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[View references \(98\)](#)**Impact of the Sachs theorem on theoretical chemistry: A participant's testimony**[Gutman, I.](#)

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Abstract

An outline is given of the role which the coefficient theorem, discovered in 1964 by Horst Sachs, played in the theoretical chemistry of conjugated molecules.

References (98)

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1. [Hückel, E.](#)
Quantentheoretische Beiträge zum Benzolproblem
(1931) *Z. Phys.*, 70 pp. 204-286 [Cited 194 times](#)
2. [Hückel, E.](#)
(1940) *Grundzüge der Theorie Ungesättigter und Aromatischer Verbindungen*, [Cited 24 times](#)
Verlag Chemie, Berlin
3. [Hückel, E.](#)
Zur modernen Theorie ungesättigter und aromatischer Verbindungen
(1957) *Z. Elektrochem.*, 61 pp. 866-890 [Cited 3 times](#)
4. [Günthard, H.H.](#), [Primas, H.](#)
Zusammenhang von Graphentheorie und MO - Theorie von Molekeln mit Systemen konjugierter Bindungen
(1956) *Helv. Chim. Acta*, 39 pp. 1645-1653 [Cited 8 times](#)
5. [Coulson, C.A.](#), [O'Leary, B.](#), [Mallion, R.B.](#)
(1978) *Hückel Theory for Organic Chemists*, [Cited 58 times](#)
Academic Press, London
6. [Yates, K.](#)
(1978) *Hückel Molecular Orbital Theory*, [Cited 28 times](#)
Academic Press, New York
7. [Conlson, C.A.](#)
On the calculation of the energy in unsaturated hydrocarbon molecules
(1940) *Proc. Cambridge Phil. Soc.*, 36 pp. 201-203 [Cited 16 times](#)
8. [Coulson, C.A.](#), [Longuet-Higgins, H.C.](#)
The electronic structure of conjugated systems. I. General theory
(1947) *Proc. Roy. Soc. London A*, 191 pp. 39-60 [Cited 91 times](#)
9. [Coulson, C.A.](#), [Longuet-Higgins, H.C.](#)
The electronic structure of conjugated systems. II, Unsaturated hydrocarbons and their hetero-derivatives
(1947) *Proc. Roy. Soc. London A*, 192 pp. 16-32 [Cited 47 times](#)

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10. [Coulson, C.A., Longuet-Higgins, H.C.](#)
The electronic structure of conjugated systems. III. Bond orders in unsaturated molecules
(1948) *Proc. Roy. Soc. London A*, 193 pp. 447-456 [Cited 26 times](#)
11. [Samuel, I.](#)
Résolution d'un déterminant seculaire par la méthode des polygones
(1949) *Compt. Rend. Acad. Sci. Paris*, 229 pp. 1236-1237
12. [Samuel, I.](#)
(1958) *Méthode des Polygones, Procédé d'Étude Graphique des Déterminants. Applications aux Problèmes de Chimie Théorique*, Thesis, Univ. Paris
13. [Coulson, C.A.](#)
Notes on the secular determinant in molecular orbital theory
(1950) *Proc. Cambridge Phil. Soc.*, 46 pp. 202-205 [Cited 13 times](#)
14. [Sachs, H.](#)
Beziehungen zwischen den in einem Graphen enthaltenen Kreisen und seinem charakteristischen Polynom
(1964) *Publ. Math. (Debrecen)*, 11 pp. 119-134 [Cited 23 times](#)
15. [Sachs, H.](#)
(1963) *Über die Anzahlen von Bäumen, Wäldern und Kreisen Gegebenen Typs in Gegebenen Graphen*, [Cited 2 times](#)
Habilitationsschrift, Univ. Halle
16. [Cvetković, D., Doob, M., Sachs, H.](#)
(1980) *Spectra of Graphs - Theory and Application*, [Cited 210 times](#)
Academic Press, New York; 2nd revised ed.: Barth, Heidelberg, 1995
17. [Gutman, I.](#)
Rectifying a misbelief: Frank Harary's role in the discovery of the coefficient-theorem in chemical graph theory
(1994) *J. Math. Chem.*, 16 pp. 73-78 [Cited 2 times](#)
[View at Publisher](#)
18. [Milić, M.](#)
Flow-graph evaluation of the characteristic polynomial of a matrix
(1964) *IEEE Trans. Circuit Theory*, 11 pp. 423-424 [Cited 2 times](#)
19. [Spialter, L.](#)
The atom connectivity matrix characteristic polynomial (ACMCP) and its physico-geometric (topological) significance
(1964) *J. Chem. Docum.*, 4 pp. 269-274 [Cited 5 times](#)
[View at Publisher](#)
20. [Graovac, A., Gutman, I., Trinajstić, N., Živković, T.](#)
Graph theory and molecular orbitals. Application of Sachs theorem
(1972) *Theor. Chim. Acta*, 26 pp. 67-78
[View at Publisher](#)
21. [Cvetković, D.M.](#)
Graphs and their spectra
(1971) *Publ. Elektrotehn. Fak. (Ser. Mat. Fiz.)*, 354 pp. 1-50 [Cited 8 times](#)
22. [Cvetković, D.M., Gutman, I.](#)
The algebraic multiplicity of the number zero in the spectrum of a bipartite graph
(1972) *Mat. Vesnik (Beograd)*, 9 pp. 141-150 [Cited 8 times](#)
23. [Gutman, I., Trinajstić, N.](#)
Graph theory and molecular orbitals
(1973) *Topics Curr. Chem.*, 42 pp. 49-93 [Cited 27 times](#)
24. [Gutman, I., Trinajstić, N.](#)
Graph spectral theory of conjugated molecules
(1975) *Croat. Chem. Acta*, 47 pp. 507-533
25. [Trinajstić, N., Gutman, I.](#)
Some aspects of graph spectral theory of conjugated molecules
(1975) *Commun. Math. Chem. (MATCH)*, 1 pp. 71-82
26. [Trinajstić, N., Živković, T.](#)
Graph theory in theoretical chemistry
(1975) *Kémiai Közlemények*, 44 pp. 460-465
in Hungarian
27. [Aihara, J.](#)

- General rules for constructing Hückel molecular orbital characteristic polynomials**
(1976) *J. Am. Chem. Soc.*, 98 pp. 6840-6844 [Cited 13 times](#)
[View at Publisher](#)
28. [Aihara, J.](#)
New approaches to aromaticity (2) - Analytical theory of aromaticity
(1976) *Kagaku no Ryoiki*, 30 pp. 379-391 [Cited 2 times](#)
in Japanese
29. [Trinajstić, N.](#)
Hückel theory and topology
(1977) *Semiempirical Methods of Electronic Structure Calculation. Part A: Techniques*, pp. 1-27
G. A. Segal (Ed.), Plenum Press, New York
30. [Trinajstić, N.](#)
Computing the characteristic polynomial of a conjugated system using the Sachs theorem
(1977) *Croat. Chem. Acta*, 49 pp. 539-633
31. [Herndon, W.C.](#), [Ellzey, M.L.](#)
Procedures for obtaining graph-theoretical resonance energies
(1979) *J. Chem. Inf. Comput. Sci.*, 19 pp. 260-264 [Cited 3 times](#)
[Abstract + Refs](#) [View at Publisher](#)
32. [Gutman, I.](#)
Mathematical investigations in organic chemistry - Success and failure
(1984) *Vestnik Slov. Kern. Društva (Ljubljana)*, 31 (SUPPL.) pp. 23-52
33. [Dias, J.R.](#)
Facile calculations of the characteristic polynomial and n-energy levels of molecules using chemical graph theory
(1987) *J. Chem. Educ.*, 64 pp. 213-216 [Cited 5 times](#)
34. [Gutman, I.](#)
Polynomials in graph theory
(1987) *Graph Theory and its Applications in Chemistry*, pp. 53-85
N. Tyutyulkov, D. Bonchev (Eds.), Nauka i Izkustvo, Sofia, in Bulgarian
35. [Trinajstić, N.](#)
Graph theory and molecular orbitals
(1987) *Graph Theory and its Applications in Chemistry*, pp. 86-120
N. Tyutyulkov, D. Bonchev (Eds.), Nauka i Izkustvo, Sofia, in Bulgarian
36. [Stankevich, I.V.](#)
Graphs in structural chemistry
(1988) *Applications of Graph Theory in Chemistry*, pp. 7-69
N. S. Zefirov, S. I. Kuchanov (Eds.), Nauka, Novosibirsk, in Russian
37. [Trinajstić, N.](#)
The characteristic polynomial of a chemical graph
(1988) *J. Math. Chem.*, 2 pp. 197-215 [Cited 8 times](#)
[View at Publisher](#)
38. [Gutman, I.](#)
Dependence of physico-chemical properties of substances on molecular structure: The example of total n-electron energy
(1990) *Glas Acad. Serbe Sci. Arts (Cl. Math. Natur.)*, 362 pp. 83-91
in Serbo-Croatian
39. [Gutman, I.](#)
Polynomials in graph theory
(1991) *Chemical Graph Theory: Introduction and Fundamentals*, pp. 133-176 [Cited 3 times](#)
D. Bonchev, D. H. Rouvray (Eds.), Gordon & Breach, New York
40. [Dias, J.R.](#)
An example of molecular orbital calculation using the Sachs graph method
(1992) *J. Chem. Educ.*, 69 pp. 695-700 [Cited 4 times](#)
41. [Graovac, A.](#), [Gutman, I.](#), [Trinajstić, N.](#)
(1977) *Topological Approach to the Chemistry of Conjugated Molecules*, [Cited 97 times](#)
Springer-Verlag, Berlin
42. [Tang, A.](#), [Kiang, Y.](#), [Di, S.](#), [Yen, G.](#)
(1980) *Graph Theory and Molecular Orbitals*,

Science Press, Beijing, in Chinese

43. [Dmitriev, I.S.](#)
(1982) *Molecules without Chemical Bonds*, [Cited 9 times](#)
Himiya, Leningrad, 1980 (Russian language edition); Mir, Moscow, 1981 (English language edition); Deutscher Verlag der Grundstoffindustrie, Leipzig, (German language edition)
44. [El-Basil, S.](#)
(1983) *On Some Mathematical Applications in Chemistry and Pharmacy*, Faculty of Pharmacy, Cairo
45. [Trinajstić, N.](#)
(1983) *Chemical Graph Theory*, [Cited 650 times](#)
CRC Press, Boca Raton; 2nd revised ed. 1992
46. [Gutman, I.](#), [Polansky, O.E.](#)
(1986) *Mathematical Concepts in Organic Chemistry*, [Cited 312 times](#)
Springer-Verlag, Berlin
47. [Tang, A.](#), [Kiang, Y.](#), [Yan, G.](#), [Tai, S.](#)
(1986) *Graph Theoretical Molecular Orbitals*, [Cited 13 times](#)
Science Press, Beijing
48. [Yu, G.](#), [Papulov, V.R.](#), [Rosenfel'd, K.](#), [Kemenova, T.G.](#)
(1990) *Molecular Graphs*, [Cited 4 times](#)
Tverskii Gosud. Univ., Tver', (in Russian)
49. [Dias, J.R.](#)
(1993) *Molecular Orbital Calculations Using Chemical Graph Theory*, [Cited 67 times](#)
Springer-Verlag, Berlin
50. [Diudea, M.V.](#), [Ivanciuc, O.](#)
(1995) *Molecular Topology*, [Cited 45 times](#)
Complex, Cluj, (in Rumanian)
51. [Diudea, M.V.](#), [Gutman, I.](#), [Jäntschi, L.](#)
(2001) *Molecular Topology*, [Cited 13 times](#)
Nova, Huntington
52. [Mallion, R.B.](#), [Schwenk, A.J.](#), [Trinajstić, N.](#)
A graphical study of heteroconjugated molecules
(1974) *Croat. Chem. Acta*, 46 pp. 171-182 [Cited 7 times](#)
53. [Mallion, R.B.](#), [Trinajstić, N.](#), [Schwenk, A.J.](#)
Graph theory in chemistry - Generalization of Sachs' formula
(1974) *Z. Naturforsch.*, pp. 1481-1484
in Rumanian
54. [Graovac, A.](#), [Polansky, O.E.](#), [Trinajstić, N.](#), [Tyutyulkov, N.N.](#)
Graph theory in chemistry. II. Graph-theoretical description of heteroconjugated molecules
(1975) *Z. Naturforsch.*, pp. 1696-1699 [Cited 4 times](#)
in Rumanian
55. [Rigby, M.J.](#), [Mallion, R.B.](#), [Day, A.C.](#)
Comment on a graph-theoretical description of heteroconjugated molecules
(1977) *Chem. Phys. Lett.*, 51 pp. 178-182 [Cited 5 times](#)
[View at Publisher](#)
56. [Kasum, D.](#), [Trinajstić, N.](#), [Gutman, I.](#)
Chemical graph theory. III. On the permanental polynomial
(1981) *Croat. Chem. Acta*, 54 pp. 321-328 [Cited 8 times](#)
57. [Gutman, I.](#), [Cash, G.G.](#)
Relations between the permanental and characteristic polynomials of fullerenes and benzenoid hydrocarbons
(2002) *Commun. Math. Chem. (MATCH)*, 45 pp. 55-70 [Cited 5 times](#)
[Abstract + Refs](#)
58. [Gutman, I.](#), [Trinajstić, N.](#)
Graph theory and molecular orbitals. Total n-electron energy of alternant hydrocarbons
(1972) *Chem. Phys. Lett.*, 17 pp. 535-538 [Cited 53 times](#)
[View at Publisher](#)
59. [Dias, J.R.](#)
Properties and derivation of the fourth and sixth coefficients of the


characteristic polynomial of molecular graphs. New graphical invariants(1985) *Theor. Chim. Acta*, 68 pp. 107-123 [Cited 11 times](#)[View at Publisher](#)

60. [Cvetković, D.](#), [Gutman, I.](#), [Trinajstić, N.](#)
Kekulé structures and topology
(1972) *Chem. Phys. Lett.*, 16 pp. 614-616 [Cited 15 times](#)
[View at Publisher](#)
61. [Gutman, I.](#), [Trinajstić, N.](#)
Graph theory and molecular orbitals. VIII. Kekulé structures and permutations
(1973) *Croat. Chem. Acta*, 45 pp. 539-545
62. [Cvetković, D.](#), [Gutman, I.](#), [Trinajstić, N.](#)
Graph theory and molecular orbitals. VII. The role of resonance structures
(1974) *J. Chem. Phys.*, 61 pp. 2700-2706
[View at Publisher](#)
63. [Graovac, A.](#), [Gutman, I.](#)
The determinant of the adjacency matrix of the graph of a conjugated molecule
(1978) *Croat. Chem. Acta*, 51 pp. 133-140 [Cited 3 times](#)
64. [Graovac, A.](#), [Gutman, I.](#)
The determinant of the adjacency matrix of a molecular graph
(1979) *Commun. Math. Chem. (MATCH)*, 6 pp. 49-73
65. [Cvetković, D.](#), [Gutman, I.](#), [Trinajstić, N.](#)
Graph theory and molecular orbitals. II
(1972) *Croat. Chem. Acta*, 44 pp. 365-374 [Cited 3 times](#)
66. [Cvetković, D.](#), [Gutman, I.](#), [Trinajstić, N.](#)
Graphical studies on the relations between the structure and reactivity of conjugated systems: The role of non-bonding molecular orbitals
(1975) *J. Mol. Struct.*, 28 pp. 289-303 [Cited 4 times](#)
[View at Publisher](#)
67. [Gutman, I.](#), [Trinajstić, N.](#)
Graph theory and molecular orbitals. IV. Further application of Sachs formula
(1973) *Croat. Chem. Acta*, 45 pp. 423-429 [Cited 3 times](#)
68. [Dyadusha, G.G.](#), [Kachkovskii, A.D.](#)
Application of graphs in the study of electrodonor property of annelated terminal groups in polymethine dyes
(1980) *Teor. Eksp. Khim.*, 16 pp. 615-619 [Cited 2 times](#)
in Russian
69. [Dyadusha, G.G.](#), [Kachkovskii, A.D.](#)
Application of graph theory to the colour of polymethine dyes
(1981) *Teor. Eksp. Khim.*, 17 pp. 393-398
in Russian
70. [Gutman, I.](#), [Trinajstić, N.](#)
Graph theory and molecular orbitals. XV. The Hückel rule
(1976) *J. Chem. Phys.*, 64 pp. 4921-4925 [Cited 6 times](#)
[View at Publisher](#)
71. [Gutman, I.](#), [Trinajstić, N.](#)
On the extension of the Hückel rule to polycyclic non-alternant conjugated hydrocarbons
(1976) *Canad. J. Chem.*, 54 pp. 1789-1794 [Cited 2 times](#)
72. [Graovac, A.](#), [Gutman, I.](#), [Trinajstić, N.](#)
A linear relationship between the total n-electron energy and the characteristic polynomial
(1976) *Chem. Phys. Lett.*, 37 pp. 471-474 [Cited 2 times](#)
[View at Publisher](#)
73. [Gutman, I.](#)
Proof of the Hückel rule
(1977) *Chem. Phys. Lett.*, 46 pp. 169-171 [Cited 2 times](#)
[View at Publisher](#)

74. [Gutman, I.](#)
Acyclic systems with extremal Hückel π -electron energy
(1977) *Theor. Chim. Acta*, 45 pp. 79-87 [Cited 32 times](#)
[View at Publisher](#)
75. [Gutman, I.](#)
The energy of a graph
(1978) *Ber. Math.-Statist. Sect. Forschungszentrum Graz*, 103 pp. 1-22
76. [Gutman, I.](#), [Yamaguchi, T.](#), [Hosoya, H.](#)
Topological index as applied to n -electronic systems. IV. On the topological factors causing non-uniform n -electron charge distribution in non-alternant hydrocarbons
(1976) *Bull. Chem. Soc. Japan*, 49 pp. 1811-1816 [Cited 3 times](#)
77. [Aihara, J.](#)
A new definition of Dewar-type resonance energies
(1976) *J. Am. Chem. Soc.*, 98 pp. 2750-2758 [Cited 115 times](#)
[View at Publisher](#)
78. [Gutman, I.](#), [Milun, M.](#), [Trinajstić, N.](#)
Topological definition of delocalisation energy
(1975) *Commun. Math. Chem. (MATCH)*, 1 pp. 171-175 [Cited 13 times](#)
79. [Gutman, I.](#), [Milun, M.](#), [Trinajstić, N.](#)
Graph theory and molecular orbitals. 19. Nonparametric resonance energies of arbitrary conjugated systems
(1977) *J. Am. Chem. Soc.*, 99 pp. 1692-1704 [Cited 106 times](#)
[View at Publisher](#)
80. [Ilić, P.](#), [Trinajstić, N.](#)
Topological resonance energies of conjugated ions, radicals and ion radicals
(1980) *J. Org. Chem.*, 45 pp. 1738-1748 [Cited 8 times](#)
[View at Publisher](#)
81. [Aihara, J.](#)
Stability of all molecular ions conceivable for C_{60} and C_{70}
(1998) *J. Chem. Soc. Faraday Trans.*, 94 pp. 3537-3540 [Cited 19 times](#)
[View at Publisher](#)
82. [Bosanac, S.](#), [Gutman, I.](#)
Effect of a ring on the stability of polycyclic conjugated molecules
(1977) *Z. Naturforsch.*, 32 A pp. 10-12 [Cited 4 times](#)
83. [Aihara, J.](#)
Resonance energies of benzenoid hydrocarbons
(1977) *J. Am. Chem. Soc.*, 99 pp. 2048-2053 [Cited 26 times](#)
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84. [Gutman, I.](#), [Stanković, M.](#)
On the Hückel ($4m + 2$) rule in polycyclic alternant hydrocarbons
(1994) *J. Mol. Struct. (Theochem)*, 309 pp. 301-304 [Cited 6 times](#)
[View at Publisher](#)
85. [Gutman, I.](#), [Ivanov-Petrović, V.](#)
Clar theory and phenylenes
(1997) *J. Mol. Struct. (Theochem)*, 389 pp. 227-232 [Cited 14 times](#)
[Abstract + Refs](#) [View at Publisher](#)
86. [Gutman, I.](#)
Cyclic conjugation in dianions: Effect of cycles on the thermodynamic stability of polycyclic conjugated dianions
(1998) *J. Mol. Struct. (Theochem)*, 428 pp. 241-246 [Cited 7 times](#)
[Abstract + Refs](#) [View at Publisher](#)
87. [Godsil, C.D.](#), [Gutman, I.](#)
Topological resonance energy is real
(1979) *Z. Naturforsch.*, 34 A pp. 776-777 [Cited 2 times](#)
88. [Heilmann, O.J.](#), [Lieb, E.H.](#)
Theory of monomer - Dimer systems
(1972) *Commun. Math. Phys.*, 25 pp. 190-232 [Cited 60 times](#)

[View at Publisher](#)

89. [Farrell, E.J.](#)
An introduction to matching polynomials
(1979) *J. Comb. Theory B*, 27 pp. 75-86 [Cited 17 times](#)
[View at Publisher](#)
90. [Farrell, E.J.](#), [Gutman, I.](#)
A note on the circuit polynomial and its relation to the μ -polynomial
(1985) *Commun. Math. Chem. (MATCH)*, 18 pp. 55-61
91. [Cvetković, D.](#), [Doob, M.](#), [Gutman, I.](#), [Torgašev, A.](#)
(1988) *Recent Results in the Theory of Graph Spectra*, [Cited 36 times](#)
North-Holland, Amsterdam
92. [Gutman, I.](#), [Polansky, O.E.](#)
Cyclic conjugation and the Hückel molecular orbital model
(1981) *Theor. Chim. Acta*, 60 pp. 203-226 [Cited 17 times](#)
[View at Publisher](#)
93. [Gutman, I.](#)
On cyclic conjugation
(1984) *Theor. Chim. Acta*, 66 pp. 43-49 [Cited 8 times](#)
[View at Publisher](#)
94. [Gutman, I.](#)
Some relations for the μ -polynomial
(1986) *Commun. Math. Chem. (MATCH)*, 19 pp. 127-137 [Cited 2 times](#)
95. [Gutman, I.](#), [Mizoguchi, N.](#)
A property of the circuit characteristic polynomial
(1990) *J. Math. Chem.*, 5 pp. 81-82 [Cited 2 times](#)
[View at Publisher](#)
96. [Li, X.](#), [Gutman, I.](#), [Milovanović, G.V.](#)
The β -polynomials of complete graphs are real
(2000) *Publ. Inst. Math. (Beograd)*, 67 pp. 1-6 [Cited 2 times](#)
97. [Gutman, I.](#)
Note on a topological property of the HOMO-LUMO separation
(1980) *Z. Naturforsch.*, 35 A pp. 458-460 [Cited 2 times](#)
98. [Gutman, I.](#), [Juranić, I.](#)
On the dependence of n-electron charge distribution on molecular topology. II
(1982) *Bull. Soc. Chim. Beograd*, 47 pp. 183-188 [Cited 2 times](#)

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