match no. 2 pp.157-158 1976

EIGENVALUE METHODS FOR IRREGULAR GRAPHS WITH APPLICATION TO SPANNING TREE ENUMERATION IN MOLECULAR GRAPHS

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(received: November 1975)

The complexity, K (G), of a graph, G, is the number of spanning trees it possesses. This useful quantity can be calculated by use of the 'Matrix Tree' Theorem often (though erroneously) attributed to Kirchhoff. Study of the eigenvalues $\{\lambda_1 = d, \lambda_2, \ldots \lambda_N\}$ of the adjacency matrix of a regular graph, G, of valency d led to the more convenient formula

$$K(G) = \frac{1}{N} \prod_{j=2}^{N} (d - \lambda_j).$$

Most graphs, however, (and particularly those which represent conjugatedhydrocarbons) are not regular; in fact, of such conjugated systems, only the annulenes have regular molecular graphs.

The 'row-regularisation' procedure introduced by one of us [D.A. Waller, Eigenvalues of Graphs and Operations, Proc. British Combinatorial Conference, 1973, London Math Soc. Lecture Notes Series 13 (1974) 177-183] involves adjoining $N - d_j - 1$ loops at each vertex of valency d_j, in order to 'make irregular graphs regular', (of valency N - 1). The loops adjoined to the vertices of G do not, of course, change

K (G); hence the eigenvalues of this associated 'row-regularised' adjacency matrix can be used in conjunction with the above formula for regular graphs of valency d (with, in this case, d = N - 1) to determine K (G), the complexity of an arbitrary graph.

The second of the present authors (R.B. Mallion, On the Number of Spanning Trees in a Molecular Graph, Chem. Phys. Letters, 36 (1975) 170-174) has applied this general formula to the sorts of molecular graphs which arise in calculation of the magnetic properties of conjugated systems and has illustrated the method by calculating the complexity of the (irregular) molecular graph of Naphthalene.