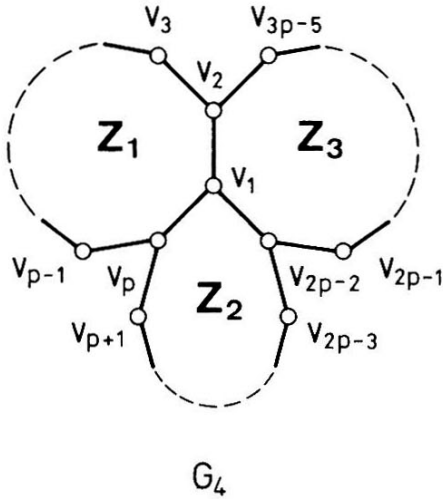
COROLLARY 4.2. The graphs considered in Theorem 4c have no H-matrix if for at least one k , $k \geq K$, $p(G_1, k) = p(G_2, k)$ and $p(G_3, k) \neq 0$.

From Theorem 4c we see that the existence of H-matrix in the case when the non-equivalent cycles Z_1 and Z_2 are of equal size is a rather complicated question. Whether the equations (16) are fulfilled or not, depends on the finer details of the structure of the graph G_0 . Both cases can occur. For example, the graph G_A fulfills all the identities (16) whereas the graph G_B does not. Therefore $H(G_A)$ exists, but $H(G_B)$ does not.



ON THE TRICYCLIC CASE

For particular tricyclic condensed molecular graphs the H-matrix exists. Let us consider the graph G_4



with three equivalent cycles Z_1, Z_2, Z_3 , i.e. with $G_5 = G_4 - Z_1$, $G_6 = G_4 - Z_2$ and $G_7 = G_4 - Z_3$ being isomorphic. Hence $G_8 = G_4 - Z_4$, $G_9 = G_4 - Z_5$ and $G_{10} = G_4 - Z_6$ are isomorphic too, where $Z_4 = Z_1 \cup Z_2$, $Z_5 = Z_2 \cup Z_3$ and $Z_6 = Z_1 \cup Z_3$, respectively. Then according to definition (10)

$$\begin{aligned}
 T(x) = & t_5^\alpha(G_5) + t_6^\alpha(G_6) + t_7^\alpha(G_7) + t_8^\alpha(G_8) + \\
 & + t_9^\alpha(G_9) + t_{10}^\alpha(G_{10}) + t_{11}^\alpha(G_{11})
 \end{aligned}
 \tag{17}$$

where $G_{11} = G_4 - Z_7$ and $Z_7 = Z_1 \cup Z_2 \cup Z_3$. Identifying $T(x)$ with zero one gets the following system of equations

$$\begin{aligned}
 t_5 + t_6 + t_7 &= 0 \\
 t_8 + t_9 + t_{10} &= 0 \\
 t_{11} &= 0
 \end{aligned}
 \tag{18}$$

because of $\alpha(G_5) = \alpha(G_6) = \alpha(G_7)$, $\alpha(G_8) = \alpha(G_9) = \alpha(G_{10})$ and using the fact that $\alpha(G_5)$, $\alpha(G_8)$ and $\alpha(G_{11})$ are polynomials of the mutually different order. Let us introduce the notation

$$\begin{aligned} \theta_{23} + \theta_{34} + \dots + \theta_{p-1,p} &= \tau_1 \\ \theta_{p,p+1} + \theta_{p+1,p+2} + \dots + \theta_{2p-3,2p-2} &= \tau_2 \\ \theta_{2p-2,2p-1} + \theta_{2p-1,2p} + \dots + \theta_{3p-5,2} &= \tau_3 \\ \theta_{p1} = \tau_4, \theta_{1,2p-2} = \tau_5, \theta_{21} = \tau_6 \end{aligned} \quad (19)$$

Then eqs. (18) read as

$$\begin{aligned} \cos(\tau_1 + \tau_4 - \tau_6) + \cos(\tau_2 - \tau_5 - \tau_4) + \cos(\tau_3 + \tau_5 + \tau_6) &= 0 \\ \cos(\tau_1 + \tau_2 - \tau_5 - \tau_6) + \cos(\tau_2 + \tau_3 + \tau_6 - \tau_4) + \cos(\tau_1 + \tau_3 + \tau_4 + \tau_5) &= 0 \\ \cos(\tau_1 + \tau_2 + \tau_3) &= 0 \end{aligned} \quad (20)$$

and the system has infinitely many solutions. A particular "symmetrical" solution is given by

$$\tau_1 = \tau_2 = \tau_3 = \frac{\pi}{2}, \tau_4 = \tau_5 = \pi, \tau_6 = \frac{\pi}{3} \quad (21)$$

In the general case of tricyclic graphs the H-matrix does not exist. In particular, it is not possible to construct the H-matrix of the molecular graph of anthracene [19].

CONCLUDING REMARKS

The main conclusion of our work is that the H(G) matrices do not exist in the general case. Therefore the idea to use the computational advantages of the determination of the

eigenvalues of $H(G)$ instead of the tedious calculation of the zeros of the matching polynomial of G , must be abandoned.

In Theorems 1 and 2 we formulated general graph-theoretical criteria of the existence of $H(G)$. Then a complete solution of the existence problem is obtained for the class of monocyclic (Corollary 1.1) and bicyclic graphs (Theorems 3 and 4).

Our method is in principle capable to treat also the case of tricyclic, tetracyclic, etc. graphs, but the mathematical difficulties of such an analysis would be considerable.

Thus the question of the reference structure in the TRE model remains without a satisfactory answer. If this problem is of any relevance [3], then a completely different approach should be invented for its solution.

ACKNOWLEDGEMENT

The authors thank Dr. R.B. Mallion, Mr. P. Pollak (The King's School, Canterbury) and Prof. O.E. Polansky (Mülheim/Ruhr) for their stimulating discussions and criticism. One of us (A.G.) gratefully acknowledges the financial support of the Max-Planck-Society.

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