Theoret. Chim. Acta (Berl.) 55, 255 (1980)

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Book Reviews

A. Graovac, I. Gutman, and N. Trinajstic: Topological Approach to the Chemistry of Conjugated Molecules (Lecture Notes in Chemistry Vol. 4). Berlin–Heidelberg–New York: Springer–Verlag 1977. 123 pp. Soft cover DM 18.—; US $8.30

Chemists have long believed that the structural formula of a molecule determines not only its geometry but also its chemical properties. The graph theory of conjugated molecules is based on this belief. A topological matrix is derived from the structural formula and, from it, quantities are defined as measures of different chemical properties. Historically the theory has grown out of Hückel theory but it is now presented as a rigorous application of graph theory and not as a poor approximation to quantum mechanics. This divorce gives the theory much greater generality while allowing it to retain its simple basic concepts.

A major objective of the theory is to define and explain the aromaticity of conjugated molecules. Aromaticity, and the related ideas of resonance and localization, does not emerge naturally from quantum mechanics because the detailed complexity of the calculations hides it. It has a much better chance of emerging from a treatment which retains only the correct topology since this is clearly very relevant and, indeed, the graph theory approach has made very considerable progress.

This book presents the elements of graph theory in a form suitable for chemists. Each of the basic concepts is directly illustrated using molecules. The more advanced concepts are reviewed briefly with appropriate references. In one respect the treatment is less than satisfactory. It makes little attempt to relate its calculated quantities to experiments and this may leave the false impression that few significant relations exist. Theoreticians will welcome a text which gives a connected, graphic account of a theory which must now be regarded as independent of quantum mechanics and a valid theory in its own right.

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Received January 21, 1980

0040–5744/80/0055/0255/$01.00

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D. Cvetković, M. Doob and H. Sachs: Spectra of Graphs—Theory and Application. New York–San Francisco–London: Academic Press, and Berlin (East): Deutscher Verlag der Wissenschaften 1980. 368 pp.

In the last few years the mathematical apparatus of graph spectral theory has been widely used in certain investigations in quantum chemistry. These efforts resulted in the so called topological theory of conjugated molecules; at least a hundred papers on this topic were published in the chemical journals after 1970. Thus graph spectral theory should be of some importance for scientists working in the field of theoretical chemistry.

The comprehensive mathematical monograph by Dragoš Cvetković (Yugoslavia), Michael Doob (Canada) and Horst Sachs (GDR) is written not only "for mathematicians working in the area of graph theory and combinatorics", but also "for chemists who are interested in quantum chemistry and, at least partly, for physicists and electrical engineers using graph theory in their work". One should note that this is the first book on the theory of graph spectra.

The book contains practically the entire knowledge about graph spectra (until early 1979). It consists of ten chapters, tables of graph spectra and bibliography.

In the first three chapters the basic properties of the graph spectrum are described. This part of the book will be of great value for chemists; they can read it without difficulties. Two other chapters will be also interesting for quantum chemists: in Chapter 5 the relations between the spectrum and the group of automorphism (i.e. symmetry) of a graph are exposed, while Chapter 8 is a short (and therefore incomplete) review of the applications of graph spectra in chemistry and physics. The book ends with an extensive collection of calculated graph spectra. For example, there is a list of the spectra and characteristic polynomicals of all trees with ten and fewer vertices.

A particularly valuable part of this monograph is the exhaustive bibliography of both mathematical and chemical publications dealing with graph spectra (consisting of nearly 700 titles and including also papers which appeared in the first half of 1979).

The "Spectra of Graphs" belongs among those mathematical books which are worth the chemists' attention.

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Received February 21, 1980

0040–5744/80/055/0256/$01.00