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COMPUTER PROGRAM FOR THE RECOGNITION OF STANDARD ISOPRENOID STRUCTURES

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Abstract. A FORTRAN IV computer program STANISO is presented, which is able to recognize whether a given chemical structure is or is not isoprenoid with standard linking (i.e. admitting at least one decomposition into isoprenoid units joined through head-to-head, head-to-tail, tail-to-head or tail-to-tail linkings). There is no other restriction as to the number of isoprenoid units or to the number of cycles in the given structure. A listing of the program is attached.

1. Introduction

A preceding paper[1] presented a computer program REGISO for the recognition of acyclic regular isoprenoid structures, i.e. of those acyclic isoprenoid structures which have head-to-tail linking (rigorous definitions will be found in the next two sections). This program had no restrictions as to the number of isoprenoid units.

Kornprobst and Harary,[2] as well as Jacquier and Kornprobst[3], developed different programs for recognizing isoprenoid structures with certain other restrictions : the number of isoprene units has to be smaller than seven, and the cyclomatic number has to be smaller than six.

The present paper describes, as announced in the previous report[1], the most general computer program sofar for the recognition of standard isoprenoid structures, whose only restriction concerns the standard linking (head-to-tail, head--to-head, tail-to-head, or tail-to-tail).

The importance of the isoprene rule in elucidating the chemical structure of natural products was discussed in the preceding paper.[1]

2. Terminology and notation

A graph G consists of a finite nonempty set X of vertices together with a prescriebed set U of unordered pairs of distinct vertices of X. Each pair u = (x, y) of vertices of 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, and no multiple edges.

More general definitions include such elements : when multiple edges between two points are allowed we have multigraphs (pseudographs) and when loops are also allowed we have general graphs. In this paper we will use neither multigraphs nor general graphs. 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

$x_0x_1 \ldots x_n$ (the lines being evident by context). It is closed if $x_0 = x_n$, and is open otherwise. It is a chain if all 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 and disconnected otherwise. The length of a walk $x_0x_1 \ldots x_n$ 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. The cyclomatic number μ of a graph with n vertices, m lines and p connected components is equal to m-n+p. For connected graphs which will be used hence p = 1, hence $\mu = m - n + 1$. The adjacency matrix $MAD = (a_{ij})_{1 \leq i,\ j \leq n}$ of a graph G with n vertices is an n x n matrix in which :

$$a_{ij} = 1 \quad \text{if} \quad (x_i, x_j) \in U$$
$$a_{ij} = 0 \quad \text{if} \quad (x_i, x_j) \in U$$

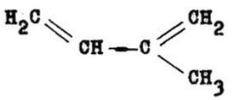
Thus there exists a one-to-one correspondence between graphs with n vertices and n x n binary matrices.

It is obvious that : (i) the degree of a vertex x_i of a 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 change of the numbering of two vertices in a graph corresponds to the permutation of the respective rows and columns; (iii) the adjacency matrix of a graph is a symmetrical one, i.e. $a_{ij} = a_{ji}$, $\forall_{i,j}$.

A graph is called acyclic if it contains no circuit, otherwise is called cyclic. The distance between two vertices is the number of edges in the smallest chain connecting these vertices. If we have a graph, we <u>cut</u> an edge by removing it from the graph, preserving its two incident vertices.

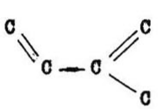
3. General algorithm for testing whether a given structure is a standard isoprenoid structure

From a graph-theoretical viewpoint, 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 disregarded). The graph has no loops because the relation between any two carbon atoms (covalent linking) is a symmetrical one, and this relation can not exist between a carbon atom and itself. Moreover, two carbon atoms may have in common 1, 2 or 3 pairs of electrons corresponding to a simple, double or triple bond, respectively. In conformity with the structural formula of the isoprene unit



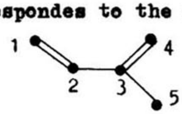
(1)

we have the carbon skeleton



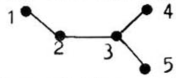
(2)

which correspondes to the connected multigraph



(3)

For the purpose we have in view, namely the clasification of a given formula as isoprenoid or not, the nature (simple, multiple) of the bond does not matter, therefore we will use instead of the multigraph (3) the simple graph

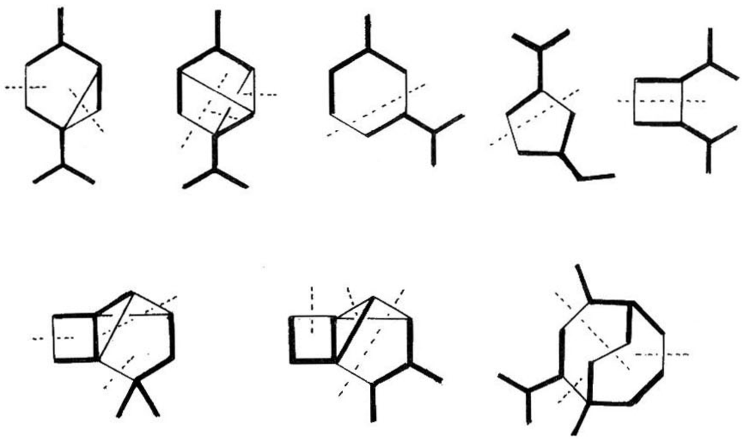


(4)

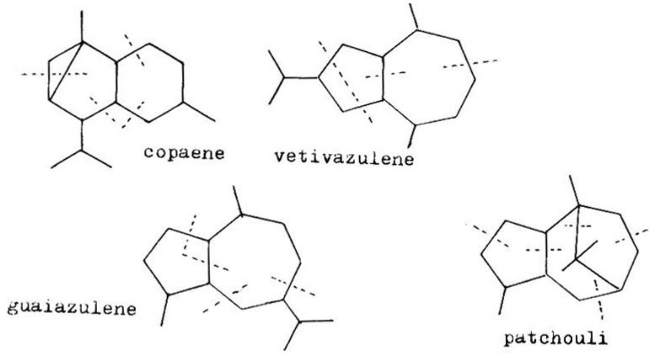
where the labelling of the vertices is arbitrary.

<u>Isoprenoid structures</u> are the structures of substances whose structural formulas are obtained by junction of n isoprene units. Thus, we shall use the term <u>isoprenoid graph</u> to define the graph with 5n vertices which can be decomposed into n subgraphs of type (4).

A few examples of isoprenoid graphs follow.

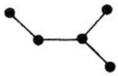


In all above examples, the cuts are indicated by broken lines, and the isoprenoid units by heavy lines. In the following examples, real terpenoid structures are indicated (double bonds are ignored, only the carbon skeleton is shown), and the isoprene units are delineated only by cuts.

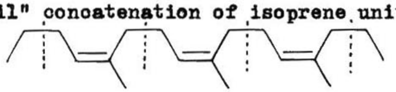


<u>Remark</u>. Because no vertex has a degree greater than four, the maximum number of egdes of a graph having 5n vertices is equal to (4 x 5n)/2.

The notation "head" and "tail" is defined as follows for an isoprenoid unit :

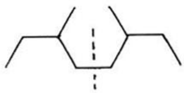
(T) tail  head (H)

The "head-to-tail" or regular linking is the most frequent one occurring in isoprenoid structures. Rubber has the following structural formula in which we can observe the "head-to-tail" concatenation of isoprene units.

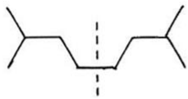


Other rules of concatenation are "head-to-head", "tail-to-head" and "tail-to-tail". For further needs we shall use the term <u>standard linking</u> to define all these four kinds of rules, which will be denoted HT, HH, TH, TT, respectively.

HT TH



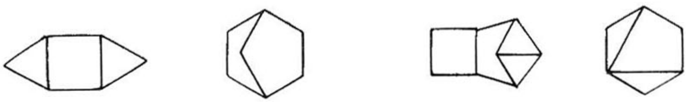
HH



TT

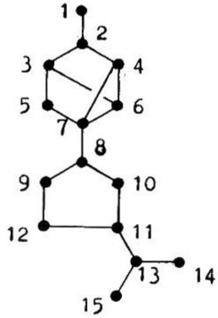
An acyclic isoprenoid graph with standard linking is an acyclic isoprenoid graph which has only standard linking in the concatenation of isoprene units. A cyclic isoprenoid graph with standard linking is a cyclic graph which admits at least one decomposition into an acyclic isoprenoid graph with standard linking.

By polycycle we define a group of circuits grafted on the same circuit; alternatively a polycycle may be viewed as a circuit having the property that it contains vertices joined by chains formed from vertices which do not belong to the circuit. Such a chain is called bridge. Examples of polycycles :



If two circuits, or two polycycles, or a circuit and a polycycle are joined by one single edge, we will call this edge an isthmus. A graph may or may have not isthmuses.

Example of graph having an isthmus (edge 7-8) :



If we have a program (an algorithm) for the recognition of acyclic standard isoprenoid structures, the cyclic problem may be reduced to an acyclic one by operating cuts into the cyclic structure in order to obtain a connected acyclic one. The number of cuts is equal to the cyclomatic number of the graph. For further needs we shall use the term <u>vertex of type A</u> to define a vertex through which at least one circuit passes.

The following <u>principles</u> are used to reduce the number of edges which must be examined for finding the cuts :

(i) we shall cut only the edges which join vertices of type A, excepting isthmus-type edges

(ii) the <u>reduced degree</u> of a vertex x of type A is defined as the number of lines which join the vertex x with other vertices of type A. We shall never cut twice around a vertex of type A with reduced degree two, three times around a vertex of type A with reduced degree three etc.

If these principles are not respected, disconnected graphs are obtained.

The steps (on which the recognition of standard isoprenoid structures are based) are :

1. If the graph of the given structure is acyclic, we apply directly the algorithm for recognition of the acyclic standard isoprenoid structures which will indicate whether the given structure is or is not, of the required type;
2. If the graph is cyclic :
   - 2.1. We determine the minimal circuits (whose number is equal to the cyclomatic number of the graph) which have to be cut. These circuits must contain all the lines which join vertices of type A, excepting isthmuses.
   - 2.2. We perform a cut into each circuit determined at the stage 2.1, taking care to respect principle (ii) and not to cut the same line in different circuits. This step will be applied many times in order to obtain all the possible combinations of such cuts.
   - 2.3. We perform the cuts indicated by each combination determined at 2.2., calling each time the algorithm for the recognition of acyclic standard isoprenoid structures. If, at least one application of this algorithm ends successfully, the given structure is a cyclic standard isoprenoid one. We also obtain its

decomposition into isoprene subunits. Otherwise, the given structure is not of the required type.

4. The FORTRAN-IV program for the recognition of standard isoprenoid structures with N carbon atoms where N is congruent to 0 modulo 5

Let be a graph with N vertices. We number its points in an arbitrary order if the graph is cyclic; if it is acyclic, the arbitrary labelling of the vertices remains valid, excepting label 1, which will be ascribed to any vertex having the degree 1. We construct the adjacency matrix MAD of the NxN type, of the given graph. The binary vector M whose length is N will specify which vertices are of type A, in the following way :

M(I) = 1, if the vertex I is of type A

M(I) = 0, otherwise

The vector MS of N1 length(where N1 is an even number) will determine the isthmuses of the graph (if they exist) indicating the pairs of vertices, which they connect, and it will be filled with zeros in case we do not have any isthmus in the graph. The order of the two endpoints of an isthmus is arbitrary. The elements N, MAD, M, N1, MS together with N3, N4, N5 which are the dimensions of working matrices and vectors, represent the input data of the program. The program includes a main program and three subroutines.

The main program verifies whether the given graph is cyclic (or acyclic) by studying the existence (or the nonexistence) of the elements equal to 1 in the input vector M. If the graph is acyclic we will construct the LS and LD vectors using the adjacency matrix MAD. Considering as starting point along the graph the vertex labelled 1, we will call the subroutine SCIA for the recognition of the acyclic standard isoprenoid structures, afterwords going to STOP. The acyclic structure (obtained by performing μ cuts in the given structure) is written as a planted out-tree (with the root being the endpoint labelled 1). Unlike the usual convention is which the plant grows upwards, the planted out-tree is written downwards). See, in this respect, Harary[4]. The LS and LD vectors will have each the length N and will contain the left linking, respectively the right one of each vertex. Constructing these vectors, which were filled with zeros, we will use the working vector B3 of length N and the following convention : if one vertex has one linking only (taking into account the direction in which we pass along the graph) it will be considered as left linking. If we have a cyclic graph we identify to zero each element of the N3 x N4 working matrix P and call the subroutine CIRCUITS. This subroutine provides the number of minimal circuits equal to the cyclomatic number of the graph, containing all the edges of the structure which join vertices of type A, excepting isthmuses. If this subroutine stops at an error message ME which has a different value than zero, the program goes to STOP. Otherwise, the program goes on calling subroutine COMB that will generate all the combinations of possible cuts in the circuits provided by the subroutine CIRCUITS, taking into account those specified in the stage

2.2. We test the value of ME again and in case this value is different from zero we go to STOP. To accomplish stage 2.3., i.e. to operate the cuts indicated by the combinations given by the subroutine COMB it is necessary to introduce the matrix MAD for each combination, in the working matrix P and the vector DG of the degrees of the vertices provided by CIRCUITS in the working vector B4 of length N. We will take into account the fact that cutting the edge determined by vertices I and J means to identify to zero the elements P(I, J) and P(J, I) and diminishing with one unit the degrees of these vertices in B4. Thus we will obtain an acyclic structure. Two of the necessary conditions for this acyclic structure to be of the required type are : the number NG1 of vertices with degree 1 must be equal to N/5 + 2 and the number NG3 of the vertices with degree 3 must be equal to N/5. These conditions result from the way the isoprene units are joined and from the fact that every isoprene unit contains one vertex with degree 3. If the first condition is not fulfilled, on the listing the error message ME = 22 appears; if the second condition is not fulfilled, the error message 23 appears. Otherwise we verify whether the vertex labelled 1 is of degree one. If this condition is not observed we will look for a vertex of degree one and we will change the labels between these two points taking into account the observation (ii) from § 1. We construct the LS and LD vectors as shown above and call the subroutine SCIA. The counter ND (equal to zero in the beginning) is increased by one unit after each successful (ME = 0) calling of the subroutine SCIA.

All these operations are to be done for each combination given by COMB, after which the normal ending of the program takes place. In the end, the value of the counter ND will be listed and will indicate the number of decompositions of the cyclic structure into an acyclic standard isoprenoid structure. The forced ending of the program determined by values different from zero of the error message ME, indicates impossible cases that result by wrongly constructing the input data.

The subroutine SCIA recognizes the acyclic standard isoprenoid structures and indicates the number of linkings of each type (HT, TH, HH, TT) as well as the edges that have to be cut in the acyclic structure in order to obtain the decomposition of the graph into the basic isoprene units. The search of subroutine SCIA ends successfully if on the listing appears the message "THE GIVEN STRUCTURE IS OF THE REQUIRED TYPE", while in the case of failure on the listing appears the message "THE GIVEN STRUCTURE IS NOT OF THE REQUIRED TYPE" followed by a value different from zero of the error label, ME, which is helpful in finding what condition was not fulfilled by the given structure to be of the required type. The subroutine has as input data the LS, LD vectors and the number N of the vertices of the graph, and as output data the variable ME which indicates the value of the error label. The vectors T(N), PR(N) and L(6) are working vectors of the subroutine. The variables NT, HT, TH, HH, TT indicate respectively the number of terminal vertices of the acyclic graph (which is regarded in the subroutine SCIA as a tree with its root labelled 1), the number of linkings of the HT, TH, HH, TT, type. Subroutine SCIA works in the following steps :

I. It calculates the number of terminal vertices NT and these vertices are introduced into the first NT positions of the T vector.

II. It constructs the PR vector which will contain the predecessors of the vertices. Convention : the predecessor of the vertex labelled 1 is denoted by zero.

III. Initially the variables HT, TH, HH and TT, the vacant positions of the T vector and all the positions of the L vector are assigned zero values.

IV. The T vector is run along taking each time two non-zero elements I and J which must fulfil one of the following conditions if the structure is of the required type :

(i) PR(T(I)) = PR(T(J))

(ii) PR(PR(T(I)) = PR(T(J))

(iii) PR(T(I)) = PR(PR(T(J))

In case (i), the predecessor of the terminal vertex T(I) is introduced into the first position of the working vector L (in cases (ii) and (iii) in the first position of L will be written the predecessor of the vertex T(J), respectively T(I)), into the next position of the L vector will be introduced the predecessor of the vertex situated in L one place behind it and so on till we have introduced either the root or a vertex having degree 3. If we meet the root and if we are in case (i), then the value K2 = K-1, where K represents the number of nonzero elements from L, must be two (for the cases (ii) and (iii) K2 must be 1). Elements T(I) and T(J) are assigned zero thus indicating that these vertices have been already studied and the step is resumed till the vector T becomes zero. If we meet a vertex having degree 3 we can have the following two possibilities : if K2 = 4 and if we are in cases (i) ((ii) or (iii)) then the number of linkings of the HT (TH) type increases with one unit; if K2 = 5 and if we are in the case (i) (K2 = 3 if we are in (ii) or (iii)) the value of TT(HH) linkings increases with one unit. The edge that must be cut in order to decompose the graph is that which joins points L(4) and L(3) in case (i) and that which joins L(3) and L(2) in cases (ii) or (iii). The counter NT increases with one and L(4) for case (i) (or L(3) for the other two cases) is introduced into the NT position of the vector T, while T(I) and T(J) are assigned zero, indicating the fact that these vertices have been studied. The process goes on resuming the same step till all the T vector's components are zero.

It is observed that because of the standard linking, in an acyclic isoprenoid structure the length between the root and the first vertex with degree 3, may be equal to 1 or 2, and the distance between two consecutive vertices with degree 3 is 3, 4 or 5. This motivates the choice of the dimension of the working vector L.

Subroutine CIRCUITS determines a number of distinct minimal circuits (equal to the cyclomatic number of the graph) whose edges cover the set of lines which join vertices of type A. The subroutine uses as input data the elements MAD, M, MS, P, N, N1, N3, N4 and supply for the main program the following elements : NCICL - the cyclomatic number of the graph, DG - the vector of degrees of vertices, D - a vector which contains the degrees of the vertices for all vertices which are not of type A, and the reduced degrees for those of type A, B - the matrix of the N3 x N4 type which contains in the first NCICL - rows the circuits which will be taken into consideration the remaining values being zero, the first element of each nonzero line indicates the number of the vertices which compose the circuits which is represented beginning with the second column, ME - the value of the error label; if this value is nonzero it determines the stopping of the main program and it may thus be used to detect the place that imposed the unnatural stopping of the program. The subroutine CIRCUITS uses the A working matrix of 5 x N type and the vector B1 of length N both of, which are initially assigned zero. The steps performed by subroutine CIRCUITS are :

I. It determines the number KC of the vertices of type A and builds the matrix A which will contain the vertices of type A on the first KC positions of the first line. The column of each such vertex contains all the vertices of type A joined by a line to the studied vertex. We have chosen the dimension 5 for the number of rows of matrix A because the highest degree is 4 for any vertex of such structure.

II. It calculates vectors DG and D whose components have been discussed, and determines the cyclomatic number NCICL.

III. It determines the circuit of minimal length which starts from each vertex situated on the first row of matrix A. If there are more than one distinct circuit of minimal length, all of them will be taken into consideration. This (these) will be transcribed in matrix B indicating (in the first position of each row which will be occupied by the vertices determining the circuit) the number of vertices which formed the circuit. Identical circuits are eliminated.

IV. If the number of circuits determined at the end of step III is equal to NCICL, then the subroutine ends by listing matrix B which will contain the circuits that will be taken into account. Otherwise, the distinct minimal circuits are pointed in the increasing order of their lengths; the first NCICL - circuits whose lines contain all the edges of the given structure which join vertices of type A will be taken into consideration.

Subroutine COMB generates all the combinations of lines which determine by cutting, the reduction of the cyclic structure into an acyclic one, making possible the application of the algorithm for recognition of the acyclic standard isoprenoid structures, i.e. the subroutine SCIA. Principles (i) and (ii) discussed above will be respected. The lines considered by subroutine COMB are those which appear in the circuits supplied by matrix B, one of the output data of the subroutine

CIRCUITS. The subroutine COMB uses as input data matrix B, vector D, as well as the elements N, N2, N4, N5, NCICL where N2 is equal to 2 x NCICL and represents the number of columns of matrix MT obtained as output data of subroutine COMB, while N5 is the number of rows of the same matrix. Each row represents a number of NCICL - distinct lines chosen one from each circuit that exists in the input data B. The choice of N2 is justified by the fact that any edge is represented by means of the two vertices which determine it. The working vectors B1 of length N and B2 (of length NCICL) are used. Initially B1 contains the values of vector D, while vector B2 is assigned component values 2. In the subroutine COMB, the element B2(I) will indicate up to which position from row I of matrix B the vertices have been taken into account. Variables T1 and T2 are counters for the number of rows and columns respectively of matrix MT, determination of all required combinations of lines take place as follows : one takes the first line from the first circuit, then the first line from the second circuit different from that already chosen and which respects principle (ii) (in this testing one takes into consideration that after each choice of an edge the degrees of the vertices incident with it diminish with one unit), and the process goes on until we reach the last circuit. Each time one indicates into vector B2 the position reached on the edges from each circuit. For each edge which observes the principle (ii) and is different from the first (NCICL-1)-edges, one obtains a combination of lines. By cutting, each of these combinations will give a connected acyclic structure. The process goes on preserving unchanged the first (NCICL-2)-edges already chosen and taking the following edge from the last but one circuit, observing thereby the mentioned conditions. Then, the last circuit is run along again, etc. We take care to assign B2(I) values 2 each time the circuit I was crossed to the last vertex. Whenever a new edge from the first circuit is taken into account, we redefine the vector B1 as vector D and the vector B2 as vector with all components equal to 2.

Comments. The present paper presents an algorithm for recognizing standard isoprenoid structures, using the reduction of cyclic graphs to the case of acyclic graphs (which were studied earlier with a more severe restriction, i.e. regular, not standard, linking). The advantage of this program consists in the fact that it can be applied to arbitrarily large structures and with an unlimited number of circuits unlike Kornprobst's program which imposed restrictions on the number of vertices (structures with more than 30 vertices were not allowed) and on the number of circuits (the structure could not have more than 5 circuits). The only restrictions of our program are those connected with the mode of concatenation of isoprene units, only standard linking being admitted. The program continues after a solution is being found, descovering thus all possible decompositions into acyclic standard isoprenoid structures, which are then tested. If an acyclic structure is isoprenoid, its decomposition is unique.

R E F E R E N C E S

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3. R. Jacquier and J.-M. Kornprobst, Math.Chem., 4, 93 (1978).

4. F. Harary, "Graph Theory", Addison-Wesley, Reading, Massachusetts, 1969, p. 201.

A P P E N D I C E S

The three appendices which follow are : the listing of the program, and (in smaller print) two computer outputs for two examples, whose formulas are given at the start of each example. Both examples are of isoprenoid structures, and the program finds that they are so, as well as the possible decompositions into isoprene units.

Appendix 1

```
* DEFINE FILE *1=1,*2=3
      IMPLICIT INTEGER (A-Z)
       DIMENSION D(15),B(20,15)
      DIMENSION MAD(15,15),M(15),MS(6),LS(15),LD(15),P(20,15),MT(200,8),
     *DG(15),B3(15),B4(15)
      READ(1,110)N,N3,N4,N5,((MAD(I,J),J=1,N),I=1,N),N1,(MS(I),I=1,N1),(
     *M(I),I=1,N)
  110 FORMAT(4I3,15(/15I1)/I2,6I1/15I1)
      WRITE(3,111)((MAD(I,J),J=1,N),I=1,N),(M(I),I=1,N),(MS(I),I=1,N1)
  111 FORMAT(40X,'THE ADJACENCY MATRIX'/40X,20('*')//15(30X,15I3/)/10X,'
     *VERTICES THROUGH WHICH CIRCUITS PASS',15I3//10X,'VERTICES WHICH DE
     *TERMINE ISTHMUSES',6I3//)
      ND=0
      DO 2 I=1,N
      IF(M(I).NE.0)GO TO 3
    2 CONTINUE
      DO 1 I=1,N
      LS(I)=0
      LD(I)=0
      B3(I)=0
    1 CONTINUE
      I1=0
      I2=0
      I=1
   20 S=0
      DO 4 J=1,N
      IF(MAD(I,J).NE.1)GO TO 4
      S=S+1
      IF(S.EQ.1)GO TO 5
      IF(S.EQ.2)GO TO 6
      ME=18
      GO TO 50
    5 LS(I)=J
      MAD(J,I)=0
      I1=I1+1
      B3(I1)=J
      GO TO 4
    6 LD(I)=J
      MAD(J,I)=0
      I1=I1+1
      B3(I1)=J
    4 CONTINUE
      I2=I2+1
      I=B3(I2)
      IF(I.NE.0)GO TO 20
      CALL SCIA(LS,LD,N,ME)
      GO TO 51
```

```
    3 DO 7 I=1,N3
      DO 7 J=1,N4
      P(I,J)=0
    7 CONTINUE
      CALL CIRCUITS(MAD,M,MS,P,D,DG,B,N,N1,N3,N4,NCICL,ME)
      IF(ME.NE.0)GO TO 51
      N2=2*NCICL
      CALL COMB(B,D,MT,N,N2,N5,NCICL)
      DO 8 I=1,N5
      IF(MT(I,1).EQ.0)GO TO 55
      WRITE(3,112)(MT(I,J1),J1=1,N2)
  112 FORMAT(//10X,'WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLI
     *C ONE OPERATING THE FOLLOWING CUTS',4(2X,I2,'-',I2))
      DO 21 I1=1,N
      B4(I1)=DG(I1)
   21 CONTINUE
      DO 22 J=1,N2,2
      B4(MT(I,J))=B4(MT(I,J))-1
      B4(MT(I,J+1))=B4(MT(I,J+1))-1
   22 CONTINUE
      NG1=0
      NG3=0
      DO 25 I1=1,N
      IF(B4(I1).EQ.1)GO TO 26
      IF(B4(I1).NE.3)GO TO 25
      NG3=NG3+1
      GO TO 25
   26 NG1=NG1+1
   25 CONTINUE
      IF(NG1-N/5-2)27,28,27
   27 ME=22
      WRITE(3,120)ME
  120 FORMAT(/25X,'THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE. E
     *RROR',I3/)
      GO TO 8
   28 IF(NG3-N/5)29,30,29
   29 ME=23
      WRITE(3,121)ME
  121 FORMAT(/25X,'THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE. E
     *RROR',I3/)
      GO TO 8
   30 DO 36 I1=1,N
      LS(I1)=0
      LD(I1)=0
      B3(I1)=0
   36 CONTINUE
      DO 9 I1=1,N
```

```
      DO 9 I2=1,N
      P(I1,I2)=MAD(I1,I2)
    9 CONTINUE
      DO 10 J=1,N2,2
      P(MT(I,J),MT(I,J+1))=0
      P(MT(I,J+1),MT(I,J))=0
   10 CONTINUE
      IF(B4(1).EQ.1)GO TO 11
      DO 12 I1=2,N
      IF(B4(I1).EQ.1)GO TO 13
   12 CONTINUE
      ME=20
      GO TO 50
   13 DO 14 I2=1,N
      P(N+1,I2)=P(I1,I2)
      P(I1,I2)=P(1,I2)
      P(1,I2)=P(N+1,I2)
   14 CONTINUE
      DO 15 I2=1,N
      P(N+1,I2)=P(I2,I1)
      P(I2,I1)=P(I2,1)
      P(I2,1)=P(N+1,I2)
   15 CONTINUE
      WRITE(3,116)I1
  116 FORMAT(/20X,'IN THE OBTAINED ACYCLIC STRUCTURE LABEL 1 IS ASSIGNED
     * TO',I3,'AND VICE VERSA'/)
   11 I3=0
      I5=0
      I4=1
   19 S=0
      DO 16 I2=1,N
      IF(P(I4,I2).NE.1)GO TO 16
      S=S+1
      IF(S.EQ.1)GO TO 17
      IF(S.EQ.2)GO TO 18
      ME=21
      GO TO 50
   17 LS(I4)=I2
      P(I2,I4)=0
      I3=I3+1
      B3(I3)=I2
      GO TO 16
   18 LD(I4)=I2
      P(I2,I4)=0
      I3=I3+1
      B3(I3)=I2
   16 CONTINUE
```

```
      I5=I5+1
      I4=B3(I5)
      IF(I4.NE.0)GO TO 19
      CALL SCIA(LS,LD,N,ME)
      IF(ME.NE.0)GO TO 8
      ND=ND+1
    8 CONTINUE
   53 IF(ND.EQ.0)GO TO 52
      WRITE(3,114)ND
  114 FORMAT(//20X,'THE GIVEN STRUCTURE IS A CYCLIC ISOPRENOID STRUCTUR
     *E WITH STANDARD LINKING'/20X,'THE NUMBER OF THE VIABLE DECOMPOSITI
     *ONS',I4)
      GO TO 51
   52 WRITE(3,115)
  115 FORMAT(//20X,'THE GIVEN STRUCTURE IS NOT OF THE REQUIRED TYPE')
      GO TO 51
   50 WRITE(3,113)ME
  113 FORMAT(20X,'ERROR',I5)
   51 STOP
      END
```

```
      SUBROUTINE CIRCUITS(MAD,M,MS,P,D,DG,B,N,N1,N3,N4,NCICL,ME)
      IMPLICIT INTEGER (A-Z)
      DIMENSION MAD(15,15),M(15),MS(6),P(20,15),A(5,15),D(15),DG(15),B(2
     *0,15),B1(15)
      ME=0
      DO 200 I=1,5
      DO 200 J=1,N
      A(I,J)=0
  200 CONTINUE
      DO 201 I=1,N
      D(I)=0
      B1(I)=0
  201 CONTINUE
      DO 202 I=1,N3
      DO 202 J=1,N4
      B(I,J)=0
      P(I,J)=0
  202 CONTINUE
      NS=0
      DO 1 I=1,N1
      IF(MS(I).EQ.0)GO TO 1
      NS=NS+1
    1 CONTINUE
      IF(NS.NE.0)GO TO 2
      M1=0
      GO TO 3
    2 M1=1
    3 KC=0
      DO 7 I=1,N
      KL=0
      IF(M(I).NE.1)GO TO 13
      KC=KC+1
      KL=KL+1
      A(KL,KC)=I
      DO 8 J=1,N
      IF(MAD(I,J).NE.1.OR.M(J).NE.1)GO TO 8
      IF(M1.EQ.0)GO TO 9
      DO 10 J1=1,NS.2
      J2=J1+1
      IF(MS(J1).EQ.I.AND.MS(J2).EQ.J)GO TO 8
      IF(MS(J1).EQ.J.AND.MS(J2).EQ.I)GO TO 8
   10 CONTINUE
    9 KL=KL+1
      A(KL,KC)=J
    8 CONTINUE
      D(I)=KL-1
   13 DG(I)=0
```

```
      DO 11 K=1,N
      IF(MAD(I,K).EQ.0)GO TO 11
      DG(I)=DG(I)+1
   11 CONTINUE
    7 CONTINUE
      WRITE(3,113)(DG(I),I=1,N),(D(I),I=1,N),((A(I,J),J=1,N),I=1,5)
  113 FORMAT(10X,'THE DEGREES OF THE VERTICES',15I3//10X,'VECTOR D',15I3
     *//50X,'MATRIX A'/50X,8('*')//5(30X,15I3/)//)
      NM=0
      DO 12 I=1,N
      NM=NM+DG(I)
   12 CONTINUE
      NCICL=NM/2-N+1
      WRITE(3,114)NCICL
  114 FORMAT(10X,'THE CYCLOMATIC NUMBER',I5///)
      M2=0
      M3=0
      M4=0
      M7=0
      DO 14 I=1,KC
      M4=M2+1
      DO 15 J=2,5
      IF(A(J,I).EQ.0)GO TO 15
      J2=A(J,I)
      K1=1
      K2=1
      F2=K1
      Z=0
      P(K1,1)=1
      K2=K2+1
      P(K1,K2)=A(1,I)
      K2=K2+1
      P(K1,K2)=J2
      P(K1,1)=P(K1,1)+1
   16 DO 17 J1=1,KC
      IF(A(1,J1).EQ.J2)GO TO 18
   17 CONTINUE
      ME=1
      GO TO 501
   18 IF(D(J2).NE.2)GO TO 19
      P1=K2-1
      DO 20 K=2,5
      IF(A(K,J1).EQ.A(1,I).AND.A(K,J1).NE.P(K1,P1))GO TO 22
      IF(A(K,J1).NE.P(K1,P1))GO TO 6
   20 CONTINUE
      ME=3
      GO TO 501
```

```
    6 K2=K2+1
      P(K1,K2)=A(K,J1)
      P(K1,1)=P(K1,1)+1
      GO TO 256
   19 DJ2=D(J2)+1
      P1=K2-1
      DO 21 K=2,DJ2
      IF(A(K,J1).EQ.A(1,I).AND.A(K,J1).NE.P(K1,P1))GO TO 22
   21 CONTINUE
      F1=F2+1
      F2=F2+D(J2)-2
      DO 23 I5=F1,F2
      DO 23 I6=1,K2
      P(I5,I6)=P(K1,I6)
   23 CONTINUE
      I5=K1
      T=0
      P1=P(K1,K2-1)
      DO 24 I6=2,DJ2
      IF(A(I6,J1).EQ.P1)GO TO 24
      T=T+1
      IF(P(I5,1).LT.4)GO TO 25
      K3=P(I5,1)-1
      DO 26 I7=3,K3
      IF(MOD(A(I6,J1)-P(I5,I7)),EQ,1)GO TO 27
   26 CONTINUE
   25 P(I5,1)=P(I5,1)+1
      P(I5,P(I5,1)+1)=A(I6,J1)
      I5=F1+T-1
      GO TO 24
   27 I9=P(I5,1)+1
      DO 28 I8=1,I9
   28 P(I5,I8)=0
      I5=F1+T-1
   24 CONTINUE
      IF(P(K1,1).NE.0)GO TO 251
      GO TO 255
   22 M3=M3+1
      DO 29 I4=1,K2
      B(M3,I4)=P(K1,I4)
      P(K1,I4)=0
   29 CONTINUE
      B(M3,1)=B(M3,1)+1
      B(M3,K2+1)=B(M3,2)
  255 IF(K1.EQ.F2)GO TO 32
      F5=K1+1
      DO 30 I5=F5,F2
```

```
      IF(P(I3,1).NE.0)GO TO 31
 30   CONTINUE
      GO TO 32
 31   K1=I3
 251  K2=P(K1,1)+1
 256  J2=P(K1,K2)
      IF(P(K1,1).LT.4)GO TO 16
      K11=P(K1,1)-1
      DO 252 I10=3,K11
      IF(MAD(J2,P(K1,I10)).EQ.1)GO TO 253
 252  CONTINUE
      GO TO 16
 253  DO 254 I11=1,K2
      P(K1,I11)=0
 254  CONTINUE
      GO TO 255
 32   M6=M3-M2
      IF(M6.LT.2)GO TO 33
      M5=B(M4,1)
      M41=M4+1
      DO 34 I4=M41,M3
      M5=MINO(M5,B(I4,1))
 34   CONTINUE
      DO 35 I4=M4,M3
      IF(B(I4,1).NE.M5)GO TO 36
      Z=Z+1
      B1(Z)=I4
      GO TO 35
 36   DO 37 I5=1,N
      B(I4,I5)=0
 37   CONTINUE
 35   CONTINUE
      IF(Z.EQ.M6) GO TO 4
      DO 38 I4=M4,M3
      IF(B(I4,1).EQ.0)GO TO 39
      DO 40 I5=1,Z
      IF(B1(I5).NE.I4)GO TO 40
      B1(I5)=0
      GO TO 38
 40   CONTINUE
      GO TO 38
 39   DO 41 I5=1,Z
      IF(B1(I5).EQ.0)GO TO 41
      M51=M5+1
      DO 42 I6=1,M51
      B(I4,I6)=B(B1(I5),I6)
      B(B1(I5),I6)=0
```

```
42 CONTINUE
   B1(I5)=0
   GO TO 38
41 CONTINUE
   GO TO 43
38 CONTINUE
   GO TO 43
 4 DO 5 I4=1,Z
   B1(I4)=0
 5 CONTINUE
   GO TO 43
33 Z=1
43 M3=M7+Z
15 CONTINUE
   IF(Z.EQ.1)GO TO 44
   M4Z=M4+Z-2
   DO 45 I5=M4,M4Z
   IF(B(I5,1).EQ.0)GO TO 45
   I51=I5+1
   M41=M4+Z-1
   DO 46 I6=I51,M41
   IF(B(I6,1).EQ.0)GO TO 46
   DO 47 I7=3,M5
   DO 48 I8=3,M5
   IF(B(I5,I7).NE.B(I6,I8))GO TO 48
   GO TO 47
48 CONTINUE
   GO TO 46
47 CONTINUE
   M51=M5+1
   DO 49 I9=1,M51
49 B(I6,I9)=0
46 CONTINUE
45 CONTINUE
   L1=0
   DO 50 I5=M4,M41
   IF(B(I5,1).EQ.0)GO TO 51
   L1=L1+1
   B1(L1)=I5
   GO TO 50
51 Z=Z-1
50 CONTINUE
   DO 52 I4=M4,M3
   IF(B(I4,1).EQ.0)GO TO 53
   DO 54 I5=1,L1
   IF(B1(I5).NE.I4)GO TO 54
   B1(I5)=0
```

```
      GO TO 52
54    CONTINUE
      GO TO 52
53    DO 55 I5=1,L1
      IF(B1(I5).EQ.0)GO TO 55
      M51=M5+1
      DO 56 I6=1,M51
      B(I4,I6)=B(B1(I5),I6)
      B(B1(I5),I6)=0
      B1(I5)=0
56    CONTINUE
      GO TO 52
55    CONTINUE
      GO TO 44
52    CONTINUE
44    M2=M2+Z
      M7=M7+Z
      M3=M4+Z-1
14    CONTINUE
      T=0
      DO 57 K=1,N
      IF(B(K,1).EQ.0)GO TO 57
      T=T+1
57    CONTINUE
      IF(T.EQ.NCICL)GO TO 500
      T2=T-1
      DO 58 I=1,T2
      IF(B(I,1).EQ.0)GO TO 58
      IS=I+1
      DO 59 J=IS,T
      IF(B(I,1).NE.B(J,1))GO TO 59
      IV=B(I,1)
      DO 60 I1=2,IV
      DO 61 J1=2,IV
      IF(B(I,I1).NE.B(J,J1))GO TO 61
      GO TO 60
61    CONTINUE
      GO TO 59
60    CONTINUE
      IV1=B(I,1)+1
      DO 62 K=1,IV1
      B(J,K)=0
62    CONTINUE
59    CONTINUE
58    CONTINUE
      C=0
      T1=0
```

```
      DO 63 I=1,T
      IF(B(I,1).EQ.0)GO TO 63
      C=C+1
      B1(C)=I
 63   CONTINUE
      WRITE(3,119)C
119   FORMAT(10X,'THE NUMBER OF DISTINCT MINIMAL CIRCUITS',I5//)
      DO 64 J=1,T
      IF(B(J,1).EQ.0)GO TO 65
      DO 66 K=1,C
      IF(B1(K).NE.J)GO TO 66
      B1(K)=0
      T1=T1+1
      GO TO 64
 66   CONTINUE
      GO TO 64
 65   DO 67 I=1,C
      IF(B1(I).EQ.0)GO TO 67
      U=B(B1(I),1)+1
      DO 68 L=1,U
      B(J,L)=B(B1(I),L)
      B(B1(I),L)=0
 68   CONTINUE
      B1(I)=0
      T1=T1+1
      GO TO 69
 67   CONTINUE
 69   IF(T1.EQ.C)GO TO 70
 64   CONTINUE
 70   WRITE(3,125)((B(E,F),F=1,15),E=1,20)
125   FORMAT(50X,'THE DISTINCT MINIMAL CIRCUITS'/50X,29('*')//20(41X,15I
     *2//)//)
      IF(C.EQ.NCICL)GO TO 500
      D1=0
 78   K=0
      R=D1+1
      M5=B(R,1)
      R1=R+1
      DO 71 I=R1,C
      M5=MIN0(M5,B(I,1))
 71   CONTINUE
      DO 72 I=R,C
      IF(B(I,1).NE.M5)GO TO 72
      K=K+1
 72   CONTINUE
      S=0
      C1=C-1
```

```
      DO 73 J=K,C1
      IF(B(J,1).NE.M5)GO TO 250
      S=S+1
      GO TO 73
250   J1=J+1
      DO 74 L=J1,C
      IF(B(L,1).NE.M5)GO TO 74
      S=S+1
      E=B(J,1)+1
      DO 75 I=1,E
      B(C+1,I)=B(J,I)
      B(J,I)=B(L,I)
      B(L,I)=B(C+1,I)
      B(C+1,I)=0
75    CONTINUE
      IF(S.EQ.K)GO TO 76
74    CONTINUE
73    CONTINUE
76    D1=D1+K
      IF(D1.EQ.C)GO TO 77
      GO TO 78
77    WRITE(3,126)((B(E,F),F=1,15),E=1,20)
126   FORMAT(20X,'THE DISTINCT MINIMAL CIRCUITS ORDERED INCREASINGLY BY
     *THEIR LENGTHS'/20X,67('*')//20(39X,15I2/)//)
      DO 79 I=1,N
      DO 79 J=1,N
      P(I,J)=MAD(I,J)
79    CONTINUE
      I=1
90    NI=I+NCICL-2
      DO 80 K=I,NI
      F=B(K,1)
      DO 81 K1=2,F
      P(B(K,K1),B(K,K1+1))=0
      P(B(K,K1+1),B(K,K1))=0
81    CONTINUE
80    CONTINUE
      SI=I+NCICL-1
      DO 82 J=SI,C
      H=B(J,1)
      DO 83 J1=2,H
      P(B(J,J1),B(J,J1+1))=0
      P(B(J,J1+1),B(J,J1))=0
83    CONTINUE
      IF(M1.NE.0)GO TO 127
      DO 84 J2=1,N
      IF(M(J2).NE.1)GO TO 84
```

```
      DO 85 J3=1,N
      IF(M(J3).NE.1)GO TO 85
      IF(P(J2,J3).NE.0.OR.P(J3,J2).NE.0)GO TO 82
   85 CONTINUE
   84 CONTINUE
      GO TO 130
  127 DO 128 J2=1,N
      IF(M(J2).NE.1)GO TO 128
      DO 129 J3=1,N
      IF(M(J3).NE.1)GO TO 129
      DO 131 J4=1,NS,2
      J5=J4+1
      IF(MS(J4).EQ.J2.AND.MS(J5).EQ.J3.OR.MS(J4).EQ.J3.AND.MS(J5).EQ.J2)
     *GO TO 129
  131 CONTINUE
      IF(P(J2,J3).NE.0.OR.P(J3,J2).NE.0)GO TO 82
  129 CONTINUE
  128 CONTINUE
  130 GO TO 88
   82 CONTINUE
      H1=C-NCICL+1
      IF(I.EQ.H1)GO TO 89
      I=I+1
      GO TO 90
   89 ME=2
      GO TO 301
   88 IF(I.EQ.1)GO TO 91
      I1=I
      H2=NCICL-1
      DO 92 K=1,H2
      DO 93 L=1,N
   93 B(K,L)=B(I1,L)
      I1=I1+1
      H3=I+NCICL-2
      IF(I1.GT.H3)GO TO 91
   92 CONTINUE
   91 IF(J.EQ.NCICL)GO TO 94
      DO 95 L=1,N
   95 B(NCICL,L)=B(J,L)
   94 H4=NCICL+1
      DO 96 L1=H4,C
      DO 97 L=1,N
      B(L1,L)=0
   97 CONTINUE
   96 CONTINUE
  300 WRITE(3,121)((B(I,J),J=1,15),I=1,20)
  121 FORMAT(40X,'THE CIRCUITS OF THE STRUCTURE WHICH WILL BE TAKEN INTO
```

```
     * CONSIDERATION'/40X,68('*')//20(5nX,15I2////)
       GO TO 302
 301   WRITE(3,122)ME
 122   FORMAT(10X,'ERROR',I3)
 302   RETURN
       END



       SUBROUTINE COMB(B,D,MT,N,N2,N5,NCICL)
       IMPLICIT INTEGER (A-Z)
       DIMENSION B(20,15),D(15),MT(200,8),B1(15),B2(15)
       DO 1 I=1,N2
       DO 1 J=1,N5
       MT(J,I)=0
   1   CONTINUE
       DO 2 I=1,N
       B2(I)=2
       B1(I)=D(I)
   2   CONTINUE
       T1=0
       T3=2*(NCICL-1)
       I1=B(1,1)
       DO 3 I=2,I1
       T1=T1+1
       T2=1
       MT(T1,T2)=B(1,I)
       T2=T2+1
       MT(T1,T2)=B(1,I+1)
       B1(B(1,I))=B1(B(1,I))-1
       B1(B(1,I+1))=B1(B(1,I+1))-1
```

```
      J=2
      IF(J.EQ.NCICL)GO TO 8
    5 L=B2(J)
      J1=B(J,1)
      DO 4 K=L,J1
      K1=K+1
      IF(B1(B(J,K)).EQ.1.OR.B1(B(J,K1)).EQ.1)GO TO 4
      DO 6 K2=1,T2,2
      IF(MT(T1,K2).EQ.B(J,K).AND.MT(T1,K2+1).EQ.B(J,K1))GO TO 4
      IF(MT(T1,K2).EQ.B(J,K1).AND.MT(T1,K2+1).EQ.B(J,K))GO TO 4
    6 CONTINUE
      GO TO 7
    4 CONTINUE
      IF(J.EQ.2)GO TO 21
   23 J=J-1
      J3=B(J,1)+1
      IF(B2(J).NE.J3)GO TO 22
      IF(J.EQ.2)GO TO 21
      B2(J)=2
      GO TO 23
   22 T2=2*(J-1)
      GO TO 5
   21 T1=T1-1
      GO TO 10
    7 T2=T2+1
      MT(T1,T2)=B(J,K)
      T2=T2+1
      MT(T1,T2)=B(J,K1)
      B1(B(J,K))=B1(B(J,K))-1
      B1(B(J,K1))=B1(B(J,K1))-1
      B2(J)=K1
      J=J+1
      IF(J.EQ.NCICL)GO TO 8
      GO TO 5
    8 T3=2*(J-1)
      J2=B(J,1)
      DO 9 K3=2,J2
      K31=K3+1
      IF(B1(B(J,K3)).EQ.1.OR.B1(B(J,K31)).EQ.1)GO TO 9
      DO 10 K4=1,T2,2
      IF(MT(T1,K4).EQ.B(J,K3).AND.MT(T1,K4+1).EQ.B(J,K31))GO TO 9
      IF(MT(T1,K4).EQ.B(J,K31).AND.MT(T1,K4+1).EQ.B(J,K3))GO TO 9
```

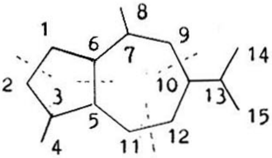
```
 10   CONTINUE
      T2=T2+1
      MT(T1,T2)=B(J,K3)
      T2=T2+1
      MT(T1,T2)=B(J,K31)
      WRITE(3,104)T1,(MT(T1,E),E=1,N2)
104   FORMAT(20X,I3,5X,8I3/)
      IF(K3.EQ.B(J,1))GO TO 11
      T1=T1+1
      DO 12 K4=1,T3
      MT(T1,K4)=MT(T1-1,K4)
 12   CONTINUE
 11   T2=T3
  9   CONTINUE
      IF(MT(T1,N2).NE.0)GO TO 13
      DO 20 K4=1,T3
      MT(T1,K4)=0
 20   CONTINUE
      T1=T1-1
 13   J=J-1
      IF(J.EQ.1)GO TO 16
      J3=B(J,1)+1
      IF(J.EQ.2.AND.B2(J).EQ.J3)GO TO 16
      IF(B2(J).NE.J3)GO TO 18
      B2(J)=2
      GO TO 15
 18   T1=T1+1
      T3=2*(J-1)
      DO 17 K5=1,T3
      MT(T1,K5)=MT(T1-1,K5)
 17   CONTINUE
      T31=T3+1
      DO 15 K6=T31,T2
      B1(MT(T1-1,K6))=B1(MT(T1-1,K6))+1
 15   CONTINUE
      T2=T3
      GO TO 5
 16   DO 19 K6=1,N
      B1(K6)=D(K6)
      B2(K6)=2
 19   CONTINUE
  3   CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SCIA(LS,LD,N,ME)
      IMPLICIT INTEGER (A-Z)
      DIMENSION LS(15),LD(15),PR(15),T(15),L(6)
      ME=0
      WRITE(3,102)(LS(I),I=1,N),(LD(I),I=1,N)
  102 FORMAT(30X,'PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES O
     *F THE OBTAINED STRUCTURE'/30X,78('-')///4X,76('*')/1X,'LS *',15(1X
     *,I2,1X,'*')/4X,76('*')/1X,'LD *',15(1X,I2,1X,'*')/4X,76('*'))
      N1=N/5
      NT=0
      DO 1 K=1,N
      IF(LS(K).NE.0.OR.LD(K).NE.0)GO TO 1
      NT=NT+1
      T(NT)=K
    1 CONTINUE
      DO 25 K=1,N
   25 PR(K)=0
      DO 26 I=2,N
      DO 27 J=1,N
      IF(LS(J).NE.I)GO TO 27
      PR(I)=J
      GO TO 26
   27 CONTINUE
      DO 28 K=1,N
      IF(LD(K).NE.I)GO TO 28
      PR(I)=K
      GO TO 26
   28 CONTINUE
      ME=3
      GO TO 50
   26 CONTINUE
      WRITE(3,108)(PR(I),I=1,N)
  108 FORMAT(1X,'PR *',15(1X,I2,1X,'*')/4X,76('*')////)
      WRITE(3,107)
  107 FORMAT(35X,'CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS
     *'/35X,54('-')//)
      HH=0
      HT=0
      TH=0
      TT=0
      N2=NT+1
      DO 5 K=N2,N
    5 T(K)=0
   15 DO 6 K=1,6
    6 L(K)=0
      N3=NT-1
      DO 7 I=1,N3
```

```
      I1=I+1
      DO 7 J=I1,NT
      IF(T(I).EQ.0.OR.T(J).EQ.0)GO TO 7
      IF(PR(T(I)).EQ.PR(T(J)))GO TO 8
      IF(PR(PR(T(I))).EQ.PR(T(J)))GO TO 9
      IF(PR(T(I)).EQ.PR(PR(T(J))))GO TO 16
    7 CONTINUE
      ME=4
      GO TO 50
    8 M1=1
      L(1)=PR(T(I))
      DO 10 K=2,6
      L(K)=PR(L(K-1))
      IF(PR(L(K)).EQ.0)GO TO 11
      IF(LS(L(K)).NE.0.AND.LD(L(K)).NE.0)GO TO 12
   10 CONTINUE
      ME=5
      GO TO 50
   12 K2=K-1
      IF(K2.EQ.4)GO TO 13
      IF(K2.NE.5)GO TO 52
      TT=TT+1
      WRITE(3,103)L(4),L(5)
  103 FORMAT(66X,2(I2,2X),'TT'/)
      GO TO 30
   13 HT=HT+1
      WRITE(3,109)L(4),L(5)
  109 FORMAT(66X,2(I2,2X),'HT'/)
   30 NT=NT+1
      T(NT)=L(4)
      T(I)=0
      T(J)=0
      GO TO 15
    9 L(1)=PR(T(J))
      GO TO 29
   16 L(1)=PR(T(I))
   29 M1=2
      DO 17 K=2,6
      L(K)=PR(L(K-1))
      IF(PR(L(K)).EQ.0)GO TO 11
      IF(LS(L(K)).NE.0.AND.LD(L(K)).NE.0)GO TO 18
   17 CONTINUE
      ME=7
      GO TO 50
   18 K2=K-1
      IF(K2.EQ.4)GO TO 19
      IF(K2.NE.3)GO TO 53
```

```
      HH=HH+1
      WRITE(3,104)L(3),L(2)
 104  FORMAT(66X,2(I2,2X),'HH'/)
      GO TO 31
  19  TH=TH+1
      WRITE(3,110)L(3),L(2)
 110  FORMAT(66X,2(I2,2X),'TH'/)
  31  NT=NT+1
      T(NT)=L(3)
      T(I)=0
      T(J)=0
      GO TO 15
  11  K2=K-1
      T(I)=0
      T(J)=0
      IF(K2.EQ.2.AND.M1.EQ.1.OR.K2.EQ.1.AND.M1.EQ.2)GO TO 21
      ME=9
      GO TO 50
  21  DO 22 K=1,NT
      IF(T(K).NE.0)GO TO 54
  22  CONTINUE
      WRITE(3,105)HH,HT,TH,TT
 105  FORMAT(15X,'THE OBTAINED STRUCTURE IS OF THE REQUIRED TYPE'/15X,46
     *('-')///15X,'THE NUMBER OF HH LINKINGS',I3//15X,'THE NUMBER OF HT
     *LINKINGS',I3//15X,'THE NUMBER OF TH LINKINGS',I3//15X,'THE NUMBER
     *OF TT LINKINGS',I3)
      GO TO 60
  52  ME=6
      GO TO 50
  53  ME=8
      GO TO 50
  54  ME=10
  50  WRITE(3,106)ME
 106  FORMAT(25X,'THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ER
     *ROR',I3)
  60  RETURN
      END
```

Appendix 2



THE ADJACENCY MATRIX

0	1	0	0	0	1	0	0	0	0	0	0	0	0	0
1	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	1	0	1	1	0	0	0	0	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0	0	1	0	0	1	0	0	0	0	1	0	0	0	0
1	0	0	0	1	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	1	0	1	1	0	0	0	0	0	0
0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	1	0	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	1	0	0	1	1	0	0
0	0	0	0	1	0	0	0	0	0	0	1	0	0	0
0	0	0	0	0	0	0	0	0	1	1	0	0	0	0
0	0	0	0	0	0	0	0	0	1	0	0	0	1	1
0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
0	0	0	0	0	0	0	0	0	0	0	0	1	0	0

VERTICES THROUGH WHICH CIRCUITS PASS 1 1 1 0 1 1 1 0 1 1 1 1 0 0 0

VERTICES WHICH DETERMINE ISTHMUSES 0 0 0 0 0 0

THE DEGREES OF THE VERTICES 2 2 3 1 3 3 3 1 2 3 2 2 3 1 1

VECTOR D 2 2 2 0 3 3 2 0 2 2 2 2 0 0 0

MATRIX A

1	2	3	5	6	7	9	10	11	12	0	0	0	0	0
2	1	2	3	1	6	7	9	5	10	0	0	0	0	0
6	3	5	6	5	9	10	12	12	11	0	0	0	0	0
0	0	0	11	7	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

THE CYCLOMATIC NUMBER 2

THE NUMBER OF DISTINCT MINIMAL CIRCUITS 2

THE DISTINCT MINIMAL CIRCUITS

6	1	2	3	5	6	1	0	0	0	0	0	0	0	0
8	7	6	5	11	12	10	9	7	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	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	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	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	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	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	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	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	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	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	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	0

THE CIRCUITS OF THE STRUCTURE WHICH WILL BE TAKEN INTO CONSIDERATION

6	1	2	3	5	6	1	0	0	0	0	0	0	0	0
8	7	6	5	11	12	10	9	7	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	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	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	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	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	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	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	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	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	0	0	0	0	0	0

1	1	2	7	6
2	1	2	6	5
3	1	2	5	11
4	1	2	11	12
5	1	2	12	10
6	1	2	10	9
7	1	2	9	7
8	2	3	7	6
9	2	3	6	5
10	2	3	5	11
11	2	3	11	12
12	2	3	12	10
13	2	3	10	9
14	2	3	9	7
15	3	5	7	6
16	3	5	6	5
17	3	5	5	11
18	3	5	11	12
19	3	5	12	10
20	3	5	10	9
21	3	5	9	7
22	5	6	7	6
23	5	6	5	11
24	5	6	11	12
25	5	6	12	10
26	5	6	10	9
27	5	6	9	7
28	6	1	7	6
29	6	1	6	5
30	6	1	5	11
31	6	1	11	12
32	6	1	12	10
33	6	1	10	9
34	6	1	9	7

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 1- 2 7- 6
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 1- 2 6- 5
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 1- 2 5-11
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 1- 2 11-12
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 1- 2 12-10
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 1- 2 10- 9
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 1- 2 9- 7
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 7- 6
IN THE OBTAINED ACYCLIC STRUCTURE LABEL 1 IS ASSIGNED TO 2AND VICE VERSA

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	6	4	0	3	5	8	0	7	9	12	10	14	0	0
LD	0	0	0	0	11	0	0	0	0	13	0	0	15	0	0
PR	0	1	5	3	6	2	9	7	10	12	5	11	10	13	13

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 6- 5

IN THE OBTAINED ACYCLIC STRUCTURE LABEL 1 IS ASSIGNED TO 2AND VICE VERSA

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	6	4	0	3	7	8	0	10	12	5	11	14	0	0
LD	0	0	0	0	0	0	9	0	0	13	0	0	15	0	0
PR	0	1	5	3	11	2	6	7	7	9	12	10	10	13	13

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 5-11

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 11-12

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 12-10

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 10- 9

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 9- 7

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 3- 3 7- 6

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 3- 3 6- 5

IN THE OBTAINED ACYCLIC STRUCTURE LABEL 1 IS ASSIGNED TO 4AND VICE VERSA

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	3	4	2	6	0	7	8	0	10	12	5	11	14	0	0
LD	0	0	0	0	0	0	9	0	0	13	0	0	15	0	0
PR	0	3	1	2	11	4	6	7	7	9	12	10	10	13	13

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   3- 5   5-11

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   3- 5   11-12

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   3- 5   14-10

IN THE OBTAINED ACYCLIC STRUCTURE LABEL 1 IS ASSIGNED TO 4AND VICE VERSA

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	3	4	2	6	11	5	8	0	10	13	12	0	14	0	0
LD	0	0	0	0	0	7	9	0	0	0	0	0	15	0	0
PR	0	3	1	2	6	4	6	7	7	9	5	11	10	13	13

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   3- 5   10- 9

IN THE OBTAINED ACYCLIC STRUCTURE LABEL 1 IS ASSIGNED TO 4AND VICE VERSA

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	3	4	2	6	11	5	8	0	0	13	12	10	14	0	0
LD	0	0	0	0	0	7	9	0	0	0	0	0	15	0	0
PR	0	3	1	2	6	4	6	7	7	12	5	11	10	13	13

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   3- 5   9- 7

IN THE OBTAINED ACYCLIC STRUCTURE LABEL 1 IS ASSIGNED TO 4AND VICE VERSA

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	3	4	2	6	11	5	8	0	0	9	12	10	14	0	0
LD	0	0	0	0	0	7	0	0	0	13	0	0	15	0	0
PR	0	3	1	2	6	4	6	7	10	12	5	11	10	13	13

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

11 12 TH

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 4

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   3- 6   7- 6

IN THE OBTAINED ACYCLIC STRUCTURE LABEL 1 IS ASSIGNED TO 4AND VICE VERSA

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	3	4	2	6	11	0	8	0	7	9	12	10	14	0	0
LD	0	0	5	0	0	0	0	0	0	13	0	0	15	0	0
PR	0	3	1	2	3	4	9	7	10	12	5	11	10	13	13

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 6 5-11

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 6 11-12

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 6 12-10

IN THE OBTAINED ACYCLIC STRUCTURE LABEL 1 IS ASSIGNED TO 4AND VICE VERSA

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	3	4	2	6	11	7	8	0	10	13	12	0	14	0	0
LD	0	0	5	0	0	0	9	0	0	0	0	0	15	0	0
PR	0	3	1	2	3	4	6	7	7	9	5	11	10	13	13

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 6 10- 9

IN THE OBTAINED ACYCLIC STRUCTURE LABEL 1 IS ASSIGNED TO 4AND VICE VERSA

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	3	4	2	6	11	7	8	0	0	13	12	10	14	0	0
LD	0	0	5	0	0	0	9	0	0	0	0	0	15	0	0
PR	0	3	1	2	3	4	6	7	7	12	5	11	10	13	13

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

2 4 HT

11 12 TT

THE OBTAINED STRUCTURE IS OF THE REQUIRED TYPE

THE NUMBER OF HH LINKINGS 0
THE NUMBER OF HT LINKINGS 1
THE NUMBER OF TH LINKINGS 0
THE NUMBER OF TT LINKINGS 1

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 6 9- 7
IN THE OBTAINED ACYCLIC STRUCTURE LABEL 1 IS ASSIGNED TO 6AND VICE VERSA
PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	3	4	2	6	11	7	8	0	0	9	12	10	14	0	0
LD	0	0	5	0	0	0	0	0	0	13	0	0	15	0	0
PR	0	3	1	2	3	4	6	7	10	12	5	11	10	13	13

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

11 12 TH
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 4

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 6- 1 7- 6
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 6- 1 6- 5
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 6- 1 5-11
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 6- 1 11-12
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 6- 1 12-10
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

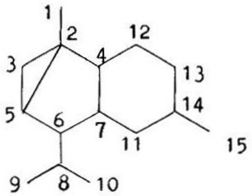
WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 6- 1 10- 9
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 6- 1 9- 7
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

THE GIVEN STRUCTURE IS A CYCLIC ISOPRENOID STRUCTURE WITH STANDARD LINKING
THE NUMBER OF THE VIABLE DECOMPOSITIONS 1

STOP

Appendix 3



RUN NL;5000,TIME;15
STARTED

THE ADJACENCY MATRIX

0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	1	1	1	0	0	0	0	0	0	0	0	0	0
0	1	0	0	1	0	0	0	0	0	0	0	0	0	0
0	1	0	0	0	0	1	0	0	0	0	1	0	0	0
0	1	1	0	0	1	0	0	0	0	0	0	0	0	0
0	0	0	0	1	0	1	1	0	0	0	0	0	0	0
0	0	0	1	0	1	0	0	0	0	1	0	0	0	0
0	0	0	0	0	1	0	0	1	1	0	0	0	0	0
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0	0	0	0	0	0	0	0	0	0	1	0	1	0	1
0	0	0	0	0	0	0	0	0	0	0	0	0	1	0

VERTICES THROUGH WHICH CIRCUITS PASS 0 1 1 1 1 1 1 0 0 0 1 1 1 1 0

VERTICES WHICH DETERMINE ISTHMUSES 0 0 0 0 0 0

THE DEGREES OF THE VERTICES 1 4 2 3 3 3 3 3 1 1 2 2 2 3 1

VECTOR D 0 3 2 3 3 2 3 0 0 0 2 2 2 2 0

MATRIX A

2	3	4	5	6	7	11	12	13	14	0	0	0	0	0
3	2	2	2	5	4	7	4	12	11	0	0	0	0	0
4	5	7	3	7	6	14	13	14	13	0	0	0	0	0
5	0	12	6	0	11	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

THE CYCLOMATIC NUMBER 3

THE NUMBER OF DISTINCT MINIMAL CIRCUITS 3

THE DISTINCT MINIMAL CIRCUITS

4	2	3	5	2	0	0	0	0	0	0	0	0	0	0
6	4	2	5	6	7	4	0	0	0	0	0	0	0	0
7	11	7	4	12	13	14	11	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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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	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	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
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	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	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

THE CIRCUITS OF THE STRUCTURE WHICH WILL BE TAKEN INTO CONSIDERATION

4	2	3	5	2	0	0	0	0	0	0	0	0	0	0
6	4	2	5	6	7	4	0	0	0	0	0	0	0	0
7	11	7	4	12	13	14	11	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	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	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	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	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	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	0	0	0	0	0	0	0
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1	2	3	4	2	11	7
2	2	3	4	2	7	4
3	2	3	4	2	4	12
4	2	3	4	2	12	13
5	2	3	4	2	13	14
6	2	3	4	2	14	11
7	2	3	2	5	11	7
8	2	3	2	5	7	4
9	2	3	2	5	4	12
10	2	3	2	5	12	13
11	2	3	2	5	13	14
12	2	3	2	5	14	11
13	2	3	5	6	11	7
14	2	3	5	6	7	4
15	2	3	5	6	4	12
16	2	3	5	6	12	13
17	2	3	5	6	13	14
18	2	3	5	6	14	11
19	2	3	6	7	11	7
20	2	3	6	7	7	4
21	2	3	6	7	4	12
22	2	3	6	7	12	13
23	2	3	6	7	13	14
24	2	3	6	7	14	11
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26	2	3	7	4	4	12
27	2	3	7	4	12	13
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30	3	5	4	2	11	7
31	3	5	4	2	7	4
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78	5	2	7	4	4	12
79	5	2	7	4	12	13
80	5	2	7	4	13	14
81	5	2	7	4	14	11

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 4- 2 11- 7
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 4- 2 7- 4
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 4- 2 4-12
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 4- 2 12-13
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 4- 2 13-14
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 4- 2 14-11
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 2- 5 11- 7
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 2- 5 7- 4

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	4	0	12	3	5	6	9	0	0	7	13	14	11	0
LD	0	0	0	0	0	8	0	10	0	0	0	0	0	15	0
PR	0	1	5	2	6	7	11	6	8	8	14	4	12	13	14

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 2- 5 4-12
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 2- 5 12-13
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

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WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 2- 5 14-11
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 5- 6 11- 7
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 5- 6 7- 4

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	4	0	12	3	8	6	9	0	0	7	13	14	11	0
LD	0	5	0	0	0	0	0	10	0	0	0	0	0	15	0
PR	0	1	5	2	2	7	11	6	8	8	14	4	12	13	14

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

11 7 HT
4 12 HT

THE OBTAINED STRUCTURE IS OF THE REQUIRED TYPE

THE NUMBER OF HH LINKINGS 0
THE NUMBER OF HT LINKINGS 2
THE NUMBER OF TH LINKINGS 0
THE NUMBER OF TT LINKINGS 0

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 2- 3 5- 6 4-12
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

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WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   2- 3   5- 6  12-13
          THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   2- 3   5- 6  13-14
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WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   2- 3   6- 7  11- 7
          THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   2- 3   6- 7   7- 4
          THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

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          THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

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          THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   3- 5   4- 2  11- 7
          THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   3- 5   4- 2   7- 4
          THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   3- 5   4- 2   4-12
          THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS   3- 5   4- 2  12-13
          THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22
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WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 3- 5 4- 2 13-14
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THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

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WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 3- 5 5- 6 14-11
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WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 3- 5 6- 7 11- 7
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 3- 5 6- 7 7- 4
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THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 3- 2 4- 2 11- 7
PREDECESSORS, LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	3	5	12	6	7	4	9	0	0	0	13	14	11	0
LD	0	0	0	0	0	8	0	10	0	0	0	0	0	15	0
PR	0	1	2	7	3	5	6	6	8	8	14	4	12	13	14

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 3- 2 4- 2 7- 4
PREDECESSORS, LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	3	5	0	6	7	11	9	0	0	14	4	12	13	0
LD	0	0	0	0	0	9	0	10	0	0	0	0	0	15	0
PR	0	1	2	12	3	5	6	6	8	8	7	13	14	11	14

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 3- 2 4- 2 4-12
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 3- 2 4- 2 12-13
THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 4- 2 13-14

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	3	5	12	6	7	4	9	0	0	14	13	0	15	0	
LD	0	0	0	0	0	8	11	10	0	0	0	0	0	0	0	
PR	0	1	2	7	3	5	6	6	8	8	7	4	12	11	14	

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 6 4- 2 14-11

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	3	5	12	6	7	4	9	0	0	0	13	14	15	0
LD	0	0	0	0	0	9	11	10	0	0	0	0	0	0	0
PR	0	1	2	7	3	5	6	6	8	8	7	4	12	13	14

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 5- 6 11- 7

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 5- 6 7- 4

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	3	5	12	0	8	6	9	0	0	7	13	14	11	0
LD	0	4	0	0	0	0	0	10	0	0	0	0	0	15	0
PR	0	1	2	2	3	7	11	6	8	8	14	4	12	13	14

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

11 7 HT

4 12 HT

THE OBTAINED STRUCTURE IS OF THE REQUIRED TYPE

THE NUMBER OF HH LINKINGS 0

THE NUMBER OF HT LINKINGS 2

THE NUMBER OF TH LINKINGS 0

THE NUMBER OF TT LINKINGS 0

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 5- 6 4-12

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 5- 6 12-13

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 5- 6 13-14

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 5- 6 14-11

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 6- 7 11- 7

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 6- 7 7- 4

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	3	5	12	6	8	0	9	0	0	7	13	14	11	0
LD	0	4	0	0	0	0	0	10	0	0	0	0	0	15	0
PR	0	1	2	2	3	5	11	6	8	8	14	4	12	13	14

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

12 13 TH

3 5 HT

THE OBTAINED STRUCTURE IS OF THE REQUIRED TYPE

THE NUMBER OF HH LINKINGS 0

THE NUMBER OF HT LINKINGS 1

THE NUMBER OF TH LINKINGS 1

THE NUMBER OF TT LINKINGS 0

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 6- 7 4-12

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	3	5	7	6	8	11	9	0	0	14	0	12	13	0
LD	0	4	0	0	0	0	0	10	0	0	0	0	0	15	0
PR	0	1	2	2	3	5	4	6	8	8	7	13	14	11	14

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

3 5 HT

7 11 TH

THE OBTAINED STRUCTURE IS OF THE REQUIRED TYPE

THE NUMBER OF HH LINKINGS 0

THE NUMBER OF HT LINKINGS 1

THE NUMBER OF TH LINKINGS 1

THE NUMBER OF TT LINKINGS 0

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 6- 7 12-13

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 6- 7 13-14

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	3	5	7	6	8	11	9	0	0	14	13	0	15	0
LD	0	4	0	12	0	0	0	10	0	0	0	0	0	0	0
PR	0	1	2	2	3	5	4	6	8	8	7	4	12	11	14

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

3 > HT

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 4

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 6- 7 14-11

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	3	5	7	6	8	11	9	0	0	0	13	14	15	0
LD	0	4	0	12	0	0	0	10	0	0	0	0	0	0	0
PR	0	1	2	2	3	5	4	6	8	8	7	4	12	13	14

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

3 > HT

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 4

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 7- 4 11- 7

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 7- 4 4-12

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 7- 4 12-13

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 22

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 7- 4 13-14

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	3	5	12	6	7	11	9	0	0	14	13	0	15	0
LD	0	4	0	0	0	8	0	10	0	0	0	0	0	0	0
PR	0	1	2	2	3	5	6	6	8	8	7	4	12	11	14

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

WE REDUCE THE CYCLIC STRUCTURE TO A CONNECTED ACYCLIC ONE OPERATING THE FOLLOWING CUTS 5- 2 7- 4 14-11

PREDECESSORS,LEFT AND RIGHT LINKINGS OF THE VERTICES OF THE OBTAINED STRUCTURE

LS	2	3	5	12	6	7	11	9	0	0	0	13	14	15	0
LD	0	4	0	0	0	8	0	10	0	0	0	0	0	0	0
PR	0	1	2	2	3	5	6	6	8	8	7	4	12	13	14

CUTS FOR DECOMPOSING THE STRUCTURE INTO ISOPRENE UNITS

THE OBTAINED STRUCTURE IS NOT OF THE REQUIRED TYPE, ERROR 6

THE GIVEN STRUCTURE IS A CYCLIC ISOPRENOID STRUCTURE WITH STANDARD LINKING
THE NUMBER OF THE VIABLE DECOMPOSITIONS 4

STOP