BOOK REVIEW

CROATICA CHEMICA ACTA

Croat. Chem. Acta **2016**, *89*(*4*), 555–557
Published online: May 9, 2017
DOI: 10.5562/cca3148

HKD 1926

Ivan Gutman

Selected Theorems in Chemical Graph Theory

Mathematical Chemistry Monographs, Vol. 18

Faculty of Science, University of Kragujevac, Kragujevac (Serbia), 2017
168 + VII pages ◦ ISBN 978-86-6009-019-5

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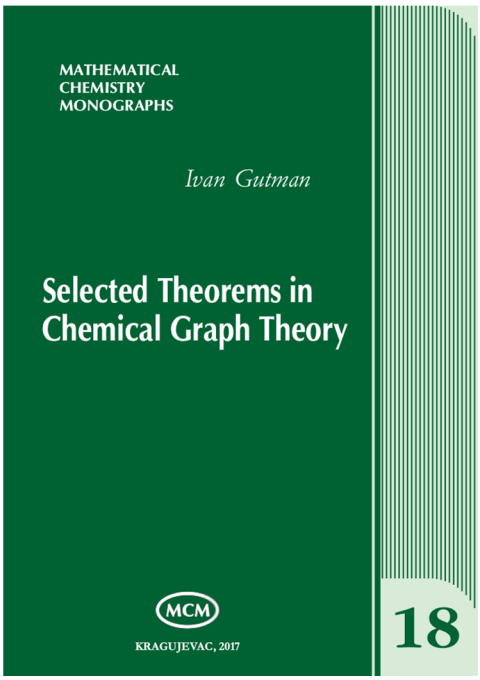
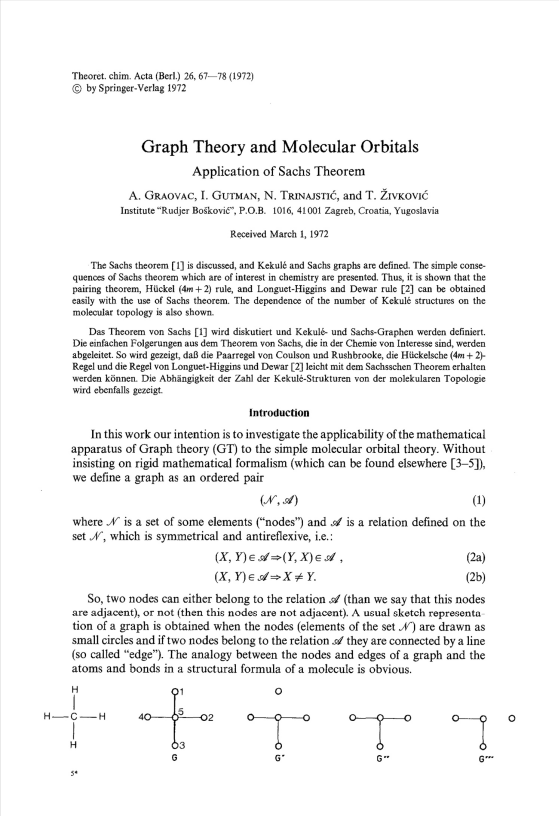
THIS monograph consists of *Preface*, *Introduction* and 16 chapters reporting theorems of interest for both mathematicians and mathematical chemists. In it, Professor Ivan Gutman collected in the form of theorems several simple, beautiful and powerful results of chemical graph theory. He was particularly interested in theorems that connect two or more mutually unrelated concepts. A very illustrative example is the Dewar-Longuet-Higgins formula which connects the determinant of adjacency matrix (a linear-algebraic concept) and the number of perfect matchings (a concept belonging to graph theory, but also to organic chemistry under the term Kekulé structures).

In *Preface* (pp. iii–vii), the autor points out what will *not* be included in this book and is supplied with 53 references. The monograph starts with *Introduction* (Chapter 1, pp. 1–3; 4 refs.). In it, the author gives definitions and illustrations of several basic graph-theoretical concepts that will be used in chapters 2–17. In the chapter 2 (pp. 5–10; 42 refs.), entitled *Degree-Based Theorems*, the author discussed the Zagreb indices, their co-indices and the connectivity (Randić) index. In the chapter 3 (pp. 11–21; 61 refs.), entitled *Distance-Based Theorems*, the theory of the Wiener number is discussed. This index has been introduced by Harold Wiener (Vienna, 1924 – New York City, 1998) in 1947 and still very much cited in the mathematical chemistry literature. In this chapter, there are also discussed the Szeged index of a graph, the relationship between the Wiener index and the Szeged index, and the Steiner-Wiener index. In the chapter 4 (pp. 23–29; 43 refs.),



entitled *Degree–and–Distance–Based Theorems*, the author discussed the degree distance, molecular topological index, the relationships between the Wiener index and the degree distance, and the Wiener index and Gutman index. The fifth chapter is entitled *Degree–and–Distance–Based Theorems for Benzenoid Systems* (pp. 31–42; 68 refs.). In this chapter, the authors discussed basic structural



Theoret. chim. Acta (Berl.) 26, 67—78 (1972)
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Graph Theory and Molecular Orbitals
Application of Sachs Theorem

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Received March 1, 1972

The Sachs theorem [1] is discussed, and Kekulé and Sachs graphs are defined. The simple consequences of Sachs theorem which are of interest in chemistry are presented. Thus, it is shown that the pairing theorem, Hückel ($4n+2$) rule, and Longuet-Higgins and Dewar rule [2] can be obtained easily with the use of Sachs theorem. The dependence of the number of Kekulé structures on the molecular topology is also shown.

Das Theorem von Sachs [1] wird diskutiert und Kekulé- und Sachs-Graphen werden definiert. Die einfachen Folgerungen aus dem Theorem von Sachs, die in der Chemie von Interesse sind, werden abgeleitet. So wird gezeigt, daß die Paarregel von Coulson und Rushbrooke, die Hückelsche ($4n+2$)-Regel und die Regel von Longuet-Higgins und Dewar [2] leicht mit dem Sachsschen Theorem erhalten werden können. Die Abhängigkeit der Zahl der Kekulé-Strukturen von der molekularen Topologie wird ebenfalls gezeigt.

Introduction

In this work our intention is to investigate the applicability of the mathematical apparatus of Graph theory (GT) to the simple molecular orbital theory. Without insisting on rigid mathematical formalism (which can be found elsewhere [3–5]), we define a graph as an ordered pair

$$(\mathcal{N}, \mathcal{A}) \quad (1)$$

where $\mathcal{N}$ is a set of some elements ("nodes") and $\mathcal{A}$ is a relation defined on the set $\mathcal{N}$, which is symmetrical and antireflexive, i.e.:

$$(X, Y) \in \mathcal{A} \Rightarrow (Y, X) \in \mathcal{A}\ , \quad (2a)$$

$$(X, Y) \in \mathcal{A} \Rightarrow X \neq Y. \quad (2b)$$

So, two nodes can either belong to the relation $\mathcal{A}$ (than we say that this nodes are adjacent), or not (then this nodes are not adjacent). A usual sketch representation of a graph is obtained when the nodes (elements of the set $\mathcal{N}$) are drawn as small circles and if two nodes belong to the relation $\mathcal{A}$ they are connected by a line (so called "edge"). The analogy between the nodes and edges of a graph and the atoms and bonds in a structural formula of a molecule is obvious.

Figure 1. The first page of the article on Sachs theorem, which appeared in *Theoret. Chim. Acta*, **1972**, *26*, 67–78.

parameters of benzenoids and gave formulae for computing their Zagreb indices, Randić index, Szeged index, Gutman index and Wiener index. In the chapter 6 (pp. 43–49; 42 refs.), entitled *Theorems related to Resistance Distance*, the author discussed the connection between the Wiener index and the Laplacian spectrum of graph, and the properties of the degree Kirchhoff index. The following chapter (pp. 51–58; 31 refs.) is entitled *Theorems of Nullity*, This chapter is dealing with graphs that possess zero(s) in their spectra.

In the chapter 8 (pp. 59–71; 64 refs.), entitled *Sachs Theorem*, the author gives account about the introduction of this theorem to mathematical chemistry and its impact on research in mathematical chemistry. The authors of the seminal paper *Graph Theory and Molecular Orbitals. Application of Sachs Theorem* (*Theoret. Chim. Acta* **1977**, *26*, 67–78) Ante Graovac (Split, 1945.), Ivan Gutman (Sombor, 1947.), Nenad Trinajstić (Zagreb, 1936.) and Tomislav Živković (Zagreb, 1943.) are now retired and Graovac unfortunately died in 2012. In this paper the terms *Sachs graph* and *Sachs theorem* were introduced (Horst Sachs, Magdeburg, 1927 – Ilmenau, 2016, was well-known Germain mathematician whose paper *Bezichungen zwischen den in einen Graphen enthaltenen Kreisen und seinen charakteristischen Polynom*, *Publ. Math*. (Debrecen) **1964**, *11*, 119–134 stimulated Graovac *et al.* to start research in what later became chemical graph theory). This paper was well-received and according to Gutman is still supstantially cited. The chapter 9 (pp. 73–77; 34 refs.) is entitled *Determinant of the Adjacency Matrix*. The interest in the determinant of the adjaceny matrix and its dependency on the structure of underlying graph goes back to two reports in 1959 and 1962 by Frank Harary (New York, 1921 – Las Cruces, New Mexico, 2005). Here belongs also already mentioned formula by Michael M. J. Dewar (Ahmednagar, 1918 – Gainesville, Florida, 1997) and Hugh Christopher Longuet-Higgins (Lenham, Kent, 1923–2004). The next chapter (pp. 79–94; 48 refs.), entitled *Algebra of Kekulé Structures*, presents some nice results for the old chemical concept of Kekulé structures. Besides Kekulé structures, the author discussed the algebraic structure count and counting Kekulé structures using approach based peaks and valleys. The necessary, but not sufficient, condition for a benzenoid structure to possess Kekulé structures is to have a number of distinct monotonic paths on the benzenoid system between its peaks and valleys. The author perhaps should have mentioned here the report by Douglas J. Klein and Trinajstić on the use of the Pascal recurrence algorithm for Kekulé-structure counts of benzenoid and coronoid hydrocarbons (*J. Mol. Struct.* (*Theochem*), **1990**, *206*, 136–142).

The chapter 11 (pp. 95–106; 57 refs.) is entitled *Matching Polynomial*. This polynomial is the key quantity in the theory of topological resonance energy. Originally the term used for this polynomial was the *acyclic* polynomial, see I. Gutman, M. Milun, N. Trinajstić, Graph theory and molecular orbitals. 19. Non-parametric resonance energies of arbitrary conjugated systems, *J. Am. Chem. Soc.*, **1977**, *99*, 1692–1704. The reason for changing from *acyclic* to *matching* is related to the meaning of this terms – *acyclic* indicates what the polynomial is not, whereas *matching* indicates a property that the polynomial possesses. In the next chapter (pp. 107–112; 35 refs.), entitled *More Real Graph Polynomials*, the author is discussed real polynomials, that is polynomials with all their zeros real numbers. In the chapter 13 (pp. 113–118; 24 refs.) is presented *Polansky's TEMO Theorem*, where TEMO stands for *topological effect on molecular orbitals*. The first contribution on TEMO entitled *Topological effect on MO energies* (*J. Mol. Struct.*, **1982**, *84*, 361–385) has been published in 1982 by Oscar E. Polansky (Vienna, 1919 – Mülheim an der Ruhr 1989) and Maximillian Zander (Berlin, 1929–2016). The second paper in the series, not cited, was O. E. Polansky, M. Zander and I. Motoc, *TEMO. II. On the MO Energies of Structurally Related Aza-arenes*, *Z. Naturforsch.*, **1983**, *38a*, 196–199. Further research on TEMO is carried out

by Polansky and several of his visitors and co-workers. Very valuable results were achieved when Polansky collaborated with Graovac and Gutman who spent some time with him in Mülheim an der Ruhr in the period 1984–1988.

The chapter 14 (pp. 119–126; 33 refs.) has an intriguing title *A Trivial Theorem with Enormous Consequences.* It contains a nice story about introducing the concept of *graph energy* and its acceptance. At the end of the chapter, the author presented two tables, the first table contains the number of papers on graph energies published in the period 1996–2016 (681 as in August 2016) and the second table contains the list of countries (46, among them is Croatia) whose researchers published at least one paper on graph energy. The next chapter, the chapter 15 (pp. 127–142; 87 refs.), is entitled *More Spectrum-Related Theorems*. In this chapter, the author discussed Coulson's integral formula, Hosoya index of trees, spanning trees of benzenoid systems, normalized Laplacian matrix and Randić matrix, and incidence matrix and Laplacian-energy-like invariant. In the chapter 16 (pp. 143–152; 81 refs.), entitled *Theorems Related to Line Graphs*, it is shown that the reformulated Zagreb indices are exactly the ordinary Zagreb indices of the line graph. The author is discussed the Wiener indices of line graphs, iterated line graphs and equienergetic line graphs. The last chapter in this monograph (pp. 153–168; 59 refs.) is entitled *Algebra of Clar Structures*. In this chapter the author discussed Clar structures of benzenoid hydrocarbons, Clar sextet, Clar number, sextet polynomial, caterpillar trees.

I enjoyed reading this book and recommend it to all who are interested in mathematical chemistry and its uses. If the reader is specially interested in chemical graph theory, this is a very useful book to have within reach. I only wonder why the author did not include the *Authors index* and the *Subject index*. However, majority of books published in the series *Mathematical Chemistry Chemistry* do not possess any of these indices. Hopefully this will be remedied in the future.

Nenad Trinajstić