

# Lecture Notes in Chemistry

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Topological Approach  
to the Chemistry  
of Conjugated Molecules

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## PREFACE

"The second step is to determine constitution, i.e. which atoms are bonded to which and by what types of bond. The result is expressed by a planar graph (or the corresponding connectivity matrix).... In constitutional formulae, the atoms are represented by letters and the bonds by lines. They describe the topology of the molecule."

VLADIMIR PRELOG, Nobel Lecture, December 12,<sup>th</sup> 1975.

In the present notes we describe the topological approach to the chemistry of conjugated molecules using graph-theoretical concepts. Conjugated structures may be conveniently studied using planar and connected graphs because they reflect in the simple way the connectivity of their pi-centers. Connectivity is important topological property of a molecule which allows a conceptual qualitative understanding, via a non-numerical analysis, of many chemical phenomena or at least that part of phenomenon which depends on topology. This would not be possible solely by means of numerical (molecular orbital) analysis.

Reader's knowledge of the formal theory of graphs is not essential for the understanding of the material presented here because these notes are "application-oriented" and the mathematical formalism is reduced to minimum. However, we would like to convince the chemical community at large that the (organic) chemists must develop their knowledge of mathematics beyond the high-school algebra because many results of (organic) chemistry may be shaped up nicely by the appropriate mathematical apparatus (group theory, graph theory, theory of polynomials, functional analysis, etc.) into concise universal laws of chemistry. A good example to support this statement is provided by the work of Prelog in chemical topology which has led him to introduce the general concept named chirality in order to understand fully the molecular architecture.

The nomenclature used in these notes has been systematically employed and developed by us. We have tried to connect the mathematical terminology with the everyday language of chemists. We shall welcome the readers' comments on the material and terminology presented in notes.

Finally, it is our pleasant duty to thank Professor Rudolf Zahradić, under whose encouragement we started this project, for useful discussions and helpful comments.

Zagreb, Croatia, June 1977.

A. Graovac, I. Gutman, N. Trinajstić

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To Professor BOŽO TEŽAK