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Graphs corresponding to reference polynomial or to circuit characteristic polynomial

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A vertex-weighted graph G^* is studied which is obtained by deleting edge e_{rs} in a circuit of a graph G and giving two vertices v_r and v_s weights $h_r = 1$ and $h_s = -1$, respectively. It is shown that if subgraph $G - v_r$ is identical with subgraph $G - v_s$, then the reference polynomial of G^* is identical with that of G and the characteristic polynomial of G^* contains the contributions due to only a certain part of the circuits found in the original graph G. This result gives a simple way to find a graph whose characteristic polynomial is equal to the reference polynomial in the topological resonance energy theory or to the circuit characteristic polynomial in the circuit resonance energy theory. This approach can be applied not only to Hückel graphs but also to Möbius graphs, provided that they satisfy a certain condition. The significances of this new type of "reference" graph thus obtained are pointed out.

1. Introduction

Reexamination of Hückel molecular orbital theory (HMO) in terms of graph theory [1] has confirmed the topological features of HMO theory [2]. One important finding is that each coefficient of the characteristic polynomial of a graph (HMO secular polynomial) can be obtained by counting the number of edges, circuits, and vertices of certain subgraphs (called Sachs graphs) [3]. This finding led to the definition of a graph-theoretical resonance energy, called the topological resonance energy TRE [4], which is the difference between the total π-electron energy of a conjugated system and that of a hypothetical acyclic reference structure. The polynomial for the hypothetical acyclic reference structure (the reference polynomial) is obtained by deleting all the cyclic component contributions to the coefficients of the characteristic polynomial.

The definition of TRE implies that the stability (or instability) of a conjugated molecule arises from cyclic conjugations of π-electrons and that the driving force for cyclic conjugations of π-electrons is each circuit found in the graph representing the molecule considered. It was verified that the sign of the contribution of each circuit (or each pair of disjoint circuits) in a graph is determined by the number of vertices in the circuit (or by the number of vertices in the two disjoint circuits) [5].

Since the TRE value of a polycyclic conjugated molecule is a complicated function of circuits and pairs of disjoint circuits, we cannot estimate from the TRE value itself the contribution of each circuit (circuit resonance energy) to the TRE of the system. In order to evaluate circuit resonance energy (CRE), Aihara introduced a new polynomial called the circuit characteristic polynomial [6]. This polynomial contains the contribution of only one circuit. It was proved that the sign of CRE for a circuit is determined by the number of vertices in the circuit [7]. The stability of Möbius annulenes shows a tendency opposite to that of Hückel annulenes [8]. It was proved both in the TRE [9] and CRE theory [7] that this is true also for polycyclic molecules.

The roots of the reference polynomial should be real numbers. A way to prove that this is true is to find a graph whose characteristic polynomial is identical with the reference polynomial under the condition that the adjacency matrix of the graph is Hermitean. Many authors in the chemistry literature have tried to find a graph whose characteristic polynomial is identical with the reference polynomial. They succeeded for monocylic graphs and nonfused polycyclic graphs, but did not succeed for fused polycyclic graphs except those with certain symmetries [10–13]. However, in the field of statistical physics, Heilmann and Lieb have proved generally that the roots of the reference polynomial are real numbers [14].

It is not evident what the "reference" structure represented by the reference polynomial is, because the definition of the reference polynomial is purely combinatorial in nature. This is another important problem associated with the reference polynomial. Finding the "reference" graph is necessary to clarify the structure represented by the reference polynomial. In previous papers, by using the knowledge of "reference" graphs, we showed that "reference" structure can be considered to be an intermediate state between Hückel and Möbius graphs [12,13].

A similar difficulty is also found in the CRE theory. It is important in the CRE theory that the roots of the circuit characteristic polynomial are real numbers. By obtaining the graph whose characteristic polynomial is identical with the circuit characteristic polynomial, it was proved that the circuit characteristic polynomial for any circuit in a polycyclic conjugated molecule has no imaginary roots if this molecule is a nonfused polycyclic conjugated molecule or a fused bicyclic system [13,15]. Further, it was shown that the graph represented by the circuit characteristic polynomial is an intermediate system between Hückel and Möbius polycyclic graphs [13]. However, a general proof of this problem has never been given [16].

There is no one-to-one correspondence between a graph and its characteristic polynomial* [18]. Therefore, there can be several different graphs whose characteristic polynomials are identical with the reference polynomial or with the circuit characteristic polynomial. So far, two different types of "reference" graphs have been obtained.

*This problem has been extensively studied as isospectral molecular graphs. See, for example, ref. [17].

The "reference" graph obtained by Herndon and Parkanyi is an edge-weighted graph which is obtained by deletion of an edge from the cyclic part of the molecular graph and weighting of the adjacent edge by the parameter $k = \sqrt{2}$ or $\sqrt{3}$ [10]. Another type of "reference" graph is a directed and edge-weighted graph which is obtained by replacing one edge in a circuit in an original graph with a pair of directed edges with the weight i or –i ($i^2 = -1$) [12, 13].

The purpose of this paper is to present an approach for obtaining a new type of "reference" graph which is a vertex-weighted graph. This approach also enables us to obtain a new type of graph whose characteristic polynomial is identical with the circuit characteristic polynomial.

2. Vertex-weighted graph

Before presenting our approach, let us define several subgraphs of a graph G and give two equations which show the relationship between the coefficients of the characteristic polynomials of the graph and these subgraphs.

Subgraph $G - v_r$ is obtained from a graph G by deleting vertex v_r and the edge(s) including this vertex. Deletion of edge e_{rs} from G gives subgraph $G - e_{rs}$. Subgraph $G - C_j$ is obtained from G by deleting all the vertices in the circuit C_j and all edges including these vertices. Figure 1 shows the subgraphs and three circuits for the naphthalene graph.

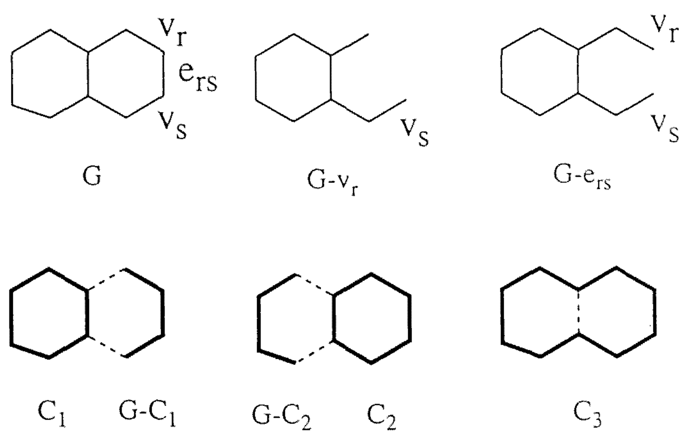

Fig. 1. Subgraphs and circuits of the naphthalene graph.

Let $a_n(G)$ be the coefficents of the characteristic polynomial of a graph G:

$$P(G; X) = \sum_{n=0}^{N(G)} a_n(G) X^{N(G)-n}, \tag{1}$$

where $N(G)$ is the number of vertices in G. Let $a_n^{\mathrm{ac}}(G)$ be the acyclic part of $a_n(G)$ arising from the contributions of acyclic Sachs graphs only, and let $a_n^{\mathrm{c}}(G)$ be the cyclic part of $a_n(G)$ arising from the contributions from cyclic Sachs graphs that contain at least one circuit. The coefficient of the reference polynomial of G is given by the acyclic part of $a_n(G)$, namely, $a_n^{\mathrm{ac}}(G)$ [4].

If G is a graph in which every edge has the weight 1 and every vertex has no weight, then by using Sachs' theorem we can obtain the following recurrence relations:

$$a_n^{\mathrm{ac}}(G) = a_n^{\mathrm{ac}}(G - e_{rs}) - a_{n-2}^{\mathrm{ac}}(G - v_r - v_s) \tag{2}$$

and

$$a_n^{\mathrm{c}}(G) = -2 \sum_j a_{n-N(C_j)}^{\mathrm{ac}}(G - C_j)$$
$$+ (-1)^2 2^2 \sum_j \sum_{k(\neq j)} a_{n-N(C_j)-N(C_k)}^{\mathrm{ac}}(G - C_j - C_k) \ldots . \tag{3}$$

In eq. (3), $N(C_j)$ denotes the number of vertices in circuit C_j, and the first and second sums run over all the circuits and over all possible pairs of disjoint circuits found in G, respectively.

Our new approach uses vertex-weighted graphs. The weighted vertex is denoted by a loop with weight h. Note that a loop is not a circuit. Sachs' theorem allows one to calculate the coefficents of the characteristic polynomial of a vertex-weighted graph G_{VW} as follows [19]:

$$a_n(G_{\mathrm{VW}}) = \sum_{s \in S_n} (-1)^{n(s)} 2^{c(s)} \prod_{r=1}^{m} h_r^{l_r(s)}. \tag{4}$$

Here, S_n is the set of all Sachs graphs of G_{VW} with n vertices; $n(s)$ is the number of the components in Sachs graphs s; $c(s)$ is the number of the circuits in Sachs graphs s; h_r is the weight of vertex v_r; l_r is the number of loops with vertex weight h_r in Sachs graphs s; m is the number of kinds of vertex weights h_r.

Let H be the graph of a (poly)cyclic conjugated molecule without bond alternation or heteroatom(s). Any vertex in H has no weight and any edge has the weight 1. Let e_{rs} be one edge contained in a circuit in H. Suppose that

$$H - v_r = H - v_s. \tag{5}$$

Let H^* be a vertex-weighted graph obtained by giving two vertices v_r and v_s in $H - e_{rs}$ weights $h_r = 1$ and $h_s = -1$, respectively (see fig. 2). We can obtain the following propositions.

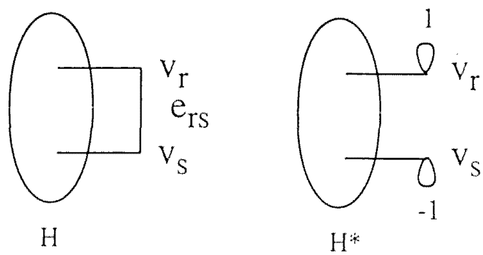

Fig. 2. Graphs H and H^*.

PROPOSITION 1

The reference polynomial of H^* is identical with the reference polynomial of the original graph H,

$$R(H^*; X) = R(H; X). \tag{6}$$

This is the case also for subgraphs such as $H^* - C_j$ and $H^* - C_j - C_k$,

$$R(H^* - C_j; X) = R(H - C_j; X), \tag{7}$$

$$R(H^* - C_j - C_k; X) = R(H - C_j - C_k; X). \tag{8}$$

Equations (6)–(8) show that the pair of vertices v_r and v_s with weight 1 and -1 acts like one edge in the calculations of the coefficients of the reference polynomials of graphs H^* and of subgraphs such as $H^* - C_j$ and $H^* - C_j - C_k$.

PROPOSITION 2

The characteristic polynomial of H^* is expressed in terms of the reference polynomials of graph H and its subgraphs such as $H - C_j$ as follows:

$$P(H^*; X) = R(H; X) - 2\sum_j R(H - C_j; X) + 2^2 \sum_j \sum_{k(\neq j)} R(H - C_j - C_k; X) - \ldots , \tag{9}$$

where the first and second sums run over all the circuits and over all possible pairs of disjoint circuits found in H^*, respectively.

Equation (9) shows that the characteristic polynomial of H^* contains the contributions due to only a part of the circuits found in H, namely the contributions due to only the circuits which do not contain the edge e_{rs} in H.

Proof of propositions 1 and 2

We divide Sachs graphs S_n for graph H^* into four groups, one which does not contain vertex v_r or v_s, one which contains vertex v_r only, one which contains vertex v_s only, and one which contains both of two vertices v_r and v_s. Then by using eq. (4), the coefficient $a_n(H^*)$ is divided into four terms corresponding to the four types of Sachs graphs,

$$a_n(H^*) = a_n(H - e_{rs}) + (-1)h_r a_{n-1}(H - v_r)$$
$$+ (-1)h_s a_{n-1}(H - v_s) + (-1)^2 h_r h_s a_{n-2}(H - v_r - v_s).$$

Since $h_r = -h_s = 1$ and $H - v_r = H - v_s$, the second and third terms of the right-hand side of the above equation cancel each other. Thus, we have

$$a_n(H^*) = a_n(H - e_{rs}) - a_{n-2}(H - v_r - v_s)$$

or

$$a_n^{\mathrm{ac}}(H^*) = a_n^{\mathrm{ac}}(H - e_{rs}) - a_{n-2}^{\mathrm{ac}}(H - v_r - v_s), \tag{10}$$

$$a_n^{\mathrm{c}}(H^*) = a_n^{\mathrm{c}}(H - e_{rs}) - a_{n-2}^{\mathrm{c}}(H - v_r - v_s). \tag{11}$$

Since graph H does not contain h_r or h_s, we can apply eq. (2) to this graph to have

$$a_n^{\mathrm{ac}}(H) = a_n^{\mathrm{ac}}(H - e_{rs}) - a_{n-2}^{\mathrm{ac}}(H - v_r - v_s). \tag{12}$$

From eqs. (10) and (12), it follows that

$$a_n^{\mathrm{ac}}(H^*) = a_n^{\mathrm{ac}}(H). \tag{13}$$

Equation (13) holds for an arbitrary positive integer n. Thus, we have proved eq. (6).

The condition of eq. (5) is satisfied also for subgraphs such as $H - C_j$ or $H - C_j - C_k$. Therefore, in a similar way, we can prove eqs. (7) and (8).

We apply eq. (3) to $H - e_{rs}$ and $H - v_r - v_s$ to have

$$a_n^{\mathrm{c}}(H - e_{rs}) = -2\sum_j a_{n-N(C_j)}^{\mathrm{ac}}(H - e_{rs} - C_j)$$
$$+ (-1)^2 2^2 \sum_j \sum_{k(\neq j)} a_{n-N(C_j)-N(C_k)}^{\mathrm{ac}}(H - e_{rs} - C_j - C_k) \ldots, \tag{14}$$

$$a_n^{\mathrm{c}}(H - v_r - v_s) = -2\sum_j a_{n-N(C_j)}^{\mathrm{ac}}(H - v_r - v_s - C_j)$$
$$+ (-1)^2 2^2 \sum_j \sum_{k(\neq j)} a_{n-N(C_j)-N(C_k)}^{\mathrm{ac}}(H - v_r - v_s - C_j - C_k) \ldots. \tag{15}$$

Equations (14) and (15) allow us to rewrite eq. (11) as follows:

$$a_n^{c}(H^*) = -2\sum_j a^{ac}_{n-N(C_j)}(H - C_j)$$
$$+(-1)^2 2^2 \sum_j \sum_{k(\neq j)} a^{ac}_{n-N(C_j)-N(C_k)}(H - C_j - C_k) + \ldots , \quad (16)$$

where we have used the following equations which are derived from eq. (2):

$$a_n^{ac}(H - C_j) = a_n^{ac}(H - e_{rs} - C_j) - a_n^{ac}(H - v_r - v_s - C_j)$$

and

$$a_n^{ac}(H - C_j - C_k) = a_n^{ac}(H - e_{rs} - C_j - C_k) - a_n^{ac}(H - v_r - v_s - C_j - C_k).$$

Equation (16) holds for an arbitrary positive integer n. From eqs. (13) and (16) we can obtain eq. (9).

So far, we have considered as graph H graphs in which each edge has the weight 1. Möbius-type conjugated molecules are represented by a graph in which some edges have the weight -1 [9]. A circuit in which an odd number of edges have the weight -1 is called a Möbius-type circuit, while a circuit in which an even number of edges have the weight -1 is called a Hückel-type circuit [9]. A Möbius graph is a graph which has at least one Möbius-type circuit [9].

The reference polynomial of any Möbius graph obtained from a parent graph is identical with that of the parent graph [9]. Therefore, proposition 1 is valid also for Möbius graphs without any changes. However, proposition 2 should be rewritten as follows:

PROPOSITION 3

If graph H is a Möbius graph, then the characteristic polynomial of H^* is expressed as follows:

$$P(H^*;X) = R(H;X) - 2\sum_j (-1)^{P(C_j)} R(H - C_j;X)$$
$$+2^2 \sum_j \sum_{k(\neq j)} (-1)^{P(C_j)+P(C_k)} R(H - C_j - C_k;X) - \ldots . \quad (17)$$

Here, $P(C_j)$ is zero for a Hückel-type circuit and 1 for a Möbius-type circuit, and the first and second sums run over all the circuits and over all possible pairs of disjoint circuits found in H^*, respectively.

To illustrate the above results, consider the graph G1 in fig. 3. Graph G1, which is a Möbius graph for anthracene, contains six circuits C_1–C_6. Three circuits C_1, C_4 $(=C_1 + C_2)$ and C_6 $(=C_1 + C_2 + C_3)$ are of Möbius type and the other three circuits C_2, C_3 and C_5 $(=C_2 + C_3)$ are of Hückel type. Two graphs G2 and G3 in fig. 3 are taken to be graphs as H^*. From proposition 2, it is seen that the reference polynomial of the three graphs are identical:

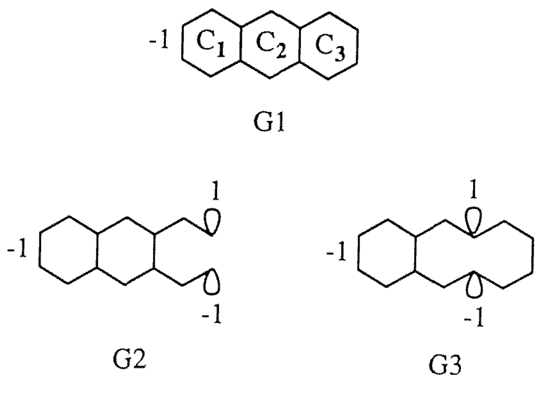

Fig. 3. Möbius anthracene graph G1 and two vertex-weighted graphs G2 and G3.

$$R(\mathrm{G1}; X) = R(\mathrm{G2}; X) = R(\mathrm{G3}; X).$$

From proposition 3, it is seen that the characteristic polynomial of graph G2 contains the contributions of the circuits C_1, C_2, C_4 only:

$$P(\mathrm{G2}; X) = R(\mathrm{G1}; X) + 2R(\mathrm{G1} - C_1; X) - 2R(\mathrm{G1} - C_2, X) + 2R(\mathrm{G1} - C_4; X)$$

and that the characteristic polynomial of graph G3 contains the contributions of the circuits C_1, C_5, and C_6 only:

$$P(\mathrm{G3}; X) = R(\mathrm{G1}; X) + 2R(\mathrm{G1} - C_1; X) - 2R(\mathrm{G1} - C_5; X) + 2R(\mathrm{G1} - C_6; X).$$

3. Graphs corresponding to reference polynomial or to circuit characteristic polynomial

The results obtained above give a simple way to find a graph whose characteristic polynomial is equal to the reference polynomial or to the circuit characteristic polynomial of a given graph.

A graph whose characteristic polynomial is equal to the reference polynomial of an original graph is called a "reference" graph for the original graph. Now it will be evident from proposition 1 that if H is a monocyclic graph, then H^* satisfies the following equation:

$$P(H^*; X) = R(H; X), \tag{18}$$

which shows that graph H^* is a "reference" graph for graph H. In this way, we can obtain a "reference" graph for any monocyclic graph as long as this graph satisfies eq. (5). Figure 4 shows three examples. Graphs on the right-hand side are "reference"

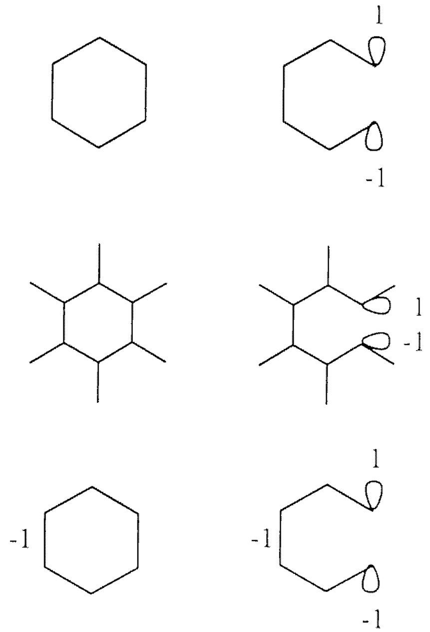

Fig. 4. "Reference" graphs for monocyclic graphs. Graphs on the right-hand side are "reference" graphs for graphs on the left-hand side, respectively.

graphs for the graphs on the left-hand side, respectively. For polycyclic graphs, we cannot obtain "reference" graphs with this method because any graph with one or more pairs of vertices with weights 1 and -1 does not satisfy eq. (5).

The circuit resonance energy for a circuit C_n in a polycyclic graph G is calculated from the roots of the circuit characteristic polynomial given by

$$P(G/C_n; X) = R(G; X) - 2R(G - C_n; X). \tag{19}$$

This polynomial contains the contribution of the circuit C_n only [6,7].

If a graph G^* satisfies

$$P(G^*; X) = P(G/C_n; X), \tag{20}$$

then G^* is a graph which represents a structure corresponding to the circuit characteristic polynomial $P(G/C_n; X)$.

Let us take the graph G4 in fig. 5 as one example. This graph contains three circuits C_1, C_2, C_3 $(=C_1 + C_2)$. From proposition 1, it is seen that for the three graphs G5–G7 in fig. 5

$$P(\text{G5}; X) = R(\text{G4}; X) - 2R(\text{G4} - C_1; X),$$

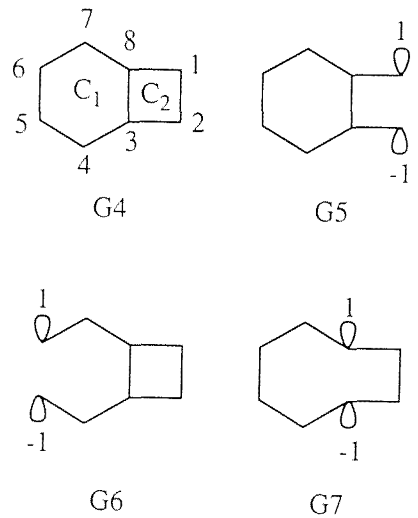

Fig. 5. Graph G4 and graphs G5, G6, and G7 corresponding to circuit characteristic polynomials for G4.

$$P(\mathrm{G6}; X) = R(\mathrm{G4}; X) - 2R(\mathrm{G4} - C_2; X),$$

$$P(\mathrm{G7}; X) = R(\mathrm{G4}; X) - 2R(\mathrm{G4} - C_3; X).$$

Thus, the characteristic polynomials of the three graphs are equal to $P(\mathrm{G4}/C_1; X)$, $P(\mathrm{G4}/C_2; X)$, and $P(\mathrm{G4}/C_3; X)$, respectively. This means that graphs G5, G6, and G7 represent structures corresponding to $P(\mathrm{G4}/C_1; X)$, $P(\mathrm{G4}/C_2; X)$, and $P(\mathrm{G4}/C_3; X)$, respectively. In this way, we can obtain a graph which represents a structure corresponding to the circuit characteristic polynomial of any bicyclic graph as long as the bicyclic graph satisfies eq. (5).

Unfortunately, we cannot apply this method to polycyclic graphs with three or more rings to obtain graphs which satisfy eq. (20) because any graph in which two or more pairs of vertices with weights 1 and -1 exist does not satisfy eq. (5).

The present approach can also be applied to Möbius graphs. If circuit C_n is of Möbius-type, then eq. (20) should be rewritten as follows [7]:

$$P(G/C_n; X) = R(G; X) + 2R(G - C_n; X). \tag{21}$$

One example is shown in fig. 6. Graph G8 is a Möbius graph for graph G4. From eq. (9), it is seen that the characteristic polynomial of graph G9 has only a contribution of the Möbius-type circuit C_1:

$$P(\mathrm{G9}; X) = R(\mathrm{G8}; X) + 2R(\mathrm{G8} - C_1; X).$$

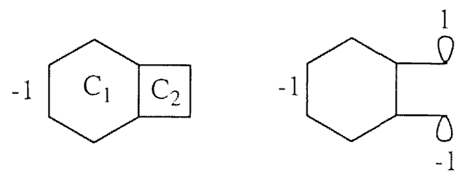

Fig. 6. Möbius graph G8 and graph G9 corresponding to the circuit characteristic polynomial for G8.

This equation shows that graph G9 represents a structure corresponding to the circuit characteristic polynomial for Möbius circuit C_1 in G8.

4. Concluding remarks

A vertex-weighted graph G^* which is obtained by deleting edge e_{rs} in a circuit of a graph G and by giving two vertices v_r and v_s weights $h_r = 1$ and $h_s = -1$, respectively, was studied. It was shown that under a certain condition, the reference polynomial of G^* is identical with that of G and the characteristic polynomial of G^* contains the contributions due to only the circuits which do not contain the edge e_{rs} in G.

From this result, we obtained a simple way to find a graph whose characteristic polynomial is equal to the reference polynomial in the TRE theory or to the circuit characteristic polynomial in the CRE theory. This approach can be applied not only to Hückel graphs but also to Möbius graphs, provided that they satisfy a certain condition.

There can be several different graphs whose characteristic polynomials are identical with the reference polynomial for a graph. Since in the present paper we have obtained a new type of "reference" graph, we now have three different types of "reference" graph. The "reference" graph obtained in the present paper is a vertex-weighted graph (type I). Herndon and Parkanyi's "reference" graph is an edge-weighted graph (type II) [10]. The "reference" graphs of type I and II have one edge less than the original graph. However, it is not always necessary that a reference structure has one edge less than the corresponding real molecular graph. In previous papers, we obtained another type of "reference" graph which is a directed and edge-weighted graph (type III). It should be noted that none of them is a simple open chain analogue of the original graph, but an edge-weighted or vertex-weighted graph with unusual weight(s).

The study of the relationship between the three systems, Hückel, Möbius, and "reference", helps us in understanding aromaticity, because the stability of Möbius systems shows a tendency opposite to that of Hückel systems. In previous papers [12,13], we pointed out that the "reference" graph of type III can be considered to be an intermediate state between Hückel and Möbius graphs and that graphs representing the circuit characteristic polynomial are intermediate systems between corresponding Hückel and Möbius polycyclic graphs. Another close relationship is also found between the "reference" graphs of types I and III and a Möbius graph. Group theory allows one to decompose the spectrum of a (Hückel) graph with certain symmetry into the spectra of smaller graphs [20]. This holds also for Möbius graphs. Knowledge of the "reference" graph is necessary in the study of the decomposition of the spectrum of the Möbius graph in order to identify the smaller graphs obtained in the decomposition. From the knowledge of the "reference" graph, for example, we can identify the graphs obtained in the decomposition of the spectrum of Möbius [$2n$]annulene graphs with plane symmetry (or with the rotation symmetry about a C_2 axis), which are the "reference" graphs of type I (or III) for an [n]annulene graph. A similar result holds also for the graphs corresponding to the circuit characteristic polynomial. Details will be given elsewhere.

The circuit resonance energy defined by Aihara [6] is given by the difference between the HMO total energy calculated from the circuit characteristic polynomial and that calculated from the reference polynomial. Another type of circuit resonance energy can be defined as the difference between the HMO total energy calculated from the characteristic polynomial and that calculated from the polynomial which does not have only the contribution of a circuit. Gutman and Bosanac used this approach and considered a polynomial given by

$$P(G/C_n; X) = P(G; X) + 2R(G - C_n; X) \tag{22}$$

to be a polynomial which does not have the contribution of a circuit C_n to the characteristic polynomial of a graph G [21]. However, it was pointed out by Herndon that the roots of the polynomial $P(G/C_n; X)$ for some molecules are imaginary numbers [22]. As shown in section 2 and in previous papers [12,13], we cannot delete only the contribution of one circuit from the characteristic polynomial of a graph G. In other words, deletion of the contribution of a ring (fundamental circuit) accompanies the deletion of other circuit(s) which contain the ring. Therefore, it is more reasonable to use, instead of eq. (22), a polynomial which does not have the contribution of a ring (and also circuit(s) which contains the ring) to the characteristic polynomial of a graph G. This polynomial is given, for instance, by the characteristic polynomial of the graph H^* discussed above. Then it is ensured that all the roots of this polynomial are real numbers because the adjacency matrix of graph H^* is Hermitean. Application of this new type of circuit resonance energy will be studied elsewhere.

References

[1] F. Harary, *Graph Theory* (Addison–Wesley, Reading, 1969).

[2] A. Graovac, I. Gutman and N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules* (Springer, Berlin, 1977);
I. Gutman and O.E. Polansky, *Mathematical Concept in Organic Chemistry* (Springer, Berlin, 1986).

[3] H. Sachs, Publ. Math. (Debrecen) 11(1963)119.
[4] J. Aihara, J. Am. Chem. Soc. 98(1976)2750;
I. Gutman, M. Milun and N. Trinajstić, J. Am. Chem. Soc. 99(1977)1692.
[5] H. Hosoya, K. Hosoi and I. Gutman, Theor. Chim. Acta 38(1975)37.
[6] J. Aihara, J. Am. Chem. Soc. 99(1977)2048.
[7] N. Mizoguchi, Chem. Phys. Lett. 158(1989)383.
[8] E. Heilbronner, Tetrahedron Lett. (1964) 1923;
H.E. Zimmerman, J. Am. Chem. Soc. 88(1966)1564; *Quantum Mechanics for Organic Chemistry* (Academic Press, New York, 1975);
M.J.S. Dewar and R.C. Dougherty, *The PMO Theory of Organic Chemistry* (Plenum Press, New York, 1975).
[9] N. Mizoguchi, J. Phys. Chem. 92(1988)2754; J. Math. Chem. 7(1991)325.
[10] W.C. Herndon and C. Parkanyi, Tetrahedron 34(1978)3419;
W.C. Herndon and M.L. Ellzey, Jr., J. Chem. Inf. Comput. Sci. 19(1979)260.
[11] J. Aihara, Bull. Chem. Soc. Japan 52(1979)1529;
L.J. Schaad, B.A. Hess, Jr., J.B. Nation and N. Trinajstić, Croat. Chem. Acta 52(1979)233;
A. Graovac, Chem. Phys. Lett. 82(1981)248;
I. Gutman, A. Graovac and B. Mohar, MATCH 13(1982)129;
A. Graovac and O.E. Polansky, MATCH 21(1986)33, 81.
[12] N. Mizoguchi, J. Am. Chem. Soc. 107(1985)4419.
[13] N. Mizoguchi, Bull. Chem. Soc. Japan 63(1990)765.
[14] O.J. Heilman and E.H. Lieb, Commun. Math. Phys. 25(1972)190.
[15] M. Lepović, I. Gutman, M. Petrović and N. Mizoguchi, J. Serb. Chem. Soc. 55(1990)193.
[16] I. Gutman and N. Mizoguchi, J. Math. Chem. 5(1990)81.
[17] N. Trinajstić, *Chemical Graph Theory* (CRC Press, Boca Raton, 1983).
[18] I. Gutman and N. Mizoguchi, Bull. Chem. Soc. Japan 63(1990)1083.
[19] N. Trinajstić, Croat. Chem. Acta 49(1977)593.
[20] R.A. Davidson, Theor. Chim. Acta 58(1981)193;
B.J. McClelland, J. Chem. Soc. Faraday Trans. II 70(1979)1453; 78(1982)911; Mol. Phys. 45(1982)189;
S.S. D'Amato, Mol. Phys. 37(1979)1363; Theor. Chim. Acta 53(1979)319;
M. Shen, Int. J. Quant. Chem. 38(1990)551.
[21] S. Bosanac and I. Gutman, Z. Naturforsch. 32a(1977)10;
I. Gutman and S. Bosanac, Tetrahedron 33(1977)1809.
[22] W.C. Herndon, J. Am. Chem. Soc. 104(1982)3541.