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COMPUTER PROGRAM FOR THE RECOGNITION OF ACYCLIC REGULAR ISOPRENOID STRUCTURES

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1. Introduction

As it was mentioned earlier,[1] in 1974-1975 a computer program was devised for recognizing whether a given carbon skeleton (connected graph) with 5k carbon atoms (vertices), where k = 1, 2 or 3) can be decomposed into isoprene subunits (isoprenoid subgraphs ). There were no restrictions on the given graph, i. e. it could be cyclic or acyclic, and the mode of linking of the isoprenoid subgraphs was arbitrary. It is hoped to extend this program to $k > 3$.[2]

Kornprobst and Harary,[3] as well as Jacquier and Kornprobst,[4] developed more recently different programs for determining isoprenoid structures obeying certain restrictions (regular, i. e. head-to-tail linking as will be discussed in more detail in the next Section ; k = 1 - 6 ;[4] cyclomatic number $\mu \leqslant 5$;[4] for monocyclic systems with $\mu = 1$, an enumeration of the smaller systems was possible [3]).

The present paper discusses the simplest case, of acyclic polyisoprenoid structures with regular (i. e. head-to-tail) linking, without any restriction on k.

The importance of the isoprene rule in the chemistry of natural products has increased continuously since Ruzicka first formulated it. Many natural compounds with biological activity obey this rule ; we will illustrate this by enumerating several Nobel prizes for chemistry awarded for elucidating the struc-

tures of these compounds : terpenes (Wallach, 1910) ; bile acids, steroids, vitamins (Wieland, 1927 ; Windaus, 1928) ; carotenoids (Karrer, 1937) ; sexual hormones (Ruzicka, Butenandt, 1939) ; rubber and other macromolecules (Staudinger, 1953) ; stereochemistry of enzymically-formed compounds (Cornforth, Prelog, 1975). The Nobel prize for physiology and medicine was awarded in 1964 to Bloch and Lynen for elucidating by means of isotopic labelling the biosynthesis of isoprenoid structures from acetate *via* mevalonic acid and isopentenyl pyrophosphate.

From the rich bibliography on the isoprene rule and isoprenoid structures we will cite only a few leading references (reviews, books, progress reports).[5-16] Though the biogenetic route *via* isopentenyl pyrophosphate ("active isoprene") normally leads to regular structures which have head-to-tail linking, notable exceptions are known,[17] as in the carotenoid field (by dimerization of the vitamin A skeleton) or the steroid field (by rearrangement on cyclization of squalene). Bacteria cyclize squalene differently.[18] The non-biological polymerization of 1-methylcyclobutene, or the metathesis of cyclic isoprene oligomers, also leads to polyisoprenoid structures.[19]

Enumerations of restricted classes of isoprenoid structures were performed by Lederberg *et al.* on the basis of the DENDRAL program (for acyclic regular dimers of isoprene with formula $C_{10}H_{16}$)[20] and by Randić on the basis of the numbers of paths in a graph.[21]

2. Terminology and notation

A *graph* G consists of a finite nonempty set X of *vertices* together with a prescribed set U of unordered pairs of distinct vertices of X. Each pair u = (x,y) of vertices in U is a *line* (*edge*) of G, and u is said to *join* x and y. We say that x and y are *adjacent vertices* ; vertex x and edge u are incident with each other, as are y and u. Note that the definition of such (simple) graphs allows no *loop*, that is, no line joining a vertex to itself. A *walk* of a graph G is an alternating sequence of vertices and edges $(x_0, u_1, x_1, \ldots, x_{n-1}, u_n, x_n)$, beginning and ending with vertices, in which each edge is incident with the

two vertices immediately preceding and following it. This walk joins x_0 and x_n, and may also be denoted $x_0x_1...x_n$ (the lines being evident by context). It is closed if $x_0 = x_n$, and is open otherwise. It is a chain if all the vertices (and thus necessarily all the lines) are distinct. If the walk is closed, and if its $n \geq 3$ vertices are distinct, it is called a circuit. A graph is connected if every pair of vertices is joined by a chain. The length of a walk $x_0x_1...x_n$ is n, the number of edges in it. The degree of a vertex x in graph G, denoted d(x), is the number of lines incident with x.

A digraph (directed graph) D consists of a finite set Y of vertices and a collection V of ordered pairs of distinct vertices. Any such pair v = (x,y) is called an arc or directed line. The arc goes from x to y and is incident with x and y. The outdegree $d^+(x)$ of a vertex x is the number of vertices adjacent from it, and the indegree $d^-(x)$ is the number of vertices adjacent to it. A (directed) walk in a digraph is an alternating sequence of vertices and arcs, x_0, v_1, x_1,..., v_n, x_n in which each arc v_i is (x_{i-1}, x_i). The length of such a walk is n, the number of occurences of arcs in it. A closed walk has the same first and last vertex. A path is a walk in which all vertices are distinct. A cycle is a closed walk with all vertices distinct, except the first and the last. If there is a path from x to y, then y is said to be reachable from x. A semiwalk is an alternating sequence x_0, v_1, x_1,..., v_n, x_n of vertices and arcs where each arc v_i may be either (x_{i-1}, x_i) or (x_i, x_{i-1}). A semipath and semicycle are defined analogously. A digraph D is strongly connected, or strong, if every two vertices are mutually reachable ; D is unilaterally connected, or unilateral, if for any two vertices at least one is reachable from the other. We say that D is weakly connected, or weak, if every two vertices are joined by a semipath.

Correspondence table for graphs and digraphs :

Graphs	Digraphs
Line (edge)	arc
walk	(directed) walk, semiwalk
chain	path, semipath
circuit	cycle, semicycle
degree	outdegree, indegree
connected	strong, unilateral, weak

The adjacency matrix $A = (a_{ij})_{1 \leq i,j \leq n}$ of a graph G (digraph D) with n vertices is an n X n matrix in which :

$a_{ij} = 1$ if $(x_i , x_j) \in U$ (V)

$a_{ij} = 0$ if $(x_i , x_j) \notin U$ (V)

Thus there is a one-to-one correspondence between graphs (digraphs) with n vertices and n X n binary matrices.

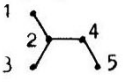
It is obvious that : (i) the degree of a vertex x_i of graph G is given by the sum of the elements on the row and column i of the adjacency matrix, i. e. $d(x_i) = a_{i1} + a_{i2} + \ldots + a_{in} + a_{1i} + a_{2i} + \ldots + a_{ni}$; (ii) the outdegree (indegree) of a vertex x_i of a digraph D is the sum of the elements of the row (column) i of the adjacency matrix : $d^+(x_i) = a_{i1} + a_{i2} + \ldots + a_{in}$ (likewise, $d^-(x_i) = a_{1i} + a_{2i} + \ldots + a_{ni}$) ; (iii) the adjacency matrix of a graph is a symmetrical one, i. e. $a_{ij} = a_{ji}$; (iv) the change of the numbering of two vertices in a graph or digraph corresponds to the permutation of the respective rows and columns.

An acyclic digraph AD contains no cycles. It is obvious that every walk of AD is a path, and that an acyclic digraph AD has at least one vertex of outdegree zero and at least one vertex of indegree zero. A source of a digraph is a vertex s which can reach all others. An out-tree (arborescence), denoted OT, is a digraph with a source and no semicycles. An out-tree is characterized by : (i) there is only one vertex, the source, in which no arc enters ; (ii) for any other vertex x, there is one path only which goes from s to x ; (iii) for all vertices excepting the source, a single arc enters each vertex. Thus we have $d^-(s) = 0$, and $d^-(x) = 1$ for any $x \neq s$. An OT is a weak digraph. A vertex x in an OT for which $d^+(x) = 0$ is said to be terminal.

3. General algorithm for testing whether a given structural formula is an acyclic regular isoprenoid structure

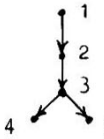
From a graph-theoretical viewpoint, structural (constitutional) formulas of hydrocarbons correspond to connected graphs with no loops, in which no vertex has a degree greater than four ; each vertex corresponds to a carbon atom (the

hydrogen atoms are not included), and each edge corresponds to a carbon-carbon bond. According to the structural formula of isoprene : $H_2C=C(CH_3)-CH=CH_2$, we have the graph :



(1)

and, respectively, the out-tree (OT) :



(2)

where the labelling of vertices is arbitrary.

Isoprenoids are substances whose structural formulas are obtained by connecting k units of isoprene. Thus we shall say that a graph with 5k vertices is isoprenoid if it can be decomposed into k subgraphs of type (1). Examples of isoprenoid graphs are presented in Figure 1, and examples of non-isoprenoid graphs in Figure 2. Since the degree of any vertex is at most four, the maximum number of edges in a graph with 5k vertices is (5k.4)/2 = 10k.

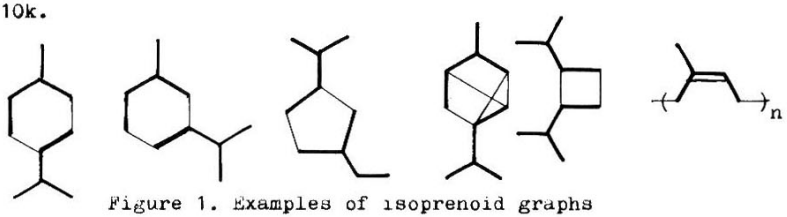


Figure 1. Examples of isoprenoid graphs

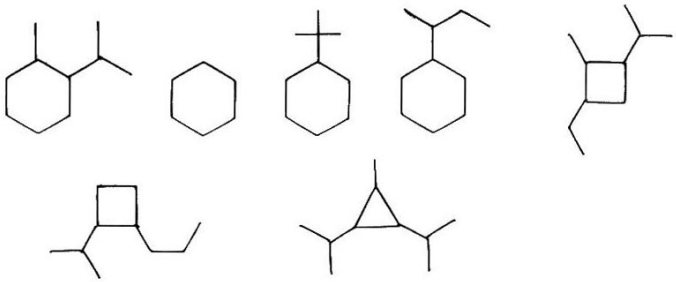


Figure 2. Examples of non-isoprenoid graphs

Our problem is the recognition of acyclic isoprenoid structures with "head-to-tail" linking, which will be called acyclic regular isoprenoid structures.* The notation "head" and "tail" is defined as follows for an isoprenoid unit :

tail  head

For further needs we shall use the term isoprenoid OT to define the out-tree with 5k vertices which can be decomposed into k out-trees of type (2). Any acyclic isoprenoid graph with "head-to-tail" connection can be represented under the form of an isoprenoid OT as follows : (i) we consider the vertices x for which $d(x) = 1$; (ii) the source of an isoprenoid OT will be the vertex x determined by the fact that it obeys (i) and that its adjacent vertex y has $d(y) = 2$; (iii) the lines of the given graph are converted into arcs respecting the properties of the OT.

The problem raised when representing a regular isoprenoid structure in the form of an isoprenoid OT is to find out which vertex will be the source of the OT. This problem is solved in two stages, as indicated above : at stage (i) we find the set of vertices of degree one, and at stage (ii) from this set we select the source of the OT. We can always represent a regular isoprenoid structure in the form of an isoprenoid OT, and this in a unique way, for the structure is acyclic. Examples of isoprenoid out-trees are presented in Figure 3.

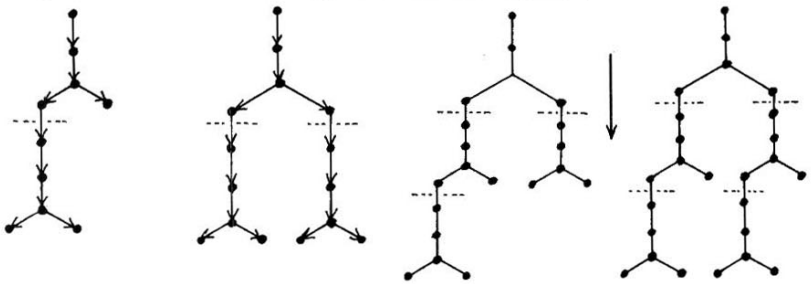


Figure 3. Examples of isoprenoid OT's

* The word "regular" originates here from chemistry, not from graph theory, and has no connotation about vertex degrees, but only indicates the "head-to-tail" linking of isoprene units.

Remarks

a) It is obvious that a necessary condition for a given OT with 5k vertices ($k \geq 1$) * to be a regular isoprenoid structure is that the number of terminal vertices equals k + 1.

b) Let us call a bifurcation any vertex of type b : 

where $d^-(b) = 1$ and $d^+(b) = 2$. Since each isoprenoid unit has one bifurcation, an OT with 5k vertices ($k \geq 1$) is an isoprenoid OT only if the number of its bifurcations is k.

c) Since for each vertex x of an isoprenoid OT we have $d^+(x) \in \{0,1,2\}$ we can find the number of vertices with the outdegree one by subtracting from the total number of vertices the number of vertices with outdegree 0 or 2.

d) Owing to the "head-to-tail" linking of isoprene units, the length of the path from the first bifurcation of the OT to any other bifurcation of the isoprenoid OT is congruent to 0 modulo 4. Thus the length of any path which has as extremities the first bifurcation and one of the terminal vertices of the isoprenoid OT is congruent to 1 modulo 4.

In the following we shall assume that n is a multiple of 5, i. e. n = 5k (where k is a positive integer).

Our algorithm for the recognition of an acyclic regular isoprenoid structure (isoprenoid OT) uses Warshall's algorithm for finding the length of the minimum path between any two vertices as well as a modification of the latter algorithm for determining the vertices of the paths of minimal length which are to be taken into account.

In order to test whether a given OT with n vertices is an isoprenoid OT we consider its adjacency matrix

$$\text{MAD} = (a_{ij}) \quad 1 \leq i,j \leq n$$

where : $a_{ij} = 1$, if $(i,j) \in V$
$a_{ij} = \infty$, if $(i,j) \notin V$

The matrix $\text{MARC} = (b_{ij})_{1 \leq i,j \leq n}$ of the arcs is given by

$b_{ij} = i$, if $(i,j) \in V$
$b_{ij} = 0$, if $(i,j) \notin V$

where i and 0 are labels for arcs.

* For the convenience of the program, henceforth n replaces 5k (the number of vertices in the graph or the OT).

We consider the concatenation operator "." for the above labels with the convention : if $\alpha = 0$ or $\beta = 0$, then $\alpha.\beta = 0$.

Applying Warshall's algorithm we obtain the matrix MDRUM = $(x_{ij})_{1 \leq i,j \leq n}$ of the lengths of minimal paths, where

x_{ij} = the length of the minimal path from i to j, if there exists a path from i to j

$x_{ij} = \infty$, otherwise;

and the matrix MNODD = $(v_{ij})_{1 \leq i,j \leq n}$ of the vertices of the paths, where

v_{ij} = the vertices which appear in the minimal path from i to j, if there exists a path from i to j

$v_{ij} = 0$, otherwise.

Warshall's algorithm for finding the length of minimal path between any two vertices of a graph and the actual determination of the vertices of this path :

1. MDRUM = MAD, MNODD = MARC
2. j = 1
3. i = 1
4. If $x_{ij} = \infty$, go to 8.
5. k = 1
6. If $x_{ik} > x_{ij} + x_{jk}$, then $x_{ik} = x_{ij} + x_{jk}$ and $v_{ik} = v_{ij} \cdot v_{jk}$
7. k = k + 1 ; if $k \leq n$, go to 6.
8. i = i + 1 ; if $i \leq n$, go to 4.
9. j = j + 1 ; if $j \leq n$, go to 3, otherwise STOP.

Comments. If the minimal path from i to j contains the sequence of vertices $i_1, i_2, \ldots, i_k$, where $i_1 = i$ and $i_k = j$, then $v_{ij} = i_1 . i_2 \ldots\ldots i_{k-1} = i, i_2 \ldots\ldots i_{k-1}$. Since in an OT there is at most one path that joins two vertices, we can omit the adjective "minimal" path.

4. The FORTRAN-IV program (named REGISO) for the recognition of regular isoprenoid OT's with N carbon atoms, where N is congruent to 0 modulo 5

Given an OT with N vertices we number these vertices arbitrarily by assigning them digits (integers) from 1 to N

and we form the adjacency matrix MAD(N,N) and the matrix MARC(N,N) of the arcs. These will also be the input data of the recognition program of isoprenoid regular out-trees.

The non-existence of an arc between two vertices is symbolized by 999. This is the equivalent to the symbol ∞ . It is chosen in such a way that it will be always greater than any other number which might appear following the calculations made by the program. The testing program for OT's contains the following stages (some of which take into account the Remarks from the previous Section) :

I. Calculate the outdegree and indegree of the vertices of the given OT (by means of theoretical considerations) and introduce these degrees into vectors GE(N) and GI(N), respectively, which appear in the listing.

II. Determine the source of the OT and denote it by SOURCE. If there are more than one vertex satisfying the conditions for being a source vertex (NS >1), an error message is signaled.

III. Determine the terminal vertices which will be put into the NODTER(NT) vector, where NT is the counter of these vertices. If NT is different from 1 + N/5 (Remark a), then the given structure is a non-isoprenoid OT. The NODTER(NT) vector is an output vector from the program.

IV. Determine the vertices with outdegree 2 and 1. These vertices will be put into the vectors NGE2(N2) and NGE1(N1), respectively, and will be displayed on the listing. Verify whether N2 is equal to N/5 (Remark b) and whether N1 is equal to N - N2 - NT (Remark c).

V. Find the first vertex after SOURCE which has the outdegree 2. Denote it by NODSEC. A necessary condition for an OT to be isoprenoid is the existence of exactly one vertex (denoted by NODPRIM) between SOURCE and NODSEC with GI(NODPRIM) = GE(NODPRIM) = 1.

VI. Calculate the matrix MDRUM(N,N) of the lengths of the paths. Calculate the matrix MNODD(N-3,N-3) of the vertices in those paths which have as extremities NODSEC and a terminal vertex. Test whether the lengths of the paths which start from NODSEC and have as endpoint a terminal vertex are congruent to

1 modulo 4 (Remark d). Every row of the matrix MNODD contains the vertices of the paths which start from NODSEC. In view of the structure of an isoprenoid OT as well as of the previous check-up, observe that MNODD is a square matrix of dimension N - 3. Both the MDRUM and MNODD matrices are obtained by a suitable adaptation of the Warshall algorithm. Indeed, we are interested in the recognition of the vertices of those paths which start from NODSEC.

VII. For every path that starts from NODSEC and has as an extremity a terminal vertex (the number of these paths is obviously equal to the number of terminal vertices, NT) verify the following stages using a DO loop : (i) the predecessor, PRED, of the terminal vertex must be a bifurcation, i. e. GE(PRED) = 2 ; (ii) the vertices of the path under consideration are decomposed into groups of four elements in the opposite sense of their order, beginning with the ante-predecessor of the terminal vertex. By introducing the vertices of each group in the above order into the vector ANTEPRED of dimension four, we test whether GE(ANTEPRED(i)) = 1, i = 1, 2, 3 and whether GE(ANTEPRED(4)) = 2. The decomposition into groups of four vertices is possible in view of Remark d. This stage is achieved by using a DO loop.

When conditions (i) and (ii) are fulfilled for all NT paths, the program ends successfully (i. e. the given structure is an isoprenoid OT). Otherwise the structure is not an isoprenoid OT. The T(N) vector used in reading and writing contains the labels of the vertices of the given structure.

This program is able to recognize regular isoprenoid OT's with 5k vertices for any k ($k \geq 1$). It can also be used for recognizing cyclic isoprenoid structures with "head-to-tail" connection containing 5k vertices, after using a modification of Kornprobst's algorithm.

Thus we can check whether a given structural formula is an acyclic isoprenoid structure with "head-to-tail" connection as follows :

- We try to convert the associated acyclic graph (hydrogen-depleted structure) into an OT whose source is one of the graph vertices with degree 1 and whose adjacent vertex has degree 2. When there is no such vertex, the structure is not of

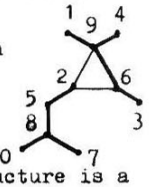
the required type ; otherwise,

- We convert the lines of the given graph into arcs respecting the properties of an OT ;

- We label in an arbitrary order the vertices of the OT obtained in the previous stages and we apply the algorithm (our REGISO program) for the recognition of isoprenoid OT's.

If the given structural formula is in the form of an OT, the testing program can be applied directly.

The algorithm presented above solves also the cyclic case since on being given a cyclic structure, by using Kornprobst's principles, the problem may be reduced to an acyclic one. The reason for using these two principles (namely, degradation of vertex degrees, and non-generation of vertices with degree zero) in Kornprobst's algorithm is to decompose the given structure into groups of five vertices, and to check whether each group coincides with an isoprenoid unit. It is our intention to devise a program for operating cuts into the cyclic structure, in order to obtain a connected acyclic structure, thus reducing the problem to one of the type solved by the REGISO program. The number of cuts which must be made in order to reduce a cyclic structure to an acyclic one, converting it into an OT, equals the cyclomatic number of the graph. No cut should fragment an isoprenoid unit. For instance, in the case of chrysanthemic acid only two of the three possible cuts are legitimate, namely 2-6 and 2-9, whereas the cut 6-9 fragments an isoprenoid unit and is therefore illegitimate. On performing the cut, an acyclic structure results. If the application of the REGISO program to this obtained OT ends successfully, then the given structure is a cyclic regular isoprenoid structure ; otherwise this stage is repeated with each of the remaining possibilities for cutting (legitimate and illegitimate). The given structural formula is not isoprenoid with "head-to-tail" connection if no application of our algorithm ends successfully.



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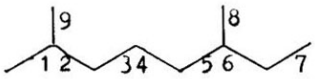
* The number of isomeric acyclic head-to-tail diterpenes $C_{10}H_{16}$ is, however, 50 and not 52 as mentioned in ref. 20. Indeed, if the nine bonds in the carbon skeleton of this diterpene are labelled as indicated below, the three pairs of π-electrons may be ascribed in the following 50 ways :



133	134	135	136	137	138	144	145	146	147
148	157	167	177	178	234	235	236	237	238
244	245	246	247	248	257	267	277	278	335
336	337	338	345	346	347	348	357	367	377
378	446	447	448	457	467	477	478	577	778

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1     * DEFINE FILE *1=1,*2=3
2           INTEGER MAD(25,25),MNODD(22,22),MDRUM(25,25),MARC(25,25),GE(25),GI
3          *(25),NODTER(25),NGE1(25),NGE2(25),ANTEPRED(4),PRED,SOURCE,T(25)
4     C
5     C      NUMBER 999 SYMBOLIZES THE NON-EXISTENCE OF AN ARC BETWEEN I*O VERT
6     C      ICES
7     C
8           READ(1,100)N,(T(I),I=1,N)
9       100 FORMAT(I2,25I2)
10          READ(1,140)((MAD(I,J),J=1,N),I=1,N)
11      140 FORMAT(25I3)
12          READ(1,141)((MARC(I,J),J=1,N),I=1,N)
13      141 FORMAT(25I2)
14          WRITE(3,135)
15      135 FORMAT(32X,'THE PROGRAM TESTS WHETHER A GIVEN STRUCTURE IS AN ACYC
16         *LIC REGULAR ISOPRENOID'/32X,76('*')///)
17          WRITE(3,124)((MAD(I,J),J=1,N),I=1,N)
18      124 FORMAT(62X,'ADJACENCY MATRIX'/62X,16('*')//25(20X,25(I3,1X)/))
19          WRITE(3,125)((MARC(I,J),J=1,N),I=1,N)
20      125 FORMAT(62X,'MATRIX OF ARCS'/62X,14('*')//25(33X,25(I2,1X)/))
21    C
22    C      CALCULATION OF OUTDEGREES
23    C
24          DO 1 I=1,N
25          GE(I)=0
26          DO 1 J=1,N
27          IF(MAD(I,J).EQ.999)GO TO 1
28          GE(I)=GE(I)+MAD(I,J)
29        1 CONTINUE
30          WRITE(3,102)(T(I),GE(I),I=1,N)
31      102 FORMAT(62X,'VERTEX I',2X,'*',2X,'OUTDEGREE'/62X,22('*')/(64X,I3,5X
32         *,'*',6X,I2))
33    C
34    C      CALCULATION OF INDEGREES
35    C
36          DO 2 J=1,N
37          GI(J)=0
38          DO 2 I=1,N
39          IF(MAD(I,J).EQ.999) GO TO 2
40          GI(J)=GI(J)+MAD(I,J)
41        2 CONTINUE
42          WRITE(3,103)(T(I),GI(I),I=1,N)
43      103 FORMAT(//62X,'VERTEX I',2X,'*',2X,'INDEGREE'/62X,21('*')/(64X,I3,5
44         *X,'*',6X,I2))
45    C
46    C      DETERMINATION OF SOURCE
47    C
48          NS=0
49          DO 3 I=1,N
50          IF(GI(I).NE.0)GO TO 3
51          SOURCE=I
52          NS=NS+1
53        3 CONTINUE
54          IF(NS.EQ.1)GO TO 25
55          WRITE(3,104)
56      104 FORMAT(15X,'ERROR-WE HAVE NOT AN OUT-TREE')
57          GO TO 50
58       25 WRITE(3,122)SOURCE
59      122 FORMAT(15X,'THE SOURCE IS:',I2/)
```

```
      C
      C     DETERMINATION OF TERMINAL VERTICES. THESE WILL BE PUT INTO NODTER
      C     VECTOR
      C
            NT=0
            DO 4 I=1,N
            IF(GE(I).NE.0)GO TO 4
            NT=NT+1
            NODTER(NT)=I
          4 CONTINUE
            WRITE(3,126)(NODTER(I),I=1,NT)
        126 FORMAT(15X,'TERMINAL VERTICES:',25(I2,1X)/)
            M=N/5+1
            IF(NT.EQ.M)GO TO 5
            WRITE(3,105)
        105 FORMAT(15X,'NON-ISOPRENOID STRUCTURE')
            GO TO 50
      C
      C     DETERMINATION OF VERTICES WHICH HAVE THE OUTDEGREE 2. THESE WILL
      C     BE PUT INTO NGE2 VECTOR
      C
          5 N2=0
            DO 6 I=1,N
            IF(GE(I).NE.2)GO TO 6
            N2=N2+1
            NGE2(N2)=I
          6 CONTINUE
            M10=N/5
            IF(N2.EQ.M10)GO TO 7
            WRITE(3,106)
        106 FORMAT(15X,'NON-ISOPRENOID STRUCTURE')
            GO TO 50
      C
      C     DETERMINATION OF VERTICES WHICH HAVE THE OUTDEGREE 1. THESE WILL
      C     BE PUT INTO NGE1 VECTOR
      C
          7 N1=0
            DO 8 I=1,N
            IF(GE(I).NE.1)GO TO 8
            N1=N1+1
            NGE1(N1)=I
          8 CONTINUE
            M1=N-N2-NT
            IF(N1.EQ.M1)GO TO 9
            WRITE(3,107)
        107 FORMAT(15X,'NON-ISOPRENOID STRUCTURE')
            GO TO 50
      C
      C     DETERMINATION OF THE FIRST VERTEX AFTER SOURCE WHICH HAS THE OUTDE
      C     GREE 2
      C
          9 IF(GE(SOURCE).EQ.1)GO TO 10
            WRITE(3,108)
        108 FORMAT(15X,'NON-ISOPRENOID STRUCTURE')
            GO TO 50
         10 DO 11 J=1,N
            IF(MAD(SOURCE,J).NE.999)GO TO 12
         11 CONTINUE
```

```
      12 NODPRIM=J
         IF(GF(NODPRIM).EQ.1)GO TO 14
         WRITE(3,109)
     109 FORMAT(15X,'NON-ISOPRENOID STRUCTURE')
         GO TO 50
      14 DO 15 J=1,N
         IF(MAD(NODPRIM,J).NE.999)GO TO 16
      15 CONTINUE
      16 NODSEC=J
         IF(GF(NODSEC).EQ.2)GO TO 17
         WRITE(3,110)
     110 FORMAT(15X,'NON-ISOPRENOID STRUCTURE')
         GO TO 50
      17 WRITE(3,128)NODSEC
     128 FORMAT(/15X,'THE FIRST VERTEX AFTER SOURCE WHICH HAS THE OUTDEGREE
        * 2,NOTED NODSEC,IS:',I2/)
C
C        CALCULATE MATRIX MDRUM OF THE LENGTHS OF PATHS AND  MATRIX MNODD
C        OF THE VERTICES OF PATHS
C
         DO 30 I=1,N
         DO 30 J=1,N
      30 MDRUM(I,J)=MAD(I,J)
         DO 31 J=1,N
         DO 31 I=1,N
         IF(MDRUM(I,J).EQ.999)GO TO 31
         DO 31 K=1,N
         IF(MDRUM(J,K).EQ.999)GO TO 31
         M6=MDRUM(I,J)+MDRUM(J,K)
         IF(MDRUM(I,K).LE.M6)GO TO 31
         MDRUM(I,K)=M6
         IF(I.NE.NODSEC)GO TO 31
         IF(K.EQ.SOURCE.OR.K.EQ.NODPRIM.OR.K.EQ.NODSEC)GO TO 31
         IF(MDRUM(I,J).NE.1)GO TO 32
         IF(MARC(I,J).EQ.0.OR.MARC(J,K).EQ.0)GO TO 31
         MNODD(K,1)=MARC(I,J)
         MNODD(K,2)=MARC(J,K)
         GO TO 31
      32 IF(MARC(J,K).EQ.0)GO TO 31
         M9=MDRUM(I,J)
         DO 34 J1=1,M9
      34 MNODD(K,J1)=MNODD(J,J1)
         MNODD(K,M9+1)=MARC(J,K)
      31 CONTINUE
         DO 111 J=1,NT
         IF(MDRUM(NODSEC,NODTER(J)).EQ.1)MNODD(NODTER(J),1)=NODSEC
     111 CONTINUE
         DO 18 I=1,NT
         M5=MOD(MDRUM(NODSEC,NODTER(I)),4)
         IF(M5.EQ.1)GO TO 18
         WRITE(3,112)
     112 FORMAT(15X,'NON-ISOPRENOID STRUCTURE')
         GO TO 50
      18 CONTINUE
         WRITE(3,129)((MDRUM(I,J),J=1,N),I=1,N)
     129 FORMAT(62X,'MATRIX MDRUM'/62X,12('**')//25(20X,25(I3,1X)/))
         WRITE(3,130)
```

```
      130 FORMAT(15X,'THE VERTICES OF EACH PATH WHICH STARTS FROM NODSEC AND
     * ENDS IN A TERMINAL VERTEX'/15X,80('*')/)
          DO 131 I=1,NT
          K2=NODTER(I)
          K1=MDRUM(NODSEC,K2)
          WRITE(3,132)K2,(MNODD(K2,J),J=1,K1)
      132 FORMAT(//15X,'THE VERTICES OF THE PATH WHICH ENDS IN',I3,5X,22(I3,
     *1X))
      131 CONTINUE
          DO 19 I=1,NT
          K1=MDRUM(NODSEC,NODTER(I))
          PRED=MNODD(NODTER(I),K1)
          IF(GE(PRED),EQ.2)GO TO 20
          WRITE(3,113)
      113 FORMAT(15X,'NON-ISOPRENOID STRUCTURE')
          GO TO 50
       20 IF(K1.EQ.1)GO TO 19
          M2=(K1-1)/4
          DO 19 I1=1,4,M2
          M4=I1+3
          DO 21 I2=I1,M4
       21 ANTEPRED(I2)=MNODD(NODTER(I),K1-I2)
          IF(GE(ANTEPRED(1)),EQ.1.AND.GE(ANTEPRED(2)),EQ.1.AND.GE(ANTEPRED(3
     *)),EQ.1.AND.GE(ANTEPRED(4)),EQ.2)GO TO 19
          WRITE(3,114)
      114 FORMAT(15X,'NON-ISOPRENOID STRUCTURE')
          GO TO 50
       19 CONTINUE
          WRITE(3,115)
      115 FORMAT(//15X,'THE STRUCTURE IS AN ACYCLIC REGULAR ISOPRENOID'/15X,
     *46('*'))
       50 STOP
          END
                                              CDC         11/11/78  11.12.29
```

THE PROGRAM TESTS WHETHER A GIVEN STRUCTURE IS AN ACYCLIC REGULAR ISOPRENOID
****

ADJACENCY MATRIX
****

999	1	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999
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MATRIX OF ARCS
****

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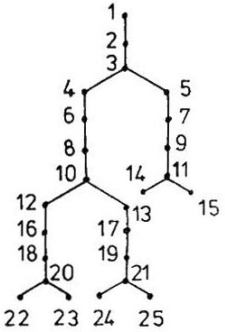
VERTEX I	*	OUTDEGREE
1	*	1
2	*	1
3	*	2
4	*	1
5	*	1
6	*	1
7	*	1
8	*	1
9	*	1
10	*	2
11	*	2
12	*	1
13	*	1
14	*	0
15	*	0
16	*	1
17	*	1
18	*	1
19	*	1
20	*	2
21	*	2
22	*	0
23	*	0
24	*	0
25	*	0



VERTEX I	*	INDEGREE
1	*	0
2	*	1
3	*	1
4	*	1
5	*	1
6	*	1
7	*	1
8	*	1
9	*	1
10	*	1
11	*	1
12	*	1
13	*	1
14	*	1
15	*	1
16	*	1
17	*	1
18	*	1
19	*	1
20	*	1
21	*	1
22	*	1
23	*	1
24	*	1
25	*	1

THE SOURCE IS: 1

TERMINAL VERTICES:14 15 22 23 24 25

THE FIRST VERTEX AFTER SOURCE WHICH HAS THE OUTDEGREE 2,NOTED NODSEC,IS: 3

MATRIX MDRUM

999	1	2	3	3	4	4	5	5	6	6	7	7	7	7	8	8	9	9	10	10	11	11	11	11
999	999	1	2	2	3	3	4	4	5	5	6	6	6	6	7	7	8	8	9	9	10	10	10	10
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999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999

THE VERTICES OF EACH PATH WHICH STARTS FROM NODSEC AND ENDS IN A TERMINAL VERTEX

THE VERTICES OF THE PATH WHICH ENDS IN 14   3 5 7 9 11

THE VERTICES OF THE PATH WHICH ENDS IN 15   3 5 7 9 11

THE VERTICES OF THE PATH WHICH ENDS IN 22   3 4 6 8 10 12 16 18 20

THE VERTICES OF THE PATH WHICH ENDS IN 23   3 4 6 8 10 12 16 18 20

THE VERTICES OF THE PATH WHICH ENDS IN 24   3 4 6 8 10 13 17 19 21

THE VERTICES OF THE PATH WHICH ENDS IN 25   3 4 6 8 10 13 17 19 21

THE STRUCTURE IS AN ACYCLIC REGULAR ISOPRENOID

THE PROGRAM TESTS WHETHER A GIVEN STRUCTURE IS AN ACYCLIC REGULAR ISOPRENOID
****

ADJACENCY MATRIX
****

999	1	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999
999	999	1	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999	999
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MATRIX OF ARCS
****

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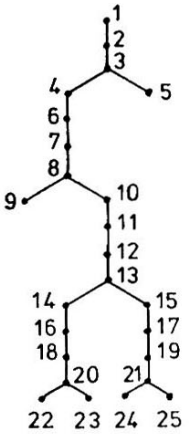
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

VERTEX I	*	OUTDEGREE
1	*	1
2	*	1
3	*	2
4	*	1
5	*	0
6	*	1
7	*	1
8	*	2
9	*	0
10	*	1
11	*	1
12	*	1
13	*	2
14	*	1
15	*	1
16	*	1
17	*	1
18	*	1
19	*	1
20	*	2
21	*	2
22	*	0
23	*	0
24	*	0
25	*	0



VERTEX I	*	INDEGREE
1	*	0
2	*	1
3	*	1
4	*	1
5	*	1
6	*	1
7	*	1
8	*	1
9	*	1
10	*	1
11	*	1
12	*	1
13	*	1
14	*	1
15	*	1
16	*	1
17	*	1
18	*	1
19	*	1
20	*	1
21	*	1
22	*	1
23	*	1
24	*	1
25	*	1

THE SOURCE IS: 1

TERMINAL VERTICES: 5 9 22 23 24 25

THE FIRST VERTEX AFTER SOURCE WHICH HAS THE OUTDEGREE 2,NOTED NODSEC,IS: 3

MATRIX MDRUM
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999	1	2	3	3	4	5	6	7	7	8	9	10	11	11	12	12	13	13	14	14	15	15	15	15
999	999	1	2	2	3	4	5	6	6	7	8	9	10	10	11	11	12	12	13	13	14	14	14	14
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THE VERTICES OF EACH PATH WHICH STARTS FROM NODSEC AND ENDS IN A TERMINAL VERTEX
****

THE VERTICES OF THE PATH WHICH ENDS IN 5   3

THE VERTICES OF THE PATH WHICH ENDS IN 9   3 4 6 7 8

THE VERTICES OF THE PATH WHICH ENDS IN 22   3 4 6 7 8 10 11 12 13 14 16 18 20

THE VERTICES OF THE PATH WHICH ENDS IN 23   3 4 6 7 8 10 11 12 13 14 16 18 20

THE VERTICES OF THE PATH WHICH ENDS IN 24   3 4 6 7 8 10 11 12 13 15 17 19 21

THE VERTICES OF THE PATH WHICH ENDS IN 25   3 4 6 7 8 10 11 12 13 15 17 19 21

THE STRUCTURE IS AN ACYCLIC REGULAR ISOPRENOID
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