A PROBLEM SOLVING MONITOR FOR A DEDUCTIVE REASONING TASK

D. H. Sleeman*

Technical Report NL 17

August 1973

*Currently visiting from the University of Leeds, U.K.

ABSTRACT

The paper discusses some of the attempts that have been made to build knowledgeable CAI programs. A distinction is made between systems which have factual data-bases and where the knowledge is expressed as an algorithm.

Much of a scientist's work is involved with making inferences and deductions from data. As this is such an important aspect of a scientist's training it was decided to consider the problems of implementing knowledgeable algorithm-based programs which can monitor students performing a task involving deductive reasoning. To pursue this broad and general problem it was necessary to choose a particular task to be investigated in some depth. The task chosen was the interpretation of Nuclear Magnetic Spectroscopy--a task encountered in university organic chemistry courses.

The paper discusses in some detail the design of this particular teaching program and includes some annotated sample student protocols. The paper concludes with a report of reactions to this program and a discussion of possible further developments.

1. Introduction

One of the major criticisms of conventional CAI is that it is only able to answer questions which have been explicitly anticipated by the person writing the material. Ideally one would provide the program with knowledge about a subject domain and for the system to generate either an appropriate response to or an appropriate question for the student. Clearly, the nature of such systems is strongly influenced by the way in which the information for a subject area can be formulated and by the teaching approach used. Both Carbonell [1] and Wexler [2] have produced systems which teach factual subjects (i.e., aspects of geography). In each of these systems the information is expressed as a semantic net and the system contains algorithms which can operate on this data base to answer specific questions. Carbonell's system also has the ability to generate questions.

The other approach has been to express the knowledge about the subject matter as an algorithm. Typically, such programs use these algorithms to generate both examples for the student and the solutions to the problems. A number of generative programs (mainly of a tutorial nature) have been reported in the literature (Uttal et al. [3], Uhr [4], Wexler [5], Koffman [6], Peplinski [7]). A significant development has been the implementation of programs whose generation/selection algorithms are guided by the student's performance on earlier questions of the same session [8]. These programs, which we have called "adaptive", are thus able to change their behavior to accomodate the student's learning rate and in some cases they include diagnostic routines to spot specific types of errors. In order to implement an adaptive program it is necessary to formulate a measure of difficulty of the task being performed and a relationship between student performance and the

task difficulty level. Further a detailed analysis of the types of errors that students make must be included if one wants to include appropriate diagnostic procedures. For a discussion of some of the experiments needed to establish these relationships in the specific instance of vertical format arithmetic teaching see [9] and [10] and for medical diagnosis teaching see [11]. As a result of this experimentation a drill-and-practice system for teaching arithmetic computation has been implemented in Leeds which is comparable in its approach to a very experienced teacher in a one-to-one relationship with a child.

Thus we are beginning to see that CAI is not a homogenous field or a single approach. It is a term which is currently used to include "page turning" programs and adaptive systems alike. In an earlier article [10] we have discussed a variety of CAI programs which have differing levels of sophistication. The significant factors seem to be the degree of the decision making which a particular program is able to make and the extent to which the "knowledge" that is being taught is accessible to the teaching program. In the earlier paper we argued that a sophisticated teaching program must have:

a representation of the teaching task

a representation of the student

a set of possible teaching operations

and a set of means-ends guidance rules.

In the least sophisticated case, the system has very limited decision-making capabilities: indeed the program is only able to guide the student through pre-stored material and does in fact not have any direct access to the knowledge in the pre-stored material. Typically, generative systems

can generate problems and analyze the student's replies: however, the difficulty of the student's next problem is not related to his previous performance. On the other hand, in the arithmetic system cited earlier the decision-making is comparable with that of a good classroom teacher and this program does in fact contain algorithms which can perform the task it is attempting to teach and contains rules (means-end guidance rules) which relate student performance and task difficulty. (In our classification this is an adaptive program.)

In general the short-comings of adaptive systems are their inability to change teaching strategy even when it is found to be unquestionably wrong (e.g., wrong rate of increase of problem difficulty). It is this problem which is addressed in a further system [12]. In this system, which we have called Self-Improving, the teaching strategy has been expressed as a set of production rules. As a result of the information collected from students' performances the self-improving algorithm makes changes in the production rules, i.e., in the strategy.

Many of the generative and adaptive systems teach subjects which are normally encountered in a pre-university mathematics education. Further these programs have often had a tutorial (question/answer) approach and teach subjects in which it is possible to use well defined algorithms (e.g. the vertical arithmetic problem). However, much of the scientist's task involves forming hypotheses from data and performing subsequent investigations which confirm or reject these hypotheses. As this approach is basic it finds its place in the curricula of science students in many forms: the objective of such teaching is twofold--to teach him something about an aspect of his subject and the way to approach such problems. Our objective

then was to produce a teaching program which was able to give the student assistance when he attempted to carry out such reasoning tasks. Clearly we needed a context for this: the task chosen involves deductive reasoning and is the interpretation of Nuclear Magnetic Resonance (NMR) spectra. This subject is normally first encountered during an intermediary level university course in organic chemistry. {Readers may have noticed the similarities between the objectives expressed above and those of HEURISTIC DENDRAL [13]. Further, the task that we consider is very similar to DENDRAL's task (the interpretation of mass spectrograms)}.

2. Nuclear Magnetic Resonance and the Determination of Molecular Structures

One of the fascinating aspects of modern chemistry is the various physical techniques which give information about molecular structures. In many of these techniques the substance under investigation is irradiated with electromagnetic waves of a reasonably homogenous nature and a record is made either of the resulting fragments (Mass Spectroscopy) or of the various absorption peaks (Nuclear Magnetic Resonance, Infra-Red, Ultra Violet Spectroscopy) or of the scatter patterns (X-Ray Crystallography). Needless to say the theories which predict the behavior of molecules in given conditions are both very complex and sometimes also incomplete. The behavior of a group often depends not only on itself but on various interacting fields which are caused by other groups. When faced with a spectrum to analyse* the chemist draws extensively on his experience: and so uses information he

---

*analyse: to propose a molecular structure (an arrangement of groups) which will successfully explain the observed data.

has for instance about the colour and the "texture" of the compound to rule out certain possibilities. In other words the chemist has a large number of pre-determined heuristics at his disposal. The other thing to bear in mind is that the chemist often uses several spectroscopic techniques when he investigates the structure of a single molecule: each technique gives a characteristic type of information.

Nuclear Magnetic Resonance is one technique which is used in structural determination. This method relies upon a nucleus changing its alignment in the applied magnetic field. Fixing the magnetic field then we are able to obtain a spectrum--i.e., a series of absorption peaks. Depending on the values of the magnetic field and the frequency one can observe different nuclei "flipping". (In fact all nuclei with non-zero spins exhibit this phenomenon.) The most commonly produced spectra are proton resonance spectra, i.e., these spectra give information about hydrogen atoms in the molecules. In the simplest theory the area of the peak is proportional to the number of equivalent protons and the peak splitting is one greater than the number of protons on adjacent centers. Here we shall talk about the number of <u>interactions</u> which is equal to the number of protons on adjacent centers.

Thus using this simple minded model we (for instance [14]) could predict that the spectrum of the molecule:

$$CH_3 - CH_2 - CH_2 - CHO$$

would be

(3,2) (2,5) (2,3) (1,2)

where using the convention outlined above the first number represents the area of the peak and the second represents the number of interacting protons

on adjacent centers.*

In the cases where the chain contains hetero-atoms it is not usually possible to observe the splitting on the hetero-atom's peak. Similarly the protons on hetero atoms do not appear to interact with protons on adjacent groups. So given the molecule

$$CH_3 - CH_2 - NH - CH_3$$

this theory would predict a spectrum in our notation of:

(3,2) (2,3) (1,0) (3,0).

Putting this succinctly we can say that if a monecule can be represented as a linear chain of groups

$$- W - X - Y -$$

where these groups have w, x and y hydrogens respectively and if I(X) signifies the interaction due to group X, S(X) is the splitting of the peak which corresponds to the group X and where A(X) is the area of the same peak.

Then $S(X) = I(W) + I(Y)$ [1]

$I(W) = w$

$A(W) = w.$

However if the group X is such that a hetero atom is part of the 'chain' then:

$I(X) = S(X) = \emptyset$. Nevertheless $A(X) = x$.

---

*In practice an NMR spectrum is a series of peaks with different splittings (see [14]). In a simple case it is relatively easy to determine the area of a particular peak and its splitting. The more complex task is to perform the reasoning to determine the structure. As we are concentrating on this aspect we have chosen to use the data format most suited to that task.

Note from equation [1] we car infer:

$$S(Y) \leq I(X).$$

Indeed [14] tells us that the NMR spectrum gives us much more information than merely the multiplicity of the peaks (the splitting). For instance the position of a peak in the spectrum gives the chemist a lot of information about the likely nature of that group, i.e., each chemical group has a range within which its spectrum normally falls if it is present. (See [14], p. 84-85.) However as we have noted earlier a large number of fairly complex rules are needed to interpret spectroscopic data. As NMR spectra are no exception to this we shall limit ourselves to discussing molecules for which the simple interaction model given earlier is known to be adequate. In fact, we shall further limit ourselves to consider only molecules which are both linear and saturated.*

In the next section we discuss the teaching approach and the Problem Solving Monitor, which has been implemented in LISP, for giving students practice with structural determination from NMR spectral data.

3. A Problem Solving Monitor for Teaching the Interpretation of NMR Spectra

In introductory courses in NMR it is usual to present a student with simple spectra and the molecular formulae and to ask him to determine the molecular structures. This exercise allows the student to become thoroughly conversant with the theory underlying NMR and with the type of reasoning which underlies structure determination in general.

In essence then the student is given some physical data and asked to

---

*That is, molecules which contain only single bonds.

make some deductions about the structure of the molecule which would give rise to such data.

When we thought about how the system should work it seemed reasonable to consider the type of interaction that would go on between a teacher and a single* student. It seemed unlikely that the teacher would hold a straight question-answer sequence; it seemed much more likely that the student would make observations/assertions about the problem and that the teacher would tell him whether his assertions were correct. The teacher might also volunteer to explain why his last assertion was incorrect. If the student was unable to think of how next to proceed the teacher might well give him some hints as to the next stage in the solution of the problem. This is the style of teaching which we have tried to incorporate in the program to be described here (we have called it a Problem Solving Monitor as it "observes" the student's assertions and provides further hints and explanations on request). Clearly such a system must be able to solve the problem in order to be able to inform the student of the next step; further, as we shall see, to be able to satisfactorily explain students' errors, the system also needs a detailed analysis of possible errors.

The Problem Solving Monitor implemented selects a problem for the

---

*In practice, the subject is treated in the lecture hall by means of an exposé of the theory and the working of several problems in fromt of the class.

student to solve, comments on the various assertions* which the student made about the problem he is investigating and provides the student with a number of socratic facilities. The general layout of the program is shown in Figure 1. The system allows the student to assert what is the equivalent form of the spectrum,** which group and which peak form the head of the molecule, which group is the next in the chain (also must state the corresponding peak in the spectrum) and what is the structure of the molecule.

The form of these assertions is:

$((e)(S_1)....(S_n))$	equivalence
$((h)(G_L)(S_J))$	head of molecule is G_L and the corresponding peak is S_J
$((J)(h)(G_L)(S_J))$	the next group in the chain is G_L and it corresponds to the peak S_J of the spectrum
$((s)(G_1)....(G_m))$	the molecular structure is $(G_1)....(G_m)$
or	or
$((s)(h)(G_k)....(G_m))$	the molecular structure is the group already spotted followed by groups $G_k....G_m$

The socratic facilities available to the student are SUMMARY, HELP and EXPLAIN. (There is also a STOP command which enables the student to leave the program.)

---

*Maybe assertions is a misleading term for these statements; these statements are also the way in which the student expresses his hypotheses about the structure.

**I.e., if the molecule contains 2 methyl, CH_3, groups which are both adjacent to CH_2 groups, then a single (6 2) peak occurs in the spectrum. The "equivalent" spectrum would contain two (3 2) peaks--it is very important to spot this equivalence.

SUMMARY gives a synopsis of the information which the student has collected about the current problem.

The HELP facility gives the student a hint as to how to go about solving the problem. The hints given depend on the information which the student has collected about the problem. (Figure 2 shows, diagramatically, HELP's structure.) Not surprisingly the structure of the HELP facility is analogous to that of the algorithm which is able to solve the problem, i.e., the BUILD function.

EXPLAIN's task is to demonstrate to the student why incorrect assertions/hypotheses are inadmissible. There are four possible types of assertions as we have seen and therefore EXPLAIN must have algorithms for each of these types. As can be seen from Figure 3 the explanation for join is the most complex; the algorithm has to check the following:

1) that the group contains the correct number of interacting protons

2) that the valency* of the group is 2 unless it is the last group

3) that the area of the peak equals the number of hydrogens in the group

4) that the splitting of a peak (if an interacting one) is greater or equal to the number of interacting protons on the last group.

Many of the errors can be spotted explicitly; others require that one demonstrates that given the molecule so far specified and the current input, it is impossible to construct a molecule which contains all the atoms in the molecular formula and which has the correct spectrum. Thus given the student's input we need to show a contradiction. In order to do this we clearly

---

*In the case of saturated molecules valency of a group is its "binding power", i.e. the number of other groups to which it can join. Thus the valency of CH_3 is 1, of CH_2 is 2, of OH is 1, etc.

need to have an algorithm which can "build" all the possible and permissible combinations given the molecule so far specified, the remaining atoms available, the spectrum still to be explained, and the spectrum which corresponds to the molecule built. (The BUILD algorithm is discussed in more detail in section 5.) In other words the program has to have the ability to perform the task that it is attempting to teach. It has been argued elsewhere (Siklossy [15], Hartley and Sleeman [10]) that any program which proports to teach in an intelligent manner must have the ability to perform the task. However, Figure 3 makes it clear that a detailed analysis of the types of errors which may arise is also necessary in order to be able to teach effectively. (After all, a simulator has a process model but such systems are not capable of performing the type of instruction we are now discussing.)

The explanations given in case of error with the "structure" and "equivalence" assertions are straightforward. The explanation given in case of erroneous "head assertions" is interesting because the algorithm creates a list of all possible uni-valent groups which could be constructed given the atoms in the molecules and the peaks in the spectrum. Again like the "join" algorithm when it does not find a specific error it attempts to show the student why such a group could not be the head of a molecule which satisfactorily explains the spectrum and complies with the molecular formula, i.e. it too accesses the "build" function.

4. Discussion of Protocols Produced by the System

Now that the main features of the system have been outlined we shall present two protocols of the system. The first of these has only carbon atoms in the chain. This protocol, Figure 5, shows clearly the function of

the HELP facility. Also note that the non-interacting groups -CO- and -O- (the carbonyl and ether groups) correspond to peaks in the spectrum of (0 0). Clearly, whatever the spectrum of the molecule it is possible to hypothesize the existance of the "null" peak.

Protocol 1 also shows the use of the build function and how by its use the system demonstrates that the student's response is inadmissible.

In fact the structure under consideration here is:

$$CH_3 - CH_2 - CH_2 - CH_2 - CO - CH_2 - CH_3$$

which using our simple model has the following spectrum:

(3 2) (2 5) (2 4) (2 2) [(0 0)]* (2 3) (3 2).

The assertion that the third group is a CH_2 and that the peak is (2 2) in fact implies the symmetric ketone:

$$CH_3 - CH_2 - CH_2 - CO - CH_2 - CH_2 - CH_3$$

which has the spectrum

(3 2) (2 5) (2 2) [(0 0)]* (2 2) (2 5) (3 2)

in view of the equivalence of the protons in the molecule this would appear as:

(6 2) (4 5) (4 2).

The EXPLAIN function as it has been implemented does not attempt to point out to the student such implications but shows the student why, given his input, a molecule cannot be formed which satisfies the various constraints.

The second protocol, Figure 6, is for a molecule which does contain hetero-atoms in the chain. (In this context hetero implies non-carbon atoms.)

---

*This peak would not occur in the spectrum.

We have already noted that protons on adjacent centers do not appear to be affected by protons on hetero atoms and similarly protons on hetero atoms are apparently unaffected by their neighbors (see section 2).

Although the addition of hetero atoms may seem to be a simple modification it does complicate both the "build" algorithm and the explanations to the student. For instance one has to be very clear to distinguish between number of protons on a center and the number of interacting protons. For example, CH_2 has two hydrogens and 2 interacting protons; on the other hand the $-NH_2$ group has also two protons but no interacting protons.

When one is starting to build a molecule the only information one has is the list of atoms in the molecule and the spectrum. Thus the only advice that HELP can give at this point (see 2nd protocol, Figure 6) is to list all possible groups which are 1-valent and whose atoms are contained in the molecular formula. (N.B. that OH- is only included in "goodlist" if the (1 0) peak is present in the spectrum.) Similarly after a non-interacting group the usual information about the number of interacting protons which are in the group is not available and so again one can only suggest that the student considers all the groups which can be formed from the remaining atoms which are consistent with the spectrum and which have the appropriate valency (1 if this group will terminate the chain; otherwise 2). As we noted earlier, the "build" function follows an identical strategy under the same circumstances. In this protocol we see the student has asserted both an incorrect non-interacting group (he asserted -CO- instead of -NH-) and the incorrect group to follow a non-interacting group. We see that both of these errors are explained by showing him that no acceptable molecules can be built incorporating these groups.

5. The "build" Function

Given a molecular formula there is an algorithm in existence due to Lederberg [16] which can produce all possible molecular structures. However, we are working in a much more constrained situation--we have chosen only to consider linear and saturated molecules (i.e., no double bonds between groups are to be allowed). Also we have further valuable information contained in the peaks of the spectrum to further constrain this choice. The "build" function uses extensively information about the valency of atoms and groups and embodies a model of molecular structure as well as the simple NMR model we discussed in section 2.

"Build" has access to a function, "goodlist", which given the molecular formula and the spectrum will produce a list of possible groups. A further selection is made from this list by the function "intvalue" which chooses from the list produced by "goodlist" the groups which have the correct interaction and which have the correct valency. The outline of the "build" algorithm is given in figure 4. The function has four parameters which are molecule built, remaining molecular formula, spectra still to be explained and spectra for the molecule built so far. Thus it is possible to call this function with partially built molecules or with the initial data.

The first phase of the algorithm is concerned with finding groups which have the correct number of interacting protons, "groupl", and the appropriate list of peaks, "peakl", which correspond to the first element of "groupl". Thus if we called "build" with data for the $CH_3CH_2CH_2CH_2COCH_2CH_3$ molecule (the molecule discussed in figure 5) the "build" function would determine that the CH_3 has to be followed by a group with 2 interacting protons and that the splitting has to be greater or equal to 3, i.e., the

number of interacting protons on the current group.

In view of the atoms in the group the only 2-valent group possible is $-CH_2-$. However there are numerous peaks in the spectrum which correspond to area 2, i.e.:

(2 5) (2 4) (2 3) (2 2).

The only one which can be eliminated on immediate inspection is (2 2) because its splitting is less than the interaction of the previous group.

Thus in this case "build" would have only $-CH_2-$ in 'group1' but 'peak1' would consist of (2 4) (2 5) and (2 3). (As we have seen if the group follows a non-interacting group or is the head then the algorithm simply has to list all permissible groups in 'group1'. The flow diagram does not show this detail but simply states that a group has to be found.) This process continues until either the solution is found or the molecule built violates a constraint (see the student protocols and Figure 7 for example of the actual "diagnostics" reported.)

When the molecule being built violates a constraint the algorithm looks to see whether backtracking is possible. If it is not then the search ceases. Otherwise the algorithm first sees whether there are any further peaks in 'peak1'. For instance in the example we gave earlier if (2 4) lead to a violation then (2 5) would be tried next. If there are no items in 'peak1' then the algorithm checks to see if an alternative group exists in 'group1'. If such a group exists then the remaining spectrum is scanned to find appropriate peaks: 'peak1' is set up and control is passed to the updating part of the algorithm. If no group remains in 'group1' then the next member of the molecule and spectrum are considered.

The interesting feature about the "build" command is how sensitive it

is to the order of the items produced by 'goodlist'. [We have noted that after non-interacting groups and for the head we have to rely on 'goodlist' to produce an appropriate list of groups.] Figure 7 shows the effect on a particular example, of giving 'goodlist' more effective heuristics.

There heuristics are:

1) If an area of 3 exists in the spectrum and C and H are in the remaining molecular formula then this very probably corresponds to the CH_3 group.

2a) If (1 0) is in the spectrum and O and H are in the molecular formula then the group very probably corresponds to the group -OH.

2b) Similarly if (1 0) is in the spectrum and N and H are in the molecular formula then the group probably corresponds to -NH.

3) It is possible to hypothesize that groups -CO- and -O- are possible groups whenever the atoms C and O are in the molecular formula. (N.B. these correspond to the null peak.)

This ordering will ensure that if a peak 3 occurs then the first group tried for a head is CH_3. In Figure 7 we give 3 sets of values for 'goodlist', the 'groupl' compiled for the head and for the non-interacting groups.

The order of the groups is really only significant when we are using "build" to create structures. When it is called by EXPLAIN it is necessary for it to consider all possibilities anyway.

6. Reactions to the Program

So far the experience that we have had with this program is limited. However, all of the students commented that it gave them very explicit help in performing the reasoning underlying structural determination from simple NMR spectra. Most of the students said that they found the input format

difficult to type but agreed when challenged that they could not think of a better format. Certainly the overall impression we got from talking with the students and faculty was that this system had met a previous need. In particular they commented upon the depth of the explanations given.

It will take further experimentation to determine whether this program has helped the students formulate an approach to deductive reasoning tasks. In particular, it would be interesting to determine whether there was transfer between this and other analogous tasks.

7. Discussion

One obvious extension would be to enhance the program such that it could deal with nonlinear and unsaturated molecules--this is clearly something which could be easily done. This would involve a more complex "build" function and more complex HELP and EXPLAIN algorithms. However, as we had stressed earlier that the model which was being used here is not very sophisticated and is not sufficient to explain the NMR spectra of the majority of chemical compounds. The obvious question then arises as to whether a more "powerful" model could be incorporated into the teaching program. Certainly, there are a number of programs in existence which can with varying amounts of human interaction solve fairly sophisticated NMR spectra. (See for instance [17].) Such programs use a large number of heuristics to solve these spectra and we would argue that even if it were possible to formulate algorithms to solve the more complex spectra it would be extremely difficult to produce explanatory dialogues which would enable the student to follow the complicated logic used by the process model.

Given a set of n heuristics--there being rules which determine how

groups interact it is possible to envisage the following type of explanatory dialogue:

> if rule r applied to groups1 and 2 and rule s to groups 3 and 4
> then the spectrum would be S.
> However, if rule s applied to group 3 and so on. . .

Such sequences might get very complex indeed.

Before a system was produced which was to teach more complex spectra intensive discussions would have to be held with NMR experts to discover the exact nature of these many rules. (In fact Feigenbaum [18] reports that the DENDRAL project has in fact helped to "clarify" the underlying rules of Mass Spectrometry.)

The system we have discussed here is essentially one which is capable of generating/selecting a spectrum and then providing the student with helpful comments and suggestions as he attempts to solve these problems. It might well be possible to analyze the task further such that the "difficulty factors" could be enumerated (these are likely to contain the number of groups in the molecule, the number of non-interacting groups). Taking into account the students performance and the various difficulty factors it would be possible to produce an adaptive system which used student performance data when it selected the next problem.

The line of development which seems most profitable for this current program, and of greatest interest from the A.I. standpoint, is to see whether it would be possible to understand the explanations students give for making assertions, particularly incorrect ones. The current program contains logic to cope with incorrect assertions (see Figure 3) and thus has the ability to give the student explanations of his mistakes. A possible extension,

which could be of considerable educational value also, would be to add an ENQUIRY mode where the student was asked various questions about a particular aspect of his last (incorrect) assertion. Many of the responses to these questions would naturally be numbers or lists of spectral peaks. Some answers, however, would most naturally be sentences, e.g., giving the reasons why a particular spectral peak was not admissible at a particular position in the molecule. It would be a challenge to build a system to understand such dialogue. However, as the context is clearly defined this would appear to be possible. Winograd [19] has shown that natural language processing requires a realistic model of the subject being discussed: we have such a model--it is the algorithm which can perform the task and which we have used here as the basis for the HELP and EXPLAIN modes.

This paper has discussed the design of a knowledgeable problem solving monitor for the interpretation of NMR spectra. There are many other areas in which the scientist, and hence the science student, encounters deductive reasoning tasks and it seems likely that a number of other teaching areas could be treated by systems with similar structures to the one described here.

It has been argued that the teaching system is as good as its underlying model and also its analysis of the subject area. We have also discussed how such a system might be used as a model on which to base a limited natural language system.

Acknowledgements

This work has benefited from discussions of NMR spectroscopy with Dr. Shoulders, of the role of NMR in undergraduate chemistry teaching with Dr. J. M. White and Dr. Culp and of algorithmic approaches to teaching with

Tim O'Shea. Various people have kindly assisted me in becoming acquinted with TAURUS. This work was carried out during the period when I was associated with Dr. R. F. Simmons' research group and was in part supported by NSF GJ 509X.

References

[1] Carbonell, Jaime. AI in CAI: An Artificial Intelligence Approach to Computer-Assisted Instruction. IEEE Trans for Man-Machine Systems, 1970, Vol MMS-11, No. 4, P. 190.

[2] Wexler, Jonathan. Information Networks in Generative CAI. IEEE Trans for Man-Machine System, 1970, Vol. MMS-11, No. 4, p. 185.

[3] Uttal, W., Rogers, M., Hieronymous, R., and Pasich, T. Generative CAI in Analytic Geometry. Entelek, Inc., 1970.

[4] Uhr, L. Teaching Machine Programs that Generate Problems as a Function of Interaction with Students. Proc. 24th ACM National Conf., 1969, p. 125-134.

[5] Wexler, J. A Self Directed Teaching Program that Generates Simple Arithmetic Problems. Univ. of Wisconsin C.S. Report 19, 1968.

[6] Koffman, E. B. A Generative CAI Tutor for Computer Science Concepts. Proc. of Spring Joint Computer Conf., 1972.

[7] Peplinski, C. A Generating System for CAI Teaching of Simple Algebra Problems. Computer Science Technical Report 24, Univ. of Wisconsin, 1968.

[8] Woods, P. M., Hartley, J. R., Lovell, K., and Sleeman, D. H. The Teaching of Arithmetic Using a Computer-Based System. In: A. P. Mann and C. R. Brunstrom (Eds.), Aspects of Educational Technology, 3, 1969.

[9] Woods, P. M., and Hartley, J. R. Some Learning Models for Arithmetic Tasks and their Use in Computer-Based Learning. British Journal of Educational Psychology, Vol. 41, No. 1, p. 35-48, 1971.

[10] Hartley, J. R. and Sleeman, D. H. Towards More Intelligent Teaching Systems. International Journal of Man-Machine Systems, Vol. 5, 1973.

[11] Hartley, J. R., Sleeman, D. H., and Woods, P. M. Controlling the Learning of Diagnostic Tasks. International Journal of Man-Machine Studies, Vol. 4, p. 319, 1972.

[12] O'Shea, T., and Sleeman, D. H. A Design for an Adaptive Self-Improving Teaching System. Proc. 2nd International Conf. on Cybernetics at Oxford, Sept. 1972. In: "Advances in Cybernetics and Systems," edited by J. Rose. Gordon and Breach, 1973.

[13] Buchanan, B., Sutherland, G., and Feigenbaum, E. A. Heuristic Dendral: A Program for Generating Explanatory Hypotheses in Organic Chemistry. In: B. Meltzer and D. Michie Eds.), Machine Intelligence, Vol. 4, p. 209. Edinburgh University Press, 1969.

[14] Dyer, J. R. Applications of Absorption Spectroscopy of Organic Compounds. Prentice Hall, 1965, p. 58-132.

[15] Siklossy, L. Computer Tutors that Know What they Teach. Proceedings of First Joint Computer Conference, 1970, p. 251-255.

[16] Lederberg, J. DENDRAL-64, A System for Computer Construction, Enumeration and Notation of Organic Molecules as Tree Structures and Cyclic Graphs. 1964. Copies available from Stanford AI Project.

[17] Pham, Chi-Cong. Analyse automatique de spectres de Resonance magnetique nucleaire par des Procèdes heuristiques. Doctoral thesis of the University of Paris, 1972.

[18] Buchanan, B. G., Sutherland, G. L., and Feigenbaum, E. A. Rediscovering Some Problems of Artificial Intelligence in the Context of Organic Chemistry. In: B. Melzer and D. Michie (Eds.), Machine Intelligence, Vol. 5, p 253. Edinburgh University Press, 1970.

[19] Winograd, T. Procedures as a Representation for Data in a Computer Program for Understanding Natural Language. Ph.D. dissertation, MIT, 1971.

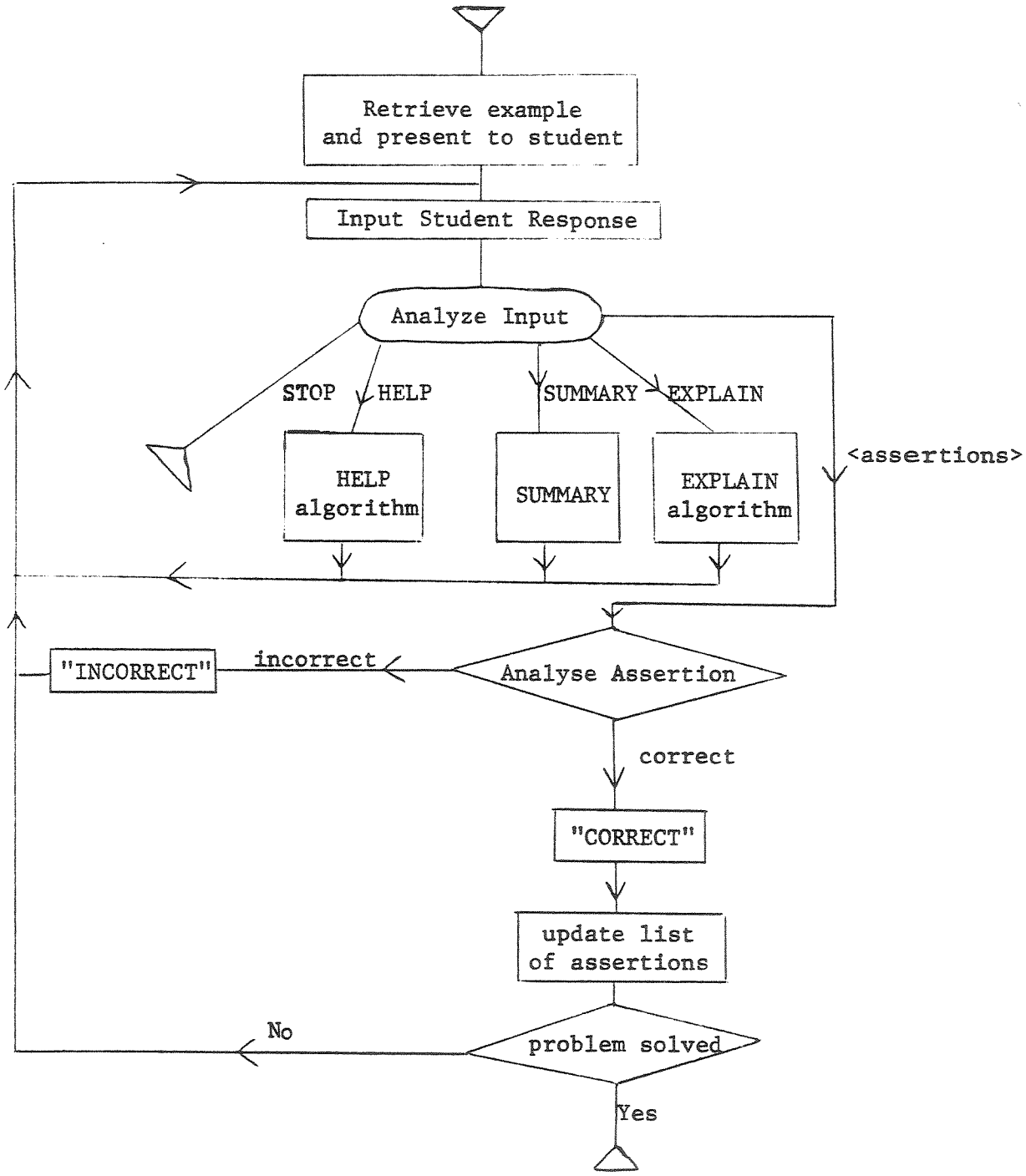


Figure 1: *Outline Structure of the NMR Problem Solving Monitor*

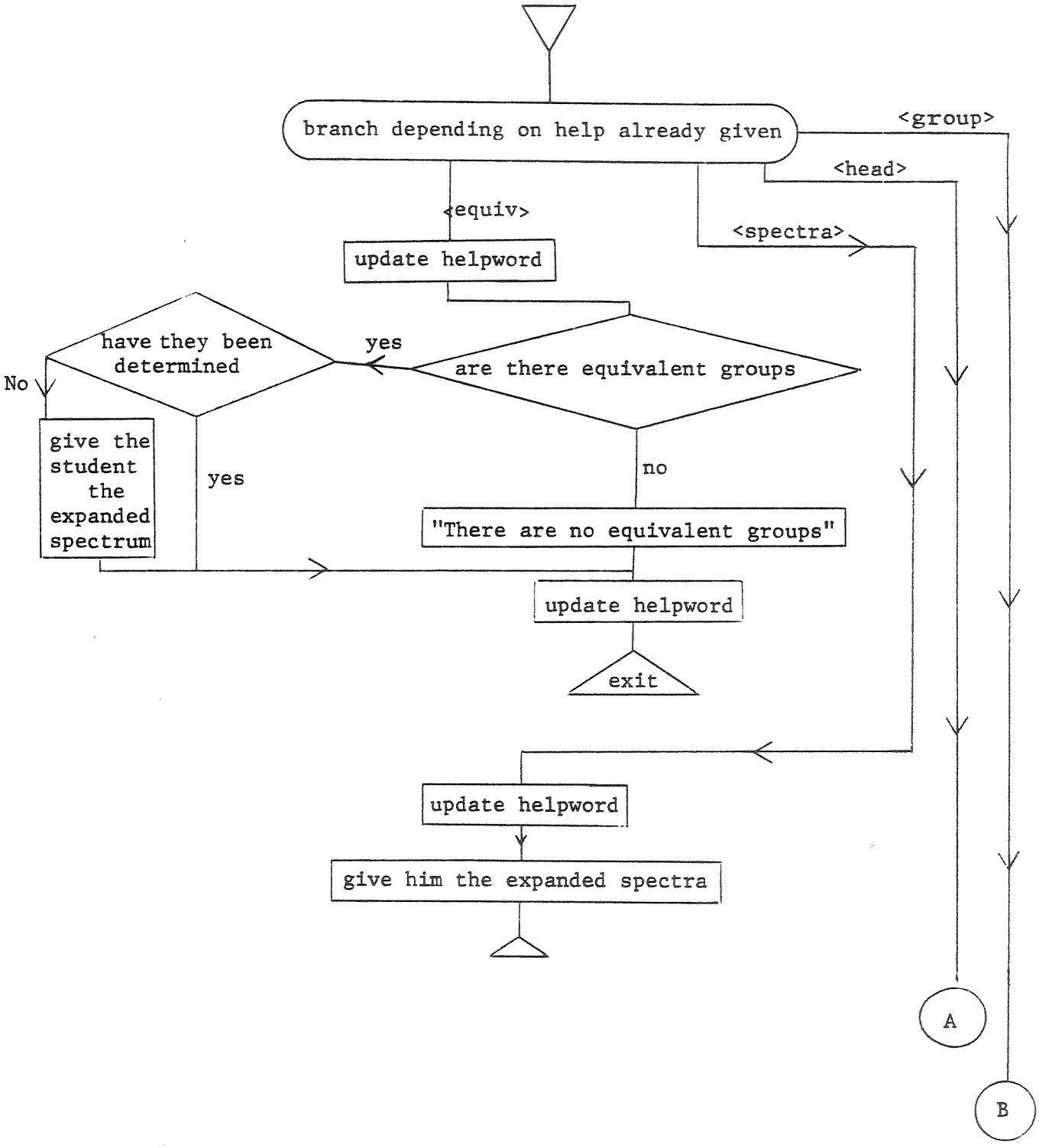


Figure 2 *The Flow Diagram for the 'HELP' Facility*

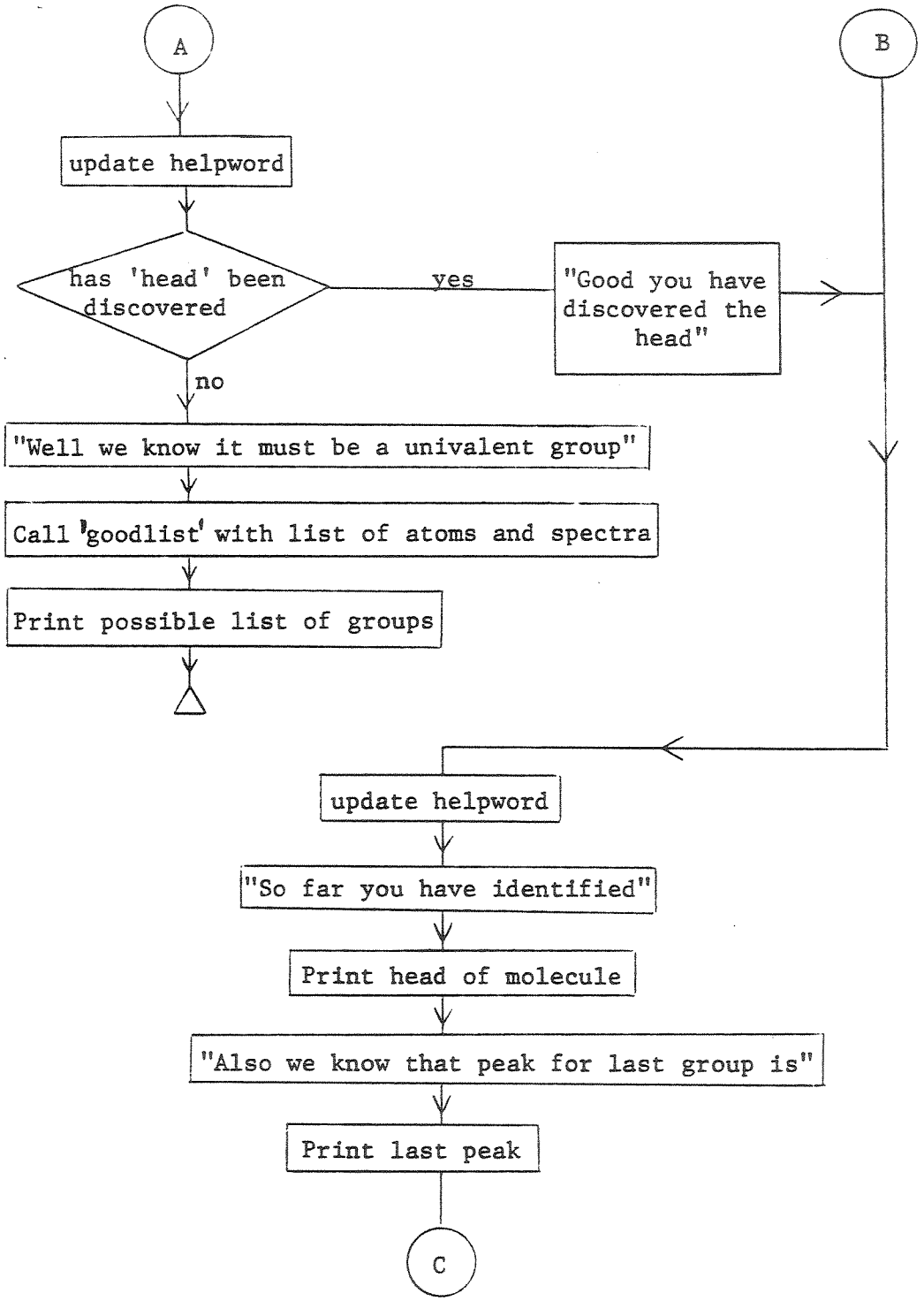
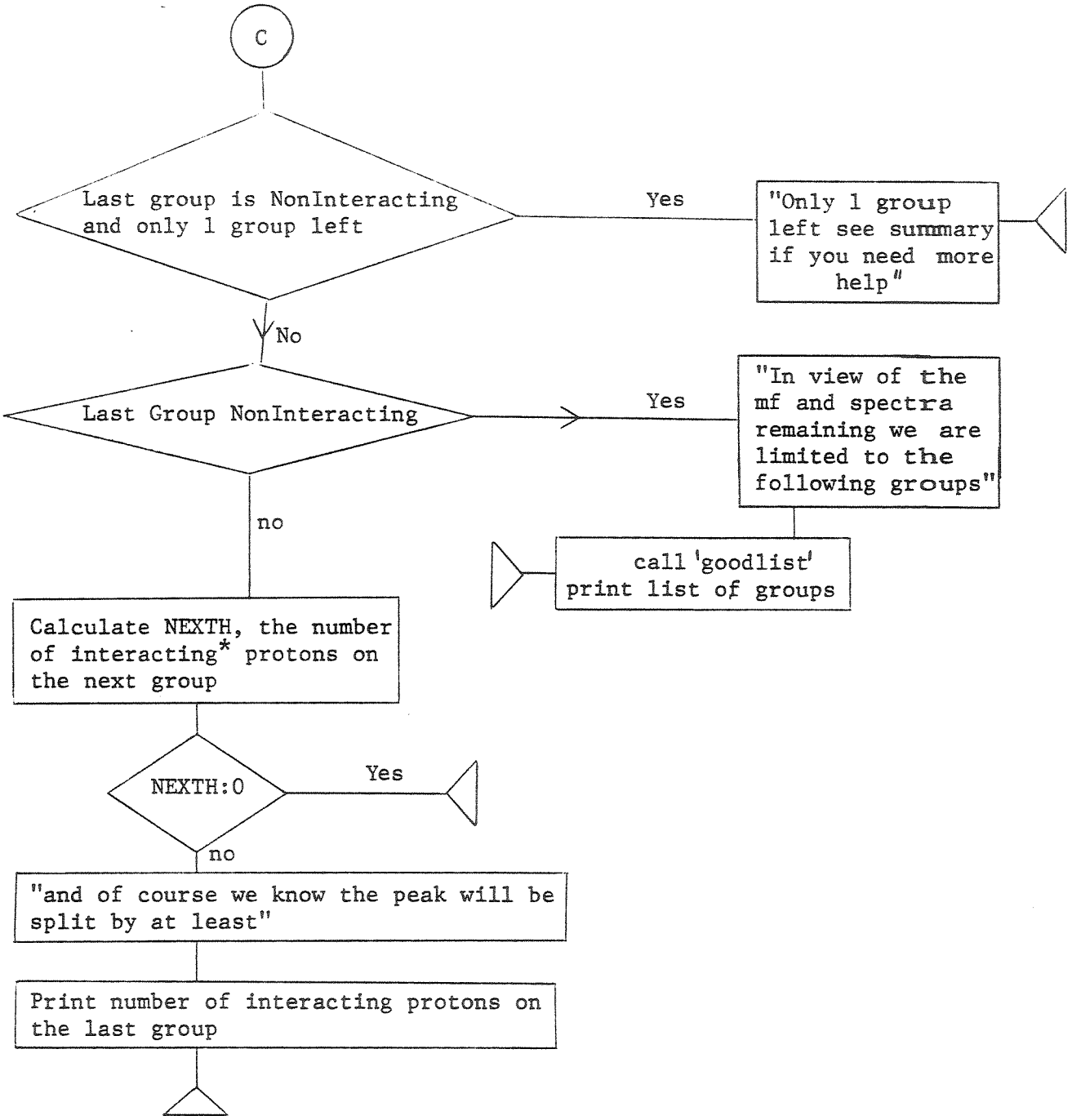


Figure 2, continued



*See formula of Section 2.

Figure 2, continued

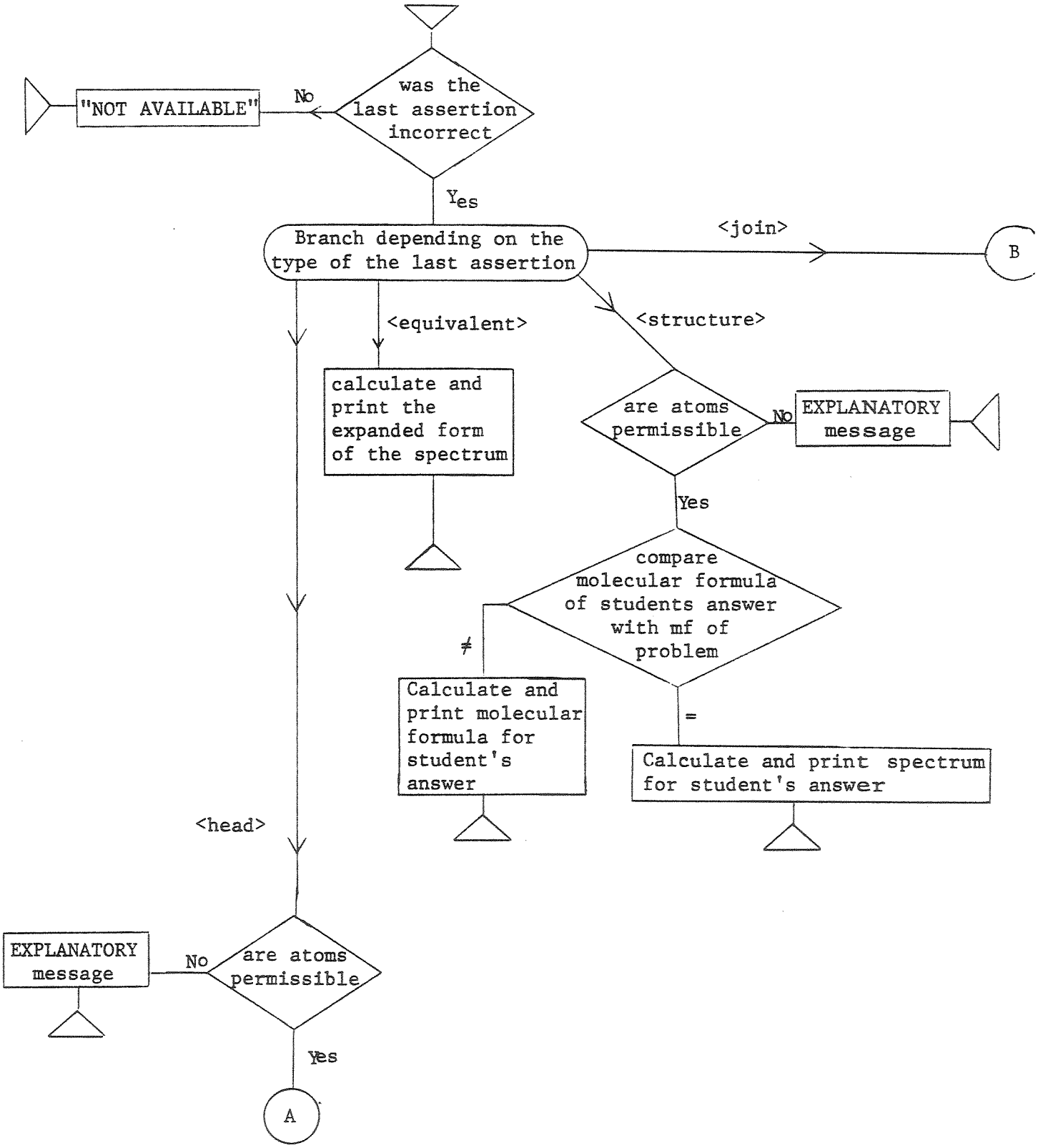


Figure 3 *The Flow Diagram for EXPLAIN*

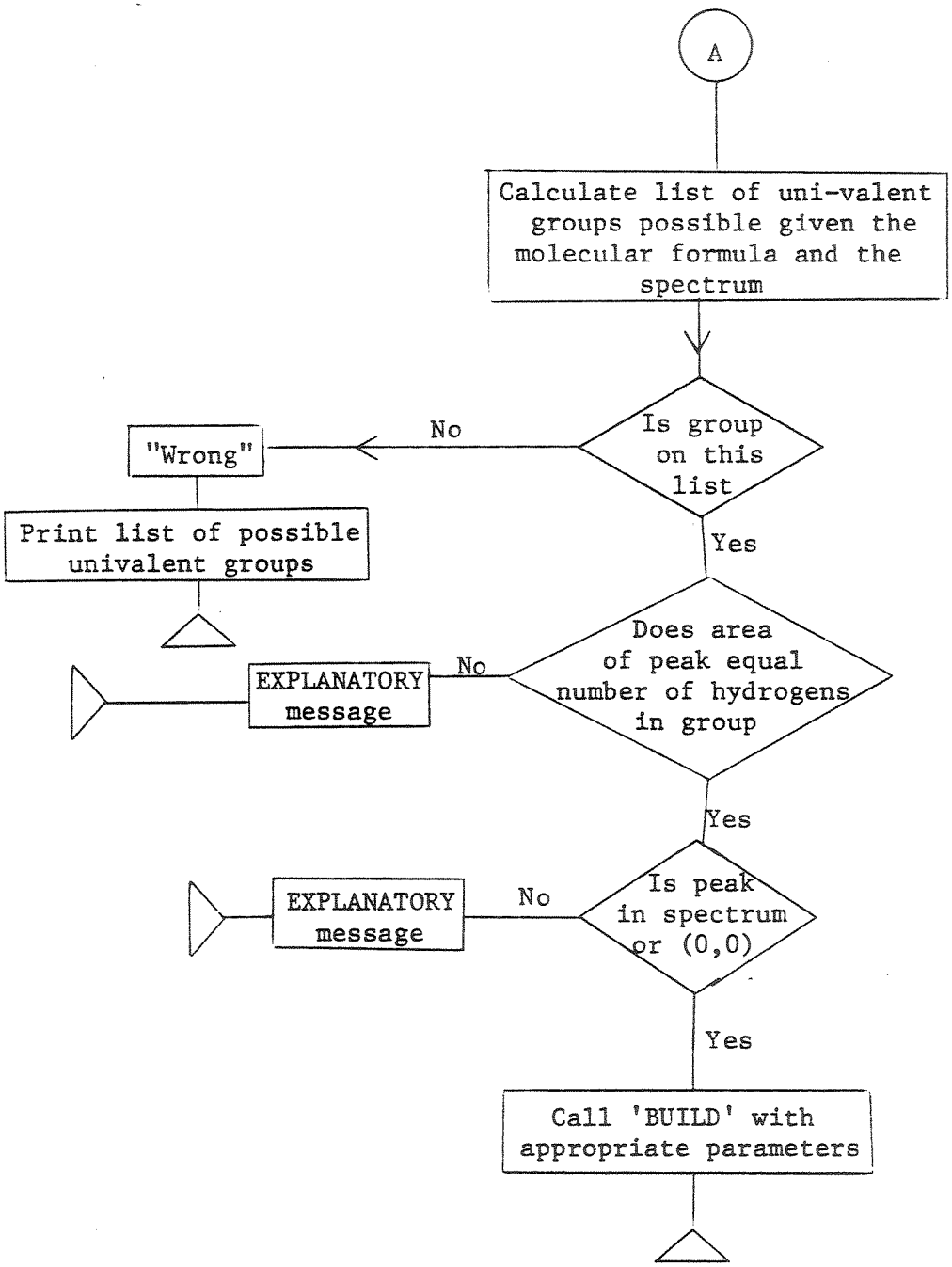


Figure 3, continued

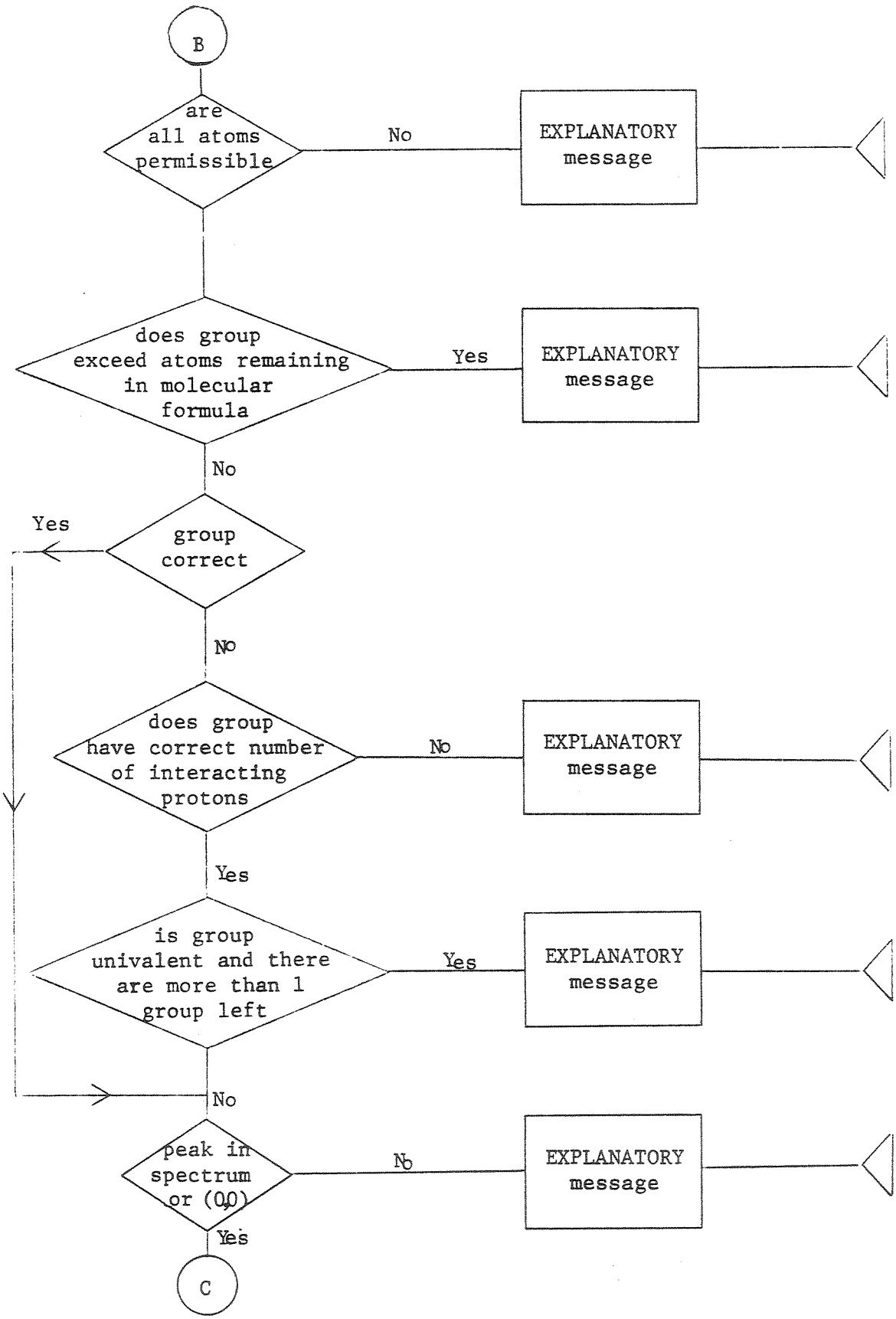


Figure 3, continued

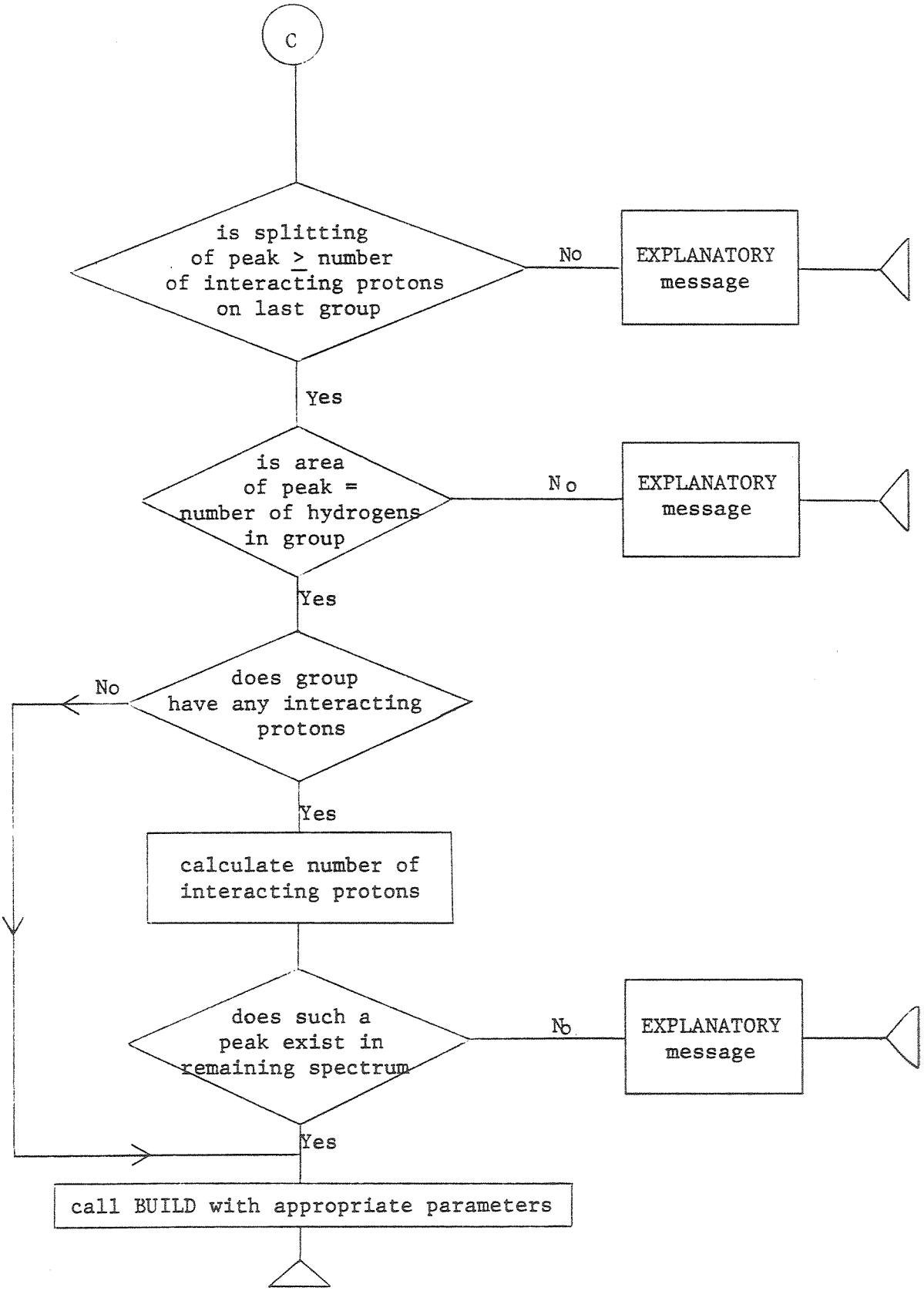


Figure 3, continued

Figure 4: *Outline of the BUILD Algorithm*

This flow diagram uses the following identifiers:

peakl: list of peaks
groupl: list of groups
rspc: spectra still to be explained
rmfr: remaining molecular formula
spc: spectra of molecule
head: structure of molecule so far built

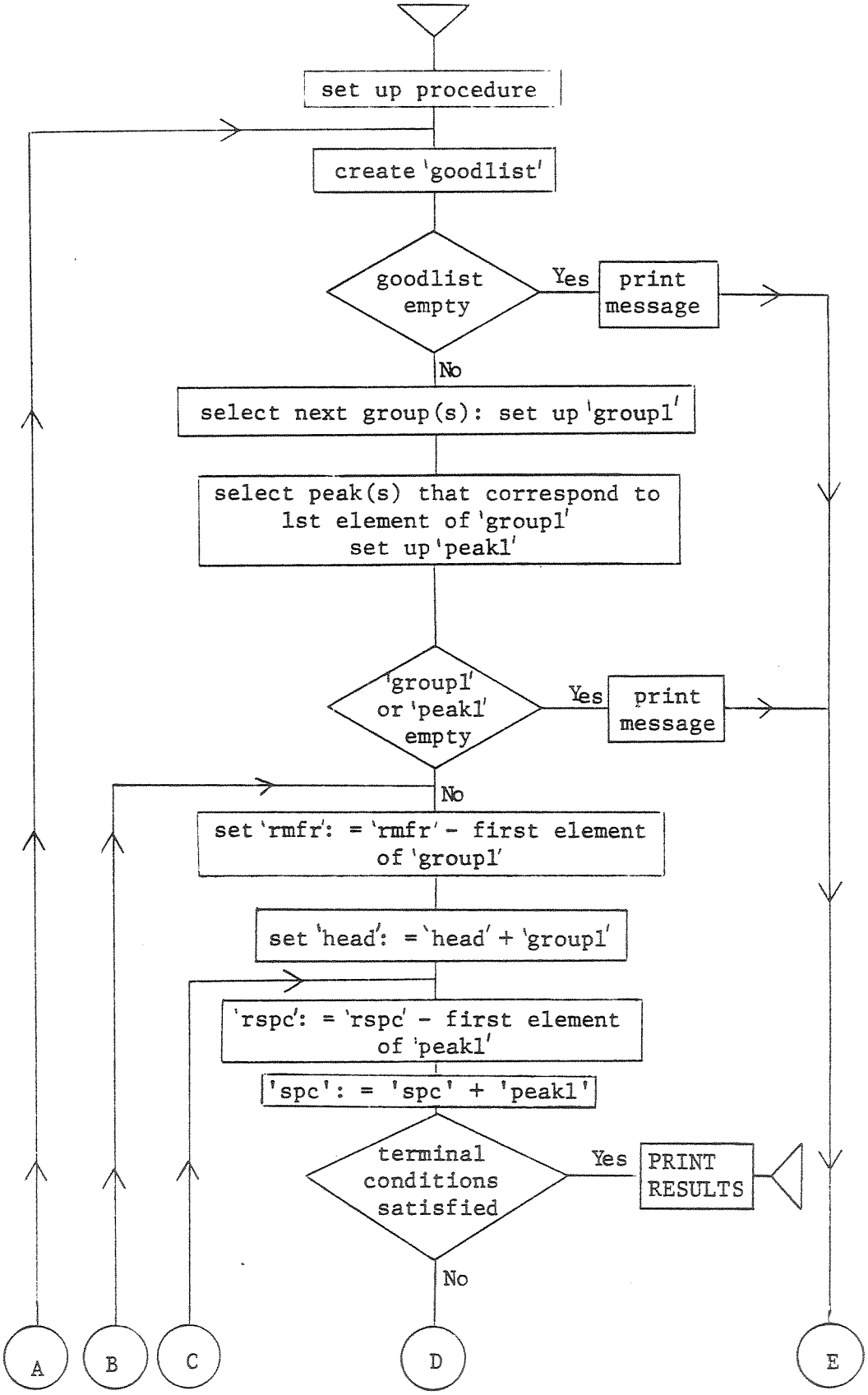


Figure 4: *Outline of the BUILD Algorithm*

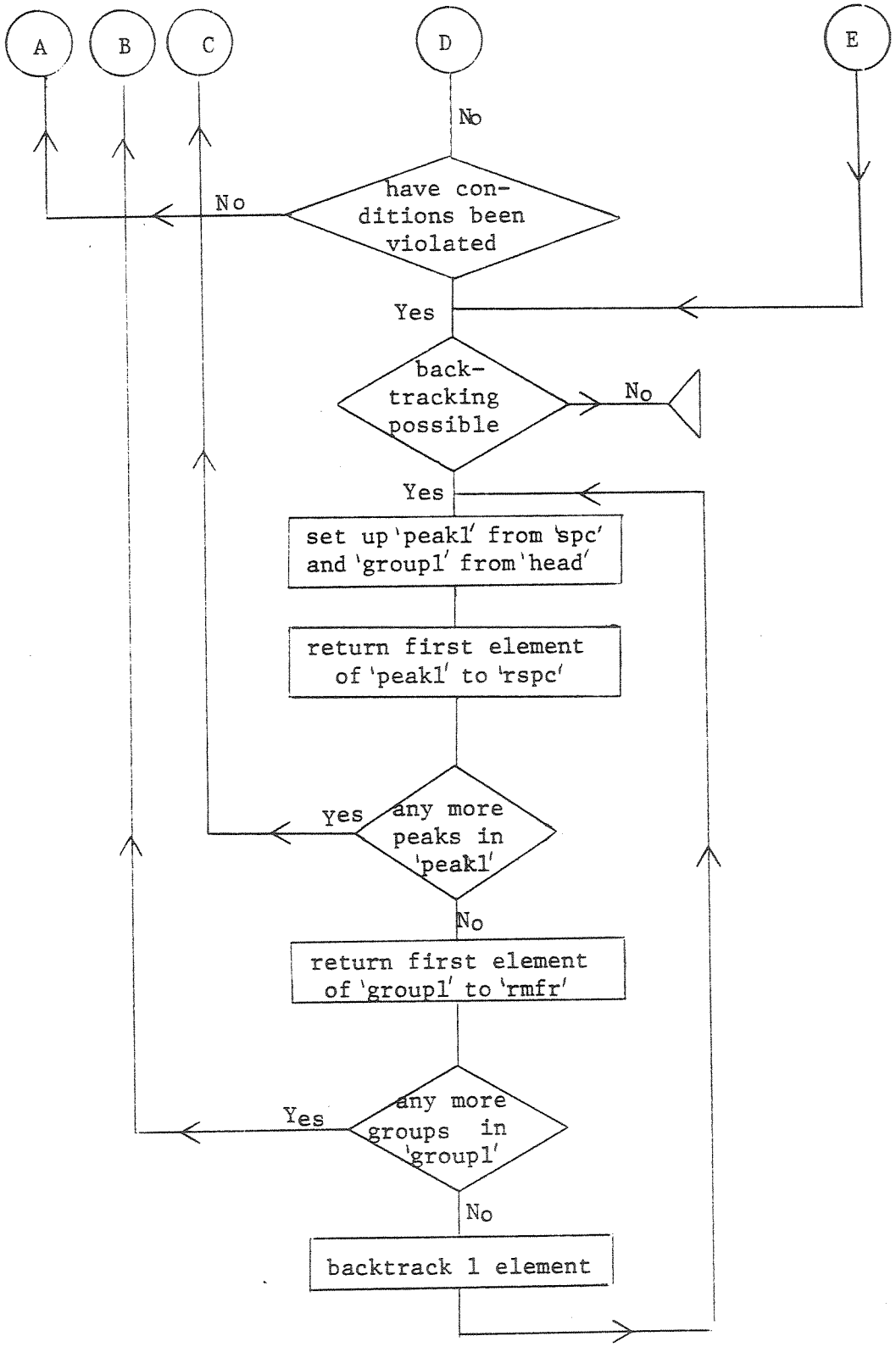


Figure 4, continued

FIGURE 5

The protocol for a session discussing the NMR spectra of $CH_3\ CH_2\ CH_2\ CH_2\ CO\ CH_2\ CH_3$

```
IN OUR NOTATION THE SPECTRUM OF YOUR MOLECULE IS
((6 2) (2 5) (2 4) (2 3) (2 2))
THE MOLECULAR FORMULA IS
(C 7 H 14 O)
*
(HELP)††
LOOP CAREFULLY AT THE SPECTRUM: DO YOU THINK THERE MAY BE EQUIVALENT
POSITIONS: ASK FOR HELP AGAIN IF YOU NEED IT
*
(HELP)
SPECTRUM IN ITS EXPANDED FORM IS
((3 2) (3 2) (2 5) (2 4) (2 3) (2 2))
*
((H)(C H 3)(3 3)
NO
*
(EXPLAIN)
GROUP SATISFIES VARIOUS CONSTRAINTS
PEAK NOT IN SPECTRUM
*
((H)(C H 3)(3 2))
CORRECT
*
(HELP)
GOOD YOU HAVE DISCOVERED THE HEAD OF THE MOLECULE
SO FAR YOU HAVE IDENTIFIED
((C H 3))
ALSO WE KNOW THAT THE PEAK FOR THE LAST GROUP IS
(3 2)
THE PREVIOUS GROUP HAS  [there was no previous group--therefore there must
0                        be ∅ interactions]
INTERACTING PROTONS: THEREFORE THE NEXT GROUP MUST HAVE
2
INTERACTING PROTONS: CHOOSE APPROPRIATE GROUPS FROM THOSE REMAINING
AND OF COURSE WE KNOW THE PEAK WILL BE SPLIT BY AT LEAST
3
HYDROGENS: IE THOSE ON THE CURRENT GROUP     [these arguments use the equations
*                                             outlined in Section 2]
((J)(H)(C H 2)(2 2))
```

---

††Student input follows on the line after the * character.

```
NO
*
(EXPLAIN)
YOUR GROUP WAS OK
WE KNOW SPLITTING HAS TO BE GREATER OR EQUAL TO
3
*
((J)(H)(C H 2)(2 4))
NO
*
(EXPLAIN)
YOUR GROUP WAS OK
WELL IF WE HAD SUCH A GROUP IT WOULD HAVE TO BE FOLLOWED BY A GROUP WITH
1
INTERACTING PROTONS
NO SUCH GROUP EXISTS IN REMAINING SPECTRA
*
((J)(H)(C H 2)(2 5))
CORRECT
*
(SUMMARY)
HEAD OF MOLECULE
((C H 3) (C H 2))
PEAK FOR THE LAST GROUP IS
(2 5)
REMAINING MOLECULAR FORMULA IS:
(C 5 H 9 O)
SPECTRA (EXPANDED FORM) STILL TO BE EXPLAINED IS
((3 2) (2 4) (2 3) (2 2))
*
((J)(H)(C H 2)(2 2))      [(2,3) is not possible for the same reasons as above]
NO
*
(EXPLAIN)
YOUR GROUP WAS OK
WELL IF WE HAD SUCH A GROUP IT WOULD HAVE TO BE FOLLOWED BY A GROUP WITH
0
INTERACTING PROTONS
WE WILL NOW ATTEMPT TO BUILD SUCH A MOLECULE

NO PEAK OF AREA
4
AND WHICH HAS SPLITTING GREATER OR EQUAL TO
2
SPECTRUM OF MOLECULE IS
((3 2) (2 5) (2 2) (0 0) (2 4))
MOLECULE BUILD WAS      [-CO- and -O- are the only non-interacting groups
((C H 3) (C H 2) (C H 2) (C O) (C H 2))                    possible]
SPECTRUM STILL TO BE EXPLAINED IS
((2 3) (3 2))
```

```
REMAINING MOLECULAR FORMULA
(C 2 H 5)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

GROUP TERMINATES CHAIN BUT ITEMS REMAIN
SPECTRUM OF MOLECULE IS
((3 2) (2 5) (2 2) (0 0) (2 3) (3 2))
MOLECULE BUILT WAS
((C H 3) (C H 2) (C H 2) (C O) (C H 2) (C H 3))
SPECTRUM STILL TO BE EXPLAINED IS
((2 4))
REMAINING MOLECULAR FORMULA
(C H 2)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

NO PEAK OF AREA        [now the algorithm tries to build a molecule with -O-
4                                                    as the non-interacting group]
AND WHICH HAS SPLITTING GREATER OR EQUAL TO
2
SPECTRUM OF MOLECULE IS
((3 2) (2 5) (2 2) (0 0) (2 4))
MOLECULE BUILT WAS
((C H 3) (C H 2) (C H 2) (O) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((3 2) (2 3))
REMAINING MOLECULAR FORMULA
(C 3 H 5)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

GROUP TERMINATES CHAIN BUT ITEMS REMAIN
SPECTRUM OF MOLECULE IS
((3 2) (2 5) (2 2) (0 0 ) (2 3) (3 2))
MOLECULE BUILT WAS
((C H 3) (C H 2) (C H 2) (O) (C H 2) (C H 3))
SPECTRUM STILL TO BE EXPLAINED IS
((2 4))
REMAINING MOLECULAR FORMULA
(C 2 H 2)
SEARCH WAS UNSUCCESSFUL
*
(SUMMARY)
HEAD OF MOLECULE
((C H 3) (C H 2))
PEAK FOR THE LAST GROUP IS
(2 5)
REMAINING MOLECULAR FORMULA IS:
(C 5 H 9 O)
SPECTRA (EXPANDED FORM) STILL TO BE EXPLAINED IS
((3 2) (2 4) (2 3) (2 2))
*
```

```
(HELP)
SO FAR YOU HAVE IDENTIFIED
((C H 3) (C H 2))
ALSO WE KNOW THAT THE PEAK FOR THE LAST GROUP IS
(2 5)
THE PREVIOUS GROUP HAS
3
INTERACTING PROTONS: THEREFORE THE NEXT GROUP MUST HAVE
2
INTERACTING PROTONS: CHOOSE APPROPRIATE GROUPS FROM THOSE REMAINING
AND OF COURSE WE KNOW THE PEAK WILL BE SPLIT BY AT LEAST
2
HYDROGENS: IE THOSE ON THE CURRENT GROUP
*
((J)(H)(C H 2)(2 4))        [(2,3) would again be rejected as there is no peak
CORRECT                      of area 1: (2,2) has also been shown to be untenable.
*                            Therefore must be (2,4)]
(HELP)
SO FAR YOU HAVE IDENTIFIED
((C H 3) (C H 2) (C H 2))
ALSO WE KNOW THAT THE PEAK FOR THE LAST GROUP IS
(2 4)
THE PREVIOUS GROUP HAS
2
INTERACTING PROTONS: THEREFORE THE NEXT GROUP MUST HAVE
2
INTERACTING PROTONS: CHOOSE APPROPRIATE GROUPS FROM THOSE REMAINING AND OF
COURSE WE KNOW THE PEAK WILL BE SPLIT BY AT LEAST
2
HYDROGENS: IE THOSE ON THE CURRENT GROUP
*
((J)(H)(C H 2)(2 2))
CORRECT
*
(HELP)
SO FAR YOU HAVE IDENTIFIED
((C H 3) (C H 2) (C H 2) (C H 2))
ALSO WE KNOW THAT THE PEAK FOR THE LAST GROUP IS
(2 2)
THE PREVIOUS GROUP HAS
2
INTERACTING PROTONS: THEREFORE THE NEXT GROUP MUST HAVE
0
INTERACTING PROTONS: CHOOSE APPROPRIATE GROUPS FROM THOSE REMAINING
*
((J)(H)(O)(0 0))            [we are told next group has no interacting protons:
NO                           student suggests -O-.  Explain shows why this is not
*                            possible.]
(EXPLAIN)

WE WILL NOW ATTEMPT TO BUILD SUCH A MOLECULE
```

```
NO PEAKS LEFT IN SPECTRA
SPECTRUM OF MOLECULE IS
((3 2) (2 5) (2 4) (2 2) (0 0) (2 3) (3 2))
MOLECULE BUILT WAS
((C H 3) (C H 2) (C H 2) (C H 2) (O) (C H 2) (C H 3))
SPECTRUM STILL TO BE EXPLAINED IS
NIL
REMAINING MOLECULAR FORMULA
(C)
SEARCH WAS UNSUCCESSFUL
*
((J)(H)(C O)(O O))
CORRECT
*
(HELP)
SO FAR YOU HAVE IDENTIFIED
((C H 3) (C H 2) (C H 2) (C H 2) (C O))
ALSO WE KNOW THAT THE PEAK FOR THE LAST GROUP IS
(0 0)
THE LAST GROUP HAD NO INTERACTING PROTONS - IN VIEW OF THE MF REMAINING AND
THE SPECTRA STILL TO BE EXPLAINED WE ARE LIMITED TO THE FOLLOWING GROUP(S)
((C H 2))    [As we have more than 1 group left it must be 2-valent]
*
((J)(H)(C H 2)(2 3))
CORRECT
*(SUMMARY)
HEAD OF MOLECULE
((C H 3) (C H 2) (C H 2) (C H 2) (C O) (C H 2))
PEAK FOR THE LAST GROUP IS
(2 3)
REMAINING MOLECULAR FORMULA IS:
(C H 3)
SPECTRA (EXPANDED FORM) STILL TO BE EXPLAINED IS
((3 2))
*
((S)(H)(C H 3))      [Structure = Molecule so far plus the (CH3) group]
CORRECT
```

FIGURE 6

The protocol for a session discussing the NMR spectra of CH_3 NH CH_2 CH_2 CHO

```
IN OUR NOTATION THE SPECTRUM OF YOUR MOLECULE IS
((3 0) (2 3) (2 2) (1 2) (1 0))
THE MOLECULAR FORMULA IS
(C4 H 9 N O)
*
(HELP)††
THERE ARE NO EQUIVALENT GROUPS IN THIS MOLECULE
*
(HELP)
WELL WE KNOW WE MUST HAVE A GROUP OF VALENCY 1 ON THE END OF A CHAIN AND IN
VIEW OF THE ELEMENTS IN THE MOLECULE AND THE PEAKS IN THE SPECTRUM OUR CHOISE
IS LIMITED TO
((O H) (C H 3) (C H O))      [-OH is mentioned because there is a (1,0) peak in
*                             the spectrum: similarly this explains selection of
((H)(C H 3)(3 2))             CHO: CH3 selected as there are peaks of area 3.
NO                            NB: -NH2 omitted as the peak (2,0) is not present
*                             in spectrum]
(EXPLAIN)
GROUP SATISFIES VARIOUS CONSTRAINTS
PEAK NOT IN SPECTRUM
*
((H)(C H 3)(3 0))
CORRECT
*
(HELP)
SO FAR YOU HAVE IDENTIFIED
((C H 3))
ALSO WE KNOW THAT THE PEAK FOR THE LAST GROUP IS
(3 0)
THE PREVIOUS GROUP HAS
0
INTERACTING PROTONS: THEREFORE THE NEXT GROUP MUST HAVE
0
INTERACTING PROTONS: CHOOSE APPROPRIATE GROUPS FROM THOSE REMAINING
*
((J)(H)(C 0)(0 0))      [Certainly this is a non-interacting group]
NO
*
(EXPLAIN)       [Explain shows why such a choice is not feasible]
WE WILL NOW ATTEMPT TO BUILD SUCH A MOLECULE
```

---

††Student input follows on the line after the * character.

```
GIVEN THE REMAINING ATOMS AND SPECTRA NO MORE GROUPS CAN BE FORMED
SPECTRUM OF MOLECULE IS
((3 0) (0 0) (1 0) (2 2) (2 3))
MOLECULE BUILT WAS
((C H 3) (C O) (N H) (C H 2) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 2))
REMAINING MOLECULAR FORMULA
(H)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

NO PEAK OF AREA
3
AND WHICH HAS SPLITTING GREATER OR EQUAL TO
2
SPECTRUM OF MOLECULE IS
((3 0) (0 0) (1 0) (2 3))
MOLECULE BUILT WAS
((C H 3) (C O) (N H) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 2) (2 2))
REMAINING MOLECULAR FORMULA
(C H 3)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

NOT POSSIBLE TO FORM FURTHER GROUP
SPECTRUM OF MOLECULE IS
((3 0) (0 0) (2 2) (2 3))
MOLECULE BUILT WAS
((C H 3) (C O) (C H 2) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 0) (1 2))
REMAINING MOLECULAR FORMULA
(H 2 N)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

NO PEAK OF AREA
3
AND WHICH HAS SPLITTING GREATER OR EQUAL TO
2
SPECTRUM OF MOLECULE IS
((3 0) (0 0) (2 3))
MOLECULE BUILT WAS
((C H 3) (C O) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 0) (1 2) (2 2))
REMAINING MOLECULAR FORMULA
(C H 4 N)
SEARCH WAS UNSUCCESSFUL
*
((J)(H)(N H)(O 0))
```

```
NO
*
(EXPLAIN)
AREA OF PEAK DOES NOT AGREE WITH NUMBER OF HYDROGENS IN THE GROUP
*
((J)(H)(N H)(1 0))
CORRECT
*
(HELP)
SO FAR YOU HAVE IDENTIFIED
((C H 3) (N H))
ALSO WE KNOW THAT THE PEAK FOR THE LAST GROUP IS
(1 0)
THE LAST GROUP HAD NO INTERACTING PROTONS - IN VIEW OF THE MF REMAINING AND
THE SPECTRA STILL TO BE EXPLAINED WE ARE LIMITED TO THE FOLLOWING GROUP(S)
((C H 2) (C O) (O))      [after a non-interacting group we must consider all
*                         possible 2-valent groups which are consistent with
((J)(H)(C O)(O O))        remaining groups and spectra (this is analagous to
NO                        the choice of the head when we could only advise
*                         student of the possibilities)]
(EXPLAIN)
WE WILL NOW ATTEMPT TO BUILD SUCH A MOLECULE

GIVEN THE REMAINING ATOMS AND SPECTRA NO MORE GROUPS CAN BE FORMED
SPECTRUM OF MOLECULE IS
((3 0) (1 0) (0 0) (2 2) (2 3))
MOLECULE BUILT WAS
((C H 3) (N H) (C O) (C H 2) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 2))
REMAINING MOLECULAR FORMULA
(H)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

NO PEAK OF AREA
3
AND WHICH HAS SPLITTING GREATER OR EQUAL TO
2
SPECTRUM OF MOLECULE IS
((3 0) (1 0) (0 0) (2 3))
MOLECULE BUILT WAS
((C H 3) (N H) (C O) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 2) (2 2))
REMAINING MOLECULAR FORMULA
(C H 3)
SEARCH WAS UNSUCCESSFUL
*
((J)(H)(C H 2)(2 2))      [So student tries the -CH2 group]
CORRECT
*
```

```
(HELP)
SO FAR YOU HAVE IDENTIFIED
((C H 3) (N H) (C H 2))
ALSO WE KNOW THAT THE PEAK FOR THE LAST GROUP IS
(2 2)
THE PREVIOUS GROUP HAS
0
INTERACTING PROTONS: THEREFORE THE NEXT GROUP MUST HAVE
2
INTERACTING PROTONS: CHOOSE APPROPRIATE GROUPS FROM THOSE REMAINING
AND OF COURSE WE KNOW THE PEAK WILL BE SPLIT BY AT LEAST
2
HYDROGENS: IE THOSE ON THE CURRENT GROUP
*
((J)(H)(C H 2)(2 2))
NO
*
(EXPLAIN)
YOUR GROUP WAS OK
PEAK IS NOT IN SPECTRUM STILL TO BE EXPLAINED
*
(SUMMARY)
HEAD OF MOLECULE
((C H 3) (N H) (C H 2))
PEAK FOR THE LAST GROUP IS
(2 2)
REMAINING MOLECULAR FORMULA IS:
(C 2 H 3 O)
SPECTRA (EXPANDED FORM) STILL TO BE EXPLAINED IS
((2 3) (1 2))    [this shows the student which peaks of area 2 are still to
*                                          be explained]
((J)(H)(C H 2)(2 3))
CORRECT
*
(SUMMARY)
HEAD OF MOLECULE
((C H 3) (N H) (C H 2) (C H 2))
PEAK FOR THE LAST GROUP IS
(2 3)
REMAINING MOLECULAR FORMULA IS:
(C H O)
SPECTRA (EXPANDED FORM) STILL TO BE EXPLAINED IS
((1 2))
*
((S)(H)(C H O))    [says molecular structure equals molecule so far constructed
CORRECT                                          plus the -CHO group]
```

FIGURE 7

How the build function performs with different goodlists

```
*EVALQUOTE:
BUILD(()(C4 H9 O N)((3 0)(2 3)(2 2)(1 2)(1 0))())

NOT POSSIBLE TO FORM FURTHER GROUP
SPECTRUM OF MOLECULE IS
((3 0) (0 0) (2 2) (2 3))
MOLECULE BUILT WAS
((C H 3) (C O) (C H 2) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 0) (1 2))
REMAINING MOLECULAR FORMULA
(H 2 N)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

NO PEAK OF AREA
3
AND WHICH HAS SPLITTING GREATER OR EQUAL TO
2
SPECTRUM OF MOLECULE IS
((3 0) (0 0) (2 3))
MOLECULE BUILT WAS
((C H 3) (C O) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 0) (1 2) (2 2))
REMAINING MOLECULAR FORMULA
(C H 4 N)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

GIVEN THE REMAINING ATOMS AND SPECTRA - NO MORE GROUPS CAN BE FORMED
SPECTRUM OF MOLECULE IS
((3 0) (0 0) (1 0) (2 2) (2 3))
MOLECULE BUILT WAS
((C H 3) (C O) (N H) (C H 2) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 2))
REMAINING MOLECULAR FORMULA
(H)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

NO PEAK OF AREA
3
AND WHICH HAS SPLITTING GREATER OR EQUAL TO
2
```

[Initial goodlist: (C H 3) (C H 2) (C H 0) (C O) (O) (N H) (OH)
Possible heads for chain: (C H 3) (C H O) (O H)
Possible non-interacting 2-valent groups: (-C O-) (-O-) (-N H-)

```
SPECTRUM OF MOLECULE IS
((3 0) (0 0) (1 0) (2 3))
MOLECULE BUILT WAS
((C H 3) (C O) (N H) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 2) (2 2))
REMAINING MOLECULAR FORMULA
(C H 3)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

NOT POSSIBLE TO FORM FURTHER GROUP
SPECTRUM OF MOLECULE IS
((3 0) (0 0) (2 2) (2 3))
MOLECULE BUILT WAS
((C H 3) (O) (C H 2) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 2) (1 0))
REMAINING MOLECULAR FORMULA
(C H 2 N)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

NO PEAK OF AREA
3
AND WHICH HAS SPLITTING GREATER OR EQUAL TO
2
SPECTRUM OF MOLECULE IS
((3 0) (0 0) (2 3))
MOLECULE BUILT WAS
((C H 3) (O) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 2) (1 0) (2 2))
REMAINING MOLECULAR FORMULA
(C 2 H 4 N)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

NOT POSSIBLE TO FORM FURTHER GROUP
SPECTRUM OF MOLECULE IS
((3 0) (0 0) (1 0) (2 2) (2 3))
MOLECULE BUILT WAS
((C H 3) (O) (N H) (C H 2) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 2))
REMAINING MOLECULAR FORMULA
(C H)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

NO PEAK OF AREA
3
AND WHICH HAS SPLITTING GREATER OR EQUAL TO
2
SPECTRUM OF MOLECULE IS
```

```
((3 0) (0 0) (1 0) (2 3))
MOLECULE BUILT WAS
((C H 3) (O) (N H) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((1 2) (2 2))
REMAINING MOLECULAR FORMULA
(C 2 H 3)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

SOLUTION IS
((C H 3) (N H) (C H 2) (C H 2) (C H O))
```

FIGURE 7B

```
*EVALQUOTE:
BUILD(()(C4 H 9 O N)((3 0)(2 3)(2 2)(1 2)(1 0))())

NOT POSSIBLE TO FORM FURTHER GROUP
SPECTRUM OF MOLECULE IS
((1 0) (2 2) (2 3))
MOLECULE BUILT WAS
((O H) (C H 2) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((3 0) (1 2))
REMAINING MOLECULAR FORMULA
(C 2 H 4 N)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

NO PEAK OF AREA
3
AND WHICH HAS SPLITTING GREATER OR EQUAL TO
2
SPECTRUM OF MOLECULE IS
((1 0) (2 3))
MOLECULE BUILT WAS
((O H) (C H 2))
SPECTRUM STILL TO BE EXPLAINED IS
((3 0) (1 2) (2 2))
REMAINING MOLECULAR FORMULA
(C 3 H 6 N)
THE SEARCH FOR A STRUCTURE WILL BE CONTINUED

SOLUTION IS
((C H 3) (N H) (C H 2) (C H 2) (C H O))
```

[initial goodlist: (NH), (OH), (CH_3), (CH_2), (CHO), (CO), (O)
possible heads for chain (1-valent): (OH), (CH_3), (CHO)
possible non-interacting 2-valent groups: (NH), (CO), (O)]