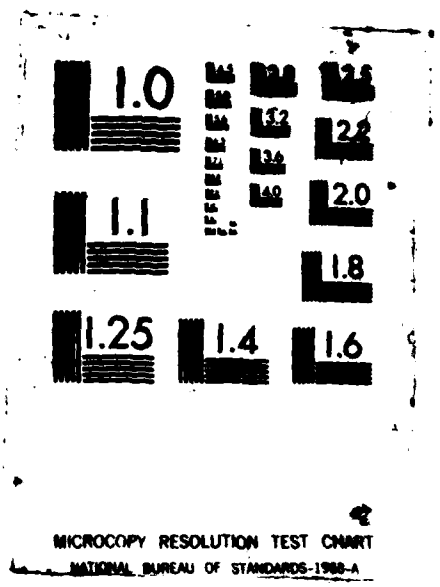
AD-A183 888 GRAPHS OF CHEMISTRY AND PHYSICS: ON DATA REDUCTION OF CHEMICAL INFORMATION(U) GEORGIA UNIV ATHENS DEPT OF CHEMISTRY S EL-BASIL 11 AUG 87 TR-49 N00014-84-K-0365 1/1

UNCLASSIFIED F/G 7/4 NL



(12)

OFFICE OF NAVAL RESEARCH

Contract N00014-84-K-0365

R&T Code 4007001-6

Technical Report No. 49

Graphs of Chemistry and Physics: On Data Reduction of Chemical Information

by

Sherif El-Basil

Prepared for Publication

in the

Proceedings of the Conference on Graph Theory and Topology in Chemisty held in Athens, GA, March 1987

University of Georgia
Department of Chemistry
Athens, Georgia 30602

August 11, 1987

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER Technical Report No. 49	2. GOVT ACCESSION NO. AD-A182 [illegible]	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Graphs of Chemistry and Physics: On Data Reduction of Chemical Information		5. TYPE OF REPORT & PERIOD COVERED Technical Report 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Sherif El-Basil		8. CONTRACT OR GRANT NUMBER(s) N00014-84-K-0365
9. PERFORMING ORGANIZATION NAME AND ADDRESS University of Georgia Department of Chemistry Athens, GA 30602		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 4007001-6
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research Department of the Navy Arlington, VA 22217		12. REPORT DATE August 11, 1987 13. NUMBER OF PAGES 7
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) 15a. DECLASSIFICATION/ DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

This document has been approved for public release and sale; its distribution is unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

To be published in the Proceedings of the Conference on Graph Theory and Topology in Chemistry held in Athens, GA, March, 1987

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Graph Theory
Data Reduction

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Five types of related graphs which are of recent use in mathematical chemistry are considered. The notion of "equivalent" graphs is introduced which seems to be of value in connection with data reduction.

(Keywords:)

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

S/N 0102-LF-014-6601

unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

International Conference on Graph Theory and Topology in Chemistry

GRAPHS OF CHEMISTRY AND PHYSICS: ON DATA REDUCTION OF CHEMICAL INFORMATION

SHERIF EL-BASIL*

Department of Chemistry, The University of Georgia, Athens, GA 30602 U.S.A.

ABSTRACT

Five types of related graphs which are of recent use in mathematical chemistry are considered. The notion of "equivalent" graphs is introduced which seems to be of value in connection with data reduction.

INTRODUCTION

The past twenty-five years witnessed serious chemical applications of discrete mathematics (mainly graph theory (ref. 1), combinatorics (ref. 2), number theory (ref. 3), and group theory (ref. 2)) which led to what is known today as "chemical" graph theory (ref. 4). The structure-resonance theory of Herndon (ref. 5), the conjugated circuits model (independently introduced by Randic (ref. 6) and by Gomes (ref. 7)) and the topological theory of resonance (refs. 8, 9) are illustrative examples of such models. An interesting combinatorial concept, the introduction of which in chemistry is mainly due to Hosoya and coworkers (ref. 10) is that of nonadjacent structures. This latter concept can be made to unify many related combinatorial polynomials in chemistry and physics (ref. 4) as shown in Chart:

NONADJACENT STRUCTURES

EDGES	VERTICES	HEXAGONS	CELLS
$p(T;k)$	$o(\Lambda;k)$	$r(B;k)$	$\kappa(P;k)$ $\rho(P_r;k)$
Matching	Color, Independence	Sextet	King Rook

*Permanent Address: Faculty of Pharmacy, Kasr El-Aini Street, Cairo, Egypt

Key words
Graph Theory
Data Reduction

The above terms are explained in Table 1 which contains polynomials of chemistry and physics. The general form of the polynomials given in Table 1 is given by

$$(G;x) = \sum_{k=0}^{m} (G;k)\, x^{(k,n)} \qquad (1)$$

EQUIVALENT GRAPHS

Fig. 1 shows five types of graphs most commonly considered in mathematical chemistry, viz., a caterpillar tree (ref. 11), T, a polyhex graph (ref. 12) of a benzenoid hydrocarbon, B, a Clar graph (ref. 13), Λ, a king polyomino graph (ref. 14), P and a rook board P_r (ref. 15).

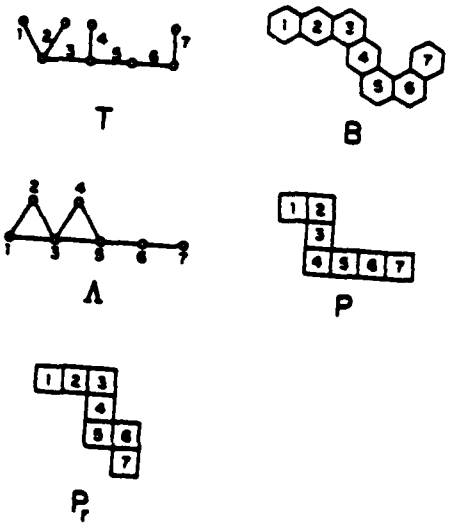


Fig. 1. A set of five equivalent graphs: a caterpillar tree, T, a polyhex graph, B, a clar graph, Λ, a king polyomino, P, and a rook board, P_r.

The following identities can easily be verified

$$H(T;x) = \sigma(B;x) = \omega(\Lambda;x) = K(P;x) = R(P_r;x)$$
$$= 1 + 7X + 13X^2 + 6x^3.$$

There is a one-to-one correspondence between any two of the invariants of each graph. For example the edges of T (arbitrarily labeled as shown) can be mapped onto the hexagons of B and so on: k edges in T are incident only if k hexagons in B are nonresonant, k vertices in Λ are adjacent or k cells in P or P_r are adjacent. In P two cells are adjacent if they share one vertex. Two cells are adjacent in P_r if they are in the same row. Fig. 2 illustrates the one-to-one correspondence between the adjacency relations of the five types of graphs for k=3. Sets of graphs such as shown in Fig. 1 will be called equivalent graphs[16].

Table 1 Polynomials, associated graphs and graph invariants in chemistry and physics.

Polynomial	ρ	Graph-Invariants	Associated Graph	$\theta(G;k)$	$f(k,n)$
1. Acyclic = Matching = $\alpha(G;x)$	$(-1)^k$	set of edges	Caterpillar Tree, T	$p(G;k)^a$	n-2k
2. Counting (of Hosoya) = $H(G;x)$	1	set of edges	Caterpillar Tree, T	$p(G;k)^a$	k
3. Sextet, = $\sigma(B;x)$	1	set of hexagons	Polyhex Graph, B	$r(B;k)^b$	k
4. King = $K(P;x)$	1	set of cells	Polyomino Graph, P	$\kappa(P;k)^c$	k
5. Rook, = $K(P_r;x)$	1 or $(-1)^k$	set of cells	Polyomino Graph, P	$\rho(P_r;k)^d$	k or n-2k
6. Independence, $\omega(A;x)$	1	set of vertices	Clar graph A	$O(A;k)^e$	k
7. Color, $C(G;x)$	1	set of vertices	Arbitrary graph, G	$\zeta(G;k)^f$	k
8. Resonance, $A(B;x)$	$(-1)^k$	set of hexagons	Polyhex graph, B	$r(B;k)^b$	2N-2k

a Number of selections of k independent edges $\in$ T(i.e. no two edges are incident)

b Number of selections of k nonadjacent but mutually resonant hexagons $\in$ B

c Number of ways of arranging k nontaking kings on a polyomino graph.

d Number of ways of arranging k non-attacking kings

e Number of selections of k independent vertices $\in$A . (No two are adjacent)

f Number of colorings in G in which there are k vertices of the same color so that no two of them are adjacent.

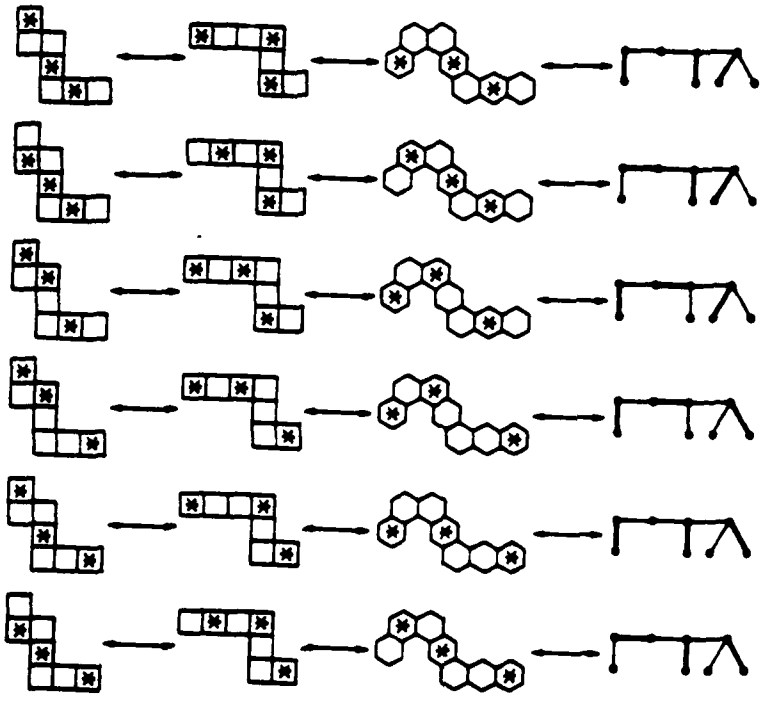


Fig. 2. One-to-one correspondence between the k-matchings of five equivalent graphs for k=3.

CONJECTURE

The graph theoretical properties (which depend only on connectivity relations between vertices) of a graph are preserved in any of its equivalent graphs. A similar conjecture applies to the physical properties (i.e. observables) which depend mainly on the graph adjacency matrix.

TEST OF CONJECTURE AND RESULTS

If our conjecture is true it would be possible (and, in fact, desirable) to study a larger graph, such as a polyhex graph of a benzenoid system in terms of much smaller equivalent caterpillar tree, or its line graph: the corresponding Clar graph. Fig. 3-5 illustrates such studies where one physical and two graph-theoretical (combinatorial) properties are studied. In all cases the molecular connectivity index of Randic (ref. 17), χ, is used and is given by

$$h\chi = \sum (v_i v_j \ldots v_{h+1})^{-\frac{1}{2}} \qquad (2)$$

where the summation is taken over all paths in the graph. Table 2 shows percent retrieval of a property for one representative case. The concept illustrated here seems to be of value in data reduction.

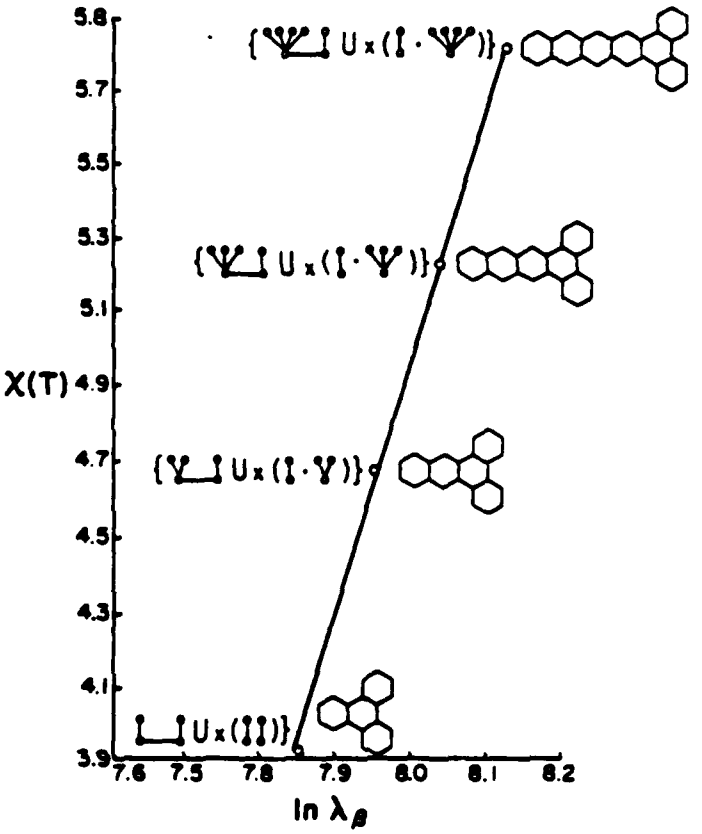


Fig. 3. A plot of electronic absorption β band, $\lambda\beta$, for a series of branched benzenoids[18] and the connectivity indices of a series of disconnected trees, (T).

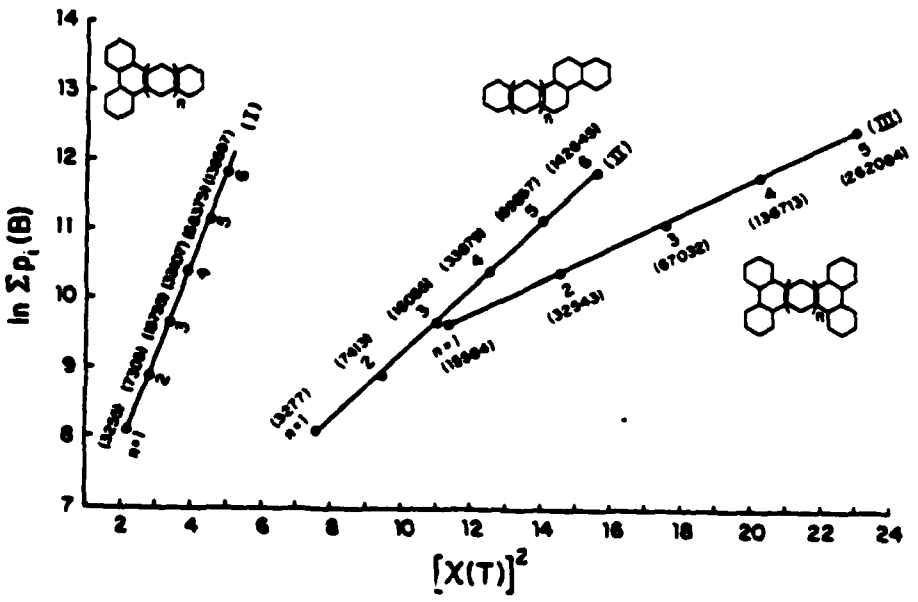


Fig. 4. Correlation between total number of self-avoiding paths,[19] $\Sigma p(B)$, (numbers of parentheses) of families of benzenoid hydrocarbons and $[\chi(T)]^2$, the squares of connectivity indices of the equivalent trees.

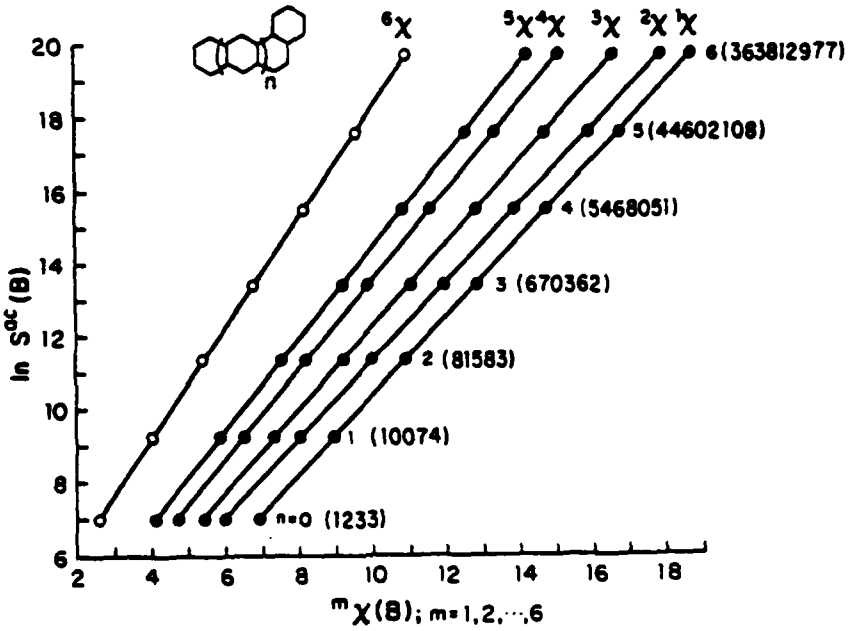


Fig. 5. Correlation between the total number of acyclic Sachs graphs,[4] S^{ac}(B), (numbers in parentheses) for a series of polyhex graphs with their molecular connectivity indices, (B) up to sixth order.

Table 2

Percent retrieval of the total number of self-avoiding paths for the series of nonbranched hydrocarbons shown in Fig. 4. The regression line is Y = 4.374 + 0.484 X with a correlation coefficient = 1.0000.

n*	% Retrieval[a]
1	99.3
2	99.7
3	100
4	99.8
5	99.7
6	98.9

*See Fig. 4

a) = 100 - 100|Calcd - Actual| /Actual.

ACKNOWLEDGMENTS

I thank the Office of the U.S. Navy for partial support of this work and Professor R.B. King for illuminating discussions. Travel assistance from Fullbright Commission in Cairo is appreciated.

REFERENCES

1 A recent account may be found in: A.T. Balaban, Ed., Chemical Applications of Graph Theory, Academic Press, New York (1976).

2 Balasubramanian revived interest in Polya Theorem c.f. K. Balsubramanian, Chem. Rev. 85, 599 (1985) and several references cited therein.

3 H. Hosoya, The Fibaonacci Quarterly, 11(3), 255 (1973); 14(2), 173 (1976); S. El-Basil, Theoret. Chim. Acta, 65, 191 (1984); 65 199 (1984).

4 c.f., N. Trinajstic, Chemical Graph Theory, CRC Boca Raton (1983).

5 W.C. Herndon and M.L. Ellzey Jr., J. Am. Chem. Soc., 96, 6631 (1974).

6 M. Randic, J. Am. Chem. Soc. 99, 444 (1977); Tetrahedron, 33, 1905 (1977).

7 J.A.N.F. Gomes, Theoret. Chim. Acta, 59, 333 (1981).

8 J. Aihara, J. Am. Chem. Soc. 98, 2750 (1976).

9 I. Gutman, M. Milun and N. Trinajstic, J. Am. Chem. Soc., 99, 1692 (1977).

10 H. Hosoya, Bull. Chem. Soc. Japan, 44, 2332 (1971).

11 F. Harary and A.J. Schwenk, Discrete Math., 6, 539 (1973), S. El-Basil, J. Chem. Soc., Farday Trans. 2, 82, 299 (1986).

12 N. Ohkami, A. Motoyama, T. Yamaguchi, H. Hosoya and I. Gutman, Tetrahedron, 37, 1113 (1981).

13 I. Gutman, Z. Naturforsch. 37a, 69 (1982); I. Gutman and S. El-Basil, Z. Naturforsch. 39a, 276 (1984); S. El-Basil, Theor. Chim. Acta, 70, 53 (1986); Discr. Appl. Math. (in press).

14 A. Motoyama and H. Hosoya, J. Math. Phys. 18, 1485 (1977).

15 C.D. Godsil and I. Gutman, Croat. Chem. Acta, 54, 53 (1981).

16 Details and mathematical proofs will be submitted elsewhere.

17 M. Randic, J. Am. Chem. Soc. 97, 6609 (1975).

18 Data are collected from E. Clar, The Aromatic Sextet, Wiley, New York, vol. 1 (1972).

19 M. Randic, G.M. Brissey, R.B. Spencer and C.L. Wilkins, Computers and Chemistry, 3, 5 (1979).

END

9-87

DTIC