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Möbius Molecules and Graphs*

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Möbius molecules and graphs are discussed. A brief discussion of the *generalized* graphs is also given. The extended Sachs formula for Möbius graphs (and generalized graphs) is reported and some examples discussed. The parity of the algebraic structure of Möbius molecules are defined.

In recent years the use of the Hückel-Möbius concept[1] is becoming increasingly popular[2-4] for studying molecules and reactions.

Möbius systems are defined[5] as cyclic arrays of orbitals in which there is *one* sign inversion, or more generally, in which there is an *odd* number of sign inversions resulting from the negative overlaps between the adjacent orbitals of different sign. Möbius cyclic polyenes (called Möbius annulenes) may appear in solution as possible twisted conformational forms of higher annulenes[6] $(CH)_n$, $n > 20$. Möbius-like structures may also appear as transition states in the electrocyclic closures of linear polyenes. For example, the conrotatory closure of butadiene and the disrotatory closure of hexatriene should prefer the Möbius transition state[1,7]. On the other hand, annulenes are composed of orbital arrays in which there is *no* sign inversion, or more generally, in which there is an *even* number of sign inversions (positive-negative overlaps) among the adjacent $2p_z$-orbitals. These molecules are called Hückel molecules because they obey the Hückel rule[8] which says that a planar cyclic polyenes with $4m + 2$ π-electrons (where m is an integer) should be stable and aromatic compounds. However, the Hückel systems with $4m$ π-electrons are predicted to be very reactive and antiaromatic species. The chemistry of annulenes is in accordance with this rule[6,9,10]. For Möbius systems it is predicted[5,11] that the systems with $4m$ π-electrons would exhibit aromatic stability whereas those with $4m + 2$ π-electrons would be antiaromatic. Therefore, the Möbius systems would display anti-Hückel properties and are indeed often called[12] »anti-Hückel systems«.

The aim of the present work is to show that graph-theoretical considerations can be extended to Möbius systems and, consequently, that a number of important pieces of information about these systems can be extracted from simple graphical (graph-theoretical) rules. Graph theory is widely applied to Hückel systems[13] and a number of interesting results are obtained[14-23]. Hückel

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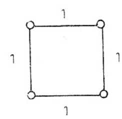
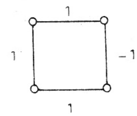
systems can be represented by *Hückel graphs* which correspond to π-network of a conjugated molecule. Thus, the correspondence between the Hückel molecules and Hückel graphs is one-to-one. Since the Hückel Hamiltonian can be written in matrix form as a unique function of the Hückel graph[24], the equivalence between the Hückel theory and the graph spectral theory is established[24-26].

In order to extend the graph-theoretical approach to Möbius systems we need to define a *new* type of graphs which we will call *Möbius graphs**. The weight of edges[13] in these graphs is either $+1$ or -1 depending on whether two $2p_z$-atomic orbitals in a Möbius molecule are in the positive-positive $(+1)$ or in the positive-negative (-1) overlap relationships, respectively. In our previous works[13] we have studied only graphs with the edge weight of $+1$. As an example, we give below graphs which correspond to Hückel (G_1) and Möbius (G_2) cyclobutadienes, respectively.





The location of the connectivity -1 between two vertices in the Möbius graphs of annulene is arbitrary. However, the important information is given that one (odd) sign inversion exists in the structure called Möbius cyclobutadiene.

Note that the Möbius graphs discussed here are a special case of more general graphs with an arbitrary number of -1 edges which we call *the generalized graphs***. Generalized graphs occur, for example, when the graph theory is applied to systems treating the relationships between the people, thus, the $+1$ edge would symbolized the attraction between two persons, 0 indifference, and the -1 edge repulsion. In another words, in the case of generalized graphs there are two distinctive, binary relations[13], but of opposite meaning between the pairs of elements of a system. The system is then fully defined when the binary relations between all pairs of elements are established.

Möbius graphs can be also described by the (vertex) adjacency matrix[28] $\mathbf{A}(G)$ of a special type, defined as follows:

$$A_{rs} = \begin{cases} 1 & \text{if there is a positive edge between the adjacent vertices r and s} \\ 0 & \text{if } r = s\text{, or if there is no edge of any kind between the vertices r and s} \\ -1 & \text{if there is a negative edge between the adjacent vertices r and s} \end{cases}$$

* There should be no confusion with the Möbius ladder graphs, which are derived from a circuit graph containing an even number of points by adding new edges joining each pair of opposite vertices (See, for example, N. Biggs, *Algebraic Graph Theory*, Cambridge University Press 1974, p. 20).

** There are some proposals to label these graphs differently such as the extended graphs[27], and consequently to call the theory the Extended Graph Theory.

The following matrices assigned to Hückel and Möbius cyclobutadiene graphs, respectively, may be considered as their vertex adjacency matrices:

$$\mathbf{A}\,(\mathrm{G}_1) = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} \qquad \mathbf{A}\,(\mathrm{G}_2) = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$

Now, we wish to demostrate how the structure of the Möbius graph is related to the various coefficients appearing in the characteristic polynomial $P\,(\mathrm{G},\,\mathrm{x})$ of the vertex adjacency matrix:

$$P\,(\mathrm{G},x) \equiv \det \left| x\,\mathbf{1} - \mathbf{A} \right| = \sum_{n=0}^{N} a_n\, x^{N-n} \tag{1}$$

of such a graph with N vertices, where a_n are the coefficients of the characteristic polynomial, and to show also that the construction of the characteristic polynomial appropriate to a Möbius graph is, once again[29], a purely combinatorial problem. Evaluation of the coefficients a_n of the characteristic polynomial corresponding to a Möbius graph may be carried out in the same way as described by Graovac *et al.*[30] for Hückel graphs using the Sachs formula[31]. However, in order to do that, we have to extend the original Sachs formula to cover both Hückel and Möbius graphs. We give below the extended Sachs formula:

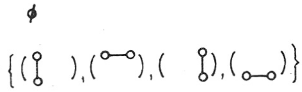
$a_0 = 1$ *(per definitionem)*

$$a_n = \sum_{\mathrm{SGS}} (-)^{c(\mathrm{s})\,+\,pr(\mathrm{s})}\; 2^{r(\mathrm{s})} \quad \text{for } 1 \leqslant n \leqslant N \tag{2}$$

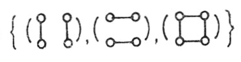
where the symbols have the following meaning: s denotes a Sachs graph[30], S_n is a set of all Sachs graphs (with n vertices) of a graph G, c(s) is the total number of components of a Sachs graphs s, r(s) is the number of rings of a Sachs graph s, and finally $\mathrm{p}_{r(\mathrm{s})}$ is the number of -1 edges in the rings of Sachs graph s. The summation in (2) is over all elements of the set S_n.

We shall illustrate the application of the extended Sachs formula to Möbius cyclobutadiene. First all Sachs graphs of G_2 should be constructed:

$S_1 = \phi$

$S_2 =$ 

$S_3 = \phi$

$S_4 =$ 

Then, we use formula (2) in order to evaluate a_n's:

$a_0 = 1$
$a_1 = 0$
$a_2 = 4\,(-)^{1+0}\,2^0 = -4$
$a_3 = 0$
$a_4 = 2\,(-)^{2+0}\,2^0 + (-)^{1+1}\,2^1 = 4$

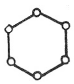
Finally, the following characteristic polynominal is obtained:

$$P(G_2, x) = x^4 - 4x^2 + 4; \ \{ x = \sqrt{2}, \sqrt{2}, -\sqrt{2}, -\sqrt{2} \}$$

It can be compared with the characteristic polynomial belonging to Hückel cyclobutadiene:

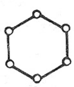
$$P(G_1, x) = x^4 - 4x^2; \ \{ x = 2, 0, 0, -2 \}$$

Obviously polynomials $P(G_1, x)$ and $P(G_2, x)$ differ only in the value of the a_N ($N = 4$) coefficient. Similar result can be also obtained for Hückel (G_3) and Möbius (G_4) benzenes:



G_3

$$P(G_3, x) = x^6 - 6x^4 + 9x^2 - 4; \ \{ x = 2, 1, 1, -1, -1, -2 \}$$



—1

G_4

$$P(G_4, x) = x^6 - 6x^4 + 9x^2; \ \{ x = \sqrt{3}, \sqrt{3}, 0, 0, -\sqrt{3}, -\sqrt{3} \}$$

A general characteristic feature of all monocyclic Hückel and Möbius systems is that they differ in the value of the a_N coefficinet only. (This is not surprising because monocyclic systems contain the cycles only in S_N set of Sachs graphs). This coefficient provides information about the chemical stability, namely, the non-vanishing a_N value indicates[30] the closed-shell stability and aromaticity, whereas $a_N = 0$ is characteristic[16,30] of monocyclic systems with open-shell reactivity and antiaromaticity. This can then be used for a very simple classification scheme of all $4m + 2 \equiv 2 \pmod 4$[31a] and $4m \equiv 0 \pmod 4$[31a] generalized monocyclic systems:

$$a_N = -4; \ e.g. \ a_N \neq 0 \ \begin{cases} \text{Hückel } (4m+2)\text{-systems} \\ \text{Möbius } (4m)\text{-systems} \end{cases}$$

$$a_N = 0 \ \begin{cases} \text{Hückel } (4m)\text{-systems} \\ \text{Möbius } (4m+2)\text{-systems} \end{cases}$$

Another property of coefficient a_N is also interesting; a_N is related[30,32] to the number of *even* (K^-, parity $= +1$) and *odd* (K^-, parity $= -1$) Kekulé structures[32] ($K = K^+ + K^-$) of Hückel molecules:

$$a_N = (-)^{N/2} \left| K^+ - K^- \right|^2 \tag{3}$$

The parity of a Kekulé structure can be obtained using the following rule[30,33,34]: *two Kekulé structures have opposite (identical) parities if the superposition of the corresponding Kekulé graphs contains odd (even) number of (4m)-membered rings.* The Eq. (3) could be applied to Möbius systems. However, it is more appropriate to call the structures of Möbius systems related to the Kekulé structures of Hückel systems *algebraic structures* (AS), because they are related to permutation matrices in exactly the same way as Kekulé structures[33,35]. Thus, Kekulé structures of Hückel molecules are just a special case of the algebraic structures which thus cover both Hückel and Möbius systems. Therefore, eq. (3) can be more appropriately rewritten as follows:

$$a_N = (-)^{N/2} \left| (AS)^+ - (AS)^- \right|^2 \tag{4}$$

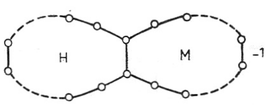
where $(AS)^+$ and $(AS)^-$ are the algebraic structures of even and odd parity. Now, we need define the parity of algebraic structures. We denote graphs corresponding to algebraic structures by h_a, h_b, ... Let the superposition graph of h_a and h_b be labelled as S_{ab}. Let also the number of Hückel-type ring components of the size 0 (mod 4) in the superposition graph S_{ab} be $H(S_{ab})$ and the number of Möbius-type ring components of size 2 (mod 4) in S_{ab} be $M(S_{ab})$. Furthermore, let $p = +1$ for even and $p = -1$ for odd algebraic structure. Then, the equation

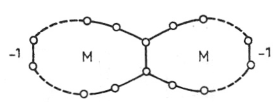
$$p_a p_b = (-)^{H(S_{ab}) + M(S_{ab})} \tag{5}$$

completely determines the parity of algebraic structures. Namely, two algebraic structures h_a and h_b are of the *same* parity if, and only if, the sum of $H(S_{ab}) + M(S_{ab})$ is *even*.
The use of formulae (4) and (5) is illustrated for Hückel and Möbius cyclobutadienes and benzenes, respectively, in Table I.

The total π-electron energies ($E = N\alpha + \sum_{i=1}^{N/2} x_i \beta$) of Hückel ($E_\pi^H = 4\alpha + 4\beta$) and Möbius ($E_\pi^M = 4\alpha + 4\sqrt{2}\,\beta'$; $\beta' = \beta \cos \pi/N$; $N = 4$) cyclobutadienes are equal ($E_\pi^H = E_\pi^M$). However, Hückel cyclobutadiene has a reactive open-shell configuration whereas Möbius cyclobutadiene has a closed-shell configuration. This is a general characteristics of 4m systems. The situation is different for $4m + 2$ systems. Thus, Hückel benzene has $E_\pi^H = 6 + 8\beta$, whereas Möbius benzene has $E_\pi^M = 6\alpha + 6\beta$ ($E_\pi^M = 6 + 4\sqrt{3}\,\beta'$; $\beta' = \beta \cos \pi/N$; $N = 6$); the difference being 2β in favour of Hückel benzene. Hückel $4m + 2$ systems have always larger values of E_π than the corresponding Möbius systems. However, this difference for a very large system is negligible ($\beta' \rightarrow \beta$ for $N \rightarrow \infty$).

We have also considered extension of these studies to some bicyclic systems which could be classified as Hückel-Möbius (G_5) and Möbius-Möbius (G_6) systems, respectively, (where the individual Möbius part has only one



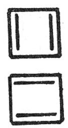
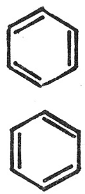
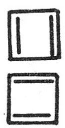
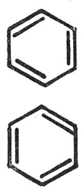


phase dislocation, *i. e.* -1 edge).* Hückel-Möbius graphs (G_5) considered here consist of two rings which have only two vertices and an edge in common. One ring is a Hückel-type cycle (H) and the other a Möbius-type cycle (M).

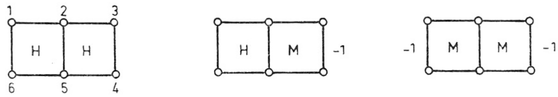
* In general, the β-parameter of the theory is different in Hückel (β) and Möbius (β′) parts of Hückel-Möbius bycyclic molecules. Since we are here interested only in giving a qualitative study, the difference between β and β′ is neglected. However, a very general Sachs formula[36] for graphs with edges of different weights could be applied.

TABLE I

Parity of algebraic structures of Hückel and Möbius cyclobutadienes and benzenes

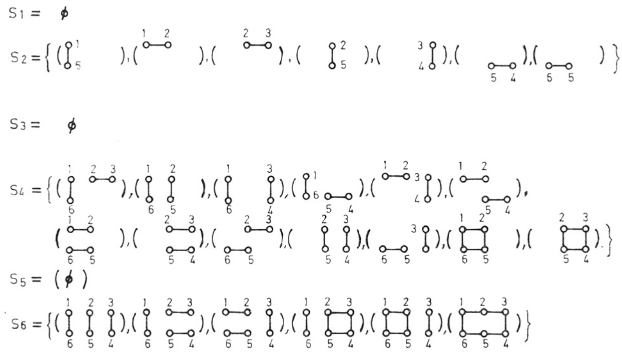
Molecule	Algebraic structure	Super-position of algebraic structues	Parity of algebraic structures	$a_N = (-)^{N/2} \mid (AS)^+ - (AS)^- \mid^2$
Hückel cyclobutadiene			assumed: + 1 calculated: — 1 $\left\{ \begin{array}{l} H\,(S_{ab}) = 1 \\ M\,(S_{ab}) = 0 \end{array} \right.$	0
Hückel benzene			assumed: + 1 calculated: + 1 $\left\{ \begin{array}{l} H\,(S_{ab}) = 0 \\ M\,(S_{ab}) = 0 \end{array} \right.$	— 4
Möbius cyclobutadiene	 — 1 — 1	 — 1	assumed: + 1 calculated: + 1 $\left\{ \begin{array}{l} H\,(S_{ab}) = 0 \\ M\,(S_{ab}) = 0 \end{array} \right.$	— 4
Möbius benzene	 — 1 — 1	 — 1	assumed: + 1 calculated: — 1 $\left\{ \begin{array}{l} H\,(S_{ab}) = 0 \\ M\,(S_{ab}) = 1 \end{array} \right.$	0

Möbius-Möbius graphs (G_6) are very closely related to Hückel-Möbius graphs except that in the former graphs both rings are of Möbius-type. We will consider, as an example, Hückel-Hückel (G_7), Hückel-Möbius (G_8), and Möbius--Möbius (G_9) bicyclohexatrienes (butylenes), respectively.



G_7 G_8 G_9

First, we give below all Sachs graphs of G_7:



Actually, these are formally all possible Sachs graphs not only of G_7, but G_8 and G_9. However, the corresponding characteristic polynomials would differ in those values of a_n coefficients for which the cycles appear in the Sachs graphs. In our case these would be a_4 and a_6 coefficients because S_4 and S_6 Sachs' graphs of G_8 and G_9 contain rings with —1 edges. Now the coefficients a_n of the characteristic polynomials $P(G_7, x)$, $P(G_8, x)$, and $P(G_9, x)$ can be evaluated using the extended Sachs formula (2):

$$a_0 = 1$$
$$a_1 = 0$$
$$a_2 = 7\,(-)^{1+0}\,2^0 = -7$$
$$a_3 = 0$$
$$a_4\,(G_7) = 11\,(-)^{2+0}\,2^0 + 2\,(-)^{1+0}\,2^1 = 7$$
$$a_4\,(G_8) = 11\,(-)^{2+0}\,2^0 + (-)^{1+0}\,2^1 + (-)^{1+1}\,2^1 = 11$$
$$a_4\,(G_9) = 11\,(-)^{2+0}\,2^0 + 2\,(-)^{1+1}\,2^1 = 15$$
$$a_5 = 0$$
$$a_6\,(G_7) = 3\,(-)^{1+0}\,2^0 + 2\,(-)^{2+0}\,2^1 + (-)^{1+0}\,2^1 = -1$$
$$a_6\,(G_8) = 3\,(-)^{1+0}\,2^0 + (-)^{2+1}\,2^1 + (-)^{2+0}\,2^1\,(-)^{1+1}\,2^1 = -1$$
$$a_6\,(G_9) = 3\,(-)^{1+0}\,2^0 + 2\,(-)^{2+1}\,2^1 + (-)^{1+2}\,2^1 = -9$$

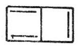
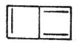
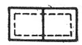
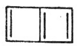
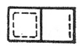
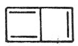
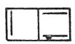
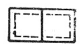
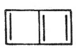
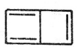
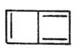
Finally, the following characteristic polynomials are obtained:

$$P\,(G_7, x) = x^6 - 7x^4 + 7x^2 - 1; \quad \{x = 2.41,\ 1.00,\ 0.41,\ -0.41,\ -1.00,\ -2.41\}$$
$$P\,(G_8, x) = x^6 - 7x^4 + 11x^2 - 1; \quad \{x = 2.17,\ 1,48,\ 0.31,\ -0.31,\ -1.48,\ -2.17\}$$
$$P\,(G_9, x) = x^6 - 7x^4 + 15x^2 - 9; \quad \{x = 1.73,\ 1.73,\ 1.00,\ -1.00,\ -1.73,\ -1.73\}$$

The value of a_N coefficients can be also obtained by using formulae (3) and (4). This is reported in Table II.

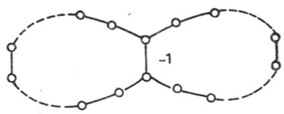
TABLE II

The calculation of a_N for G_7, G_8, and G_9 (see text)

Molecule	Algebraic structure	Superposition of algebraic structure	Paritiy of algebraic structures	$a_N = (-)^{N/2} \mid (AS)^{+} - (AS)^{-} \mid^2$
Hückel-Hückel bicyclohexa-triene (G_7)			assumed: + 1	
			calculated: + 1 H $(S_{ab}) = 0$ M $(S_{ab}) = 0$	— 1
			calculated: — 1 H $(S_{ab}) = 1$ M $(S_{ab}) = 0$	
Hückel-Möbius bicyclohexa triene (G_8)	 — 1		assumed: + 1	
	 — 1	 — 1	calculated: — 1 H $(S_{ab}) = 0$ M $(S_{ab}) = 1$	— 1
	 — 1	 — 1	calculated: + 1 H $(S_{ab}) = 0$ M $(S_{ab}) = 0$	
Möbius-Möbius bicyclohexa-triene (G_9)	— 1  — 1		assumed: + 1	
	— 1  — 1	— 1  — 1	calculated: + 1 H $(S_{ab}) = 0$ M $(S_{ab}) = 0$	— 9

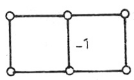
a_N values from Table II are, of course, identical with those appearing in $P(G_7, x)$, $P(G_8, x)$, and $P(G_9, x)$, respectively.

A final point we wish to discuss is this: under which conditions our procedure is invariant with respect to the position of a -1 edge in the Möbius-type graphs described here. For monocyclic graphs, because of the high symmetry of annulenes, the invariance on the position of the -1 edge is easily seen. However, this is not so evident for Hückel-Möbius (G_5) and Möbius-Möbius (G_6) graphs. Let us first consider the bicyclic graphs G_{10} with -1 common edge.



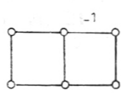
G_{10}

It becomes apparent from the inspection of Sachs graphs containing rings that G_{10} belongs to the class of Möbius-Möbius bicyclic graphs. Thus, for example, Möbius-Möbius graph G_{11} has the characteristic polynomial, $P(G_{11}, x)$ identical with the one of G_9, $P(G_9, x)$.

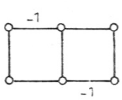


G_{11}

Similarly, it could be easily shown by inspection of the S_4 and S_C Sachs graphs that the characteristic polynomials of Hückel-Möbius graph G_{12}, $P(G_{12}, x)$, and Möbius-Möbius graph G_{13}, $P(G_{13}, x)$ are identical with $P(G_8, x)$ and $P(G_8, x)$ respectively.



G_{12}



G_{13}

Therefore, it follows from the inspection of G_{11}, G_{12}, and G_{13} that two Hückel--Möbius or Möbius-Möbius graphs are invariant with respect to the position of the -1 edge if the Sachs graphs containing rings are in both graphs identical.

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SAŽETAK

Möbiusove molekule i grafovi

A. Graovac i N. Trinajstić

Uveden je pojam Möbiusovog grafa, koji je pridružen Möbiusovim strukturama. Dana je i kratka diskusija o poopćenim grafovima. Coulson-Sachsova metoda je proširena da uključuje i Möbiusove grafove (i poopćene grafove). Definirana je parnost algebarskih struktura Möbiusovih molekula.

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