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UNIQUE DESCRIPTION OF CHEMICAL STRUCTURES BASED ON HIERARCHICALLY ORDERED EXTENDED CONNECTIVITIES. IV.[1] RECOGNITION OF GRAPH ISOMORPHISM AND GRAPH SYMMETRIES

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Abstract. After a brief review of the important problem (both for chemistry and for graph theory) of establishing whether two given graphs are, or are not, isomorphic, it is shown that the Unique Topological Representation (UTR) resulting from the HOC algorithms provides a simple means to reach this goal : the UTR's of the given graphs are obtained, and then either compared directly (in the manually-implemented procedure), or converted into adjacency matrices or topological codes (for graphs) and correspondingly into SHOC codes (for chemical compounds) which can be processed by computer programs for matching in order to decide whether the given graphs are, or are not, isomorphic.

The order of the symmetry group of a graph results automatically from a simple relationship, during the course of the iterations for the HOC-3 algorithm. One can also obtain easily the order of the symmetry group for non-planar graphs which are used as reaction graphs. Examples are provided both for chemical compounds (molecular or constitutional graphs), and for reaction graphs : the highly symmetrical Petersen graph (5-cage) is the example for the latter type of graphs.

A list of abbreviations is appended after the bibliography.

1. INTRODUCTION

The Hierarchically Ordered extended Connectivity (HOC) algorithm [2] succeeds in a simple manner to discriminate unambiguously all vertices in a graph according to their topological equivalence and to order them into ranks (levels) of a Unique Topological Representation (UTR), by applying the first part of this algorithm : HOC-1, HOOC and / or HOC-2, HOC-2A. The second part, HOC-3, succeeds in assigning numbers to all vertices of the graph ; when topologically equivalent vertices exist in the graph, several topologically equivalent numberings (TEN's) are possible, each of which is reducible to the same UTR. By converting the UTR into its adjacency matrix, one can thus obtain for any graph a unique form of its adjacency matrix.

It is therefore logical to use the advantages of the HOC algorithm, which are discussed in a previous part of this series,[2] for recognizing isomorphism in graphs and for deriving their symmetry properties, in addition to other uses which are described in the first three parts of this series. In particular, the second part has presented how to use the result of the HOC algorithm for devising in linear notation a topological code for graphs, and a chemical and stereochemical code (SHOC) for chemical compounds.[3]

Briefly, the differences between the variants of the HOC algorithm are as follows : HOC-1 deals with the large majority of chemical structures and ranks vertices according to their hierarchically ordered extended connectivities. For regular graphs, the HOOC algorithm ranks vertices by taking into account overextended connectivities which involve more distant neighbours than adjacent vertices. For graphs with peri-condensed rings of different sizes, the HOC-2 algorithm has as additional criterion for ranking vertices by sizes of all rings to which the given vertex belongs. For rare cases of compounds having more than six peri-condensed rings with additional restrictions as to ring size, or for strongly regular graphs, one has to use the HOC-2A algorithm.

Both the above variants (HOC-2 and HOC-2A algorithms) are topological in nature ; however, for the same types of excep-

tional graphs which cannot be treated by HOC-1, one can use the HOC-4 algorithm whose nature is different : it searches the "best name" for finding the canonical numbering and the corresponding orbitally equivalent vertices ; the resulting set of best names is an analog of the TEN's.

Normally, after applying HOC-1 (or in the appropriate cases HOC-2 or HOC-2A) algorithm, the numbering of vertices is effected by using the HOC-3 algorithm which results in an unambiguous and non-subjective set of TEN's.

2. BRIEF REVIEW ON THE RECOGNITION OF GRAPH ISOMORPHISM

As expressed in the title of a recent paper by Read and Corneil,[4] (cf. also [5]), the "graph isomorphism disease" gave rise to a still continuing search for graph invariants which could uniquely characterize graphs without degeneracy and without involving complicated matching procedures, in order to establish whether a pair of given graphs with the same numbers of vertices and edges, respectively, are or are not isomorphic, irrespective of the way they are drawn. Two graphs are isomorphic if there is a one-to-one correspondence between their vertices which conserve all adjacencies. Necessary, but insufficient conditions for isomorphism are equalities of the numbers of vertices, edges, and partition of vertex degrees.

That the problem is of interest also to chemists and not only to graph theorists, is demonstrated by proved cases of failures to recognize the identity of bridged polycyclic systems and therefore to assign correct IUPAC names to such systems when using the A. von Baeyer system of nomenclature ; this in turn has led to erroneous indexing of the same classes of compounds prepared by different research groups and named differently.[6]

So far, the search for simple criteria for graph isomorphism has met with little success when trying to use such reduced forms of the adjacency matrix as the spectrum of the graph, since it was shown that the graph spectrum or the characteristic polynomial do not characterize unambiguously the molecular topology, so that there exist non-isomorphic cospectral graphs.[7]

However, Randić argued that the adjacency may be read sequentially as a binary number with the condition that among

all permutations of rows and columns, a unique permutation can be selected which results in the smallest binary number.[8-10] Ideas about selecting uniquely extremal forms of the adjacency matrix nad existed earlier,[11-13] but it is the merit of Randić to have demonstrated the scope of the smallest binary number (SBN) algorithm for obtaining a graph invariant, and to have used it for ordering graphs,[14] for devising canonical numbering systems,[15] and for obtaining symmetry properties of graphs.[16] Notwithstanding the theoretical importance of this approach, for prectical applications it is difficult to implement by hand and is rather time-consuming by means of computer programs (which sometimes with pairwise permutations do not arrive at the SBN but at false (local) minima,[9] so that triple permutations have to be tested).

Many other approaches have been used, mainly by mathematicians, for recognizing graph isomorphism. We shall not review exhaustively the literature, but shall give a selective overview highlighting mainly the chemically relevant aspects, and attempting to group together related procedures in some cases.

A. Procedures based on matchings.

a. To avoid the necessity of the N! possible mappings of one graph on another, if N is the number of vertices, each time one tests for isomorphism, an algorithm was proposed for attempting a vertex-to-vertex matching for coincidence,[17] which is still time-consuming because the choice of vertices is arbitrary, involves considerable back-tracking, lacks criteria in the decision-making step, and consumes space in the computer memory for being able to restart from the last point of agreement.

b. Matching of the Fourier maxima to specified entities of the known graph, also in chemical contexts.[18]

c. Sussenguth [19] combined a selection of simple graph properties with a subsequent matching algorithm, and applied it to chemical problems.

d. Other matching procedures.[20-24]

B. Procedures based on comparing global or local characteristics of graphs.

a. An approach was proposed on the basis of comparing vertices after ordering them according to their degree and to the degree of their adjacent vertices.[25] Here belongs also Penny's connectivity code [26] which has been used for describing chemical structures.

b. The determinant of the adjacency matrix supplemented with atomic symbols along the main diagonal was proposed as a preliminary screening in testing isomorphism of chemical systems.[27] However, as indicated earlier,[7] the identity of such determinants is insufficient.

c. Topological indices such as J,[28] or the superindex [29] which have a low degeneracy are of assistance in testing isomorphism. The following paper in this series,[30] which introduces two new topological indices, $\mathcal{N}$ and $\mathcal{M}$, with low and practically nil degeneracy, respectively, also belongs here. However, as in the preceding case, topological indices which are of considerable use in chemical correlations, are mathematically not free of degeneracy.

C. Other procedures.

We list here only a few other procedures and indicate that more information may be found in some of the references already cited,[4-29] and especially in graph-theoretical papers. Of considerable interest are bibliographies for graph theory, the simplest of which is Turner's [31] because it employs the "keyword in context system", and the most recent of which are Berman's "forward citations in graph theory" [32] and Ruiz's "graph theory newsletters".[33] Some references on graph isomorphism found through these bibliographies follow.[34-39]

3. RECOGNITION OF GRAPH ISOMORPHISM

To find out whether a pair of graphs are or are not isomorphic, after testing the simple graph invariants (number of vertices and the partition of their degrees, number of edges, number of circuits with 2, 3, 4, etc. vertices - cf. [40] for a computer program giving the numbers of rings with all sizes), we apply separately the HOC algorithm to each of these two graphs, in order to find the rank (topological equivalence level) structure, and the canonical numbering. Then we construct the two

UTR's. If the testing for isomorphism is effected manually, visual comparison of the two UTR's will show by vertex-to-vertex matching if the two graphs as UTR's are, or are not, isomorphic. The matching should be done for correspondingly numbered vertices, on correspondingly numbered levels, and the UTR's should be identical if the two graphs are isomorphic.

If the search is made by means of a computer program, the UTR's should be compared by using a specially devised program (incorporating also the rules for constructing the UTR's), or they can be cenverted into their correspondingly ordered adjacency matrices, which can be easily compared by the computer. An alternative approach, valid for graphs and for chemical compounds, is to convert them, through the HOC algorithm into UTR's and hence into topological or SHOC codes, respectively,[3] which can again be compared symbol by symbol for isomorphism which must result in the identity of the codes.

Thus the HOC and SHOC algorithms are useful not only for organizing and storing information about graphs and molecules, respectively, but also for comparing such structures. Since these algorithms are based on objective, clear and unambiguous rules, their outcome does not depend on how the graph has been drawn or on its initial arbitrary numbering, and each graph results in a Unique Topological Representation which makes the recognition of graph isomorphism a tractable problem, at least for graphs which are relevant in chemical contexts.

4. RECOGNITION AND ENUMERATION OF GRAPH SYMMETRIES USING THE HOC ALGORITHM AND THE UTR

The first paper in this series,[2] describing the HOC algorithm, indicated how the hierarchically ordered extended connectivities and the ranks of adjacent vertices arranged in increasing order can discriminate vertices in a graph till a complete ordering results according to their ranks (levels) of topological equivalence. It was proved [2] that HOC-1, HOOC and HOC-2(A) procedures were necessary and sufficient for finding the topologically equivalent vertices (or orbitally equivalent vertices, OEV's) and for obtaining a unique topological representation (UTR) on the basis of levels provided by OEV's. The topmost level of the UTR thus obtained is occupied by the vertex or

vertices with the lowest numbering(s), i. e. the highest rank, as resulted from HOC-1, HOOC, HOC-2 or HOC-2A (which provide the ranks or levels) and from HOC-3 (which provides the vertex numberings). To this effect, at the end of HOC-1, HOOC, HOC-2 or HOC-2A, if there exist OEV's in the graph, HOC-3 introduces artificial discriminations among OEV's with the highest rank ; we thus end up in one of the possible topologically equivalent numberings (TEN's) of all vertices, so that in the presence of topological (orbital) equivalence, the UTR corresponds to more than one topologically equivalent numbering (TEN).

The levels of the UTR are populated with the vertices of the graph arranged in increasing numerical order from top right to bottom left. The position of each vertex is thus determined by (i) its rank according to HOC-1, HOOC, HOC-2 or HOC-2A algorithms ; the rank determines the level on which the vertex is placed, and (ii) its numbering according to HOC-3, which determines the relative position (more to the right or to the left) on the level. If one wishes to avoid as far as possible crossing lines in UTR's, elaborate conventions are necessary ; this problem will be discussed in a separate paper.

The UTR is isomorphic with the given graph. Since, however, the numbering obtained by the HOC algorithms has no apparent order (because it does not conserve the adjacency of vertices, this numbering has hardly any logical order, except for very simple cases), the UTR compensates this fact by drawing the given graph in such a manner that the resulting numbering acquires a logical order : in the UTR, the numbering increases, as indicated above, from top right to bottom left, regularly. Truly, this gives rise sometimes to awkward structural formulas, as the examples in the first part of this series [2] or in the present paper show, but the connectivity is easy to be recognized. At the same time, this manner of drawing the given graph, although "ugly" with respect to its geometry, is "beautiful" with respect to its HOC-dictated topological nature.

While the levels of the UTR (corresponding to the graph orbits) are non-subjective and uniquely dictated by the graph topology, the disposition of vertices on the same level needs further conventions to make the resulting geometrical represen-

tation of the graph truly unique. Ideally, the UTR should avoid crossing lines for planar graphs ; this is feasible (with some conventions which will be presented in detail in a separate paper) only for acyclic, monocyclic and bicyclic graphs. For polycyclic planar graphs, it is still an open problem to devise a general method yielding UTR's devoid of crossings, or to prove that this is impossible. At present we think that in such cases a UTR is useful even if it has crossing lines.

The reason why several TEN's may exist for a single UTR is the presence of topologically equivalent vertices, i. e. of symmetry. The number of TEN's depends on the symmetry of each graph. We shall discuss as an example the constitutional formula of 2,3,5,6-tetramethylbicyclo [2.2.1] heptane (1) , ignoring its stereochemistry, as indicated in Figure 1, where the numbering is according to the HOC-3 procedure.

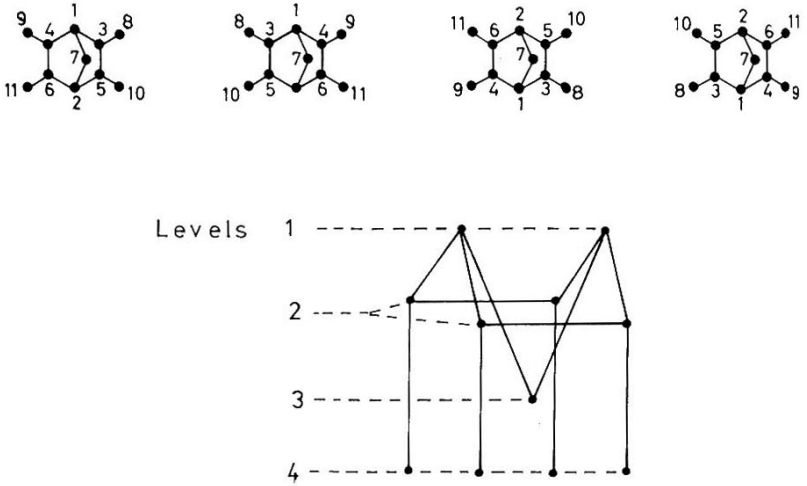

Fig. 1. The four TEN's and the UTR (unique topological representation) of 1 , presented with crossing lines

Pairwise permutations between vertices can be classified as follows according to several criteria :

A. Vertex permutations between different levels of UTR's.

B. Vertex permutations on the same level of the UTR.

By convention, we start from top to bottom and from right to left in the UTR.

a. Independent vertex permutations.

b. Dependent vertex permutations, i. e. those caused by the former ones and by the connectivity of the graph.

If we admit as valid permutations only those which are compatible with the graph connectivity and we ignore the permutations which violate this connectivity, we have to reject all permutations of type A. We exemplify with the UTR of 1 , and we present examples of independent (B.a) and dependent (B.b) valid permutations of vertices on the same level ; under each independent permutation we list the dependent permutations, which may be either on lower levels, e. g. those triggered by the independent permutation (1,2), or on the same level, e. g. the first of those triggered by the independent permutation (3,4) :

B.a :	(1,2)	(3,4)
B.b :	(3,5) and (4,6)	(5,6)
	(8,10) and (9,11)	(8,9) and (10,11)

The product of the number of independent permutations (B.a - type ones) determines the number of TEN's, namely 2 x 2 = 4 in the example discussed here (1).

In chemical examples, the independent permutations are of two types : permutations which correspond to the point-group symmetry operations (rotation, reflection, etc. of the whole rigid skeleton as in the example 1), and permutations which correspond to symmetry operations involving a molecular fragment (i. e. a component of a separable, or weakly-connected, graph), e. g. (i) permutation of carbon atoms in an isopropyl group, corresponding to rotation of this fragment relatively to the remaining part of the molecule, or (ii) permutations in spiro-compounds, where the symmetry operation involves inversion of configuration at the spiranic atom.

Every TEN will correspond to the same UTR and therefore will have the same adjacency matrix. This may seem paradoxical in view of the fact that for a complete numbering we have introduced with HOC-3 arbitrary discriminations of one or several vertices with the highest rank(s) once, or several times, during this algorithm. However, the nature of the HOC procedure is such that the connectivity of all TEN's is the same, because all TEN's are derived from one another by symmetry operations applied to the whole molecule or to fragments thereof , including products of these permutations, so that the UTR and the adjacency matrix of any TEN are unique and identical for any given graph.

The order of the symmetry group of any graph results from the HOC-3 algorithm by counting all topologically equivalent numberings (TEN's) compatible with the UTR : these TEN's are derived from the independent vertex permutations of type B.a. Thus the order h(G) of the automorphism group of a graph G is [2]

$$h(G) = \prod_i p_i \qquad (1)$$

In the stepwise HOC-3 procedure for obtaining the UTR and the TEN's, artificial discrimination of vertices must occasionally be introduced i times between a set of equivalent vertices ; p_i is the cardinality of this current set of equivalent vertices having the highest HOC rank.

When the graph has weakly connected components which are separable by a bridge (cut-edge) or a cut-point, then automorphisms involving separately these components must be taken into account.

The second example is a molecule where stereoisomerism would exclude free rotation around the double bond, yet constitutional isomerism requires a symmetry operation which corresponds to such a process : all carbon atoms of 2,3,4,4-tetramethyl-2-pentene (2) are numbered from 1 to 9 as shown in Fig. 2. The automorphisms are indicated in Table 1, and they correspond to symmetry operations classified in terms of rotations (C_3 and powers thereof), reflections (σ), or combinations of such operations. One can see from Table 1 that the number of 12

automorphisms agrees with formula (1) where $p_1 = 3$, $p_2 = 2$, and $p_3 = 2$. The numbers p_1 and p_2 refer both to symmetry operations involving the methyl group ; in this case and in general for weakly connected components having a total of m_j equivalent vertices in component j, the number of local automorphisms is $m_j!$ For such cases all local automorphisms are expressed by

$$h(G) = \prod_j m_j! \qquad (2)$$

and indeed this formula together with (1) leads for molecule 2 to $h(2) = 2! \times 3! = 12$.

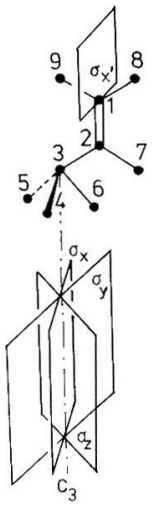

Fig. 2. Numbering and symmetry elements of 2

Table 1. Automorphisms and point group symmetry operations for constitutional graph 2

Automorphism	Operation
(1)(2)(3)(4)(5)(6)(7)(8)(9)	E
(1)(2)(3)(4)(5)(6)(7)(8,9)	$\sigma_{x'}$
(1)(2)(3)(4,5)(6)(7)(8)(9)	σ_y
(1)(2)(3)(4,6)(5)(7)(8)(9)	σ_z
(1)(2)(3)(4)(5,6)(7)(8)(9)	σ_x
(1)(2)(3)(4,5,6)(7)(8)(9)	C_3
(1)(2)(3)(4,6,5)(7)(8)(9)	C_3^2
(1)(2)(3)(4,5)(6)(7)(8,9)	$\sigma_y \sigma_{x'}$
(1)(2)(3)(4,6)(5)(7)(8,9)	$\sigma_z \sigma_{x'}$
(1)(2)(3)(4)(5,6)(7)(8,9)	$\sigma_x \sigma_{x'}$
(1)(2)(3)(4,5,6)(7)(8,9)	$C_3 \sigma_{x'}$
(1)(2)(3)(4,6,5)(7)(8,9)	$C_3^2 \sigma_{x'}$

For a very symmetric graph we take as a last example the 5-cage, also known as the Petersen graph (Fig. 3), 3, which appeared in several chemical contexts as a reaction graph.[41-43] The Petersen graph is vertex- and edge-transitive, actually it is 3-unitransitive or 3-regular in Tutte's terminology.[44,45] The first artificial discrimination during the HOC-3 algorithm is

made in the first stage of the iteration of Step 7 (Table 2), since the HOOC algorithm shows, as known, the topological equivalence of all ten vertices in this cubic non-planar graph. The first discrimination is thus made among $p_1 = 10$ topologically equivalent vertices.

Table 2. Application of the HOC algorithm to the Petersen graph 3 starting with an arbitrary numbering and ending after 7 stages in the final numbering (one of the 120 TEN's). Whenever two succeeding stages result in the same vertex ranking, the highest degenerate rank K is artificially increased by 1, according to Step 7 of the HOC algorithms, yielding an underlined rank K'. The numbers p_i of vertices having the highest degenerate rank are shown in brackets. The ranks of vertices adjacent to each degenerate vertex are displayed in increasing order (IOR) at various stages for obtaining the new rank, removing degeneracy.

Stage	HOOC		1		2			3	
Vertex	K	K'	IOR	^{1}K	IOR	^{2}K	^{2}K'	IOR	^{3}K
1	1(10)	2		3		3	4		5
2	1	1	1,1,2	2	1,1,3	2(3)	3		4
3	1	1	1,1,1	1	1,1,2	1	1	1,1,3	2
4	1	1	1,1,1	1	1,1,2	1	1	1,1,2	1
5	1	1	1,1,2	2	1,1,3	2	2	1,1,4	3
6	1	1	1,1,1	1	1,1,2	1	1	1,1,2	1
7	1	1	1,1,1	1	1,1,2	1	1	1,1,3	2
8	1	1	1,1,1	1	1,1,2	1	1	1,1,2	1
9	1	1	1,1,2	2	1,1,3	2	2	1,1,4	3
10	1	1	1,1,1	1	1,1,2	1	1	1,1,2	1

Stage	4			5		6			7	
Vertex	IOR	^{4}K	^{4}K'	IOR	^{5}K	IOR	^{6}K	^{6}K'	IOR	^{7}K
1		5	6		7		7	8		10
2		4	5		6		6	7		9
3	1,1,4	2	2	1,1,5	3	1,2,6	3(2)	4		6
4	1,2,3	1	1	1,2,4	2	1,3,5	2	2	1,4,6	4
5	1,1,5	3(2)	4		5		5	6		8
6	1,2,3	1	1	1,2,4	2	1,3,5	2	2	1,3,6	3
7	1,1,4	2	2	1,1,5	3	1,2,6	3	3		5
8	1,2,3	1	1	1,2,3	1	2,3,4	1	1	2,3,5	1
9	1,1,5	3	3		4		4	5		7
10	1,2,3	1	1	1,2,3	1	2,3,4	1	1	2,4,5	2

The second discrimination is made in stage 3 of the iteration among $p_2 = 3$ vertices, the third discrimination in stage 4 among $p_3 = 2$ vertices, and the fourth and last discrimination in stage 6 among $p_4 = 2$ vertices, ending up in complete removal of degeneracy in ranks ${}^{k}K$ at stage $k = 7$. All these four artificial discriminations of one vertex with the highest rank during the course of the HOC-3 algorithm are indicated in Table 2 by underlined ranks, and they lead to the numbering shown on the right-hand graph in Fig. 3.

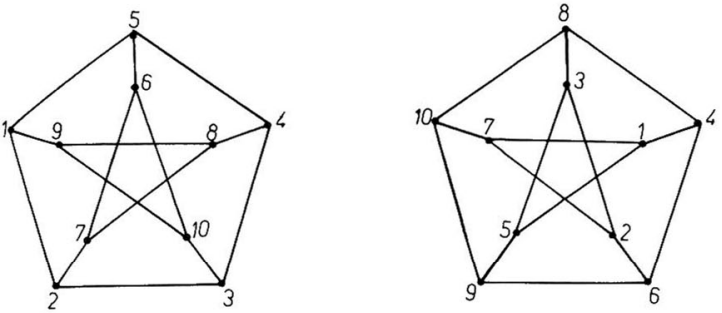

Fig. 3. The Petersen graph $\underline{3}$ with arbitrary numbering (Hamiltonian path) at left, and with HOC-3 numbering at right

Thus the order of the symmetry group for the Petersen graph is, as known from literature data :[16,44]

$$h(\underline{3}) = 10 \times 3 \times 2 \times 2 = 120.$$

As a final comment on the HOC-3 numbering of the Petersen graph vertices (Fig. 3, right-hand graph), any of our 120 TEN's for the Petersen graph has two adjacent consecutive numberings (2 and 3, 9 and 10), similarly to the final numbering for the same graph obtained by the procedure of Randić for recognizing graph symmetry.[16]

As seen above, simultaneously with the progress of the HOC-3 algorithm ending up in one of the TEN's with a full numbering of all N vertices in the graph with digits from 1 to N, the order of the symmetry group of the graph is obtained directly, without any additional special, elaborate calculations. This

is a considerable advantage of the present procedure over other procedures. In addition, the presence of symmetry (topological equivalence) is easily recognized during the HOC algorithm by the nature of its step 7, which counts the n ranks obtained at the end of HOC-1, HOOC, HOC-2 or HOC-2A algorithms : if n = N, the graph has no symmetry, but if n<N, the graph with N vertices has symmetry. Thus, both the manually-implemented and the computer-implemented versions of HOC algorithms lead automatically to recognizing the presence of, and counting the number of operations in, symmetry.

5. CONCLUDING REMARKS

It is indeed a very simple procedure to apply the HOC or SHOC algorithms in order to find whether two given graphs or two chemical structures are, or are not, isomorphic, irrespective of the way they are drawn. The advantages of our procedure have been discussed in the first two parts of this series [2,3] and will not be repeated here, but it should be mentioned that all these advantages are conserved when HOC algorithms are applied to decide about graph isomorphism.

One limitation in this respect is common both to our method and to the Morgan and improved Morgan algorithms ; it concerns, however, a different problem, namely substructure search (fragment matching). Though it is easily possible by our method to find out whether two graphs are isomorphic, it is not possible by the HOC or Morgan algorithms to locate substructures common in two graphs. This is due to the fact that the ordering and numbering of levels and vertices depend on the connectivity of the whole graph. On the other hand, some of the linear notation systems or coding procedures are better suited to the problem of substructure search.

For the problem of enumerating graph symmetry operations, it should be said as a conclusion that during the course of the implementation of the HOC procedure with the special types of algorithms dictated by the nature of the graph (HOC-1, HOOC, HOC-2 or HOC-2A on one hand, and HOC-3 on the other hand), the symmetries appear automatically and may be counted without any extra specially devised additional features of the algorithm.

puters in Chemical Research and Education, Ljubljana-Zagreb, 1973, paper 3/1 (cited in ref. 8).

19. E. H. Sussenguth Jr., Ph. D. Thesis, Harvard Univ. 1964 ; J. Chem. Docum. 5, 36 (1965).
20. D. R. Garey and D. S. Johnson, "Computers and Intractability. A Guide to the Theory of NP-Completeness", Freeman, San Francisco, 1979 ; P. Kelly, Pac. J. Math. 14, 191 (1964) ; S. Unger, Comm. ACM, 7, 26 (1964).
21. V. A. Koptyug, G. P. Ulyanov, V. N. Piottukh-Peletsky, B. G. Derendyev and M. I. Podgornaya, Codata Bull. No. 40, 45 (1981).
22. N. S. Zefirov, N. P. Zhidkov, B. M. Shchedrin and S. S. Trach, in "Matematicheskie Voprosy Strukturnogo Analiza" (N. P. Zhidkov and B. M. Shchedrin, eds.), Moscow Univ., 1978, p. 68.
23. M. Uchino, J. Chem. Inf. Comput. Sci. 22, 201 (1982) ; M. Razinger, Theor. Chim. Acta, 61, 581 (1982).
24. A. Lubiw, SIAM J. Comput. 10, 11 (1981).
25. H. Bouman, J. Chem. Docum. 3, 92 (1965).
26. R. Penny, J. Chem. Docum. 5, 113 (1965).
27. L. Spialter, J. Amer. Chem. Soc. 85, 2012 (1963).
28. A. T. Balaban, Chem. Phys. Letters, 89, 399 (1981) ; Pure Appl. Chem. 55, 199 (1983) ; A. T. Balaban and L. V. Quintas, Math. Chem. 14, 213 (1983).
29. D. Bonchev, O. Mekenyan and N. Trinajstić, J. Comput. Chem. 2, 127 (1981).
30. Part 5 in the series : O. Mekenyan, D. Bonchev and A. T. Balaban, submitted for publication to J. Comput. Chem.
31. J. Turner, in "Proof Techniques in Graph Theory", Proc. 2nd Ann Arbor Conf. Feb. 1968 (F. Harary, ed.), Academic Press, New York, 1969, p. 189.
32. G. Berman, J. Graph Theory, 1, 175 (1977) ; "Forward Citations in Graph Theory", Univ. of Waterloo, 1975 ; "Applied Graph Theory Bibliography with Forward Citations" Univ. of Waterloo, 1977.
33. S. Ruiz (ed.), "Graph Theory Newsletter", 12 (1982) ; 13 (1983) ; previous volumes had other editors ; Dept. of Mathematics, Western Michigan Univ., Kalamazoo, Michigan.
34. H. Whitney, Amer. J. Math. 54, 150 (1932) ; P. Kelley, Pac.

REFERENCES

1. Preceding part in the series, O. Mekenyan, A. T. Balaban and D. Bonchev, J. Chem. Inf. Comput. Sci. (in press).
2. Part 1 in the series, A. T. Balaban, O. Mekenyan and D. Bonchev, J. Chem. Inf. Comput. Sci. (in press).
3. Part 2 in the series, idem, ibid. (in press).
4. R. C. Read and D. G. Corneil, J. Graph Theory, 1, 339 (1977).
5. R. C. Read, in "Selected Topics in Graph Theory" (L. W. Beineke and R. J. Wilson, eds.), Academic Press, London, 1978, p. 417 ; D. G. Corneil, Ph. D. Thesis, Univ. of Toronto, 1968.
6. A. T. Balaban, Rev. Roumaine Chim. 18, 635 (1973) ; J. Meinwald and J. K. Crandall, J. Amer. Chem. Soc. 88, 1292 (1969), Appendix ; K. Conrow, J. Chem. Docum. 6, 206 (1966).
7. A. T. Balaban and F. Harary, J. Chem. Docum. 11, 258 (1971) ; W. C. Herndon, ibid. 14, 150 (1974) ; Tetrahedron Letters, 671 (1974) ; T. Živković, N. Trinajstić and M. Randić, Mol. Phys. 30, 517 (1975) ; M. Randić, N. Trinajstić and T. Živković, J. Chem. Soc. Faraday Trans. II, 72, 244 (1976) ; N. Trinajstić, "Chemical Graph Theory", chapter 7, vol. 1, p. 97, CRC Press, Boca Raton, Florida, 1983.
8. M. Randić, J. Chem. Phys. 60, 3920 (1974).
9. A. L. Mackay, J. Chem. Phys. 62, 309 (1975).
10. M. Randić, J. Chem. Phys. 62, 309 (1975).
11. F. Harary, in "Combinatorial Theory and Its Applications" (P. Erdös, A. Rényi and V. T. Sos, eds.), János Bólyai Math. Soc. Budapest, and further references therein.
12. J. F. Nagle, J. Math. Phys. 7, 1588 (1966).
13. R. P. Tewarson, "Sparse Matrices", Academic Press, New York, 1973, p. 68.
14. M. Randić, J. Amer. Chem. Soc. 97, 6609 (1975).
15. M. Randić, J. Chem. Inf. Comput. Sci. 17, 171 (1977).
16. M. Randić, Acta Cryst.(in press) ; Croatica Chem. Acta, 49, 643 (1977) ; Chem. Phys. Letters, 42, 283 (1976) ; Math. Chem. 7, 5 (1979).
17. L. C. Ray and R. A. Kirsch, Science, 126, 814 (1957).
18. J. C. J. Bart and N. Giordano, Proc. Internat. Conf. on Com-

J. Math. 7, 961 (1957).

35. F. Harary and E. M. Palmer, J. Math. Mech. 15, 623 (1966) ; L. Weinberg, TEEE Trans. CT, 13, 142 (1966).
36. J. Jakubik, Slovak Acta Fac. Nat. Univ. Comenian, 1 (4), 255 (1953).
37. R. Halm and H. Jung, J. London Math. Soc. 42, 254 (1967) ; C. Bohm and A. Santolini, ICC Bull. 3, 57 (1964).
38. M. M. Syslo, Theoret. Comput. Sci. 17, 91 (1982) ; E. A. Smolenskii, USSR Comput. Math. & Math. Phys. 21, 396 (1963).
39. C. J. Colbourn, Networks, 11, 13 (1981) ; M. K. Goldberg, Graph Theory Newsletter, 10, No. 6, 1 (1981).
40. A. T. Balaban, Rev. Roumaine Chim. 11, 1097 (1966) ; 15, 463 (1970) ; Math. Chem. 1, 33 (1975) ; chapter 5 in "Chemical Applications of Graph Theory" (A. T. Balaban, ed.), Academic Press, London, 1976, p.63 ; M. Banciu and A. T. Balaban, Chem. Scripta, 22, 188 (1983) and a further paper to appear in the same journal.
41. A. T. Balaban, D. Fărcaşiu and R. Bănică, Rev. Roumaine Cheim. 11, 1205 (1966).
42. J. D. Dunitz and V. Prelog, Angew. Chem. Internat. Ed. Engl. 7, 725 (1968).
43. A. T. Balaban, Rev. Roumaine Math. Pures Appl. 17, 3 (1972).
44. W. T. Tutte, "Connectivity in Graphs", Univ. of Toronto Press, 1966, p. 74.
45. F. Harary, "Graph Theory", Addison-Wesley, Reading, MA, 1969.

APPENDIX. LIST OF ABBREVIATIONS

HOC = Hierarchically Ordered extended Connectivities
HOOC = Hierarchically Ordered Overextended Connectivities
IOR = Increasing ORder
OEV = Orbitally Equivalent Vertex (vertices) ; the term "orbit" is used here in the graph-theoretical acceptance.
SBN = Smallest Binary Number
SHOC = Stereochemical Hierarchically Ordered extended Connectivity
TEN = Topologically Equivalent Numbering
UTR = Unique Topological Representation