match no. 16 pp. 153-162 1984

MATRIX INVERSE OF CHEMICAL GRAPHS

II SINGULAR GRAPHS

Sherif El-Basil

Faculty of Pharmacy, Kasr El-Aini Street,
Cairo , Egypt

(Received: August 1983)

ABSTRACT

Three theorems are stated and proved which allow generation of infinite number of singular graphs i.e. graphs whose adjacency matrices have no inverses. An observation is cited in relation to antiaromatic and non-kekulean hydrocarbons. A fourth theorem is given which relates the spectrum of the eigenvalues of the adjacency matrix to the non-existence of an inverse.

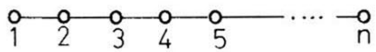
The importance of the inverse of the adjacency matrix, $\underline{A}^{-1}$, of a graph arose many years ago in connection of the relation between resonance and MO theories[1]. In part I of this work[2] we showed the potential of the $\underline{A}^{-1}$ matrix in coding of chemical graphs. The problem is related to important topics such as order, comparability and similarity among a set of (chemical) graphs and thus allowing the study of molecular properties from information obtainable from the $\underline{A}^{-1}$ matrix. The conditions necessary for the existence of an inverse of a given matrix is that the determinant of this matrix does not vanish i.e. it has a non-zero value[3]. In this work we present three theorems by which one might generate an infinite number of singular graphs i.e. graphs whose adjacency matrices possess no inverses. A fourth theorem is presented which relates the spectrum of eigenvalues to the singularity of $\underline{A}$.

Theorem 1

The adjacency matrix corresponding to a linear chain containing an odd number of vertices is singular.

Proof

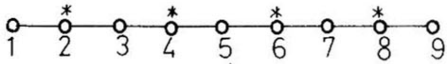
We number the vertices of the linear chain arbitrarily from left to right 1, 2, ... , n, where n is the number of vertices in the chain.



Then we perform the following row operation on the determinant of the corresponding $\underline{A}$, $r_3 - r_5 + r_7 - \ldots \pm r_n$ where r_i is ith row. By this operation the value of det $\underline{A}$ remains unchanged. Since the third an fifth rows are now identical, then from a well known theory in algebra follows that det A = 0, hence the original matrix $\underline{A}$ is singular.

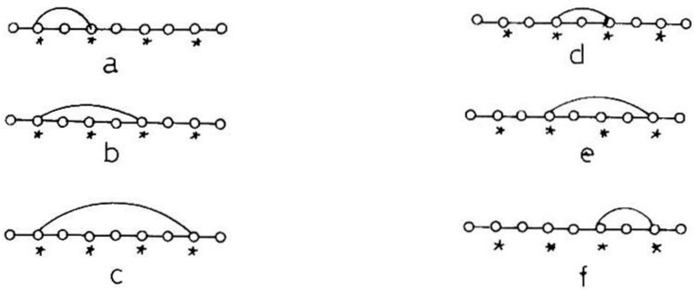
Corollary 1

Theorem 1 allows the construction of an infinite number of singular graphs: Since the row operations involve only the vertices with odd numbers $(r_1, r_3, r_5, \ldots, r_n)$ substitutions on vertices with even numbers will yield singular graphs. Also, linking tuplets of "even" vertices will introduce ones only in rows with even labels i.e. in r_2, r_4, ..., r_{n-1}. The resulting graphs will be, also, singular. Suppose, e.g., we have L_9 i.e.

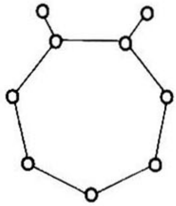


L_9

We are allowed to introduce ones between pairs (or higher tuplets) of the even set $\{2,4,6,8\}$. We shall have, therefore $\binom{4}{2}$ selections i.e. $4!/(4-2)!2! = 6$ structures for the pair-wise selections. These structures are shown below



However it is clear that a = f and b = e therefore the net number of pair-wise connections of "even" vertices is only four singular graphs. It might be observed that the above representations correspond to graphs of chemical interest, e.g. (c) corresponds to the following cycloheptatriene radical:



c

The above singular graphs (a-f) might be used to generate another group of singular graphs with two additional ones in their matrices. The resulting matrices might in turn be used to generate other singular matrices and so on. Fig 1 shows such graphs after deletion of the equivalent ones.

<u>Theorem 2</u>

The adjacency matrix of a cycle containing 4n vertices (n = 1, 2, 3, ...) is singular.

<u>Proof</u>

We assign numbers to the vertices of the cycle in the natural order of the real numbers starting at any vertex. Let $j = 4n$ be the number of vertices in the cycle. We perform the following row operations on the corresponding determinant $r_1 - r_m + r_{m-2} - r_{m-4} + \ldots\ldots + r_5$ where $m = j-1$. The resulting determinant has $r_1 = r_3$ whence the corresponding matrix is singular. This proves the theorem.

<u>Corollary 2</u>

If we divide the vertices of a C_{4n} into two groups of different parities one might easily generate graphs with singular matrices by connecting vertices of identical parities. The following general types of singular graphs result from theorem 2.

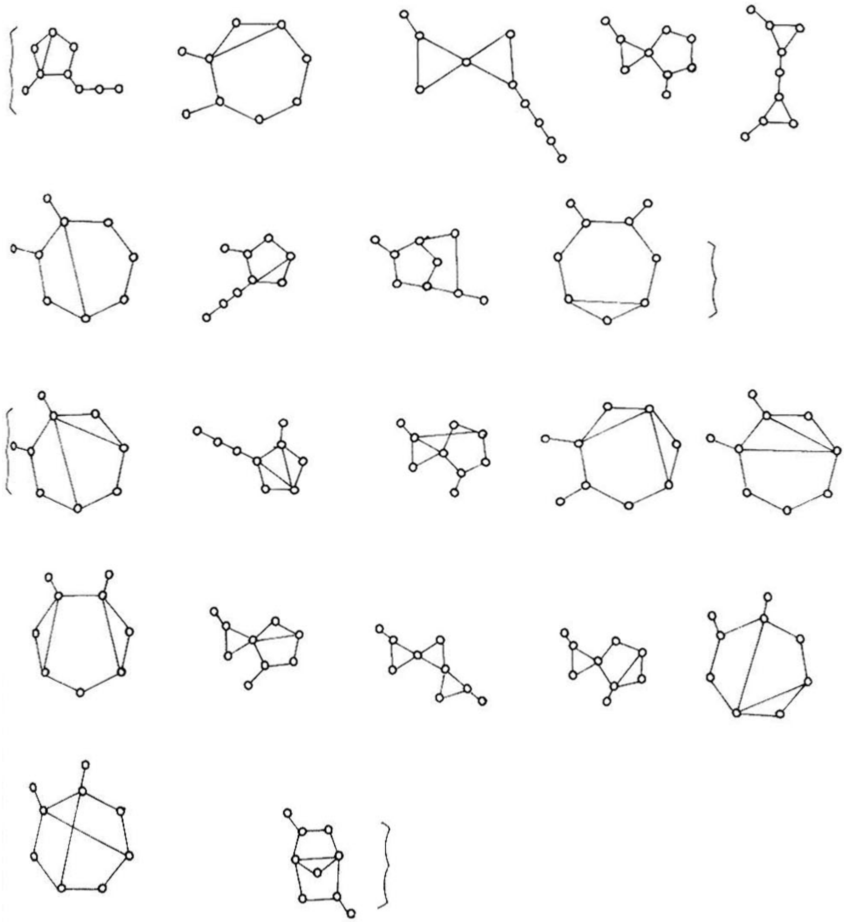


Fig 1.

Singular graphs on nine vertices generated from graphs a-f by appropriate additions of two and three ones to their adjacency matrices.

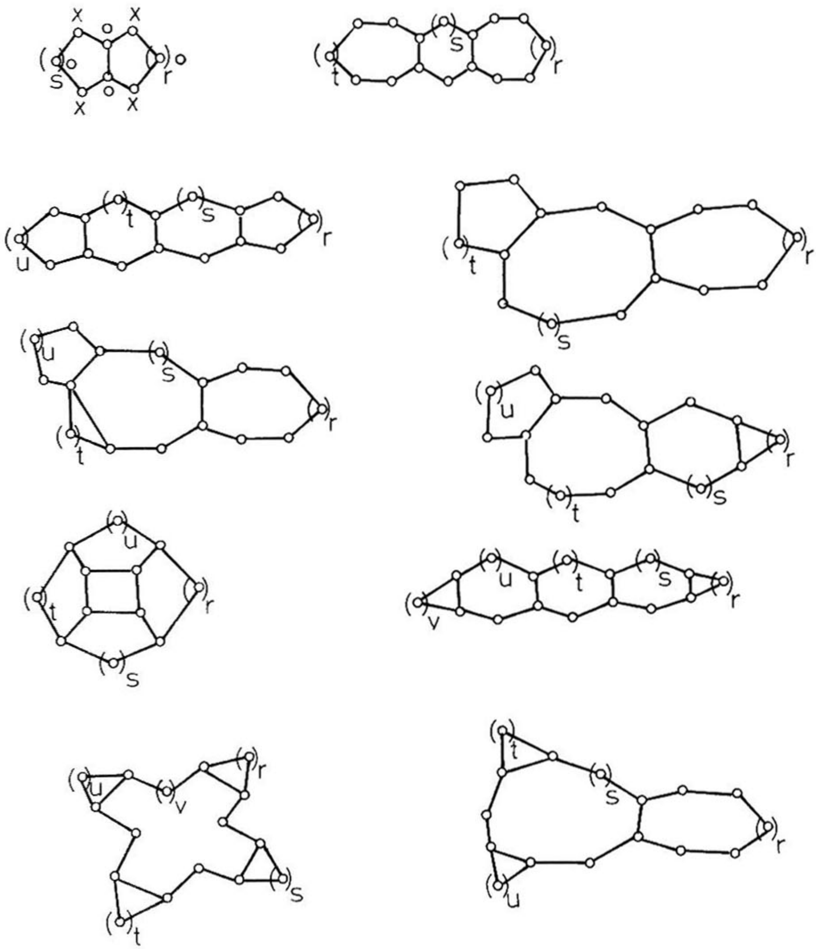


Fig 2

Examples of singular graphs which are constructed using theorem 2. The parameters r, s, t, u, v take values of 1, 5, 9, 13, ...

Theorem 3

The adjacency matrix of a wheel[4], W_{4n+1} $(n = 1, 2, 3, ...)$ is singular.

Proof

Label the vertices of the periphery of the wheel 1, 2, 3, ..., 4n while the central vertex is assigned the number 4n+1. Perform the following row operation: $r_1 - r_j + (r_{j-2}) - (r_{j-4}) + ... - r_3$; where $j = 4n-$. The resulting determinant will have zeros in all the enteries of the first row; whence the original $\underline{A}$ must be singular.

Corollary 3

Graphs obtainable by deleting edges connecting the central vertex of W_{4n+1} to vertices of like parities are singular. I.e., their $\underline{A}$'s possess no inverses. Fig 3 contains several examples of such types of graphs.

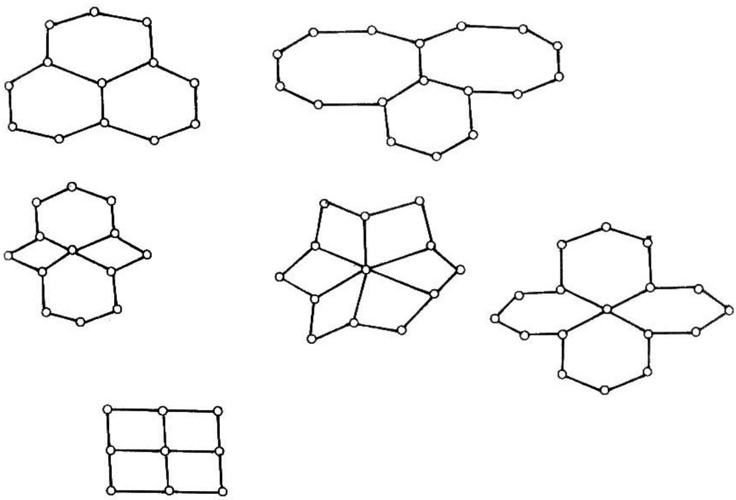
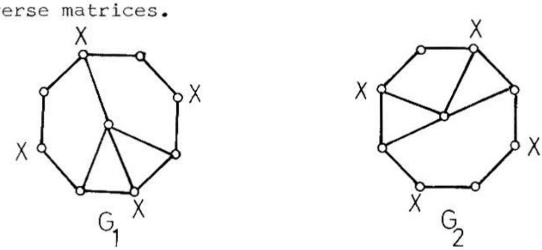


Fig 3

Some illustrative examples of singular graphs generated using theorem 3.

It is interesting to observe that the two cospectral graphs G_1 and G_2 discovered sometime ago by Schwenk et al.[5] are both derived from W_9; by deleting edges connecting the central vertex to vertices of <u>different</u> parities and thus do not satisfy corollary 3. Indeed both G_1 and G_2 possess inverse matrices.



Finally one observes that theorem 2 generate fully antiaromatic having only 4n conjugated circuits[6] (e.g. the first three graphs of Fig 2), while theorem 3 generate non-kekulean hydrocarbons, i.e. systems for which no Kekule structures might be written (e.g. the first two graphs of Fig 3).

<u>Theorem 4</u>[7]

Let G be a simple graph on n vertices , $\underline{A}$ its adjacency matrix and spec (G) the spectrum of the eigenvalues, λ , of G. The following holds :
Iff $0 \in$ spec (G) , then $\underline{A}$ is singular (iff = " if and only if").

<u>Proof</u>

The eigenvalues, λ , of G follow the equation

$$\det \left\| \lambda \cdot \underline{1} - \underline{A} \right\| = 0 \qquad (1)$$

In case of $\lambda = 0$, the expression becomes

$$\det \left\| - \underline{A} \right\| = \det \left\| \underline{A} \right\| = 0$$

Hence A is singualr, when $\lambda = 0$ is an eigenvalue of G as supposed. In order to prove the assertion " only if ", let us assume $0 \notin$ spec (G). Because there are only n distinct values of λ , and no one of these equals zero, then in order to satisfy eqn. 1, we have $\det \left\| -A \right\| \neq 0$

<u>q.e.d</u>

Using this theorem one might apply the Coulson-Rushbrooke rules[8] in case of bipartite graphs[9]: the path graphs P_{2m+1} used in theorem 1 as well as the cycles C_{4m} (m=1,2, 3,...) in theorem 2. The construction of the derived graphs provide interesting extensions to these rules.

Acknowledgment

I deeply thank Professor Dr. O.E. Polansky for kindly directing my attention to theorem 4, its proof and possible future extensions.

References

(1) N.S. Ham and K. Ruedenberg, J. Chem. Phys. 29, 1215 (1958).

(2) S. El-Basil and A. Hussean, Match, submitted for publication (1983).

(3) See, e.g., H. Anton, Elementary Linear Algebra, John Wiley & Sons (1981).

(4) A wheel W_n is defined to be the graph $K_1 + C_{n-1}$, C.f. F. Harary, Graph Theory, Reading, Mass. Addison-Wesley (1972).

(5) A.J. Schwenk, W.C. Herndon and M.L. Ellzey, Jr., Annals of the New York Academy of Sciences, 319, 494 (1979).

(6) M. Randić, J. Am. Chem. Soc., 99, 444 (1977).

(7) O.E. Polansky, Private communication (1984), C.f., acknowledgment

(9) C.A. Coulson and G.S. Rushbrooke, Proc. Camb. Phil. Soc. 36 , 193 (1940) ; See also K. Higasi, H. Baba and A. Rembaum, Quantum Organic Chemistry, Interscience Publishers (1965), Chapt. 6.
An interesting book dealing with these rules is written by I.S. Dmitriev, Molecules Without Chemical Bonds- "Essays on Chemical Topology ", Mir Publishers, Moscow (1981) , Chapter 3.

(9) For some graph-theoretic definitions, see I. Gutman and N. Trinajstić, Top Curr. Chem. 42 , 60 (1973).