

A COMPLETE LIST OF FUNCTIONS USED IN DENDRAL

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The following pages contain an alphabetical listing of all LISP functions used in the program called DENONE (Dendral with Graph Matching). Each function description includes a statement of the purpose of the function and a list of arguments. Associated with each function is an index number telling where to find the function on the symbolic tape (Dectape #115 or #116). The index numbers are in two parts. The first part specifies the file number and the second part specifies the line number within the file.

There are four files:

- 1- DENDRL - contains functions for basic Dendral
- 2- ADDEND - contains functions for partitions, spectrum, histogram
- 3- ADDISO - contains main functions for graph matching
- 4- SUBGRF - contains secondary functions for graph matching

The functions are written in Q32 Evalquote format which by itself is not compatible with PDP-6 LISP. Thus, a fifth file on tapes 115 and 116 contains versions of the functions EVALQUOTE and DEFINE. These must be read in and EVALQUOTE must be executed before LISP will properly read the other four files. A file called UTILS contains these functions.

The other functions in DENONE which are not a part of LISPXY are certain tracing functions which are obtained from the system tape on DTA7 (in a file called TRACE). These functions are described in the writeup dated January 16, 1967 describing use of the Dendral program.

File Number

↙ ↘ Line Number

1-14770 ABSVAL - 1 argument

X - a number

ABSVAL returns the absolute value of the number X.

1-840 ADDICT - 0 arguments

ADDICT calls for one radical at a time in dot notation from the teletype and adds each radical onto the front of the proper dictionary list. The radical and all similar radicals with greater afferent link will be added to the dictionary list. Implied radicals will cause an error. Typing "END," will terminate ADDICT.

1-1330 ADDNAM - 2 arguments

RAD - a radical or molecule

NAME - an atomic symbol - the print name for RAD

ADDNAM adds the pair (RAD . NAME) to the name list. Any radical in implied format should not have the number after the apical node telling the number of that radical on the dictionary list.

3-1780 ADDSH - 4 arguments

S - a number

SS - a list of numbers

H - a list of lists of numbers

HS - a list of lists of numbers

ADDSH returns revised versions of H and HS which include the information in S and SS. If $SS=HS_i$, then H_i becomes $MERGE(S H_i)$. Otherwise $LIST(S)$ and SS are placed on the end of H and HS respectively.

2-780 ALLMEMBERS - 1 argument

R - a radical in list notation

ALLMEMBERS checks the total radical and all its subparts for inclusion of molecular weights in the list "SPECTRUM". If any part is not included, the value NIL is returned. Otherwise the value is T.

2-1880 APPORTION - 2 arguments

CL - a composition list

NL - a list of numbers

APPORTION returns a list of composition lists, each of which has the number of atoms specified by the corresponding element in NL. The composition lists are in non-decreasing order.

3-2450 ASSIGN1 - 1 argument

A - a number or NIL

ASSIGN1 finds a possible correspondent of node X in set SS.
(Both X and SS are global to ASSIGN1, being set within NEWABLEK
and NEXTASSIGN which are the functions which can call ASSIGN1.)
If A is not NIL, then it is the last correspondent used for X,
and the search for a new correspondent starts with the successor
of A in list SS. The new correspondence X:SS is checked for
validity against the sets of V and VS.

1-1651 ATOMWEIGHT - 1 argument

ATM - the letter name of an atom

ATOMWEIGHT returns the atomic weight of the atom. This is
obtained from the global variable "WEIGHTLIST".

1-14710 BLANKS - 1 argument

N - a number

BLANKS causes the appropriate number of blank spaces to appear
on the output line.

4-6660 BVAL - 1 argument

G - a graph

BVAL returns a list of the form $\{(S \text{ node node..})(D \text{ node node..})$
 $(T \text{ node node ..})$ where the nodes are the node numbers of those
nodes adjacent to bonds of the types S, D, and T respectively.
Other bond types are ignored.

1-11580 CANNONIZE - 1 argument

STR - a string of Dendral polish notation

CANNONIZE prints the canonical form of STR in dot notation.

1-2850 CHANGELIST - 3 arguments

XX - an atom

NN - a number

CL - a composition list

The value of CHANGELIST is a new composition list which is the
same as CL except that NN XX's have been added to (or subtracted
from) the list *depending on the sign of NN). Trying to subtract
more XX's from the list than are actually on it will cause that
atom to be deleted from the list (unless the XX is a "U" in which
case an erroneous result will occur).

4-9360 CHBND - 1 argument

B - a number

CHBND translated Dendral bond notation (1, 2, or 3) to notation appropriate for subgraph matching (S, D, or T).

4-9420 CHECKDEN - 1 argument

R - a structure in Dendral list notation

CHECKDEN searches R for occurrences of terminal oxygen atoms, terminal nitrogen atoms, and nitrogen atoms with only one attached hydrogen atom. In the first case, the "O" is replaced by "OH". In the other cases, "N" is replaced by "NHR". This allows the subgraph matching process to distinguish between certain occurrences of oxygen and nitrogen which are forbidden in some positions and not in others.

2-610 CHECKMATCH - 1 argument

R - a structure in list notation

Normally CHECKMATCH checks the structure for forbidden substructures. This dummy version assumes that no substructures are forbidden, and thus bypasses all subgraph matching.

4-8460 CHECKMATCH - 1 argument

R - a structure in list notation

This is the driver function for searching structures for forbidden substructures. It is responsible for cycling through the elements of BADLIST and determining whether R contains any of the forbidden structures. The value of checkmatch is T if R contains forbidden structures, NIL otherwise.

2-4860 CHNOPSXVQW - 1 argument

LARG - a list of the following ten arguments

CC - the number of carbon atoms

H θ the number of hydrogen atoms

NN - the number of nitrogen atoms

OO - the number of oxygen atoms

PP - the number of phosphorus atoms

SS - the number of sulfur atoms

X - an atomic symbol, any new atom you want to define

V - the valance of X

Q - the number of X atoms

W - atomic weight of an X atom

CHNOPSXVQW will apply WORKLIST to a composition list made from the above arguments. It compares the total weight of the composition to the spectrum (if present) and resets the masterlist and weightlist to account for X type atoms if present.

4-8990 CHNOT - 3 arguments

RAD - a structure in Dendral list notation

NUM - a number, initially equal to 1

NAT - a number or "RAD"

CHNOT converts the structure RAD to a notation acceptable by the graph matching algorithm. NUM is the next node number to be assigned, and NAT is the number of the node to which this structure is connected. If RAD is a molecule, or if RAD is a radical and CHNOT is being called for the first time, NAT is set to "RAD" indicating that the structure is not connected to anything else. On successive calls (CHNOT calls itself both iteratively and recursively), NAT will be a node number (integer). The value of CHNOT is a list of two elements, the first being the structure in translated form and the second being the next value of NUM.

2-2950 CLFAIL - 1 argument

CL - a pseudo composition list (hydrogens at end)

CLFAIL calculates the molecular weight and composition name of the composition list. If the molecular weight is not contained in the spectrum, or if the dictionary indicates an impossible composition, then the composition list fails the test and the value T is returned.

2-70 CLPRIN - 1 argument

PCL - a pseudo composition list (hydrogens at end)

CLPRIN return a list of character objects corresponding to the atom names and numbers of atoms in PCL.

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1-2750 COMBLIST - 1 argument

LSTCL - a list of composition lists

The value of COMBLIST is a composition list combining all of the lists in LSTCL.

4-3360 COMMON - 2 arguments

X1 - a list of numbers

X2 - a list of numbers

COMMON returns the list of elements which appear in both X1 and X2. (This is the "intersection" of X1 and X2.)

1-4330 COMPARLIST - 2 arguments

CL1 - a composition list

CL2 - a composition list

COMPARLIST compares the Dendral orders of CL1 and CL2 and returns "LSS", "EQL", or "GRT" according to whether CL1 is less than, equal to, or greater than CL2.

1-4350 COMPARL1 - an auxiliary function for COMPARLIST

1-4380 COMPARL2 - an auxiliary function for COMPARL1

1-1770 COMPATIBLE - 2 arguments

NODES - a list of the atoms at the nodes of the radical prior to RAD

RAD - a radical

COMPATIBLE is a predicate. The value is T if NODES and RAD will form a legal string of atoms (not containing any forbidden strings).

1-4410 COMPRAD - 2 arguments

R1-a radical

R2-a radical

COMPRAD compared the Dendral order of R1 and R2. If R1 is greater than R2 then the value is "GRT", if R2 is greater the value is "LSS", and if they are equal then the value is "EQL". The implied form of a radical has a lower Dendral value than any of its structured forms.

3-690 CONNEC - 0 arguments

CONNEC examines the lists V and VS and adds new corresponding sets to L and LS. The elements added to L and LS are the result of finding the connectivity of corresponding elements on V and VS. The n-connectivity of a list of nodes is the union of all nodes which can be reached by a path of length n (with direct back-tracking disallowed) from the given nodes. Connectivity is established for n=1 and n=2.

4-6240 CONSET - 3 arguments

G - a graph

M - an integer

S - a list of nodes

CONSET computes the list of nodes which are connected to the elements of S by paths of length M. It does this by calling CONSET1 M times.

4-6280 CONSET1 - an auxiliary function for CONSET

1-2340 CONTAINED - 2 arguments

CL1 - a composition list

CL2 - a composition list

The value of CONTAINED is T if all of the elements of CL1 are contained in CL2 and F (NIL) otherwise.

1-2010 COUNT - 1 argument

R - a radical or molecule

The value of COUNT is the total number of atoms in R.

1-3980 CPRCAL - an auxiliary function for CPRCOMPAT

1-4280 CPRCNTCL - 2 arguments

CL1 - a composition list

CL2 - a composition list

CPRCNTCL compares the number of atoms in CL1 and CL2. If CL1 has more than CL2 the value is "GRT". If CL2 has more than CL1 the value is "LSS". Otherwise the value is "EQL".

1-4300 CPRCNTCL1 - an auxiliary function for CPRCNTCL

1-3960 CPRCOMPAT - 2 arguments

AT1 - an atom in orderlist

AT2 - an atom in orderlist

CPRCOMPAT uses the global constant ORDERLIST to compare AT1 and AT2. If AT1 equals AT2 then the value is "EQL". If AT1 is greater than AT2 then the value is "GRT". Otherwise the value is "LSS".

1-4070 CPRCOMPCL - 2 arguments

CL1 - a composition list

CL2 - a composition list

CPRCOMPCL uses the global constant ORDERLIST to compare the compositions of CL1 and CL2. An equal number of atoms from both lists are compared, with the shortest list terminating the comparison. If CL1 has a higher composition value than CL2 the value is "GRT". If CL1 is lower than CL2, the value is "LSS". Otherwise the value is "EQL".

1-4130 CPRCOMPCLL - an auxiliary function for CPRCOMPCL

1-4030 CPRUNSATCL - 2 arguments

CL1 - a composition list

CL2 - a composition list

CPRUNSATCL compares the unsaturation parts of CL1 and CL2. If CL1 has more unsaturations then the value is "GRT". If CL2 has more then the value is "LSS". Otherwise the value is "EQL".

1-4690 DECOMPOSE - 1 argument

R - a radical or molecule

DECOMPOSE uses the global constant ORDERLIST to obtain the composition list of R.

1-1860 DEGREE - 1 argument

RAD - a radical or molecule

The Value of DEGREE is the number of efferent radicals of RAD.

4-6090 DEGS - 3 arguments

S - a list of numbers or atoms

Z - a dummy variable - initially NIL

I - a dummy variable - initially 1

S is a list with one element for each node of a graph. Each element is the value of a node for a property. The output is a list with one element for each different value, the elements being of form (value node node . . .). Z and I are dummy variables used for accumulating the result.

4-6130 DEGL - an auxiliary function for DEGS

1-1410 DELETE - 2 arguments

XX-any valid S-expression or number

LL-any list

The value of DELETE is a list the same as LL except that the first occurrence of XX, if it occurs at all, has been deleted. This affects only the top level of the list.

1-1380 DELLAST - 1 argument

LL - a list with at least one element

The value of DELLAST is the list LL with the last element deleted.

1-13220 DANDRAL - 0 arguments

DANDRAL presents the user with a number of options to be used in generating chemical structures. The user must respond to these questions. DANDRAL generates a composition name, calls structure generation routines, and cycles back to review the options and read other composition names if desired by the user.

4-7010 DINDEX - 2 arguments

G - a list (graph)

I - a number

DINDEX returns the remainder of G starting with the I-th element. (Applies CDR I-1 times)

1-3080 DISTRIB - 2 arguments

LCL - a list of composition lists

LN - the least number of unsaturations for any list

DISTRIB checks the first two composition lists in LCL and assures that the second has no more than its upper limit of unsaturations. This upper limit is determined by MAXUNS or by LN (whichever is greater). Any extra unsaturations are put into the first list on the list LCL.

1-48600 DIVIDE - 2 arguments

X - a number

Y - a number

DIVIDE returns a list of two elements. The first is a number equal to (QUOTIENT X Y) and the second is a number equal to (REMAINDER X Y). (i.e., X is divided by Y)

1-11630 DOTORD - 0 arguments

DOTORD reads in from the teletype the dot notation for a radical and prints out the canonical form.

1-1580 EFFACE - 2 arguments

XX - an element

LL - a list

EFFACE deletes the first appearance of item XX from the list LL. It is the same function described in the LISP 1.5 manual.

4-4160 EXCEPT - 2 arguments

X1 - a list of numbers

N - a number

EXCEPT returns the "complement" of the "set" X1 with respect

to a "universe" of size N. All positive numbers less than N and not in X1 are placed on the current list.

2-2860 FAILTEST - 1 argument

LCL - a list of composition lists.
FAILTEST uses the subsidiary function FAIL to test each element of LCL for certain failures.

3-800 FF - 0 arguments

FF uses the lists L and LS to form families of corresponding nodes. Each pair of elements (L_i , LS_i) are examined for useful information. Known corresponding nodes are removed (by the function REMK) from L_i and LS_i . If exactly one node remains in each, then this becomes a new known correspondence and the nodes are placed on K and KS respectively and the new correspondence is used to remove nodes from all lists V and VS (by the function REMNEMK). Otherwise, the elements L_i and LS_i are placed on lists V and VS (by the function MERGESET), provided they do not contradict (no isomorphism) or duplicate any pair of elements (V_j , VS_j).

After FF has considered all elements on L and LS, the length of lists K and KS determine the future action of the subgraph matching algorithm. If the number of correspondences (length of K) is equal to the number of nodes of graph G, an isomorphism is found and FF terminates with a value of 1. If the length of K is greater than the number of nodes of G, then a contradiction must exist and no isomorphism will be possible. In such a case FF exits with a value of 0. Otherwise, FF terminates with a value of 2 indicating that more work needs to be done.

1-2230 FINDVALENCE - 2 arguments

NN - a number

CL - a composition list

The value of FINDVALENCE is the first atom in CL whose valence is greater than or equal to NN.

3-6040 FIRSTEST - 2 arguments

L - a list of lists

X - any LISP construct

FIRSTEST RETURNS THE CDR of the first element of L whose CAR is EQUAL to X. If none is found, the result is NIL.

1-10740 FIRSTRAD - 1 argument

STR - a string of Dendral list notation starting with an atom

The value of FIRSTRAD will be a list of atoms. The first element will be the first atom mentioned in STR expression in list notation but without the "CAR" link. The second element will be the remainder of the string.

4-8730 FIXBADLIST - 3 arguments

I - either "ADD" or "REMOVE"

R - a structure in Dendral list notation

P - a predicate

FIXBADLIST is a function called by the user of Dendral from the top level of LISP. FIXBADLIST adjusts the global variable BADLIST according to the parameters I, R, and P. The structure R is accordingly added or removed. If P is true, then R is first converted to a notation which takes account of "OR" and "NHR" substructures. P is the first element on the BADLIST entry for structure R.

2-220 FIXFORM - 2 arguments

LCL - a list of pseudo-composition lists

D - the original number of elements in LCL

FIXFORM converts composition lists with hydrogens at the end to the proper composition list form with unsaturations at the beginning.

2-3770 FIXLIST - 1 argument

L - a list of dotted pairs

FIXLIST returns a list composed of the CAR's of all elements of list L.

1-3350 FLATEN - 1 argument

CL - a composition list

The value of FLATEN is a list of the characters from the elements of CL. Any number greater than 99 in CL will be represented by X and its last digit. All other numbers will be represented by two digits.

1-1370 FNIL - 0 arguments

The value of FNIL is NIL.

4-6190 FNODE - 1 argument

N - a node-element

The form of N is (node number, node element, list of connections).
FNODE returns the set of nodes connected to this node.

1-1660 FORBIDEN - 2 arguments

AT - a chemical atom

NODES - a list of the atoms at the nodes of the radical prior to AT

FORBIDEN is a predicate which determines if an atom should be put at a node in a radical, given the list of nodes appearing before AT in the radical. The value is T if AT is not acceptable at the node.

4-6380 GAMDEG - 4 arguments

G - a graph

M - a number

I - a dummy variable, initially equal to 1

L - a number - the length of graph G

GAMDEG computes the gamma=M degree of all nodes of graph G. The gamma=M degree of a node is the number of distinct nodes of G that can be reached by a path of length exactly M from the given node. Output is a list of values appropriate for use by DEGS ((value, node, node, . . .) (value, node, node, ..) ...)

1-4890 GENMOL - 1 argument

CL - a composition list

The value of GENMOL is the lowest Dendral molecule which can be made from CL. If none can be made then the value is NIL. CL must contain three or more atoms.

1-13620 GENRAD - 4 arguments

NODES - a list of the atoms at the nodes of the radical prior to the one about to be made

CL - a composition list

LN - a number

HN - a number

The value of GENRAD is a dotted pair of the lowest Dendral radical made from the elements of CL with afferent link no less than LN and no greater than HN, and a predicate telling whether the radical was obtained from a dictionary list or not (T means the origin was a dictionary list).

1-3904 GETNAM - 1 argument

RAD - a radical or molecule

GETNAM searches the NAMELIST for the name of RAD. If it finds a name, then it returns it, if none is found it returns NIL.

1-3560 GETNEX - 5 arguments

NODES - a list of the atoms at the nodes of the radical prior to RAD

RAD - a radical

LR - a list of radicals containing RAD

LN - a number

the following two arguments must be in a dotted pair

HN - a number

NN - a list of numbers

The value of GETNEX is the rest of LR which follows RAD.

The list starts with a radical which has an afferent link not greater than HN or less than LN or in the list NN and whose nodes are comparable with the previous NODES. If RAD is NIL then the value will be the rest of LR starting at the first such radical on the list.

This version of GETNEX checks the radical obtained from the dictionary to insure that any radical it returns for purposes of printed output conforms to the spectrum requirements (if any). If the spectrum is NILL or if dictionary construction is being performed, then this check is not made.

2-3830 GETSCORE - 1 argument

E - a partition (list of pseudo-composition lists)

1-3450 GETVAL - 1 argument

CL - a list of character objects

The value of GETVAL is a dotted pair of the value of the atomic symbol made from the characters in CL, and either IMP if it has the indicator IMP on its property list or NIL. If this atomic symbol has no value, then the value of GETVAL is NIL.

2-2330 HDISTRIB - 5 arguments

CL - a list of composition lists

NH - the number of hydrogens to be used

D - the length of the original CL

TOT - the total number of atoms in the original CL

NO - the total number of combinations in the original CL

HDISTRIB distributes NH hydrogens among the elements of CL. All possible distributions are generated, and the ultimate value of HDISTRIB is a list of partitions (thus, a list of lists of composition lists is generated).

2-3230 HSTGRM - 1 argument

R - a structure in list notation

HSTGRM returns a list of weights of all substructures of R. The first of the list is the molecular weight of R itself.

2-3340 HST1 - 1 argument

R - a structure in list notation

HST1 returns a list of weights of all radicals in R.

2-540 INDEX - 2 arguments

G - a list

I - a number

INDEX returns the I-th element of list G.

1-10390 INDOT - 0 arguments

INDOT will take a string of characters in legal dot notation and return the corresponding polish (list) notation.

1-2790 INSETPR - 2 arguments

PR - a dotted pair of atom and number

CL - a composition list not containing any atom the same as PR

The value of INSETPR is a composition list the same as CL except that PR has been inserted in the proper place.

1-2810 INSETPR1 - an auxiliary function for INSETPR

3-20 ISOLISP - 2 arguments

G - a graph

GS - a graph

ISOLISP is the driver function for the subgraph matching algorithm. It calls other functions to construct and use the lists L, LS, V, VS, K, and WS to find an isomorphism between G and any part of GS. ISOLISP recognizes when an isomorphism has been found or denied and calls for assignments to be made in case multiple isomorphisms are possible.

1-12940 ISOMERS - 1 argument

COMP - a composition name

ISOMERS converts a composition name into a list of numbers of atoms and calls the structure generating function.

3-1700 ISS - 5 arguments

I - a number

SS - a list of numbers

V - a list of lists of numbers

VS - a list of lists of numbers

CNVS - a list of dotted pairs (each dotted pair contains a predicate and a list of numbers)

ISS returns the list of correspondents for node I. This list is the intersection of SS with VS_j (if I is in V_j) or with the complement of VS_j (if CAAR(CNVS) is true). The complement of VS_j is stored in CDAR(CNVS_j).

1-14830 LAST - 1 argument

X - a list

LAST returns the last element of list X.

1-2300 LCOUNT - 1 argument

CL - a composition list

The value of LCOUNT is the total number of atoms in CL.

1-2310 LCT1 - an auxiliary function for LCOUNT

1-260 MAKCOM - 1 argument

CL - a composition list

(uses the global constants MASTERLIST, VALENCELIST, and ORDERLIST) MAKCOM will take the unordered composition list and place the pairs in the proper Dendral order according to the constant MASTERLIST. At the same time MAKCOM will set the constants ORDERLIST and VALENCELIST so that they contain only the atoms in CL.

1-3170 MAKECL - 3 arguments

LCL - a composition list with at least IN unsaturations

MCL - a composition list

LN - a number

MAKECL makes a new composition list from the elements of LCL. The new list will have the same number of atoms as LCL which is greater than or equal to LN. The new list will have at least LN unsaturations. If it is not possible to make such a list then the value is NIL. If such a list is made then the value of MAKECL will be a dotted list whose first element is the new list and whose second element is a composition list of the elements of MCL which were not used.

1-3170 MAKECLSUB - 3 arguments

KX - a number

NN - a number

CL - a composition list containing at least NN atoms

The value of MAKECLSUB is a composition list having KX unsaturations and made from the elements of CL.

1-4820 MAKELIST - 1 argument

LR - a list of radicals or molecules

The value of MAKELIST is a composition list of all the elements of LR.

1-6710 MAKELSTCLS - 5 arguments

D - a number

CL - a composition list

LCL - a composition list

LN - a number

AL - the greatest number of atoms that any list can contain

The value of MAKELSTCLS is a list of D composition lists made from the elements of CL, each of which is greater than or equal to the preceding one, with the first being greater than or equal to LCL. Each list contains at least LN unsaturations, and each list except for the last is the lowest that is still greater than or equal to the preceding one. If no such list can be made, the value is NIL.

1-5280 MAKERADS - 5 arguments

NODES - a list of the atoms at the nodes of the radical prior to the start of these radicals

D - a number - the number of radicals to be made

NN - a number - the greatest possible sum for the efferent links to all radicals

CL - a composition list - the elements from which to make the radicals

the following four arguments must be in a single list

LCL - the lowest starting composition list

LN - a number - the least efferent link for any radical

HN - a number - the greatest afferent link for any radical
NL - the greatest number of links that any radical can contain
The value of LINKED is a list of links according to
the specifications in the list of links. If the value is a
list, then the value is link.

1-1740 MATCH - 2 arguments

N1 - a list of atoms

N2 - a list of atoms

MATCH is a predicate which determines if all the elements of
N1 are the same as a like number of elements from the top
of N2. If N1 matches N2 the value is T. If N2 is shorter
than N1 the value is NIL.

1-48550 MAX - 2 arguments

A - a number

B - a number

MAX returns the maximum of its arguments

2-2730 MAXHYD - 1 argument

AL - a list of atoms (a composition list without the
unsaturation part)

MAXHYD calculates and returns the maximum number of hydrogen
atoms that can be accommodated when making a structure out
of this group of atoms.

1-2490 MAXUNS - 1 argument

CL - a composition list

The value of MAXUNS is an upper bound on the number of
unsaturations that a composition list can have and still be
converted into some radical.

1-6040 MCLCOMFG - 3 arguments

LCL - a composition list

LCL - a composition list

LN - a number

The value of MCLCOMFG is a composition list with LN unsatu-
rations, made from the elements of LCL with the same number
of atoms as LCL, and whose composition is the next greater
than LCL. If it is not possible to make this list then
the value is NIL.

HN - a number - the greatest afferent link for any radical
NL - the greatest number of links that any radical can contain
The value of LINKED is a list of links according to
the specifications in the list of links. If the value is a
list, then the value is link.

1-1740 MATCH - 2 arguments

N1 - a list of atoms

N2 - a list of atoms

MATCH is a predicate which determines if all the elements of
N1 are the same as a like number of elements from the top
of N2. If N1 matches N2 the value is T. If N2 is shorter
than N1 the value is NIL.

1-48550 MAX - 2 arguments

A - a number

B - a number

MAX returns the maximum of its arguments.

2-2730 MAXHYD - 1 argument

AL - a list of atoms (a composition list without the
unsaturation part)

MAXHYD calculates and returns the maximum number of hydrogen
atoms that can be accommodated when making a structure out
of this group of atoms.

1-2490 MAXUNS - 1 argument

CL - a composition list

The value of MAXUNS is an upper bound on the number of
unsaturations that a composition list can have and still be
converted into some radical.

1-6040 MCLCOMP - 3 arguments

LCL - a composition list

LCL - a composition list

LN - a number

The value of MCLCOMP is a composition list with LN unsatu-
rations, made from the elements of LCL with the same number
of atoms as LCL, and whose composition is the next greater
than LCL. If it is not possible to make this list then
the value is NIL.

2-5260 MINUSP - 1 argument

N - a number

The value of MINUSP is a predicate which is true if N is negative and false otherwise.

2-890 MOLCLIST - 1 argument

M - a molecule in list notation

MOLCLIST returns a list of composition lists made from a molecule. One composition list is made for the central atom (if present) and one composition list is made for each efferent radical.

2-960 MOLCL - 1 argument

LR - a list of radicals

MOLCL returns a list of composition lists, one for each radical in LR.

1-11170 MOLORD - 1 argument

M - a molecule

The value of MOLORD will be the Dendral canonical form of M. M must have a count greater than 2 and any molecules with an odd count cannot be written as central bond molecules.

3-2250 NEWABLK - 0 arguments

NEWABLK adds a new assignment block to ASTACK. An assignment block is a list of the form (XS X SS V VS K KS) where the correspondence (assignment) X:XS was made from set SS which is part of list VS. Values of V, VS, K, and KS are prior to assignment so they can be restored if the assignment fails. X is added to ASLIST, and lists K, KS, V, and VS are updated using the new assignment.

2-4310 NEWGENMOL - 1 argument

PCL - a composition list

NEWGENMOL returns a molecule made from the elements of PCL. If the partition option is not being exercised, then the result is the value of GENMOL (i.e., the lowest molecule). If partitions are being used, however, the function takes the next partition from PARTLIST and generates radicals for each part of the current partition and combines them into a molecule.

2-4760 NEWUPMOL - 1 argument

M - a molecule in list available
NEWUPMOL attempts to return the next most allowable molecule. It first tries the current partition system by calling UPMOL. If the partition option is not being exercised then this is the final result of NEWUPMOL. With the partition option, however, the result of UPMOL must be checked to be sure it is consistent with the current partition (saved in CURPART). If it does not, then all variations of CURPART have been tried, and the program then uses the next partition by calling NEWGENMOL.

3-2650 NEXTASSIGN - 0 arguments

NEXTASSIGN makes the next assignment in the current block. The current block is the first element of ASTACK, which has kept track of all assignments made in the current attempt to locate an isomorphism.

1-2270 NEXTATOM - 2 arguments

AT - an atom

CL - a composition list

The value of NEXTATOM is the next atom after AT in CL. If AT does not occur in CL then the value is NIL.

4-6960 NINDEX - 2 arguments

G - a list of node-elements (graph)

I - a number (node index)

NINDEX finds node element I of list G by finding an element of G whose CAR is I. The CDR of the node element is returned.

1-2130 NUMBEROFATOMS - 2 arguments

XX - an atom

R - a radical or molecule

The value of NUMBEROFATOMS is the number of times that the atom XX appears in structure R.

2-1690 NUMLIST - 4 arguments

MN - a number - the minimum element to be returned

MX - a number - the maximum element to be returned

TOT - a number - the number to be divided

D - a number - the number of elements to be returned

NUMLIST returns a list of D elements whose sum is TOT, given in non-decreasing order of size, with values no less than MN and no greater than MX.

1-3510 NUMRAD - 3 arguments

NODES - a list of atoms

NN - a number

LR - a list of radicals

The value of NUMRAD is the number of radicals with an afferent link of NN that occur in the list LR.

4-6430 NVAL - 1 argument

G - a graph

NVAL returns a list of the values of all nodes in graph G.

1-1198 OLDSETDICT - 5 arguments

NODES - a list of the atoms at the nodes of the radical prior to RAD

CL - a composition list

LN - the least afferent link for RAD

EN - the greatest afferent link for RAD

RAD - a radical - the output of GENRAD

SETDICT and OLDSETDICT establish the dictionary list for CL the first time it is encountered by GENRAD (if no dictionary list already exists). The value of SETDICT is RAD. RAD must be checked for forbidden substructures. If any are found, RAD is incremented by calling UPRAD until an acceptable radical or NIL is generated.

1-1450 ONEP - 1 argument

NN - a number

If NN is 1 then the value of ONEP is T, otherwise the value is F.

1-11040 ORDEFF - 1 argument

LR - a list of radicals

The value of ORDEFF will be the list of radicals with each of the radicals put into canonical form and all of the radicals listed in increasing order.

2-3700 ORDEREDLIST - 2 elements

L - a list of dotted pairs of numbers

E - a dotted pair of numbers

E is inserted into L in such a way that the CDR's of all elements are in decreasing order.

1-12361 OUTDEN - 1 argument

RM - a radical or molecule

OUTDEN will convert RM from list to dendration and then print the result. If a non-null radical is present, OUTDEN will also print a list of the radical names that were not used in generating this structure.

3-1880 PAR - 0 arguments

PAR examines elements of V and VS and combines sets (using operations similar to union, intersection, and complement) to find single node correspondences. PAR returns 0 if an isomorphism is impossible, 1 if an isomorphism is found, and 2 if more work needs to be done.

2-1020 PARTITION - 1 argument

CLIST - a composition list for a molecule

This function sets the global variable PARTLIST by calling PARTN2(CLIST) which returns a list of partitions. The word "STOP" is appended to the end of this list so that generating functions will notice that the end of the list has been reached.

2-1090 PARTN2 - 1 argument

CL - a composition list

PARTN2 calculates and prints a list of all allowed partitions of a composition. The allowed partitions have been checked against the dictionary and against the spectrum. A partition is a list of composition lists. The number of lists varies from two to five, and the order of each list corresponds to the Dendral order for generating structures (one radical will be generated from each list.) In partitions with length greater than two, the first list contains only one atom (other than hydrogens) and specifies the central atom of the molecule.

2-3560 PLAUSORDER - 0 arguments

PLAUSORDER calculates a plausibility score for each partition on PARTLIST. It returns a list of numbers which determine the rearranged order of partitions by plausibility. The actual score calculation is performed by GETSCORE.

4-6330 PRDWN - 1 argument

L - a list of numbers

PRDWN returns a copy of L in which multiple occurrences of items are deleted.

1-3820 PRINDICT - 0 arguments

PRINDICT calls for each radical name from the teletype in the same manner as PRINDICTL and then prints out the composition name of this radical in the dictionary list with it.

1-3891 PRINDICTLIST - 0 arguments

PRINDICTLIST prints a list of all compositions for which dictionary entries have been made.

1-13120 PRINFCN - 1 argument

L - a list of atoms

PRINFCN prints the list as a paragraph preceded by an asterisk. It is used for printing messages from within Dendral.

2-10 PRINFORM - 1 argument

LCL - a partition - a list of composition lists

PRINFORM takes a list of pseudo-composition lists and converts them to suitable form for printing. The lists are "pseudo" in the sense that instead of having unsaturations at the beginning they have number of hydrogens at the end. PRINFORM uses the subsidiary function CLPRIN to convert each individual element of LCL.

1-1470 PROPI - 2 arguments

LR - a list of radicals

RAD - a radical

PROPI searches the list LR for an item EQUAL to RAD. If such an element is found, the value of PROPI is the rest of the list after RAD. An error results if RAD is not found in LR.

1-2570 QUANH - 2 arguments

AFL - the afferent link

CL - a composition list

The value of QUANH is the number of hydrogen atoms that a linear radical would have if it were made from CL with the specified afferent link.

1-11130 RADORD - 1 argument

R - a radical

The value of RADORD will be R in its canonical form.

2-650 RADWEIGHT - 1 argument

R - a radical in list notation
RADWEIGHT calculated the radical weight of the radical
by adding the atomic weights of the atoms.

1-13530 READIT - 0 arguments

READIT returns a character object read from the
teletype. If it reads a percent sign (left arrow) then
it allows the user to input a pair of S-expressions
before reading another character which it will return
as the value of READIT.

2-1960 REAPPORTION - 3 arguments

CL - a list of composition lists
L - a list of numbers
PT - a predicate, the first element of which called itself.
REAPPORTION takes a list of composition lists and switches
atoms between lists so that the list of composition lists
resulting from the switch will be "higher" than CL.
REAPPORTION always attempts to switch atoms between the
last two elements of CL. If this is not possible then
the function APPORTION is called for the last elements
past the switch in order to put these composition lists
in lowest order.

2-430 REARRANGE - 2 arguments

NL - the name of a list to be rearranged
L - a list of numbers
REARRANGE returns a rearranged version of list NL. The
list L specifies the order of rearrangement. If, for example,
L is (3 1 4), then the new order is third element, first
element, fourth element. The new list is terminated by the
word "STOP".

1-3690 REFDICT - 0 arguments

REFDICT calls for a radical in dot notation from the
teletype and then returns a list of: the composition name,
to which the radical belongs, the radical in list notation,
the dictionary list for the composition name (or "NONE" if
there is no dictionary list for the radical).

1-48570 REMAINDER - 2 arguments

A-a number
B-a number
REMAINDER returns the remainder that occurs when A is divided
by B.

3-1100 REMK - 4 arguments

K - a list of numbers (known nodes)
KS - a list of numbers (known correspondents)
S - a list of numbers
SS - a list of numbers

REMK removes numbers from S and SS which are contained in corresponding positions on K and KS. In conditions which cause the value NIL to be returned indicating a contradiction (i.e., if K_1 is on S but KS_1 is not on SS). The value of REMK is the two element list containing the "edited" S and SS.

1-2950 REMLIST - 2 arguments

NN - a number
PCL - a partial composition list

The value of REMLIST is the same as PCL with the first NN atoms removed from the composition.

3-1430 REMNEWK - 3 arguments

PR - a list of two arguments, each is a list of numbers
V - a list of lists of numbers
VS - a list of lists of numbers

REMNEWK removes CAR(PR) from V and CADR(PR) from VS, checking for contradictions as in REMK. NIL is returned if a contradiction is found; (NIL) is returned if V and VS do not change. Otherwise the result is the list (T V VS TK TKS) where T is the predicate (true), V and VS are the revised lists of lists of numbers, and TK and TKS (if present) are to be added to the lists of known node correspondences.

4-8130 REMOVE - 2 arguments

X - an element
L - a list of lists

REMOVE returns a copy of L in which one occurrence of X is removed from each element of L.

4-8170 REM1 - 2 arguments

X - an element
S - a list

REM1 returns a copy of S in which the first occurrence of X is deleted. (This differs from EFFACE in that it returns a copy rather than changing the original list.)

1-11640 REPRND - 1 argument

RAD - a radical

REPRND provides for the conversion of a radical from the list into dot notation. Single bonds are represented as ., double bonds as =, and triple bonds as ≡. Anything else will be represented as X.

1-11690 REPEFF - 1 argument

LR - a list of radicals

REPEFF will place the proper representation for the afferent links of LR into the character buffer.

1-11750 REPRAD - 1 argument

RAD - a radical

REPRAD will take a radical represented as a list structure and pack characters which will represent that radical in Dendral dot notation into the end of the character buffer. Hydrogen atoms will be filled in for all unsatisfied valences. Radicals represented implicitly (as a composition) will be printed as a formula enclosed in parentheses and preceded by a number telling the number of radicals implicitly represented.

1-3030 REVLIST - 2 arguments

CL1 - a composition list

CL2 - a composition list

The value of REVLIST is a composition list obtained by taking the elements of CL1 away from CL2.

1-7930 RSET - 5 arguments

NODES - a list of the atoms at the nodes of the radical prior to CR and LRS

LRS - a list of radicals (not null)

CR - base radical

TV - greatest total allowed for sum of all afferent links
the next two arguments must be in a dotted pair

LN - lowest possible afferent link for any radical

HN - greatest possible afferent link for any radical

The value of RSET is a list of radicals having the same elements as the radicals in LRS and reset to the lowest radicals possible which are at least equal to CR, which satisfy the valence requirements of TV, LN, and HN, and which are not forbidden by NODES.

1-1139 SETDICT - 5 arguments

NODES - a list of the atomic weights of the radical prior to FAN

CL - a composition list

LN - the least different list for FAN

HN - the greatest different list for FAN

RAD - a radical - the output of FAN

This function provides for generated structures to be checked against an input spectrum. If the atomic weight is in the spectrum, then the radical may be given as output. In any case, the radical needs to be entered into the dictionary. Because SETDICT is recursive, the global variable called DICTWORK is necessary to distinguish between initial calls on SETDICT (from GENRAD) and calls which result from attempting to create all appropriate dictionary entries for the composition.

3-250 SETFORM - 0 arguments

SETFORM uses set generating (property generating) functions to set L and LS to lists of corresponding nodes of G and GS. The properties are: gamma degree = 1, gamma degree = 2, node value, branch value, and quasi-order. (Quasi-order is not included when using linear Dendral.)

3-380 SETPAIRS - 3 arguments

W1 - a list of properties from G

W2 - a list of properties from GS

Z - a number

W1 and W2 are lists whose elements are lists of the form (value node node ...). Lists of nodes with equal values for the same properties are placed in corresponding positions on L and LS. If Z = 1 then the corresponding sets may have nodes with unequal properties (as in the case of gamma degree where the number of nodes reached from node n of graph G may be fewer than the number reached from its correspondent on GS.)

3-570 SETRIGHT - 1 argument

LN - a list of numbers

SETRIGHT returns a reordered version of LN in which the numbers are in increasing order with duplicates eliminated.

4-5960 SPSUB1 - 2 arguments

V - a number

W2 - a list of properties of nodes

SPSUB1 is an auxiliary function for the program. Each property on W2 is a list of the form (value name ...). SPSUB1 returns a list of nodes from all properties whose value is greater than or equal to V.

1-12730 STARTDENDRAL - 0 arguments

This function prints descriptive information and instructions about running the program.

1-1350 SUBNAM - 2 arguments

RAD - a radical or molecule

NAME - its print name

SUBNAM removes the first occurrence of the radical and its print name from the name list.

1-2090 SUMAFL - 1 argument

LR - a list of radicals or molecules

The value of SUMAFL is the sum of all of the afferent links of all the radicals or molecules in LR.

2-5270 TEREAD - 0 arguments

Returns NIL.

1-9755 TESTDENDRAL - 1 argument

M - a molecule in list notation

TESTDENDRAL causes all of the succeeding molecules after M to be generated and printed. It provides for the user to interrupt the output at periodic intervals and also checks each molecule (before printing) to be sure no forbidden structures are contained within it.

1-10670 TOPEFFS - 1 argument

STR - a string of Dendral Polish (list) notation

STR must start with a bond. The value of TOPEFFS will be a dotted pair. The first element will be a list of all the consecutive bonds at the head of the string. The second element will be the remainder of the string after removing these bonds.

1-12150 TOPMOL - 1 argument

MOL - a molecule

TOPMOL starts the conversion of a radical from list into dot notation.

1-12120 TOPRAD - 1 argument

RAD - a radical

TOPRAD starts the conversion of a radical from list into dot notation.

1-2410 TOTVAL - 1 argument

CL - a composition list

The value of TOTVAL is the total of all of the valences of all of the atoms in CL.

1-9670 TSTRAD - 2 arguments

R - a radical

PRED - a predicate

TSTRAD causes all of the succeeding radicals after R to be generated and printed in Dendral order. If pred is T then radicals with all possible afferent links will be generated, otherwise only those with an afferent link of 1 will result.

1-1010 UNADDICT - 0 arguments

UNADDICT calls for one radical at a time in dot notation from the teletype. The first occurrence of each radical (and all similar radicals with greater afferent link) are removed from the dictionary list. Typing END will terminate UNADDICT.

1-380 UNDICT - 1 argument

LCN - a list of composition names

UNDICT will unset each of the dictionary lists of the composition names in LCN.

1-1890 UNSATURATION - 1 argument

R - a radical or molecule

The value of UNSATURATION is the number of saturations in R.

1-10910 UNSTRING - 1 argument

STR - a string of Dendral radical notation
The value of UNSTRING is the list of radicals corresponding to STR.

1-7150 UPCOMPNODE - 4 arguments

NODES - a list of the atoms at the nodes of the
radical prior to R

HN - a number

R - a radical

LN - a number

The value of UPCOMPNODE is a radical made from the same elements as R, having the same degree as R, with afferent link no greater than HN and no less than LN, and whose apical node is the next greatest in composition from R (providing it is not forbidden by NODES).

1-7600 UPDEGNODE - 4 arguments

NODES - a list of the atoms at the nodes of the
radical prior to R

HN - a number

R - a radical

LN - a number

The value of UPDEGNODE is a radical made from the same elements as R with degree one greater than R, an afferent link no greater than HN or less than LN, and a string of atoms not forbidden by NODES.

1-6940 UPLINKNODE - 3 arguments

NODES - a list of the atoms at the nodes of the
radical prior to R

HN - a number

R - a radical

The value of UPLINKNODE is a radical the same as R with an afferent link one greater than R but less than HN. If this is not possible then the value is NIL.

1-9080 UPMOL - 1 argument

M - a molecule

The value of UPMOL is the next greater Dendral molecule.

2-1500 UPUNLIST - 1 argument

L - a list of numbers

UPUNLIST returns a list of numbers of the same length as L and with the same total as the original L. The new list is obtained by moving one unit from one element to another element earlier in the list. The elements of the new list must be monotonically non-decreasing, and if the length of L is greater than 2, then the first element of the list must always be 1.

1-8280 UPRAD - 5 arguments

NODES - a list of the atoms at the nodes of the radical prior to R and HCR

NUM - the greatest sum total of afferent links that R and HCR are allowed

R - the radical to be incremented

HCR - a list of all radicals connected with R and of higher Dendral value

The remaining three arguments must be in a single list.

LN - the least afferent link for any radical

HN - the greatest afferent link for any radical

AL - the greatest number of atoms that any radical can contain

The value of UPRAD is a list of radicals with the first element of the list being the next higher radical after R and the rest of the list being the new set of HCR. If R is in the implied format, then the next higher radical would be one with an afferent link at least one more than that of R. If it is not possible to increment the radical and find a new HCR, then the value is NIL.

1-1640 VALENCE - 1 argument

AT - a chemical atom

VALENCE uses the global constant VALENCELIST. If AT is "H" then the value of VALENCE is 1. Otherwise the value of VALENCE is the number associated with AT on VALENCELIST. The value is NIL if AT is not H or not the first element of one of the pairs in VALENCELIST.

1-9840 WORKLIST - 5 arguments

CL - a composition list

LCL - a composition list or NIL

L - a number - the least number of atoms wanted

H - a number - the greatest number of atoms wanted

The following three arguments must be in a single list.

LN - a number - the least number of unsaturations

PRED - a predicate - NIL indicates molecules while
T specifies radicals

P2 - a predicate - whether or not to let unsaturations
go to 3

WORKLIST produces all possible combinations of the atoms in CL starting with the list LCL and within the limits of L, H, and LN. If LCL is NIL then the lowest list is created. Depending on the value of PRED it then applies TESTDENDRAL or TSTRAD to each of the compositions, starting with the lowest molecule (or radical) possible from that composition. If P2 is NIL then TSTRAD is to be used to obtain only radicals with an afferent limit of 1. WORKLIST also presents the user with the option (for molecules only) of whether or not to construct and observe a list of partitions from which the structures will be generated. It provides the user with the opportunity to delete members of the partition list and to rearrange the elements of the list. Structures that are generated are checked for forbidden substructures before proceeding.

USE OF DENDRAL PROGRAMS ON THE PDP-6

Georgia Sutherland
January 16, 1967

At long last Dendral is installed on the PDP-6. Hopefully the current version is similar to the last version which worked on the Q32. The new version has been recoded (in portions of the graph matching algorithm) to increase speed of execution.

The program is a LISP program which contains many functions in interpretive form. The core image is saved on Dectape #182 and is called "DENONE". The program is loaded and started by typing

```
RUN DTAn DENONE
```

to the monitor system of the PDP-6 after mounting tape 182 on tape drive n.

The program contains several hundred LISP functions, most of which are described in a document entitled "A COMPLETE LIST OF FUNCTIONS USED IN DENDRAL" and dated January 10, 1967. Additional functions include EVALQUOTE, DEFINE, and some general purpose tracing functions. The program was constructed by the following set of commands:

```
R LISPXY 40
*(INC (INPUT DTAm: UTILS DENDRL ADDEND ADDISO SUBGRF))
bell
(INC (INPUT DTA7: TRACE))
C
.SAVE DTAn DENONE
```

The symbolic files called UTILS, DENDRL, ADDEND, ADDISO and SUBGRF are located on Dectape #115 (with 116 as backup). The file called UTILS contains the functions EVALQUOTE and DEFINE and also contains a call of EVALQUOTE so that LISP will correctly read the rest of the symbolic files (which are in Q32 Evalquote format). The files called DENDRL and SDDEND contain the LISP functions for pure Dendral (with a dummy version of CHECKMATCH which bypasses the subgraph matching). The files called ADDISO and SUBGRF contain the LISP functions for subgraph matching. The file called TRACE contains general purpose tracing functions. The main tracing functions are described below.

(TRACE F1 F2 F3 ...) causes the functions named F1 F2 F3 ... to be traced. A teletype printout is made every time a traced function is entered or exited.

(UNTRACE F1 F2 F3 ...) causes tracing to be deleted on the functions named F1 F2 F3 ...

(RESET) causes certain numbers to be reset to their lowest values. These numbers are associated with traced functions because each time a trace printout is printed, the level (of recursion) of the traced function is printed also. If an error occurs, LISP takes the program back to the top level without executing the rest of the code, and these level numbers will remain set at the value they had when the error was encountered. Thus RESET must be called to correct them.

(SLST V1 V2 V3...) causes the variables V1 V2 V3... to be monitored. Any time a variable is the object of SETQ, this fact will be noted along with the value which is to be assigned to the variable.

(USLST V1 V2 V3 ...) causes monitoring of variables V1 V2 V3 ... to be discontinued.

(TRACET) is a function which must be called before the function SLST is called. It sets up certain variables and parameters which allow monitoring to proceed.

As it exists on the PDP-6, LISPHY uses EVAL as its top level. This has several consequences:

- 1) Typing an atom name (followed by a blank) results in the value of the atom being printed on the teletype. (This works if the atom is a global variable or if the atom was currently bound when an error occurred.)
- 2) Arguments of functions are evaluated rather than being quoted. Most top level Dendral functions thus require an explicit QUOTE of their arguments.
- 3) The user can call the function EVALQUOTE before calling the Dendral functions. Any function call to EVALQUOTE must have a space between the name of the function and the first left parenthesis.

The functions which are usually called from the top level are listed below. A description of each of these functions may be found in the memorandum dated January 10.

STARTDENDRAL, DENDRAL, ISOMERS, CHNOPSXVQW, HSTGRM, ADDICT, UNADDICT, UNDICT, PRINDICTLIST, CHECKMATCH, FIXBADLIST, INDOT, RADORD, REPRAD, ADDNAM, SUBNAM, UNSTRING.

For the new user of the program or for someone who has not used the program for a while, an initial call of STARTDENDRAL is advised. This will print a description of the current version of the program and instruct the user to call the function DENDRAL in order to exercise the available options.

It is not necessary to call DENDRAL, however. The function of DENDRAL is to ask questions about the options and then ask for a composition name to give to the function ISOMERS. The options which are asked about are:

- 1) Whether to turn off the dictionary. (SETQ DICTSWITCH (QUOTE OFF)) if dictionary is not to be built. (QUOTE ON) will allow the dictionary to be built as usual.
- 2) Whether to allow dialog (intermediate printout within the function GENRAD). (SETQ DIALOG (QUOTE OFF)) if

no dialog is to be allowed. (QUOTE OFF) causes dialog to be given.

3) Whether to control the amount of output. A global variable called AMT determines how often the program will pause in listing output. The usual value is AMT=11 which causes the program to pause after every 11 structures and request permission to continue. The global variable called OUTCONTROL is set to (QUOTE OFF) if the output is to be uninterrupted.

These variables may be set by the user and then a call on ISOMERS may be made without first calling DENDRAL. The function ISOMERS takes a composition name as its argument. Remember that this composition name must be quoted if EVAL is being used as the top level of LISP. The composition may contain any number of carbon, hydrogen, nitrogen, oxygen, phosphorus, and sulfur atoms. If a different type of atom is to be introduced, the user must call the function CHNOP SXVQW (note the new "W" at the end of the name of this function) directly.

If the structure specified by the composition name is a molecule, the program will ask if the partitions are to be observed. The single character response "N" will bypass the partition option and cause structures to be generated in increasing Dendral order. The single character response "Y" will cause a list of partitions to be printed. The user will then be requested to enter a list of numbers or "NIL" or "PLAUSIBLE". The list of numbers defines a reordering of the partition list. NIL specifies that the partition list is to be unchanged. And the word PLAUSIBLE causes the function PLAUSORDER to be called to obtain a reordering of the whole partition list on the basis of plausibility, with the most plausible partition being first on the list. Structure generation will then proceed by calculating all structures implied by the first partition, all structures implied by the second partition, and so on.

One option must be exercised by the user before calling any structure generating functions (i.e., it must be exercised at the top level). This is the spectrum option. If the global variable called "SPECTRUM" is set to a list of numbers, then only those structures whose molecular weight is contained in the list of numbers will be generated. This includes all radicals and subradicals which are checked against the spectrum before being attached to the partially built structure. (Remember to set the SPECTRUM to NIL when done with that structure or else the spectrum option will continue to be exercised where it may not be meaningful.)

In order to obtain the numbers to use for the spectrum option the user may call the function HSTGRM with one argument which is the structure in list notation. This function will return the list of numbers which represents the first order spectrum of the structure. The function INDOT will convert dot notation to list notation if the user is in doubt about

about the correct list notation.

Other handy bits of knowledge:

- 1) If the dictionary is being built while a spectrum is current, the dictionary building apparatus ignores the spectrum so that the dictionary is independent of any spectra data.
- 2) Building the dictionary takes quite a while and interrupts the basic flow of the program. So, if a demonstration is being given, or if only one or two structures are being observed and building a dictionary for future reference is not important, it is better to turn off the dictionary (SETQ DICTSWITCH (QUOTE OFF)) before generating structures.
- 3) The function PRINDICTLIST will allow the user to see which compositions have been included in the dictionary.
- 4) An error during execution will cause the program to return to the top level (EVAL). Typing bell will also cause the program to return to the top level. Typing control C will cause the program to be interrupted and the user will then be talking to the PDP-6 monitor. Typing S to the monitor will then take the user back into Dendral, but the point at which the program was interrupted will not be resumed. Instead, the user will be talking to EVAL.