match no. 30 pp. 153-169 1994

Calculating the characteristic polynomial and the eigenvectors of a weighted hexagonal system (benzenoid hydrocarbon with heteroatoms)

Peter E.John
Technische Hochschule Ilmenau, Germany
(received: July 1992)
first version

Abstract

Two simple and easily computable algorithms of low complexity are described (without proofs):
Algorithm $\bar{\mathbf{A}}$ enables the characteristic polynomial and the eigenspaces (eigenvalues,eigenvectors) to be calculated for all hexagonal systems.
Algorithm $\bar{\mathbf{B}}$ enables the same to be done, in a more efficient way, for those hexagonal systems whose dualist graph (the inner dual graph) is a tree (representing catacondensed benzenoid hydrocarbons).
Both algorithms are variants of a simple summation procedure following the edges in a (cycle-free) directed graph.

1 Introduction

1.1 Definitions and notation

A **hexagonal cell** (briefly: a **cell**) is a closed plane region bounded by a regular hexagon of unit side length.
A **hexagonal system** (HS) is a finite 2-connected plane graph in which the closed hull of every finite region is a cell.
A **catacondensed hexagonal system** (CHS) is a HS in which no vertex belongs to more than two cells.
Let $G = (V, E)$ be a graph with vertex set $V = V(G) = \{v_1, v_2, ..., v_n\}$ and edge set $E = E(G)$ and let $w(u)$ be a function, defined on $U = V \cup E$.

assigning non-negative weights to the vertices and positive weights to the edges of G; call the pair $\bar{G} := (G, w)$ a "weighted graph".
Let $\bar{A} = (\bar{a}_{ij})$ denote the weighted adjacency matrix of $\bar{G}$, where

$$\bar{a}_{ij} = \begin{cases} w(v_i) & if\ i = j \\ w(e_{ij}) = w(v_i, v_j) & if\ i \neq j\ and\ vertices\ v_i, v_j \\ & are\ connected\ by\ the\ edges\ e_{ij} \in E \\ 0 & if\ i \neq j\ and\ vertices\ v_i, v_j \\ & are\ non-adjacent \end{cases}$$

Let I be the $n \times n$ unit matrix. The polynomial

$$det(\lambda I - \bar{A}) \tag{1}$$

of $\bar{A}$ and its roots are called the characteristic polynomial of $\bar{G}$, denoted by $P_{\bar{G}}(\lambda)$, and the eigenvalues of $\bar{G}$, respectively. Let λ^0 be an eigenvalue of $\bar{G}$ and let $\mathbf{0}$ denote the zero vector on n components. The set $\mathbf{S}(\lambda^0)$ of all solutions $\mathbf{x}$ of the equation

$$(\lambda^0 I - \bar{A}) \cdot \mathbf{x} = \mathbf{0} \tag{2}$$

forms the eigenspace of $\bar{G}$ belonging to λ^0; every non-zero $\mathbf{x}^0 \in \mathbf{S}(\lambda^0)$ (with $| \mathbf{x}^0 |= 1$) is a (normalized) eigenvector of $\bar{G}$ belonging to λ^0. (In connection with the Hückel theory, these vectors are called "molecular orbitals" by chemists .) If $G = H$ is a HS then call $\bar{G} = \bar{H}$ a **weigthed hexagonal system** (WHS).
A **horizontally fixed WHS** is a WHS in which some of its edges are horizontal.

1.2 Chemical background

The structural formula of a benzenoid hydrocarbon $\bar{B}$ with heteroatom(s) consits of a weighted hexagonal system $\bar{H}$ spanned by the carbon and heteroatoms and some hanging edges which represent bonds with hydrogen atoms (Fig.1); let us call $\bar{H}$ the **skeleton** of $\bar{B}$.

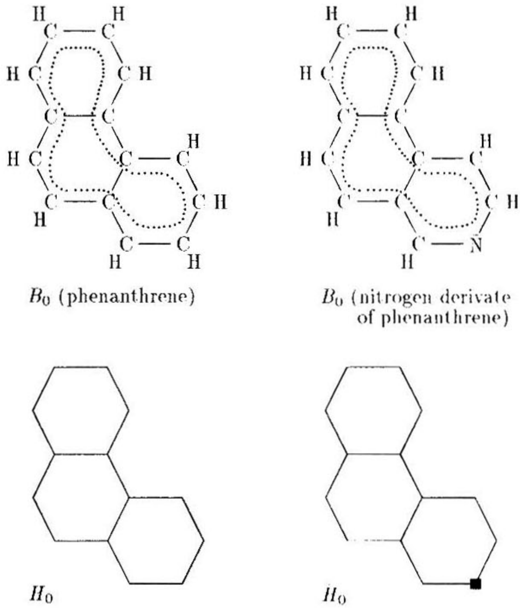


Figure 1

1.3 Literature

The fundamentals of a general theory of graph spectra were independently elaborated by L.M.Lihtenbaum [1] (1956) and L.Collatz and U.Sinogowitz [2] (1957). Also independently, M.Milić [3],H.Sachs [4], and L.Spialter [5] (1964) established a formula expressing the coefficients of the characteristic polynomial of a graph in terms of its cyclic structure.
Much information about the early approaches to the Hückel theory of (aromatic) hydrocarbons are contained in the books "Dictionary of π - Electron Calculation" by C.A.Coulson and A.Streitwieser.Jr. [6] (1965) and "Hückel Theory for Organic Chemists" by C.A.Coulson, B.O'Leary and R.B.Mallion

[7] (1978). After the publication of [6] many papers on weighted graphs have appeared from which we mention only A.Graovac, O.E.Polansky, N.Trinjastić and N.Tyutyulkov [8] (1975), N.Trinjastić [9] (1977), M.J.Rigby, R.B.Mallion and A.C.Day [10, 11] (1977,1978), and P.Křivka, R.B.Mallion and N.Trinjastić [12] (1988). For more details, the reader is referred to the monographs of D.M.Cvetković, M.Doob and H.Sachs [13] (1980) and D.M.Cvetković, M.Doob, I.Gutman and A.Torgašev [14] (1988).
In this paper, an algrithm $\bar{\mathbf{A}}$ is developed (see also [15, 16, 17, 18]); this algorithm is based on a general graph-theoretical procedure for calculating determinants and solving systems of linear equations, see Kh.Al-Khnaifes and H.Sachs [19] (1990); $\bar{\mathbf{A}}$ allows the eigenvalues and eigenspaces of any WHS to be simultaneously calculated.

2 An algorithm for the general case

Let $\bar H$ be an horizontally fixed WHS. In $\bar H$ we find a set of "zigzag lines", $\bar Z_1, \bar Z_2, ..., \bar Z_p$, say, where $\bar Z_i$, is a maximal monotone (weighted) path (non-interrupted zigzag line) in $\bar H$ connecting a top point t_i with a bottom point b_i, as indicated in Fig.2.

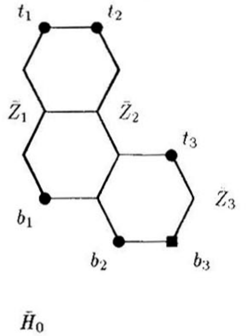


Figure 2

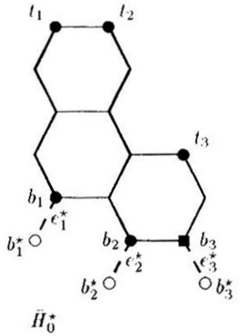
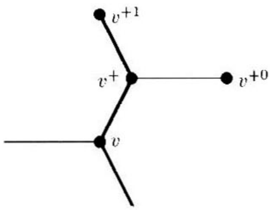


Figure 3

Let $Z = Z(H)$ denote the subgraph of H whose components are the zigzag lines $\bar Z_1, \bar Z_2, ..., \bar Z_p$ and put $\bar Z = (Z, w^*)$ where $w^* = w\,|_{V\cup E(Z)}$ is the restriction of w to the elements of Z. Put

$$w(Z) = \prod_{e \in E(Z)} w(e) \tag{3}$$

The points t_i, $i = 1, 2, ..., p$, are called the top vertices of $\bar{H}$. Every zigzag line Z_i of $\bar{H}$ is prolonged beyond its bottom point b_i by one unit segment e_i^* of weight $w(e_i^*) = 1$ connecting b_i with an additional "virtual" vertex b_i^* of weight $w(b_i^*) = 0$; thus H is turned into a weighted graph $\bar{H}^*$, see Fig.3. For any vertex v of $\bar{H}^*$ let v^+ denote its unique upper neighbour (if it exists) and let $N^+(v) := N(v^+) - \{v\}$ be the set of neighbours of v^+ of $\bar{H}^*$ which are different from v (Fig.4).



$N^+(v) = \{v^{+0}, v^{+1}\}$

Figure 4

Algorithm $\bar{\mathbf{A}}$:
To every vertex v of $\bar{H}^*$ assign a vector

$$\bar{\mathbf{d}}(v, \lambda) = (\bar{d}_1(v, \lambda), \bar{d}_2(v, \lambda), ..., \bar{d}_p(v, \lambda))$$

according to the following rules.
($\bar{\mathbf{A}}$.1) For top vertex t_k, put

$$\bar{\mathbf{d}}(t_k, \lambda) = (\delta_{1k}, \delta_{2k}, ..., \delta_{pk}),$$

where $\delta_{ii} = 1$, $\delta_{ik} = 0$ if $i \neq k$ $(i, k = 1, 2, ..., p)$;
($\bar{\mathbf{A}}$.2) for any vertex v of $\bar{H}^*$ which is not a top vertex, put

$$\bar{\mathbf{d}}(v, \lambda) = \frac{1}{w(v, v^+)} \Big\{ (\lambda - w(v^+)) \bar{\mathbf{d}}(v^+, \lambda) - \sum_{v' \in N^+(v)} w(v^+, v') \bar{\mathbf{d}}(v', \lambda) \Big\}$$

where $w(v^+)$ and $w(v^+, v')$ are the weights of vertex v^+ and of the edge connecting v^+, v', respectively.
It is easy to see that, running through $\bar{H}^\star$ from top to bottom, we have no difficulty in successively calculating the vectors $\bar{\mathbf{d}}(v, \lambda)$ which, by ($\bar{\mathbf{A}}$.1) and ($\bar{\mathbf{A}}$.2), are uniquely determined.
Form the $n \times p$ matrix

$$D(\bar{H}, \lambda) = (\bar{\mathbf{d}}^T(v_1, \lambda), \bar{\mathbf{d}}^T(v_2, \lambda), \ldots, \bar{\mathbf{d}}^T(v_n, \lambda))^T$$
$$= (\bar{d}_k(v_j, \lambda))$$
$$(j = 1, 2, \ldots, n; \; k = 1, 2, \ldots, p)$$

and the $p \times p$ matrix

$$D^\star(\bar{H}, \lambda) = (\bar{\mathbf{d}}^T(b_1^\star, \lambda), \bar{\mathbf{d}}^T(b_2^\star, \lambda), \ldots, \bar{\mathbf{d}}^T(b_p^\star, \lambda))^T$$
$$= (\bar{d}_k(b_i^\star, \lambda))$$
$$(i, k = 1, 2, \ldots, p).$$

Theorem 1

$$P_{\bar{H}}(\lambda) = \varepsilon \cdot w(\bar{Z}) \cdot \det D^\star(\bar{H}, \lambda), \qquad \varepsilon \in \{+1, -1\}. \tag{4}$$

Theorem 2 *Let λ^0 be an eigenvalue of $\bar{H}$, let $\bar{\mathbf{y}}^0$ be an solution of*

$$D^\star(\bar{H}, \lambda^0) \cdot \bar{\mathbf{y}}^0 = \mathbf{0} \tag{5}$$

and put

$$\bar{\mathbf{x}}^0 = D(\bar{H}, \lambda^0) \cdot \bar{\mathbf{y}}^0. \tag{6}$$

Then the vector $\bar{\mathbf{x}}^0$ is an eigenvector of $\bar{H}$ belonging to λ^0, and all eigenvectors (in fact: the eigenspace) belonging to λ^0 can be obtained this way.

Both theorems are slight modifications of theorems in [19].
Example 1.
For the WHS depicted in Fig.1 (see also Fig.5 with labelled vertices), we obtain the following Table 1 (the weights to be used are: $w(v_j) = 0, j = 1, 2, \ldots, 13$; $w(v_{14}) = \alpha$, $w(v_{12}, v_{14}) = w(v_{13}, v_{14}) = \beta$; all other edges e of $\bar{H}^\star$ have weight $w(e) = 1$).

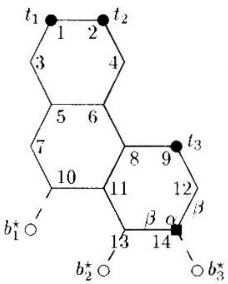


Figure 5

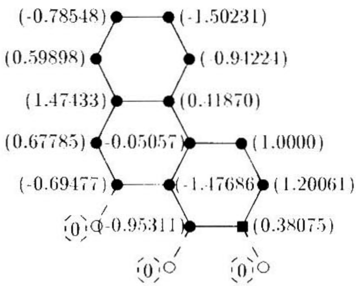


Figure 6

Thus

$$
\begin{aligned}
P_{\bar{H}_0}(\lambda) &= (+1)\cdot w(\bar{Z}_0)\cdot \det D^\star(H_0,\lambda) \\
&= \beta \cdot \det D^\star(\bar{H}_0,\lambda) \\
&= \lambda^{14} - \alpha\lambda^{13} - (14+2\beta^2)\lambda^{12} + 14\alpha\lambda^{11} \\
&\quad +(72+26\beta^2)\lambda^{10} - 72\alpha\lambda^9 - (174+123\beta^2)\lambda^8 \\
&\quad +174\alpha\lambda^7 + (207+272\beta^2)\lambda^6 - 207\alpha\lambda^5 \\
&\quad -(113+294\beta^2)\lambda^4 + 113\alpha\lambda^3 + (21+145\beta^2)\lambda^2 \\
&\quad -21\alpha\lambda - 25\beta^2
\end{aligned} \tag{7}
$$

In the case of the nitrogen derivate of phenanthrene (B_0'), the weights are $\alpha = \alpha' = 0.5$, $\beta = \beta' = 1$ [20, 21], therefore, the characteristic polynomial is

$$
\begin{aligned}
P_{\bar{H}_0'}(\lambda) &= \lambda^{14} - 0.5\lambda^{13} - 16\lambda^{12} + 7\lambda^{11} \\
&\quad +98\lambda^{10} - 36\lambda^9 - 297\lambda^8 + 87\lambda^7 + 479\lambda^6 \\
&\quad -103.5\lambda^5 - 407\lambda^4 + 56.5\lambda^3 + 166\lambda^2 - 10.5\lambda - 25.
\end{aligned} \tag{8}
$$

All roots of $P_{\bar{H}_0'}(\lambda)$ (see Table 2) are simple.
λ_5 =1.150039 is a single root of $P_{H_0'}(\lambda)$, i.e., λ_5 is a simple eigenvalue of the nitrogen derivate $\bar{B}_0'$. In this case,

$$
D^\star(\bar{H}_0',\lambda_5) = \begin{pmatrix} -0.65937 & 1.0104 & 1 \\ 0.01196 & -0.43571 & -0.64518 \\ -1.17326 & 0.75302 & 0.2097 \end{pmatrix}
$$

Table 1: $\bar{d}_k(v_j, \lambda)$ and $\bar{d}_k(b_i^*, \lambda)$ values of $\bar{H}_0$

$\bar{d}_k(v_j, \lambda)$:

k / j	1	2	3
1	1	0	0
2	0	1	0
3	λ	-1	0
4	-1	λ	0
5	$\lambda^2 - 1$	$-\lambda$	0
6	$-\lambda$	$\lambda^2 - 1$	0
7	$\lambda^3 - \lambda$	$-2\lambda^2 + 2$	0
8	$-2\lambda^2 + 2$	$\lambda^3 - \lambda$	0
9	0	0	1
10	$\lambda^4 - 2\lambda^2 + 1$	$-2\lambda^3 + 3\lambda$	0
11	$-2\lambda^3 + 3\lambda$	$\lambda^4 - 2\lambda^2 + 1$	-1
12	$2\lambda^2 - 2$	$-\lambda^3 + \lambda$	λ
13	$-3\lambda^4 + 7\lambda^2 - 3$	$\lambda^5 - \lambda^3 - \lambda$	$-\lambda$
14	$\frac{1}{\beta}(2\lambda^3 - 2\lambda)$	$\frac{1}{\beta}(-\lambda^4 + \lambda^2)$	$\frac{1}{\beta}(\lambda^2 - 1)$

$\bar{d}_k(b_i^*, \lambda)$:

k / i	1	2	3
1	$\lambda^5 - \lambda^3 - \lambda$	$-3\lambda^4 + 7\lambda^2 - 3$	1
2	$-3\lambda^5 + 7\lambda^3 - 4\lambda$	$\lambda^6 - \lambda^4 - 1$	$-2\lambda^2 + 2$
3	$\frac{\lambda-\alpha}{\beta}(2\lambda^3 - 2\lambda)$	$\frac{\lambda-\alpha}{\beta}(-\lambda^4 + \lambda^2)$	$\frac{\lambda-\alpha}{\beta}(\lambda^2 - 1)$
	$-\beta(-3\lambda^4 + 9\lambda^2 - 5)$	$-\beta(\lambda^5 - 2\lambda^3)$	

Table 2: The eigenvalues of the nitrogen derivate of phenanthrene ($\bar{B}_0'$):

λ_1	=	2.451078	λ_{14}	=	-2.426279
λ_2	=	2.019018	λ_{13}	=	-1.913331
λ_3	=	1.550860	λ_{12}	=	-1.502878
λ_4	=	1.388331	λ_{11}	=	-1.238253
λ_5	=	1.150039	λ_{10}	=	-1.128276
λ_6	=	0.833920	λ_9	=	-0.686649
λ_7	=	0.605804	λ_8	=	-0.603384

and because of Theorem 2,

$$\bar{\mathbf{y}}_5 = \begin{pmatrix} -0.78548 \\ -1.50231 \\ -1.00000 \end{pmatrix}$$

and

$$D(\bar{H}_0', \lambda_5) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1.150039 & -1 & 0 \\ -1 & 1.150039 & 0 \\ 0.32259 & -1.150039 & 0 \\ -1.150039 & 0.32259 & 0 \\ 0.370991 & -0.645179 & 0 \\ -0.645179 & 0.370991 & 0 \\ 0 & 0 & 1 \\ 0.104064 & 0.408058 & 0 \\ 0.408058 & 0.104064 & -1 \\ 0.645179 & -0.370991 & 1.150039 \\ 1.010397 & -0.659370 & -1.150039 \\ 0.741981 & -0.426654 & 0.32259 \end{bmatrix}$$

In Fig.6 the components $x_i(\lambda_5)$ of the (non-normalized) eigenvector (molecular orbital) belonging to λ_5 (see Theorem 2) are given in brackets, close to vertex v_i ($i = 1, 2, ..., 14$). The zeros in the dotted brackets only serve for checking the correctness of the calculation.

3 The algorithm for a weighted catacondensed benzenoid system

Let $\bar{H}$ be a weighted CHS with at least two cells. An edge of $\bar{H}$ is called **internal** if it is the intersection of two cells, and **external** otherwise. Cell c is an **end cell** (**bifurcation cell**) of $\bar{H}$ if and only if the boundary of c has exactly one (three) internal edges. An **end edge** of $\bar{H}$ is an edge of an end cell c which lies opposite to the internal edge of c (Fig.7).

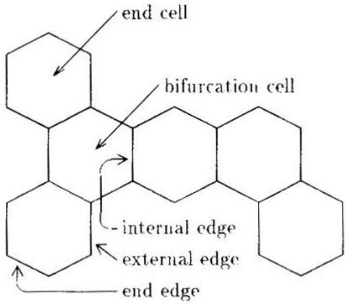
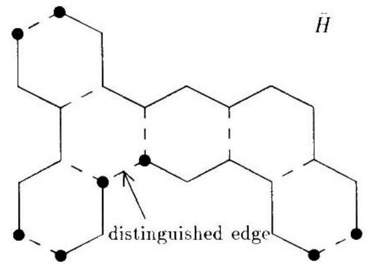


Figure 7

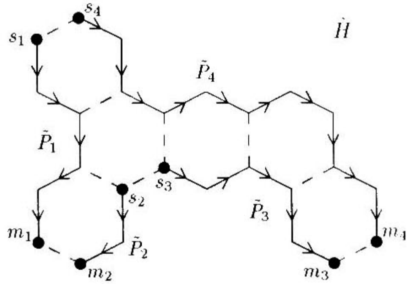
If $\bar{H}$ has eyactly b bifurcation cells, $b \in \{0, 1, 2, ...\}$, then it has exactly $b + 2$ end cells.
For every bifurcation cell $c^\star$, arbitrarily distinguish precisely one of the three external edges which lie on the boundary of $c^\star$. Delete all internal edges, end edges, and distinguished edges of $\bar{H}$; what remains is a set of $2(b+1)$ disjoint paths $\bar{P}$ lying on the periphery, and covering all vertices, of $\bar{H}$(Fig.8.1). Put $2(b+1) = q$.
Arbitraryly specify one of the paths $\bar{P}$ as $\bar{P}_1$ and, following the periphery in the positive sense, number the paths $\bar{P}$ consecutively from 1 to q. Let $P = P(H)$ denote the subgraph of H whose components are the paths $P_1, P_2, ..., P_q$ and put $\bar{P} = (P, w^\star)$ where $w^\star = w\,|_{V \cup E(P)}$ is the restriction of w to the elements of P.
Put

$$w(\bar{P}) = \prod_{\epsilon \in E(P)} w(\epsilon) \qquad (9)$$

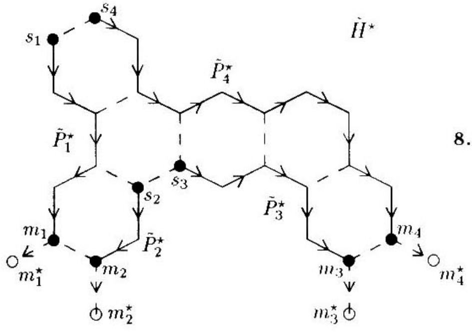
Direct paths $\bar{P}_1, \bar{P}_3, ..., \bar{P}_{q-1}$ in the positive and paths $\bar{P}_2, \bar{P}_4, ..., \bar{P}_q$ in the negative sense; denote the directed path obtained from $\bar{P}_j$ by $\tilde{P}_j$ and the source vertex and the month vertex of $\tilde{P}_j$ by s_j and m_j, respectively. Denote the resulting figure by $\tilde{H}$ (see Fig.8.2). The subgraph $\tilde{P} = P(\tilde{H})$ is the union of all paths $\tilde{P}_j$ of $\tilde{H}$.



8.1



8.2



8.3

Figure 8

To each path $\tilde{P}_j$ from $\tilde{H}$, add a new "virtual" vertex $m_j^\star$ and a directed edge $(\overrightarrow{m_j, m_j^\star})$ from m_j to $m_j^\star$ with weight 1: Thus $\tilde{P}_j$ is turned into a directed path $\tilde{P}_j^\star$ from s_j to $m_j^\star$, and $\tilde{H}$ is turned into a figure which we call $\tilde{H}^\star$ (Fig.8.3).
Further, in $\tilde{H}^\star$ every vertex v which is not a source vertex has a unique immediate predecessor which we denote by v^0; let $N^0(v) := N(v^0) - \{v\}$ be the set of neighbours of v^0 in H which are different from v.
Algorithm $\tilde{\mathbf{B}}$:
To every vertex v of $\tilde{H}^\star$ assign a vector

$$\tilde{\mathbf{d}}(v, \lambda) = (\tilde{d}_1(v, \lambda), \tilde{d}_2(v, \lambda), ..., \tilde{d}_q(v, \lambda))$$

by means of the following recursive procedure.
($\tilde{\mathbf{B}}$.1) For source vertex s_k put

$$\tilde{\mathbf{d}}(s_k, \lambda) = (\delta_{1k}, \delta_{2k}, ..., \delta_{qk}),$$

where $\delta_{ii} = 1$, $\delta_{ik} = 0$ if $i \neq k$ $(i, k = 1, 2, ..., q)$,
($\tilde{\mathbf{B}}$.2) for any vertex of $\tilde{H}^\star$ which is not a source vertex, put

$$\tilde{\mathbf{d}}(v, \lambda) = \frac{1}{w(v, v^0)}\left\{(\lambda - w(v^0)) \cdot \tilde{\mathbf{d}}(v^0, \lambda) - \sum_{v'' \in N^0(v)} w(v^0, v'') \cdot \tilde{\mathbf{d}}(v'', \lambda)\right\}$$

Running through $\tilde{H}^\star$ following the directed paths $\tilde{P}_j^\star$ from the source vertices s_j to the virtual vertices $m_j^\star$, we have no difficulty in successively calculating the vectors $\tilde{\mathbf{d}}(v, \lambda)$, which by ($\tilde{\mathbf{B}}$.1) and ($\tilde{\mathbf{B}}$.2) are uniquely determined.
Form the $n \times q$ matrix

$$\begin{aligned} D(\tilde{H}, \lambda) &= (\tilde{\mathbf{d}}^T(v_1, \lambda), \tilde{\mathbf{d}}^T(v_2, \lambda), ..., \tilde{\mathbf{d}}^T(v_n, \lambda))^T \\ &= (\tilde{d}_k(v_j, \lambda)) \\ &(j = 1, 2, ..., n; \;\; k = 1, 2, ..., q) \end{aligned}$$

and the $q \times q$ matrix

$$\begin{aligned} D^\star(\tilde{H}, \lambda) &= (\tilde{\mathbf{d}}^T(m_1^\star, \lambda), \tilde{\mathbf{d}}^T(m_2^\star, \lambda), ..., \tilde{\mathbf{d}}^T(m_q^\star, \lambda))^T \\ &= (\tilde{d}_k(m_i^\star, \lambda)) \\ &(i, k = 1, 2, ..., q). \end{aligned}$$

Using these matrices, calculate the characteristic polynomial $P_{\bar{H}}(\lambda) = P_{\tilde{H}}(\lambda)$ and the eigenspaces of $\bar{H}$ in exactly the way as described in Theorems 1 and 2 with $\bar{H}, \bar{Z}, p, \bar{\mathbf{y}}^0, \bar{\mathbf{x}}^0$ replaced by $\tilde{H}, \tilde{P}, q, \tilde{\mathbf{y}}^0, \tilde{\mathbf{x}}^0$, respectivly.

Example 2:

For the weighted CHS depicted in Fig.1 (see also Fig.9 with labelled vertices) with weights as in Example 1, we obtain the following Table 3.

$P_{\tilde{H}_0}(\lambda) = \varepsilon \cdot w(\bar{P}_0) \cdot \det D^\star(\tilde{H}_0, \lambda)$ is identical with the polynomial $P_{H_0}(\lambda)$ given in (7) (Note that the order of the determinant to be calculated reduced from $\frac{n}{2}$ to $q = 2(b+1)$).

For the nitrogen derivate of phenanthrene ($\bar{B}_0'$), $P_{\tilde{H}_0'}(\lambda)$ is identical with the polynomial given in (8).

λ_5 =1.150039 is a single root of $P_{\tilde{H}_0'}(\lambda)$. Here we have

$$D^\star(\tilde{H}_0', \lambda_5) = \begin{pmatrix} -1.30375 & 0.68167 \\ 0.41345 & -0.21617 \end{pmatrix}.$$

$$\tilde{\mathbf{y}}_5 = \begin{pmatrix} -0.78548 \\ -1.50231 \end{pmatrix},$$

and

$$D(\tilde{H}_0', \lambda_5) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1.150039 & -1 \\ -1 & 1.150039 \\ 0.32259 & -1.150039 \\ -1.150039 & 0.32259 \\ 0.370991 & -0.64518 \\ 0.10406 & 0.40806 \\ -0.25131 & 1.11446 \\ -0.64518 & 0.37099 \\ 0.2521 & 0.50263 \\ 0.65937 & -1.0104 \\ 1.40348 & -1.53299 \\ 0.54123 & -0.53642 \end{bmatrix}$$

The components of the eigenvector belonging to λ_5 are, of course, the same as given in Fig.6.

Table 3: $\tilde{d}_k(v_j, \lambda)$ and $\tilde{d}_k(m_i^\star, \lambda)$ values of $\bar{H}_0$

$\tilde{d}_k(v_j, \lambda)$:

k / j	1	2
1	1	0
2	0	1
3	λ	-1
4	-1	λ
5	$\lambda^2 - 1$	$-\lambda$
6	$-\lambda$	$\lambda^2 - 1$
7	$\lambda^3 - \lambda$	$-2\lambda^2 + 2$
8	$\lambda^4 - 2\lambda^2 + 1$	$-2\lambda^3 + 3\lambda$
9	$\lambda^5 - 3\lambda^3 + 2\lambda$	$-2\lambda^4 + 5\lambda^2 - 2$
10	$-2\lambda^2 + 2$	$\lambda^3 - \lambda$
11	$\lambda^6 - 4\lambda^4 + 6\lambda^2 - 3$	$-2\lambda^5 + 6\lambda^3 - 4\lambda$
12	$-\lambda^5 + \lambda^3 + \lambda$	$3\lambda^4 - 7\lambda^2 + 3$
13	$-\lambda^6 + \lambda^4 + 3\lambda^2 - 2$	$3\lambda^5 - 8\lambda^3 + 4\lambda$
14	$\frac{1}{\beta}(\lambda^7 - 5\lambda^5 + 9\lambda^3 - 5\lambda)$	$\frac{1}{\beta}(-2\lambda^6 + 8\lambda^4 - 9\lambda^2 + 2)$

$\tilde{d}_k(m_j^\star, \lambda)$:

k / i	1	2
1	$\frac{\lambda-\alpha}{\beta}(\lambda^7 - 5\lambda^5 + 9\lambda^3 - 5\lambda)$ $+\beta(3\lambda^4 - 9\lambda^2 + 5)$	$\frac{\lambda-\alpha}{\beta}(-2\lambda^6 + 8\lambda^4 - 9\lambda^2 + 2)$ $+\beta(-\lambda^5 + 2\lambda^3)$
2	$-2\lambda^7 + 7\lambda^5 - 7\lambda^3 + 2\lambda$	$5\lambda^6 - 19\lambda^4 + 20\lambda^2 - 5$

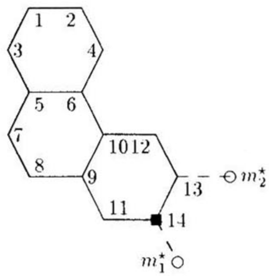


Figure 9

4 Concluding remarks

4.1 In order to minimize the calculation expenditure, before applying algorithm $\bar{\mathbf{A}}$ for a given WHS H, put H in a fixed position such that the number p of zigzag lines is minimum.

4.2 In a following paper a computer program (for algorithm $\bar{\mathbf{A}}$) will be introduced, in which the remarks of [17] will be considered.

The help of Dr.R.Hennecke (TH Ilmenau) and Dr.B.Jaggi (Uni Bern) in the calculation of the roots of (8) and (7), respectively, is gratefully acknowledged.

This paper was supported by the DFG(Jo 231/1-2).

References

[1] Lihtenbaum,L.M.,*Trudy 3-go Vses.Matem.S"ezda*,tom 1,135(1956)

[2] Collatz.L. and U.Sinogowitz,*Hambg.math.Abhandlg.*,**21**,63(1957)

[3] Milić,M.,*IEEE Trans.Circuit Theory CT-11*,423(1964)

[4] Sachs,H.,*Publ.Math.Debrecen*,**11**,119(1964)

[5] Spialter,L.,*J.Chem.Docum.*,4,269(1964)

[6] Coulson,C.A. and A.Streitwieser,Jr.,*Dictionary of π-Electron Calculations*, Pergamon Press,Oxford,1965

[7] Coulson,C.A.,B.O'Leary and R.B.Mallion,*Hückel Theory for Organic Chemists*, Academic Press,London-New York-San Francisco,1978

[8] Graovac,A.,O.E.Polansky,N.Trinajstić and N.Tyutyulkov, *Z.Naturforsch.* **30a**,1696(1975)

[9] Trinajstić,N.,*Croat. Chem. Acta* **49**(4),593(1977)

[10] Rigby,M.J.,R.B.Mallion and A.C.Day.*Chem. Phys. Letters*, **51**,178(1977)

[11] Rigby,M.J.,R.B.Mallion and A.C.Day.*Chem. Phys. Letters*, **53**,418(1978)

[12] Křivka,P.,R.B.Mallion and N.Trinajstić,*J.Mol.Struct.(Theochem.)*, **164**,363(1988)

[13] Cvetković,D.M.,M.Doob and H.Sachs,*Spectra of Graphs - Theory and Application*, Academic,New York,1980

[14] Cvetković,D.M.,M.Doob,I.Gutman and A.Torgašev, *Recent Results in the Theory of Graph Spectra*,North-Holland,Amsterdam (Annals of Discrete Mathematrics,36),1988

[15] John,P.,*33 IWK TH Ilmenau*,24.-28.10.1988,H.4, Vortragsreihen C1/C2,p.195

[16] John,P. and H.Sachs,*J.Chem.Soc.Faraday Trans.II*,**86**(7),1033(1990)

[17] John,P. and H.Sachs, In: *Advances in the Theory of Benzenoid Hydrocarbons, I.Gutman and S.J.Cyvin (Edts), Topics in Current Chemistry, Nr.153*, Springer - Verlag,Berlin - Heidelberg,1990,p.145

[18] John,P.,In: *International Conference "Discrete Mathematics"*,March 12-16, 1990,Eisenach,p.34

[19] Al-Khnaifes,Kh. and H.Sachs,In: *Contemporary Methods in Graph Theory*, R.Bodendiek(Ed.),B.I.-Wissenschaftsverlag Mannheim - Wien - Zürich,1990,p.47

[20] Heilbronner,E. and H.Bock,*Das HMO - Modell und seine Anwendung*, Verlag Chemie,GmbH,Weinheim/Bergstraße,1968,p.155

[21] Scholz,M. and H.-J.Köhler,*Quantenchemie, Ein Lehrgang*,Band 3, VEB Deutscher Verlag der Wissenschaften,Berlin,1981,p.158