Topological analysis of some special classes of graphs. II. Steps, ladders, cylinders

Shyi-Long Lee [a] and Yeong-Nan Yeh [b]

[a] *Department of Chemistry, National Chung-Cheng University, Chin-Yi, Taiwan 621, ROC*
[b] *Institute of Mathematics, Academia Sinica Taipei, Taiwan 11529, ROC*

Received 1 November 1990; revised 19 August 1991

A general strategy is proposed for generating the eigenvectors and the eigenvalues of some special classes of graphs from the well-known chemical graphs such as lines and cycles which are isomorphic to the hydrogen-suppressed linear and cyclic polyenes. This method is applied to step graphs, ladders, cylinders, etc. Net sign analyses are then performed for all these special classes of graphs.

1. Introduction

During the last two decades, there has been a growing interest in the application of graph theory to topological analysis of external [1] and internal [2] connectivities of chemical graphs. The research activities in this field have been extended to various fields of chemistry, such as organic conjugated systems [3], organometallics [4], clusters [5], drug research and design [6], heterocyclic compounds [7], isomer enumeration [8], the quantitative-structure–activity relationship [9], toxicity studies [10], etc. Applications of graph theory to molecular orbital theory have also been advanced by Gutman et al. [11]. However, some fundamental studies concerning the internal connectivity of molecular orbital graphs [12] are still of interest. In this paper we have applied a general strategy proposed by the authors [13] for generating the eigenvectors and eigenvalues of some special classes of graphs from well-studied chemical graphs, e.g. lines and cycles which are isomorphic to linear and cyclic polyenes. This strategy was successfully applied to the class of hypercubes [14] which are direct products of a series of complete graphs of order 2, K_2, the isomorphic counterpart of the hydrogen-depleted ethene. Linear and cyclic polyenes, whose eigenvectors and eigenvalues were fully studied and were expressed in analytic formulas in ref. [15], are used as the starting point in this paper to show the elegance of our method.

Net sign analysis was proposed by Lee et al. [2] to study the topological properties of Hückel molecular orbital graphs. One of the important results of net sign analysis is the parallel relationship between the ordering of net signs and the ordering of eigenvalues, especially for one-dimensional quantum systems [16]. Only partial agreement was found for two-dimensional systems [16,17]. It was pointed out that the Euclidean 3-dimensional hypercubes obey the parallel relationship rigorously [14]. For the purpose of the net sign analysis, it is necessary to have some ways to obtain the eigenvectors and eigenvalues without too complicated calculations. The strategy proposed in this paper seems to serve our purpose quite well. Besides, it is intriguing to trace out the graphical criteria for a graph to obey the parallel relationship rigorously.

This paper is composed as follows. A brief introduction of our method is given in section 2. A detailed description will be published elsewhere [13]. Applications of this method to graphs belonging to the special class of graphs such as steps, combs and torus are given in section 3. Results of net sign analyses of these graphs are also presented and discussed in section 3. Conclusions are drawn in section 4.

2. Method

The central theme of this general strategy is to obtain analytic expressions or generating formulas for the eigenvectors and eigenvalues of a special class of graphs which can be defined through some of operations, say direct products from a certain known graph whose eigenvectors and eigenvalues are well-studied. For a detailed description of this method, the reader is referred to ref. [13]. Only the essence of this method is briefly stated here.

Let us start from the class of cyclic graphs which is familiar to most chemists and is a well-studied class of graphs whose eigenvectors and eigenvalues have analytic expressions [15]. The adjacency matrix of the n-cycle graph C_n is given by

$$A(C_n) = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 & 1 \\ 1 & 0 & 1 & \dots & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 & 0 \\ \dots & \dots & \dots & & \dots & \dots \\ 0 & 0 & 0 & & 0 & 1 \\ 1 & 0 & 0 & & 1 & 0 \end{bmatrix}. \tag{1}$$

An interesting cyclic permutation exists between any two successive rows of the adjacency matrix $A(C_n)$. A square matrix having the above property is called a circulant matrix or a circulant. Thus,

$$A = \begin{bmatrix} a_1 & a_2 & a_3 & \dots & a_n \\ a_n & a_1 & a_2 & \dots & a_{n-1} \\ a_{n-1} & a_n & a_1 & \dots & a_{n-2} \\ \dots & \dots & \dots & \dots & \dots \\ a_2 & a_3 & a_4 & \dots & a_1 \end{bmatrix} \quad (2)$$

is a circulant, denoted by $[[a_1, a_2, \dots, a_n]]$. A theorem [18] concerning the eigenvectors and eigenvalues of a circulant A states that $\{V_1, V_2, \dots, V_n\}$ is the complete set of eigenvectors of A, where $V_k = (1, x^k, x^{2k}, \dots, x^{(n-1)k})$ and $k = 0, 1, 2, \dots, (n-1)$, provided $x = e^{i2\pi/n}$ and $i = \sqrt{-1}$. The corresponding eigenvalue λ_k of eigenvector V_k is given by

$$\lambda_k = \sum_i a_i x^{(i-1)k}, \quad (3)$$

Therefore, the class of cycles is a special case whose adjacency matrices are circulants having the form of eq. (1). The kth eigenvector, V_k, of $A(C_n)$ is expressed as $V_k = (1, x^k, x^{2k}, \dots, x^{(n-1)k}), k = 0, 1, 2, \dots, (n-1)$. The corresponding eigenvalue λ_k of the eigenvector V_k is $2\cos(2k\pi/n)$, which is the same as that obtained by Coulson et al. [15] using a different method.

A short remark should be made on the spectrum of a graph and the labelling of a graph before we proceed further. Different label assignments would certainly produce different adjacency matrices. If A_1 and A_2 are adjacency matrices which arise from two different labellings of the same graph, then $A_1 = P^{-1}A_2P$ holds for some permutation matrix P. According to the theorem [19] which states that *the spectrum of the characteristic polynomial of matrix A is the same as that of $B^{-1}AB$*, where B is any *nonsingular matrix*, the spectrum of a graph is invariant with respect to the labelling of the graph.

The class of graphs whose adjacency matrices are circulants are called step or circulant graphs [20]. A step graph, denoted by $C_n(n_1, n_2, \dots, n_p)$ and $1 < n_1 < n_2 < \dots < n_p < (n+1)/2$, is defined as a graph on n vertices, $\{v_i, i = 1, 2, \dots, n)$, with the vertex v_i adjacent to each vertex $v_{i \pm nj}$ (mod n), where n_j is called the jump size. Therefore, the set of eigenvectors can be written by corollary as $\{V_k | k = 0, 1, 2, \dots, n-1\}$, where $V_k = (1, x^k, x^{2k}, \dots, x^{(n-1)k})$ and x has the same meaning as mentioned earlier. The corresponding eigenvalue λ_k of eigenvector V_k is given by

$$\lambda_k = 2 \sum_{p \geqslant i \geqslant 1} \cos(2n_i\pi k/n) \qquad \text{if } n_p \neq n/2 \quad (4a)$$

and

$$\lambda_k = \cos(2n_p\pi k/n) + 2 \sum_{p > i \geqslant 1} \cos(2n_i\pi k/n) \quad \text{if } n_p = n/2. \quad (4b)$$

Thus, cycles of n vertices are special cases of step graphs with a single jump size of

1. Complete graphs, which are denoted by K_n, are also special cases of step graphs with multiple jump sizes ranging from 1, 2 to $[(n-1)/2]$ where $[f]$ is the greatest integer less than or equal to f. The kth element of the set of eigenvectors is written as $V_k = (1, x^k, x^{2k}, \ldots, x^{(n-1)k})$, where $k = 0, 1, 2, \ldots, (n-1)$ and x has the same meaning as mentioned earlier, and the corresponding eigenvalue λ_k is given by

$$\lambda_k = \begin{cases} n-1 & \text{if } k = 0, \\ -1 & \text{if } k \neq 0, \end{cases} \tag{5}$$

where the eigenvectors whose eigenvalues are equal to -1 are $n-1$ degenerate.

Now let us define the Cartesian direct product of two graphs G_1 and G_2 by $H = G_1 \times G_2$. Consider any two vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ in $U = U_1 \times U_2$, where U, U_1 and U_2 are the sets of vertices of H, G_1 and G_2, respectively. Then u and v are adjacent in H when every $[u_1 = v_1$ and $u_2v)2 \in E(G_2)]$ or $[u_2 = v_2$ and $u_1v_1 \in E(G_1)]$ where $E(G_1)$ and $E(G_2)$ are the sets of edges of G_1 and G_2. The Cartesian product of $G_1 = K_2$ and $G_2 = L_3$ is shown in fig. 1. Other examples can be taken from the class of hypercubes, such as a square is the direct product of $(K_2 \times K_2)$ and a cube is the direct product of (square $\times K_2$). Assuming G_1 and G_2 are graphs on m vertices and n vertices, respectively, the adjacency matrix of the Cartesian product of $A(H)$ is defined as

$$I_n \otimes A(G_1) + A(G_2) \otimes I_m , \tag{6}$$

where I_n is a unit matrix of dimension n. The definition of the Kronecker product of two matrices is given in appendix A.

If the set of eigenvectors and eigenvalues of graphs G_1 are denoted by $\{U_i | i = 1, 2, \ldots, m\}$ and $\{\alpha_i | i = 1, 2, \ldots, m\}$ and those of G_2 by $\{V_i | i = 1, 2, \ldots, n\}$ and $\{\beta_i | i = 1, 2, \ldots, n\}$, then the set of eigenvectors of $G_1 \times G_2$, $\{W_i | i = 1, 2, \ldots, mn\}$, can be constructed easily from $\{U_i\}$ of G_1 and $\{V_i\}$ of G_2. V_i and U_i are $1 \times n$ and $1 \times m$ row vectors and denoted by the coefficients on each vertex as $[V_{i1} V_{i2} \ldots V_{in}]$ and $[U_{i1} U_{i2} \ldots U_{im}]$, respectively. The elements of $\{W_i\}$ are given by

$$W_{(k-1)n+j} = V_j \times U_k = [V_{j1} U_k, V_{j2} U_k, \ldots, V_{jn} U_k] \tag{7}$$

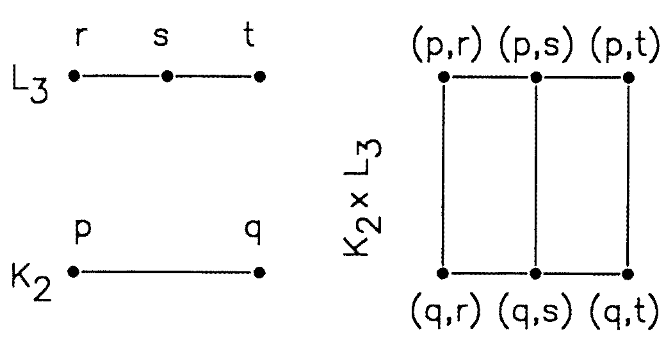


Fig. 1. The Cartesian product of K_2 and L_3.

for $m \geqslant k \geqslant 1, n \geqslant j \geqslant 1$. The corresponding eigenvalues are given by

$$\lambda_{(k-1)n+j} = \alpha_k + \beta_j . \tag{8}$$

The eigenvalues in eq. (8) were also obtained by Cvetković et al. in ref. [21], where they defined the graph sum corresponding to the Cartesian direct product in this paper. Now we can discuss the general feature concerning the eigenvalues and eigenvectors of graphs which can be obtained via some operations on the line graphs, circulant graphs and some well-studied graphs. Let us concentrate on the class of graphs whose adjacency matrices can be written in the following partitioned form:

$$A(H) = \begin{bmatrix} C & I \\ I & C \end{bmatrix}, \tag{9}$$

where the off-diagonal block is an identity matrix of order n and C is the adjacency matrix of lines, circulants or well-studied graphs. The adjacency matrix in eq. (9) is the result of Cartesian product of a graph with K_2, the complete graph of order 2. Applications of these formulas using cycles and lines as the starting point are presented in the next section.

3. Examples

A hypercube is a special class of graphs which can be constructed by the direct product of a series of K_2, the complete graph of order 2. For example, an n-cube, H_n, is expressed as

$$H_n = \overbrace{K_2 \times K_2 \times \ldots \times K_2}^{n\,\text{times}} . \tag{10}$$

The adjacency matrix of H_{n+1} obeys the following recurrence relation:

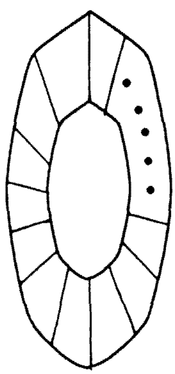
$$H_{n+1} = \begin{bmatrix} H_n & I \\ I & H_n \end{bmatrix}, \tag{11}$$

where I is the identity matrix of order n whose eigenvalues are 1. We have applied the method mentioned above to hypercubes. The eigenvalue set of H_n is composed by eigenvalues of $n - 2i$, where $i = 0, 1, \ldots, n$, and the degeneracy of each eigenvalue is $n!/(n-i)!i!$. A binomial distribution was found to exist among the distribution of eigenvalues. The eigenvectors can be easily constructed from a recurrence formula and can be expressed as $2^n \times 1$ row vectors $W(H_n) = (W_1, W_2)$, where W_1, W_2 are $2^{n-1} \times 1$ row vectors and $W_1 = \pm W_2$ [13]. Net sign analysis [14] revealed that a simple relation exists between net signs and eigenvalues of hypercubes, i.e.,

$$S_i(H_n) = 2^{n-1}\lambda_i(H_n) , \tag{12}$$

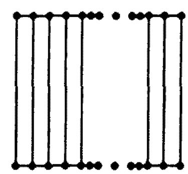
where S_i is the net sign of the edge-signed graph of the ith eigenvectors and, so far, the set of hypercubes is found to be the first class of graphs which obeys rigorously the parallel relationship between net signs and eigenvalues, in addition to the one-dimensional quantum systems [16].

Annulus(n)



1

Ladder(n)



2

Annulus (1) is a class of graphs which can be constructed by the direct product of cycles with K_2. The adjacency matrix of the annulus, $A(\mathrm{Annulus}(n))$, is given by

$$A(\mathrm{Annulus}(n) = \begin{bmatrix} A(C_n) & I \\ I & A(C_n) \end{bmatrix} . \tag{13}$$

The complete set of eigenvectors is $\{V_i | i = 1, 2, \ldots, 2n\}$ where n is the number of vertices of the constituent cycles and V_i can be expressed pairwisely by the eigenvectors of cycles $\{W_k\}$, i.e.,

$$\{V_{2k-1}, V_{2k}\} = \{[W_k W_k], [W_k \; -W_k]\}, \quad k = 1, 2, \ldots, n . \tag{14}$$

The corresponding eigenvalues are also written pairwisely by

$$\{\lambda_{2k-1}, \lambda_{2k}\} = \{1 + 2\cos(2k\pi/n), -1 + 2\cos(2k\pi/n)\} . \tag{15}$$

Net sign analysis of the class of annulusus leads to an expression of the net sign of the ith eigenvector of annulusus in terms of the net sign of the ith eigenvector of cycles,

$$(S_{2i}(Annulus(n)), S_{2i-1}(Annulus(n))) = 2S_i(C_n) \pm n , \tag{16}$$

where "+" and "−" are for the in-phase and out-phase combinations in eq. (14), respectively. Results of net sign analysis of the first five members of annulusus (see fig. 2) are presented in table 1.

One can write down relationships for the ladder (**2**) as done for the annulus. Accordingly, one has for the adjacency matrix (cf. eq. (13))

$$A(\text{Ladder}(n)) = \begin{bmatrix} A(L_n) & I \\ I & A(L_n) \end{bmatrix} \tag{17}$$

and the eigenvectors and the corresponding eigenvalues will be given as (cf. eqs. (14) and (15))

$$\{V_{2k-1}, V_{2k}\} = \{[W_k W_k], [W_k \; -W_k]\}, \quad k = 1, 2, \ldots, n, \tag{18}$$

$$\{\lambda_{2k-1}, \lambda_{2k}\} = \{1 + 2\cos(2k\pi/n+1), -1 + 2\cos(2k\pi/n+1)\}, \tag{19}$$

respectively. In this case, $W_k, k = 1, 2, \ldots, n$, are the eigenvectors of lines. Similarly, the net sign of the ith eigenvector of ladders is given by

$$(S_{2i}(Ladder(n)), S_{2i-1}(Ladder(n))) = 2S_i(L_n) \pm n, \tag{20}$$

where the meaning of "+" and "−" is similar to that for the annulus. Results of net sign analysis of the first five members of ladders are presented in table 2.

The above idea can be easily extended to the much more complicated graphs, such as grids and cylinders, for the study of their eigenvectors and eigenvalues. For example, an $n \times m$ rectangular grid is a direct product of $L_n \times L_m$ and its adjacency matrix is given by

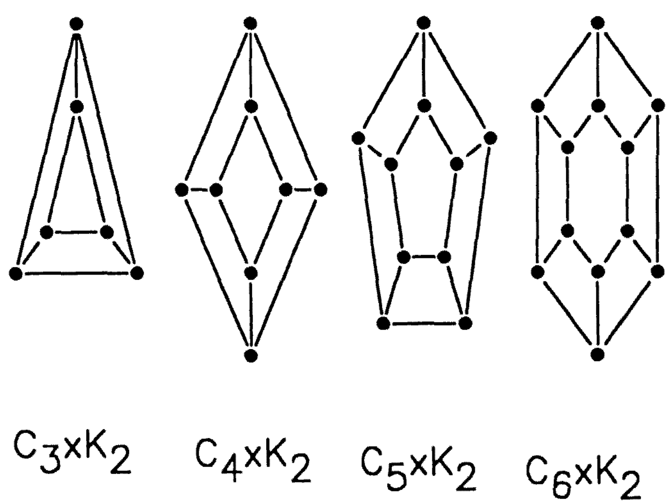


Fig. 2. Graphs of the first four members of the class of annulusus.

Table 1
Net signs and eigenvalues of first five members of the class of annulusus.

Cylinders	Eigenvalues	Net signs
$C_2 \times K_2$	$3, 1, 0, 0, -2, -2$	$9, 3, 1, 1, -5, -5$
$C_4 \times K_2$	$3, 1, 1, 1, -1, -1, -1, -3$	$12, 4, 4, 4, -4, -4, -4, 12$
$C_5 \times K_2$	$3, 1, 1.62, 1.62, -0.38, -0.38$ $-0.62, -0.62, -2.62, -2.62$	$15, 5, 7, 7, -3 - 3, -1, -1,$ $-11, -11$
$C_6 \times K_2$	$3, 1, 2, 2, 0, 0, 0, 0, -2, -2,$ $-1, -3$	$18, 6, 10, 0, 0, 0, 0, -10, -10,$ $-6, -18$
$C_7 \times K_2$	$3, 1, 2.25, 2.25, 0.25, 0.25, 0.56,$ $0.56, -1.45, -1.45, -0.80$ $-0.80, -2.8, -2.8$	$21, 7, 13, 13, -1, -1, 5, 5, 9,$ $-9, -3, -3, -17, -17$

$$A(\mathrm{Grid}(n,m)) = \begin{bmatrix} L_n & I & & & & \\ I & L_n & I & & 0 & \\ & I & L_n & I & & \\ & & & \ddots & & \\ & 0 & & & I & \\ & & & & I & L_n \end{bmatrix}. \tag{21}$$

Table 2
Net signs and eigenvalues of first five members of the class of ladders.

Ladders	Eigenvalues	Net signs
$L_2 \times K_2$	$2, 0, 0, -2$	$4, 0, 0, -4$
$L_3 \times K_2$	$2.41, 0.41, 1, -1, -0.41, -2.41$	$7, 1, 3, -3, -1, -7$
$L_4 \times K_2$	$2.62, 0.62, 1.62, -0.38,$ $-0.38, -1.62, -0.62, -2.62,$	$10, 2, 6, -2,$ $2, -6, -2, -12$
$L_5 \times K_2$	$2.73, 0.73, 2, 0, 1, -1,$ $0, -2, -0.73, -2.73$	$13, 3, 9, -1, 5,$ $1, -9, -3, -13$
$L_6 \times K_2$	$2.8, 0.8, 2.25, 0.25,$ $1.45, -0.56, 0.56, -1.45,$ $-0.25, -2.245, -0.8, -2.8$	$16, 4, 12, 0,$ $8, -4, 4, -8,$ $0, -12, -4, -16$

The net sign of the grid is given as

$$S_{(k-1)n+j}(Grid(n,m)) = S_k(L_n) \times m + S_j(L_m) \times n\,. \tag{21a}$$

Equation (20) is a special case of eq. (21a) as $m = 2$ and $S_k(L_2)$ is either 1 or -1. A cylinder, Cylinder (n, m), is a direct product of n-cycle with m-line and its adjacency matrix is given by

$$A(\text{Cylinder}(n,m)) = \begin{bmatrix} C_n & I & & & & \\ I & C_n & I & & 0 & \\ & I & C_n & I & & \\ & & & \ddots & & \\ & 0 & & & I & \\ & & & & I & C_n \end{bmatrix}. \tag{22}$$

$$= \begin{bmatrix} L_n & I & & & & I \\ I & L_n & I & & 0 & \\ & I & L_n & I & & \\ & 0 & & \ddots & & \\ I & & & & I & L_n \end{bmatrix}.$$

The net sign of the cylinder is given as

$$S_{(k-1)n+j}(\text{Cylinder}(n,m)) = S_k(L_m) \times n + S_j(C_n) \times m\,. \tag{22b}$$

Equation (16) is a special case of eq. (22b) as $m = 2$ and $S_k(\text{L}_2)$ is either 1 or -1.

4. Conclusions

A general strategy was proposed to generate the eigenvectors and eigenvalues of some special classes of graphs from well- studied chemical graphs such as lines and cycles. Ladders and cylinders, constructed from the Cartesian products of lines and cycles with the complete graph of order 2, were used as examples to demonstrate this strategy. This strategy is currently applied to study the topological properties of star graphs, spider graphs, and full binary trees.

Net sign analyses of ladders and cylinders were performed. A simple expression of net sign for each molecular orbital of the product graph can be derived in terms of the constituent graphs in both cases. Ladders and cylinders also provide us classes of graphs which obeys rigorously the parallel relationship between the ordering according to net signs and the ordering according to eigenvalues.

Acknowledgements

We thank the referees for very helpful suggestions. This work was supported financially by the National Science Council, Taiwan, Republic of China.

Appendix A

KRONECKER PRODUCT OF TWO MATRICES

For a matrix $A = [a_{ij}]$ of dimension $m \times n$ and a matrix $B = [b_{ij}]$ of dimension $p \times q$, the Kronecker product of two matrices $A \otimes B = [c_{ij}]$ is defined a matrix of order $mp \times nq$ with elements

$$c_{(i-1)p+j(t-1)q+k} = a_{ik} b_{jt} ,$$

where $i = 1, 2, \ldots, n$ and $t = 1, 2, \ldots, m$. $A \otimes B$ can thus be written in the partitioned form as

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \ldots & a_{1n}B \\ a_{21}B & a_{22}B & \ldots & a_{2n}B \\ \ldots & \ldots & \ldots & \ldots \\ a_{m1}B & a_{m2}B & \ldots & a_{mn}B \end{bmatrix} .$$

References

[1] N. Trinajstić, *Chemical Graph Theory*, Vols. I & II (CRC Press, Boca Raton, Florida, 1983).
[2] S.-L. Lee, R.R. Lucchese and S.-Y. Chu, Chem. Phys. Lett. 137 (1987) 279;
S.-L. Lee and I. Gutman, Chem. Phys. Lett. 157 (1989) 229.
[3] A. Graovac, I. Gutman and N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules* (Springer, Berlin, 1977).
[4] R.B. King, J. Phys. Chem. 92 (1988) 4452; J. Comput. Chem. 8 (1987) 341.
[5] Y. Wang, T.F. George, D.M. Lindsay and A.C. Beri, J. Chem. Phys. 86 (1987) 3493;
S.-L. Lee, Theor. Chim. Acta 81 (1992) 185.
[6] L.B. Kier and L.H. Hall, *Molecular Connectivity in Chemistry and Drug Research* (Academic Press, New York, 1976).
[7] M.J. Rigby, R.B. Mallion and A.C. Day, Chem. Phys. Lett. 51 (1977) 178; 53 (1978) 418.
[8] R.C. Read, in: *Chemical Applications of Graph Theory*, ed. A.T. Balaban (Academic Press, New York, 1976) ch. 4;
A.T. Balaban, in: *Chemical Applications of Graph Theory*, ed. A.T. Balaban (Academic Press, New York, 1976) ch. 5.
[9] L.B. Kier and L.H. Hall, *Molecular Connectivity in Structure-Activity Analysis* (Research Studies Press, Letchworth, England, 1986).
[10] L.H. Hall and L.B. Kier, J. Pharm. Sci. 66 (1977) 642.

[11] I. Gutman and O.E. Polansky, *Mathematical Concepts in Organic Chemistry* (Springer, Berlin, 1986).
[12] S.-L. Lee and F.-Y. Li, J. Mol. Struct. (THEOCHEM) 207 (1990) 301.
[13] S.-L. Lee and Y.-N. Yeh, J. Math. Chem. 12 (1993) 121.
[14] S.-L. Lee and Y.-N. Yeh, Chem. Phys. Lett. 171 (1990) 385.
[15] C.A. Coulson and A. Streitweiser, *Dictionary of π-electron Calculations* (Freeman, San Francisco, 1965).
[16] S.-L. Lee, F.-Y. Li and F. Lin, Int. J. Quant. Chem. 39 (1991) 59.
[17] E.B. Wilson, J. Chem. Phys. 63 (1975) 4870.
[18] M.L. Mehta, *Elements of Matrix Theory* (Hindustan Publ., Delhi, 1977) p. 93.
[19] F. Buckley and F. Harary, *Distance in Graphs* (Addison-Wesley, New York, 1990) p. 118.
[20] M. Marcus and H. Min, *A Survey of Matrix Theory and Matrix Inequalities* (Allyn and Bacon, Boston, 1964).
[21] D.M. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs: Theory and Application* (Academic Press, New York, 1980) p. 70.