United States Patent [19]

Feldman

[11] **Patent Number: 4,967,372**

[45] **Date of Patent: Oct. 30, 1990**

[54] **AUTOMATIC ORIENTATION AND INTERACTIVE ADDRESSING OF DISPLAY**

[75] Inventor: **Alfred P. Feldman**, Columbia, Md.

[73] Assignee: **The United States of America as represented by the Department of Health and Human Services**, Washington, D.C.

[21] Appl. No.: **863,981**

[22] Filed: **May 16, 1986**

[51] **Int. Cl.**[5] **G06F 15/66**

[52] **U.S. Cl.** **364/518**; 340/721; 400/110

[58] **Field of Search** .... 364/518, 521, 522; 346/139 R; 340/703, 923; 400/110, 484; 382/44–47

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Primary Examiner—H. R. Herndon

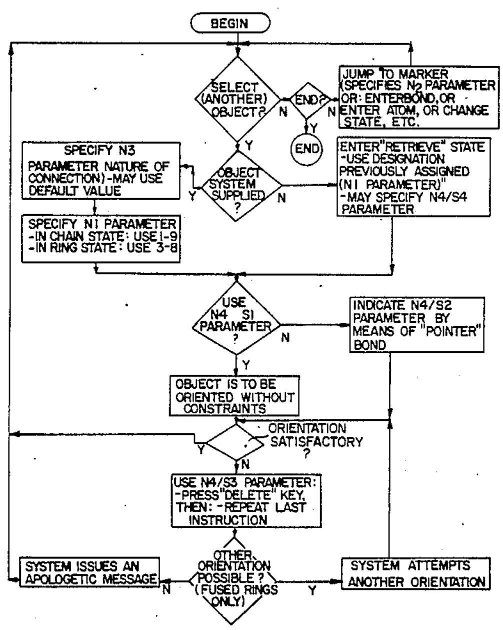
Assistant Examiner—H. R. Herndon

Attorney, Agent, or Firm—Glenna Hendricks; Marc A. Miller

[57] **ABSTRACT**

Automatic orientation of predefined chemical structures in conjunction with a computer terminal employs respective protocols corresponding to a system state. The system states can include a chain state, ring state, library state, and retrieve state. Upon orientation, the object is attached according to a specified attachment command to a parent graph. The protocols corresponding to connection of the object to the parent includes rules regarding angles at which the structures can be attached to one another, and another protocol governs rules respecting rotation of the stored object through predetermined angles. Nodes of the object recalled are automatically provided with markers in alphabetic order from the most recently used marker corresponding to a letter of alphabet. Multiple alphabet sequences are used. Specification of position is indicated by inputting the lower case letter of the alphabet corresponding to the location desired. Bonds can be specified between two markers.

21 Claims, 9 Drawing Sheets



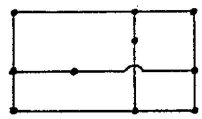


FIG. 1(a)

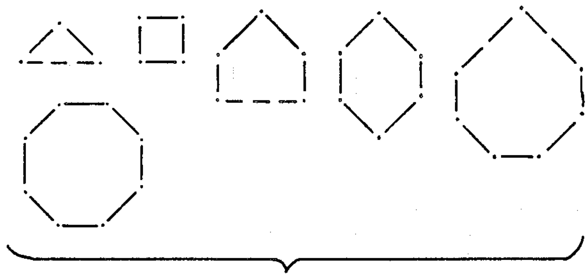
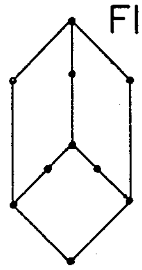


FIG. 2(a)

FIG. 1(b)



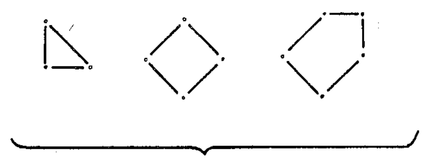
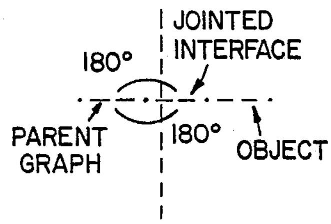


FIG. 2(b)

FIG. 3(a)



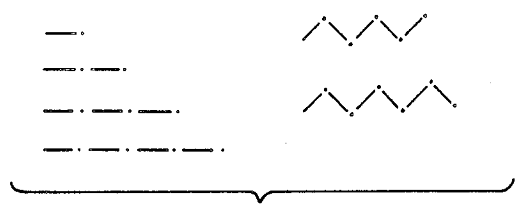


FIG. 2(c)

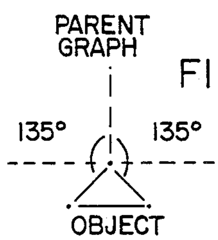


FIG. 3(b)

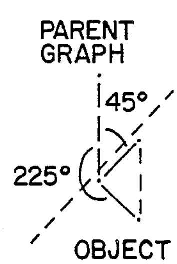


FIG. 3(c)

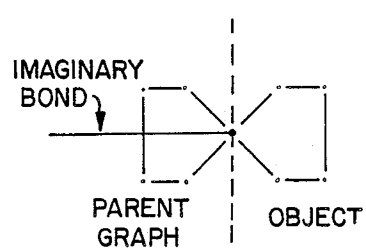


FIG. 4(a)

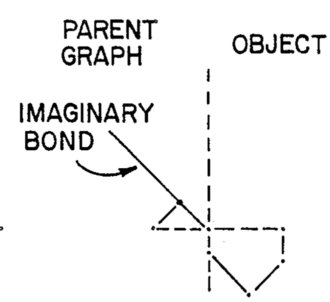
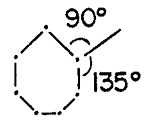
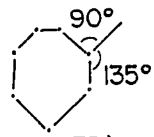


FIG. 4(b)



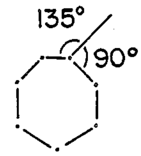
(NOT OBTAINED)

FIG. 5(a)



(OBTAINED)

FIG. 5(b)



(NOT OBTAINED)

FIG. 5(c)

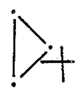


FIG. 6(a)

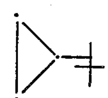
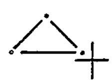
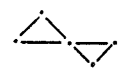
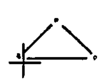
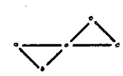


FIG. 6(b)

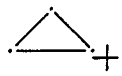
PARENT GRAPH	ENTER *	RESULT	
	3		FIG. 7(a)
	03		FIG. 7(b)
	03		FIG. 7(c)
	03		FIG. 7(d)

* FIRST DIGIT = N_3 CONNECTION CODE - SECOND DIGIT = N_1 IDENTIFICATION CODE.

PARENT GRAPH ENTER RESULT

3

FIG. 8(a)



13 OR 3

FIG. 8(b)

13 OR 3

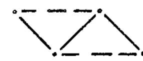
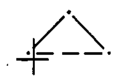


FIG. 8(c)



13 OR 3

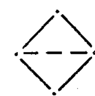
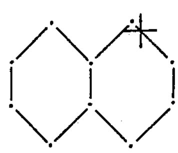


FIG. 8(d)

PARENT GRAPH ENTER RESULT



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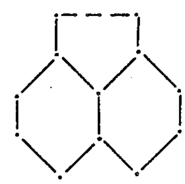
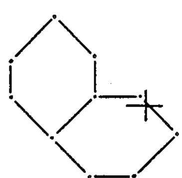


FIG. 9(a)



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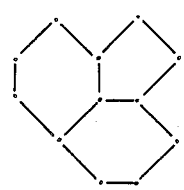


FIG. 9(b)

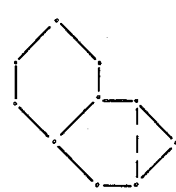


FIG. 9(c)

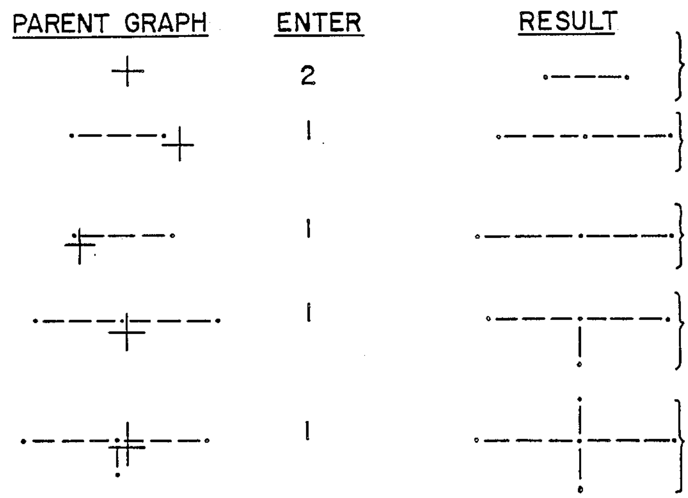


FIG. 10(a)
FIG. 10(b)
FIG. 10(c)
FIG. 10(d)
FIG. 10(e)

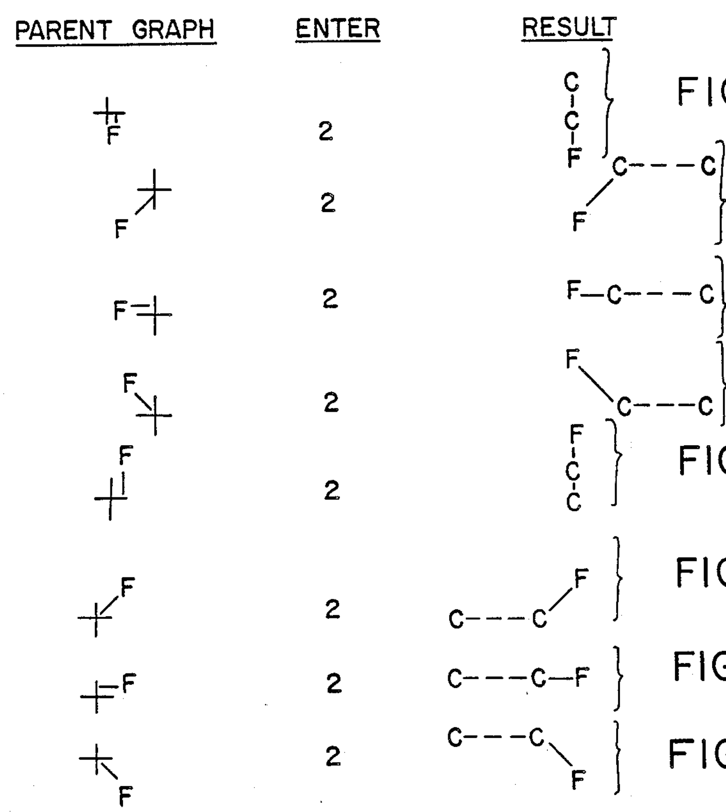


FIG. 11(a)
FIG. 11(b)
FIG. 11(c)
FIG. 11(d)
FIG. 11(e)
FIG. 11(f)
FIG. 11(g)
FIG. 11(h)

PARENT GRAPH ENTER* RESULT

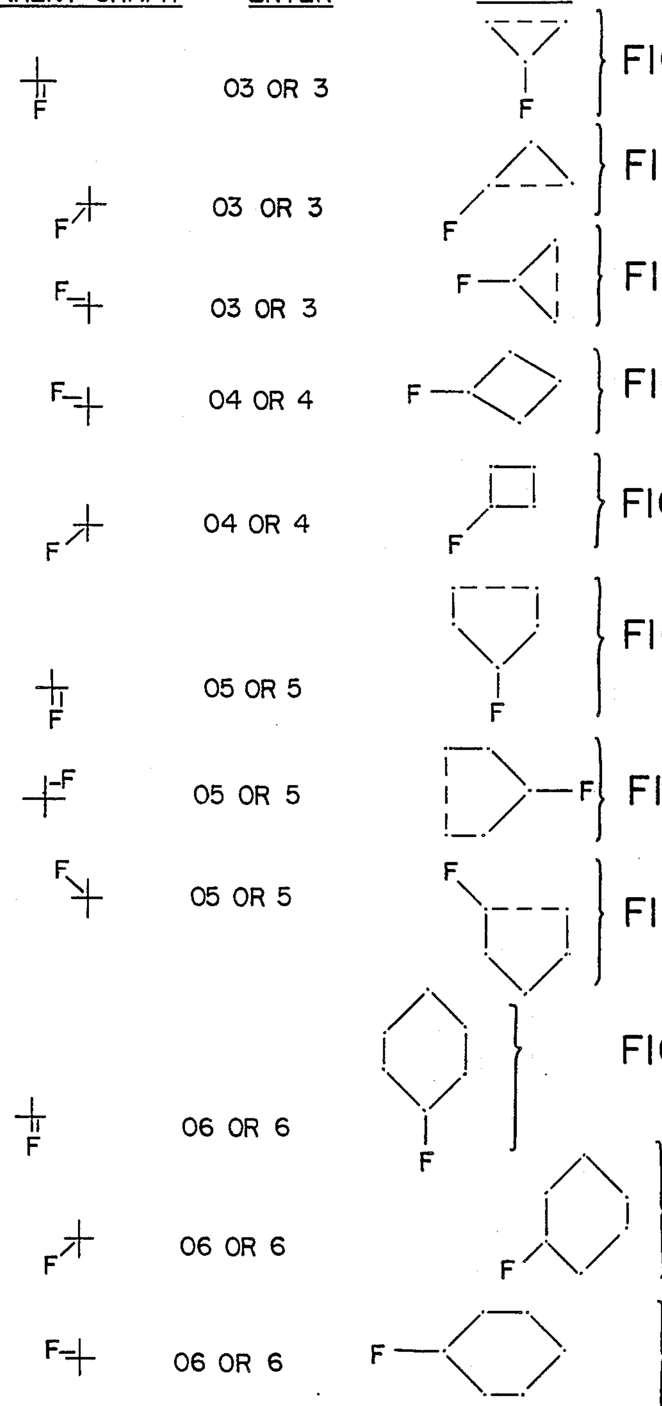


FIG. 12(a)

FIG. 12(b)

FIG. 12(c)

FIG. 12(d)

FIG. 12(e)

FIG. 12(f)

FIG. 12(g)

FIG. 12(h)

FIG. 12(i)

FIG. 12(j)

FIG. 12(k)

07 OR7

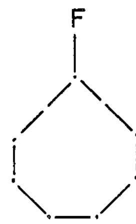


FIG. 12(l)

07 OR 7

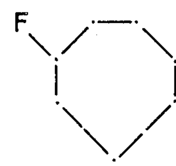


FIG. 12(m)

07 OR 7

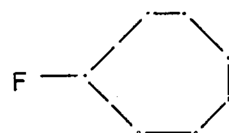


FIG. 12(n)

08 OR 8

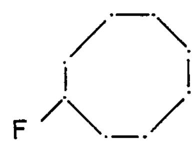


FIG. 12(o)

08 OR 8

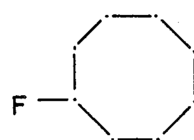
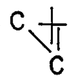
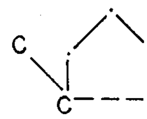
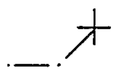
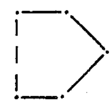
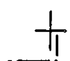
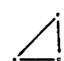


FIG. 12(p)

PARENT GRAPH	ENTER *	RESULT	
	15	 (FORCES SHARP ANGLE)	FIG. 13(a)
	25	 (FORCES NON-STANDARD ORIENTATION)	FIG. 13(b)
	23	 (FORCES USE OF ALTERNATIVE SHAPE)	FIG. 13(c)

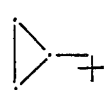
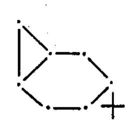
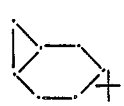
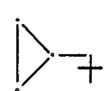
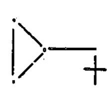
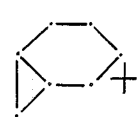
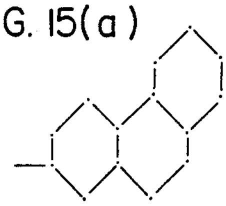
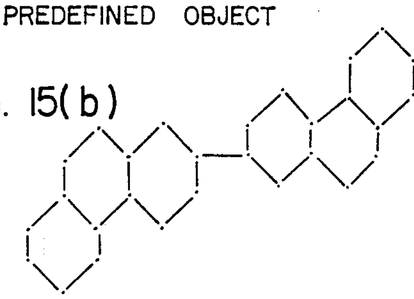
PARENT GRAPH	ENTER *	RESULT	
	26		FIG. 14(a)
	DE		FIG. 14(b)
	26		FIG. 14(c)

FIG. 15(a)



PREDEFINED OBJECT

FIG. 15(b)



ATTACHED TO ITSELF WITHOUT FLIP

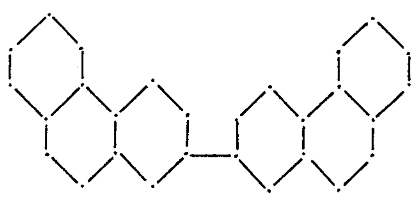


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FIG. 15(c)

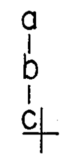


FIG. 16

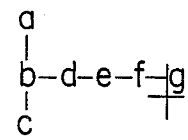


FIG. 18

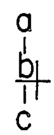


FIG. 17

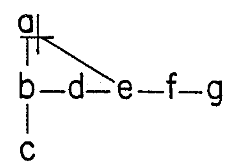


FIG. 19

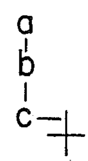


FIG. 20

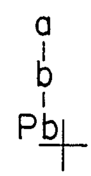


FIG. 21

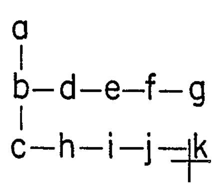


FIG. 24

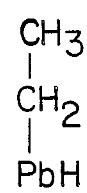


FIG. 22

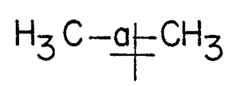
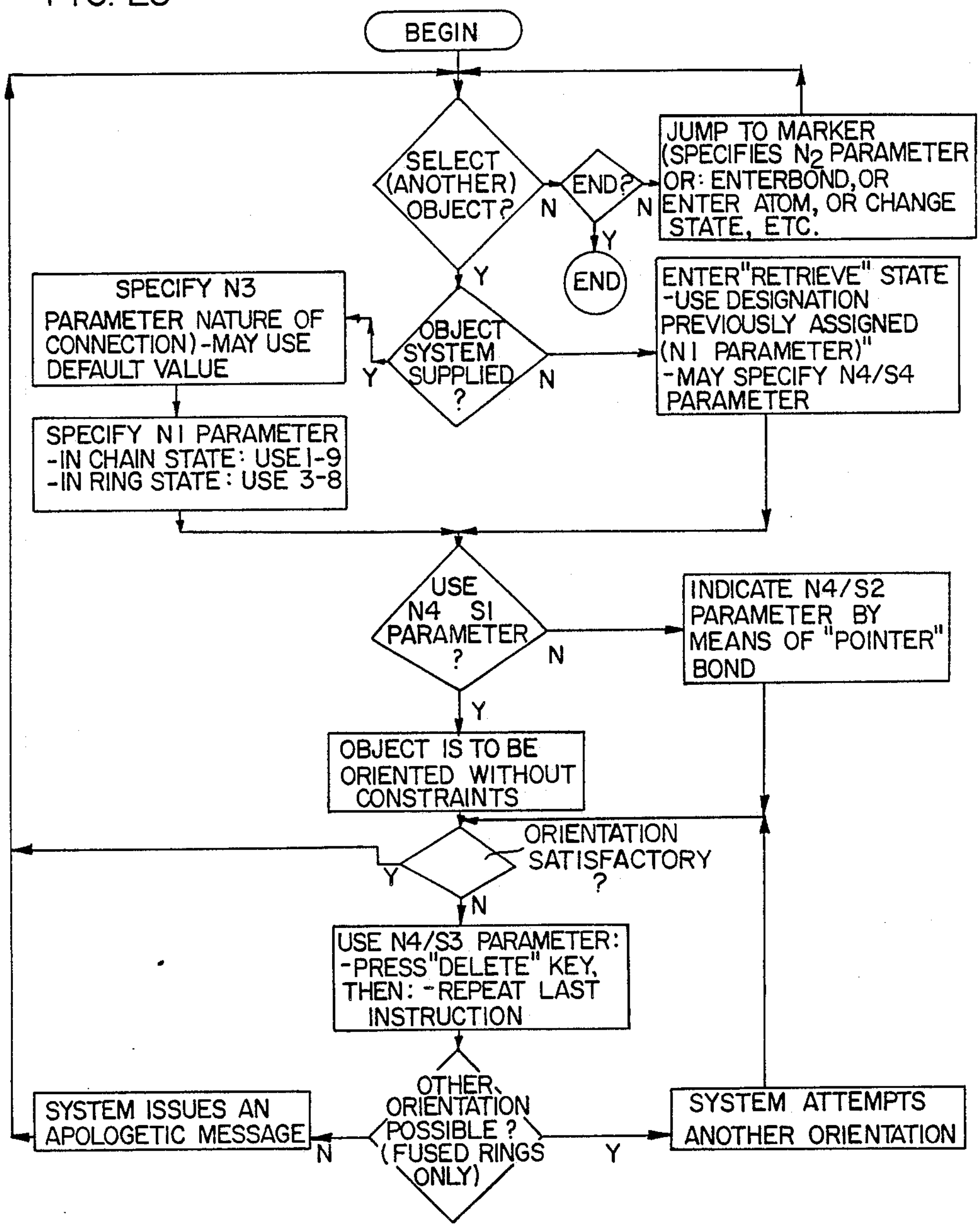


FIG. 23

FIG. 25


BEGIN
SELECT (ANOTHER) OBJECT?
END?
END
JUMP TO MARKER (SPECIFIES N_2 PARAMETER OR: ENTERBOND, OR ENTER ATOM, OR CHANGE STATE, ETC.
SPECIFY N3 PARAMETER NATURE OF CONNECTION)-MAY USE DEFAULT VALUE
OBJECT SYSTEM SUPPLIED ?
ENTER "RETRIEVE" STATE -USE DESIGNATION PREVIOUSLY ASSIGNED (N1 PARAMETER)" -MAY SPECIFY N4/S4 PARAMETER
SPECIFY N1 PARAMETER -IN CHAIN STATE: USE 1-9 -IN RING STATE: USE 3-8
USE N4 S1 PARAMETER ?
INDICATE N4/S2 PARAMETER BY MEANS OF "POINTER" BOND
OBJECT IS TO BE ORIENTED WITHOUT CONSTRAINTS
ORIENTATION SATISFACTORY ?
USE N4/S3 PARAMETER: -PRESS "DELETE" KEY, THEN: -REPEAT LAST INSTRUCTION
OTHER ORIENTATION POSSIBLE ? (FUSED RINGS ONLY)
SYSTEM ISSUES AN APOLOGETIC MESSAGE
SYSTEM ATTEMPTS ANOTHER ORIENTATION
Y
N

AUTOMATIC ORIENTATION AND INTERACTIVE ADDRESSING OF DISPLAY

BACKGROUND OF THE INVENTION

1. The Technical Field

This invention is an improvement in display encoding, and deals in particular with the orientation of the objects by the addition of which a diagram is built up. As described herein, the invention relates to chemical structures, but the concept is usable with other applications, such as drafting and composition.

This invention is also to an improvement in display encoding, a technique for interactively entering graphic data into a computer. The improvement is due to a simplification in the orientation, marking, and display of structures on the screen of a CRT computer terminal. As described herein, the invention relates to chemical structures, but the concept is applicable to other types of diagrams, such as logical and electrical diagrams.

A computer may be used not only to process data, but also to facilitate the entry of these data into the computer With text input, for example, the user seemingly enters depictions of characters. In reality, he enters bit patterns, which are the codes that the computer needs. The machine translates these to graphic characters which are displayed. The input of visible graphics instead of arcane code is known as "display encoding". The term, however, is usually not applied to the input of common text, but is reserved for two-dimensional constructions, such as a diagram.

In display encoding, an entity is entered, as is text, by being assembled—on the face of a graphic computer **13** terminal—from smaller constituents. Ease of input, however, is not the sole advantage of display encoding. Throughout the process of assembly, the unfinished entity is visible, so that it can be determined, at a glance, what has been completed, and what remains to be done. The coupling between code and display further ensures that the visible structure accurately reflects the corresponding machine code. If one is correct, so will be the other. Any errors are apparent, and may be corrected prior to the entity's completion. A further, and not insignificant advantage, is that the input structure can be saved for re-display. Coded text is always translatable into visible, legible graphics; but with other applications, reconstruction of the display may require more than the data whose entry the display facilitated. Saving the code generating the display in addition to these data, will make it possible, in subsequent retrieval, to always view the graphic representation of these data, instead of their arcane codes.

A characteristic facilitating the graphic encoding of chemical structures is their flexibility. The appearance of a chemical structure bears as little resemblance to the shape of the molecule as does an electric wiring diagram to the layout of the actual wires This leaves such diagrams insensitive to the distortions, that are unavoidable in display encoding. There is, however, a limit. In FIG. **1**, two diagrams are shown, representing the molecule, adamantane. Both diagrams are chemically correct, as they show all the atoms and all their bonds. But this identity will not be revealed by a casual glance, nor even by closer scrutiny. Considerable practice, or pencil and paper, will be required. This difficulty is normally circumvented by an artificial similarity, a "traditional" appearance, that has been adopted for many classes of chemical compounds. Very subtle, and often very personal considerations, determine what distortions are innocuous, and what distortions are objectionable.

Display encoding offers considerable latitude in the manner an entity is assembled. A diagram might wholly be constructed line by line. But it is more efficient to use simple lines only as a last resort, and to construct an entity, when possible, with larger building blocks. Indeed, the efficiency of the typewriter results from its capability of composing text with ready made and well formed characters, which are building blocks preassembled from simple lines.

A computer may be used not only to process data, but also to facilitate the entry of these data into the computer. This is commonly done for the input of graphic data, such as diagrams. The data are entered by seemingly being drawn on the face of the screen of a graphic computer terminal. This is an interactive process, in which the human user repeatedly issues commands, which the machine executes, and in so doing builds the diagram. Able to work with visible graphics instead of arcane code, the user's task is facilitated. Even so, the specification to the computer of the graphic elements (or objects) to be displayed, and of the location of these elements on the face of the screen, together with the orientation of these elements, is not a trivial matter. A variety of methods have been developed to facilitate these tasks. The present invention represents an improvement in two of these, namely orientation of these elements, and screen addressing.

The locations on a display can be specified precisely by means of Cartesian or other coordinates. This is one form of screen addressing. It would however be tedious to have to determine the value of these coordinates, and to have to key them in. Coordinates may, however, be obtained implicitly, thereby avoiding the necessity of keying them in, relieving even the operator from having to know their values. A number of approaches have been developed for obtaining coordinates implicitly. On a typewriter, for example, the type-guide indicates the location where a typed character will be printed. This location can be changed by depressing certain keys, called "function" keys: the space bar, the back space, the carriage-return, and others. On computer terminals, these same keys move a cursor. The cursor's coordinates can be determined by the computer's program as needed, without the human operator having to be importuned, or even being aware of this.

The drawing of a diagram, positioning all lines and characters by means of the above keys, would still be very cumbersome, even-though coordinates are obtained implicitly. The cause is the limited range of motions allowed by the above function keys. These permit the operator to progress only horizontally or vertically, usually in increments not exceeding the width or the height of a character. Graphic terminals, therefore, are often provided with additional function keys, called "cursor" keys. There are several of these, each engraved with an arrow, one pointing up, one down, one left and one right. If one is depressed, the cursor moves continuously, until the key is released, in the direction of the arrow.

More sophisticated yet is the "light pen". The computer senses the motion of the "pen" on the face of the terminal. Internally, it detects and computes the corresponding coordinates. It then displays a trace at the pen's location, the process being executed so rapidly that the input operator is under the impression of drawing free-hand. The user may also use the light pen to point at items (these are called "primitives" or "fragments" or "building blocks") on the screen, thereby selecting one of them, and even to drag it to another location on the screen While this goes on, the computer records, unobtrusively, both the identity and the new coordinates of the repositioned item.

Notwithstanding such sophistication, the light pen is not ideal. For example, keeping the hand raised to the screen for any length of time causes fatigue. Consequently, a number of alternatives to the light pen have developed: "Rand" or "graphic tablet", "joy stick", "mouse", "thumbwheel", "knee controls", "track ball", "touch pad", "touch screen", etc. The variety of these approaches is evidence of the effort to the facilitation of graphic input.

And yet, none of these devices overcomes all the problems inherent in the light pen. Because a character can be typed faster than it can be drawn with a pen, the keyboard cannot be dispensed with. Yet keyboard and light pen (or its equivalents) do not, from the ergonomics point of view, mix well. The alternation between light pen and keyboard taxes the operator. Typing, often done blindly, by "touch", must be interrupted to pick up the pen, requiring the typist to look away from the screen. The keyboard is a digital device, whereas the light pen is an analog device. Touch typists are able to type blindly because typewriter keys are located at fixed positions, evenly spaced, not too far apart yet sufficiently separated to be distinct. With the light pen, in contrast, the target that must be reached on the screen can have many positions It cannot be reached blindly; it requires hand-eye coordination. Unlike the keys, it cannot be reached with a simple motion. Studies in human factor analysis have revealed that subjects waver when pointing at an object. Initially, the target is overshot or undershot, requiring a number of adjustments to "zero in" on it with the required precision.

A difficulty in the construction of graphs from various predefined objects is the fitting of such objects to the parent graph. An object is not allowed to come too near, nor to touch, any part of the graph except through its point of attachment. Therefore, a fit may not always be possible, no matter what the object's orientation.

With complex graphs such as those used in chemistry, parameters can be used which are hereinafter referred to as N4 parameters, which define the orientation of objects to be attached to the parent graph, and are the most troublesome to specify. Commands such as 'rotate by 30 degrees' may not provide sufficient flexibility; if expanded to permit specification of the actual number of degrees, the user is generally unable to estimate that number, so that multiple trials may be necessary. Nudging an object with a light pen is slow and requires skill. The same object may be made available in different orientations, but, the larger the number of objects shown, the more extensive will be the menu wanderings required to locate any object. If, to reduce clutter, fewer objects are offered in menus, more of the input will have to be entered by means of simple lines or simple objects, thereby reducing the speed of the input process and rendering it more tedious. All these difficulties increase with the complexity of the graphs.

2. The Prior Art

U.S Pat. No. 4,085,443 to Dubois et al relates to a keyboard operated apparatus for coding and display of chemical structure and other graphical information. A cursor indicates on the display the part of a structural formula which is subject to the next keyboard operation. Alphanumeric characters identify atoms at nodes. The type of bond in any of eight directions from a node toward another node can be registered and displayed. Registering a bond at a particular node, by character and direction, causes the cursor to relocate to the node at the other end of the designated bond. Other movements of the cursor can be effected by the space bar, with the use of directional keyed instructions. FIG. **4** is noteworthy. This patent does suggest entering of graphical information on the keyboard of chemical structures, position by position, by operation of a direction key **5**. This would evidently permit attachment of additional input figures, element-by-element, from a predetermined initial cursor position.

U.S Pat. No. 4,205,391 to Ulyano et al teaches inputting to a computer alphabetic as well as topological graphic data, and in particular, the structural formula of chemical compounds. An encoding tablet is provided, as well as an electronic writing means. FIG. **2** is noteworthy. In this device, graphical data is obtained by inputting the graphical data using a pickup sensor **5**, symbol generator **17**, coordinate pickup **4**, and changeable writing member **38**. The sensor **24** is used to check that the changeable writing member **38** touches the surface of the writing tablet **1**. Other sensors **41**,**42** indicate axial position of the writing member **38**.

U.S. Pat. No. 3,256,422 to Meyer et al relates to an apparatus for automatic encoding and retrieval of topological structures, such as chemical structures. In Meyer, as seen in FIG. **6**, a scanning means is employed for coding the structures desired. A coded sheet having a standardized grid is required in order to encode the structures. Optical or light-sensitive scanning means are employed in this patent.

U.S Pat. No. 4,473,890 Araki, teaches a method and device for storing stereochemical information about chemical compounds. Three-dimensional structures of compounds are stored by supplying the coordinates of the atoms in a three-dimensional space represented by X,Y, and Z coordinates.

The entire disclosure of U.S. Pat. No. 4,476,462 to Feldman, issued Oct. 9, 1984 and filed on Nov. 16, 1981, which has been assigned to the U.S. Department of Health and Human Services, as described hereinabove, is expressly incorporated herein by reference in its entirety.

SUMMARY OF THE INVENTION

Automatic orientation is shown of chemical structures in conjunction with a computer terminal or the like. The invention is not limited to use with a computer terminal nor to use with chemical compounds, but can be extended to any computer-driven display for displaying any type of graphical information wherein graphical units (i.e. predetermined structures, such as for electrical diagrams, architectural diagrams, and the like) are stored, and detailed rules are provided regarding the angles at which such structures can be attached to one another. Such rules also determine the precise location at which additional structures can be added.

In this invention, each object specified has a "standard" orientation. Orientations are then automatically rotatable by 90 degrees as required for the computer to fit the object selected to the attachment points specified. All 90 degree rotations possible are tried by the computer before selection of a new, alternative shape for the structure will be specified. In chemistry especially, this is possible since there usually are a variety of ways of showing a particular chemical structure, other than the "standard" shape.

Furthermore, once a site has been selected for adding an object, a computer list is maintained of the angle pairs possible with the new structure. This permits precise determination of preferred orientations of chemical structures in readily identifiable standard manner. Automatic orientation takes into account all of the rules specified for each of the stored structures. Furthermore, user-defined structures are used within the program by reference thereto. Flipping of such structures is permitted to make mirror-images thereof.

Thus, a graphical display is made by positioning a cursor, whether by a light pen, cursor control from a keyboard, or the like, to move a cursor to a particular position, and an object is then selected. Automatically, the cursor is re-positioned at a predetermined point on the object specified. Alternatively, predetermined attachment points can be readily moved to by cursor control if necessary. From any predetermined attachment point, a new object can be specified and added, while being automatically oriented, without additional input from the user.

Another aspect of the invention shown herein relates to storage of icons or figures, each of which has labels thereon. Once recalled from storage, the stored figure permits positioning of the cursor thereon at selected locations thereof, by depression of a keyboard character, which corresponds to an identical character on the stored figure. Upon depression of the character, the cursor relocates there and permits attachment of the figure to another entity or figure selected. This permits precise attachment of one entity to the following entity, the attachment being automatic and precise.

This invention is particularly useful for specifying chemical structures, but is also useful in mechanical diagrams, electrical diagrams, and logical diagrams among many other uses.

An actual example of display encoding is the input of chemical structures. A chemical structure is a labeled graph, representing the architecture of a molecule in that each of its nodes represent an atom—each denoted by a chemical symbol—and each of its edges represents a chemical bond. It has been found that, in chemical structures, particular groupings of atoms tend to recur more frequently than others. Notable examples are rings and chains. These can be made into building blocks for the purpose of display encoding.

Dealing with a larger number of "objects" than the letters of the alphabet, dealing with two-dimensional space rather than with the linear arrangement of text, display encoding must surmount difficulties that can be far greater. These difficulties are reflected in the parameters that must be specified. These parameters define specific functions. They are listed below and numbered for later reference.

N1-This parameter defines identity. The potential variety of subassemblies or objects from which graphs may be constructed is very large. Furthermore, different sets of subassemblies are likely to be useful. To be selected in the construction of a diagram, these must all be identified.

N2-This parameter defines the intended location at which the above objects are to be placed. With text input, one letter usually follows the preceding one. In display encoding, the desired location must usually be specified explicitly. Requiring x- and y-coordinates, this is an example of a parameter using multiple items of data.

N3-This parameter defines the connection at the locus given by N2. Implied is the rigidity of the connection. The junction between the characters of text is rigid; only one orientation is acceptable. But the subassemblies of a graph can be connected with the parent graph through a single point, or by sharing a line, or in a number of other ways. There are degrees of rigidity, or degrees of attachment; several orientations may be compatible with the specified connection.

N4-This represents one or more parameters that indicate the orientation of the subassembly. In text, the normal orientation of a character is assumed. But if the character should be part, for example, of a caption that labels the y-coordinate of a graph, then its orientation will be changed by 90 degrees from the horizontal. This will have to be explicitly indicated.

Given a character, the purpose of its orientation is to make it agree with the orientation of the other characters on its line of text. In display encoding, as mentioned, the connection specified by N3 may be so rigid, that it allows for but a single orientation. But frequently, the connection specified by N3 is loose enough to allow for several orientations. The purpose of orientation then becomes different. Its purpose then is to fit the irregular contour of an object into the space available for it on the parent graph.

N5-This is required in systems that allow users to define objects for subsequent use. Such objects may be constructed normally, and may be identified with a N1 type parameter. But it is necessary to indicate, in addition, that they be stored for recall, and how they should attach to the parent graph. This requires additional parameters.

It is evident that the potential difficulties inherent in the specification of so many and so diverse a set of parameters may be formidable. Considerable ingenuity has been devoted to facilitate their specification.

The input of text is so common, that much of the logic required for the translation of key codes to character depictions is "hard wired" in terminals. So far, this has not been done for the capabilities required for display encoding. The required logic is normally implemented by means of programs running on a computer.

With simple displays, such as text, it is often possible to use "default" values for the required parameters. Default values are assigned beforehand, and take effect unless explicitly changed. Thus, in text, a character will always be placed to the right of the preceding character (parameter N2), unless a carriage-return, a tabulator, or similar command is used to override it.

Where the use of default values is impractical, other stratagems may be resorted to. A typewriter facilitates the selection of characters (parameter N1) by providing one key to each, and by further arranging these keys in such a manner that the most frequently used ones will be located in the most accessible part of the keyboard.

Because of their numbers, their variety, and their volatility, it is generally not practical to assign "dedicated" keys to all the objects used in the construction of a chemical structure or other graph. An alternative is to designate them by name or by code. A more ingenious approach is to allow the user to "pick" such objects from a "menu" that appears on the terminal's screen.

The N2 parameter may be specified by keying in actual coordinates. It may also be done by pointing at the desired location with a light pen, or by keying the symbol of a marker that has previously been positioned there.

The values used to specify the N4 parameters exhibit, perhaps, the widest variety. There are specific commands, such as "rotate" and "flip". An object may also be oriented by nudging it with the light pen, not unlike a tugboat maneuvering a large vessel into its berth. For a line whose starting point has been specified, both length and orientation are determined by its end point. And an object may appear on a menu in multiple orientations, so that one has to pick the desired object in the desired orientation.

One aspect of the invention is a method to facilitate the specification of one of the above parameters, namely **N4**, which specifies the orientation and to orient recalled objects with sequentially indicated nodes.

The orientation method performed automatically according to one aspect of the present invention has the following advantages.

The command structure, as described below, is simpler. With simpler and fewer commands, the encoding process is faster. Because of the symmetry inherent in automatic orientation, the layout of the graphs obtained with the method of the present invention tends to be more regular, hence more esthetically pleasing, than graphs generated by the usual methods.

The present inventive improvement in screen addressing takes advantage of the fact that, in display encoding, diagrams are constructed by attaching new entities to those already in place on the screen. A graph is begun by bringing up on the screen an entity, a character, a line, or any other building block. This first entity, of necessity a standalone, need not be positioned with the maximum precision afforded by the resolution of which the display is capable. Usually, the entity is placed roughly either in the center of the display, or in the top left quadrant. But the entities entered subsequently must be attached, and therefore need to be positioned with precision.

Another aspect of the present invention relates to marking of potential attachment sites, use of the markers for positioning of the cursor, and use of the markers for automatic replacement by a chemical symbol.

If an entity is to be attached to a point of the graph on display, then that point's coordinates are already known to the computer program that manages this display. As described below, the present invention implements a strategy for marking each potential attachment site. To attach an entity at a particular site on a diagram, it is then necessary only to identify that entity, and to specify the marker indicating the site of the attachment. That specifies the corresponding coordinates with precision.

The marker is a character, and it is selected by depressing, on the keyboard, the key bearing that character. Depressing this key will not, as is normal, cause that character to print. Instead, the computer program will cause the cursor to jump to the site marked with that character. The user next identifies the entity to be placed there. For example, if a four-atom chain is wanted, that chain—assuming everything else to be set up correctly—can be specified by entering the number **4**. That will cause a four-atom chain to be drawn, attached to the site indicated by the cursor. In this manner, that chain (or other entity) is accomplished with precision, quickly, without wavering, without requiring the operator to remove either the hands from the keyboard, or the not least, the expensive hardware that is associated with the light pen, or, its equivalents, is superfluous.

The automatic system of the present invention is capable of fitting more objects into a graph than systems currently available for including chemical structure. This is due to the fact that, in the event of a failed test, the system of the present invention may make available an alternate object which, though diagramatically equivalent, has a different shape. The system will try to fit this by orienting it, as it did for the primary object. Therefore, the chances of achieving a fit are improved.

No manual system can practically have recourse to this solution, since even if objects were to be supplied in a menu in alternate shapes, it would be very difficult to translate and rotate an object mentally to gauge which shape, if any, and in what orientation, the shape is likely to fit.

Should the system of the present invention fail to fit an object onto the parent structure, an apologetic message will be issued. The user is still then able, by means of single bonds and atoms, to enter the object although in a distorted but chemically correct manner.

Although the orientation of objects is automatic, the system of the present invention produces structures in their traditional appearance. When generated directly from code, structures tend to lose their traditional appearance. That is because a structure's code, which is a connection table, is devoid of information concerning what constitutes a traditional appearance. The present inventive method works because it merely orients objects that tend to correspond to traditional subassemblies. It thereby retains the traditional appearance of chemical structures. FIG. **1** illustrates the difference.

FIG. **1** illustrates two equally correct representations of the molecule adamantane. FIG. **1**(*a*) shows an unconventional but correct representation of the molecule; FIG. **1**(*b*) illustrates a more conventional and recognizable representation of the same molecule. As discussed above, the identity of these two figures (a) and (b) is not apparent at a single glance.

The system of the present invention requires a "graphic" computer terminal, discussed in detail hereunder, of medium or high resolution. It does not require accessories such as a "light pen" or a "mouse", which are available on only some terminals, and then usually as expensive options.

The system of the present invention provides two types of objects for attachment to the parent graph. These are objects which are supplied by the system, and objects that have been created by the user which are stored in anticipation of future use. The objects supplied by the system include chains of atoms and rings of atoms. Some of the objects stored have alternate permissible shapes, which are also stored and selected by the system when the primary object will not fit, or cannot be fitted. The chains, at one of their extremities, have a bond, called the "merging" bond. That is, the bond is unattached at one end. Through this bond, these chains will connect to the parent graph.

Users can also create partial structures and store them in anticipation of future need, thereby increasing the variety of objects available for attaching to the parent graph. These are called "user-defined" or "predesigned" objects. These objects are of necessity entered with only a single orientation. This becomes their "standard orientation".

The system alters neither stored objects nor their orientation. In attempting to attach an object to the parent graph, it will manipulate only a copy of the object. The original remains available for subsequent use.

While system-supplied objects and user-defined objects differ in their origin. they do not differ in their interactions with the parent graph.

BRIEF DESCRIPTION OF THE DRAWINGS

FIGS. **1**(*a*)-(*b*) shows two representations of a molecule;

FIGS. **2**(*a*)-(*c*) illustrates system-supplied objects;

FIGS. **3**(*a*)-(*c*) illustrates computation of angle-pairs;

FIGS. **4**(*a*) and (*b*) illustrate the imaginary bond of spiro connections;

FIGS. **5**(*a*), (*b*), and (*c*) illustrate three similar angle-pairs which are obtained with different ring orientations or attachment points;

FIGS. **6**(*a*) and (*b*) illustrate implied commands;

FIGS. **7**(*a*)-(*d*) illustrate unconstrained orientation in the "ring" state where the object has no merging bond and the connection code is 0;

FIGS. **8**(*a*)-(*d*) illustrate unconstrained orientation when the system is in the ring state where the object has no merging bond and the connection code is 1;

FIGS. **9**(*a*)-(*c*) illustrate unconstrained orientation in the ring state where the object has no merging bond and the connection code is 2;

FIGS. **10**(*a*)-(*e*) illustrate unconstrained orientation where the object has a merging bond in a chain state;

FIGS. **11**(*a*)-(*h*) illustrate constrained orientation with a bond-interfacing object in a chain state;

FIGS. **12**(*a*)-(*p*) illustrate constrained orientation in a ring state with an atom-interfacing object;

FIGS. **13**(*a*)-(*c*) illustrate constrained orientation in a ring state with an atom-interfacing object and a different connection code from FIG. **12**;

FIGS. **14**(*a*)-(*c*) illustrate correction of automatic orientation in a ring state;

FIGS. **15**(*a*)-(*c*) illustrate use of a "flip" command;

FIG. **16** illustrates a chain before addition;

FIG. **17** illustrates movement of the cursor to marker "b";

FIG. **18** illustrates attachment of a four-atom chain at marker "b" of FIG. **17**;

FIG. **19** illustrates connection of a line between two specified locations;

FIG. **20** shows addition of a bond to a marker;

FIG. **21** shows alteration of a diagram to include a chemical symbol;

FIG. **22** shows substitution of markers by atoms;

FIG. **23** shows assignment of markers upon request;

FIG. **24** shows automatic assignment of alphabetic letters to recalled chains; and

FIG. **25** shows a flowchart illustrating the choices available to the user.

DETAILED DESCRIPTION OF THE INVENTION

The present invention is disclosed in a preferred embodiment utilizing a standard version of the Model HP 2623A Graphics Terminal Keyboard manufactured by the Hewlett-Packard Company of Palo Alto, Calif. in conjunction with a DEC SYSTEM 10 computer manufactured by the Digital Equipment Corporation. A listing of instructions for a specific program embodying the present invention with the aforementioned equipment is provided in Appendix I attached hereto. It is to be understood that the equipment and program specifically described and illustrated herein are examples of a preferred embodiment only; in other words, the present invention can be performed with other equipment and other programs and should not be limited to the specific embodiment disclosed herein.

FIG. **2**(*a*) illustrates system supplied objects having standard ring shapes. The number of atoms in a ring ranges from 3–8 atoms connected by corresponding bonds, and includes one element having seven atoms and two double-length bonds. Other ring-shaped objects could also be used, and the addition of any such ring-shaped objects as system supplied objects are contemplated as being within the scope of the present invention.

FIG. **2**(*b*) illustrates secondary ring shapes for the three atom ring, the four atom ring, and the five atom ring. These secondary ring shapes are to be used by the computer in the present invention when the standard ring having the same number of atoms cannot be placed or added to the parent graph in a proper fashion, e.g. without touching other structures except at the connection point, or without going off the page, etc. Thus, it is seen that these secondary ring shapes are rotated through an angle relative to the corresponding shapes of the preceding FIG. **2**(*a*).

FIG. **2**(*c*) illustrates system-supplied objects having chain form. Both short (linear) and long (jagged) chains are stored in the computer system. Upon recall, as described hereunder, the dots appearing between the dashed bonds would be replaced by alphanumeric characters. This replacement is discussed hereunder with respect to FIGS. **16–24**.

Before an object can be attached to the parent graph, the common boundary between them, called an "interface", must be specified. A number of parameters must be specified, among them the **N2** and **N3** parameters.

Interfaces can range from simple to complex. The simplest ones consist of a bond, the more complex ones share one or more atoms. If the interface is constituted solely of a bond, then all the atoms of the parent graph lie to one extremity of this bond, and all the atoms of the object lie to its other extremity. If one or more atoms participate in the interface, then these atoms, as well as any bonds connecting them, will have belonged, before the connection was made, separately to both parent graph and object. The connection was made by overlapping, or "fusing" these atoms and bonds. Atom interfaces involving a single atom are referred to, in common chemical parlance, as "spiro"; atom interfaces involving two or more atoms are denoted as "fused".

TABLE I

Interactions between objects and parent graphs

parent-graph interface	connection code	object interface	interface obtained	illustrated in FIG.
bond	—	bond	jointed	11, 15
atom	—	bond	jointed	10
bond	0	atom	jointed	12
atom	1 or 2	atom	hinged	13, 14
atom	0	atom	spiro	7
atom	1 or 2	atom	hinged	8, 9

As for the site of the interface, the N2 parameter, it must be specified independently both for the parent graph, and for the stored object. For the stored object, this specification could be made either at the time it is used, or when it is stored. The former renders these objects more versatile, because any atom or bond then can serve as interface; the latter simplifies their use, because it avoids the necessity of specifying that interface when requesting the object. In the present system, the location of the interface—the N2 parameter—is specified when a predefined object is stored, but the nature of the interface—the N3 parameter—is specified when the object is used.

A. ORIENTATION OF OBJECTS

When recalled from storage, objects can be oriented. The number of potential orientations varies. It depends, in part, on what the specified interface, the N3 parameter, allows. Atom interfaces that consist of two points permit the object to be placed only against either one side or the other of the hinge line connecting these points. Bond and spiro interfaces, which consist of a point, accommodate orientations obtainable by rotating the object around this point. Rotations, however, are performed only in increments that are multiples of 90 degrees. Potential orientations are further limited by available space; as mentioned, an object is not allowed to come too near, nor to touch, any part of the graph except through its point of attachment. Automatic orientation consists of the selection of one orientation from these potential ones.

The system of the present invention selects one of the potential orientations on the basis of coupling rules. There are two such rules. One is applicable to objects that are rotated around a point or joint, hereafter called a "jointed" interface, the other is applicable to objects that have a "hinged" interface. Not all orientations are automatic. In addition to being rotated or hinged, objects may be changed into their mirror-images, or flipped, as illustrated in FIG. **15**. The user accomplishes this by entering a "flip" command, as described hereunder. Flips, useful only with asymmetric objects, are rarely executed, however. Most orientations are automatic.

B. COUPLING RULES

B1. Coupling Rules for Jointed Interfaces

FIGS. **3**(*a*)–(*c*) illustrate computation of angle-pairs. The order in which angle pairs are selected is governed by a preference list (protocol), as follows:

Preference List for angle-pairs (in degrees)

180,180
135,225 or **225,135**
135,135
90,90
135,90 or **90,135**
135,180 or **180,135**

As an example, in FIGS. **3***b* and **3***c*, the two joints shown yield the angle-pairs **135,135** and **45,225**, respectively. The former, being higher on the preference list, determines the corresponding orientation. This is an example of the use of a protocol.

If, because of an obstruction, the object, in the orientation determined from the preference list (protocol), cannot be fitted on the parent graph, then the system will attempt another orientation, provided it has the same angle-pairs. Failing that, it will attempt to use an alternate object, if available. Failing that, it will issue an apologetic message. Under no circumstance will it use an orientation with an angle-pair lower than the best.

With jagged chains, interpretation of the protocol becomes somewhat more complex, as the system will attempt not only to orient the chain in the appropriate direction, but will also try to keep the pucker regularly alternating, avoiding any discontinuities.

On system-supplied rings, the interface is not indicated. Any atom may be used, as they are all equal members of the rings. Nevertheless, because of graphic considerations, the appearance of the rings' sides and angles is uneven. The rings, consequently, can be oriented according to evaluation by the preference list. Should the same angle-pairs be obtained with different orientations, as in FIGS. **5** and **10**(*d*), secondary considerations are deciding, namely equality of length of the adjoining sides (FIG. **5***b*) and, should that not suffice, the preference criteria of the list of rotations, below. Arbitrary considerations, based merely on aesthetics, may additionally be used (see FIG. **5**).

B2. Coupling Rules for Hinged Interfaces

Hinged interfaces are obtained by rotating the object (a ring or ring system) until the designated side is lined up with the corresponding side of the parent graph.

The order in which successive orientations are attempted by the system is also governed by a preference list, which follows:

Preference list for rotations:
first, try standard orientation
rotate standard object by 180 degrees
rotate standard object by −90 degrees
rotate standard object by 135 degrees

Note that the object may appear on either side of the hinge line (cf FIG. **14**). In the absence of impediments, placement of the object against either side is at the system's discretion. If the wrong side was selected by the system, the user may remedy this with the retry command. The retry command, which is described below, rejects the current orientation, then allows the same rules to apply again while preventing rejected orientations from appearing.

C. THE COMMANDS

C1. Implied Commands

It is the burden of commands used in display encoding that not only must they convey the many parameters mentioned above, with their diversity, their multiple elements of data, and their complex definitions; but they must further do this efficiently, minimizing the inconvenience to the user.

The explicit specification of all necessary parameters is consequently intolerable. Prominent among the alternatives that have been devised is the already mentioned use of default values. Further, since the selection of an object is easier by pointing at it on a display than by alternative N1 specifications, many systems offer the use of a "light pen", or an equivalent.

With orientation being performed automatically, the parameter load according to the present invention is reduced. For the remaining conventional commands, default values are, of course, provided. In addition, the system of the present invention offers the use of "implied" commands.

Implied commands are defined by the position of the cursor relative to an atom or a bond. They work as follows. If the cursor's position adjoins an atom, that expresses an "**S1**" command, resulting in a requested object becoming oriented in a particular manner. If the cursor's position adjoins the unattached end of a bond, that expresses an "**S2**" command, resulting in a requested object becoming oriented in a different manner (see FIG. 6). The **S1** and **S2** commands convey **N4** parameters. Their meaning is explained hereunder.

To be executed, implied commands must be activated. They are activated by another command that requires depressing a key, such as a request for an object. This is also discussed hereunder.

These implied commands have been devised in the present invention because, on the average, they will require fewer keystrokes than conventional commands. If, for example, an **N4** parameter—specified by implied command—requires the cursor to be located at the unattached end of a particular bond, it may not be necessary to place it there deliberately. The cursor may already be there, having gotten there as a consequence of entering that particular bond. If now this bond is to be used as a jointed interface to a chain, it will be necessary only to depress the key that calls the chain; no further command will have to be entered to specify its **N4** parameter. Similarly, if the cursor is to be located next to an atom, there is at least a probability that it did not have to be placed there on purpose, but got there as a consequence of the preceding command. In these instances, the depression of a single key, to obtain, say, a system-supplied object, triggers a series of automatic operations that result in the assignment of default values to command, and consequently in the selection, interfacing, orientation and display of the requested object.

C2. Express Commands Requesting Objects

Inasmuch as one aspect of the present application is concerned with the orientation of objects, and not with an entire system of coding chemical compounds, detail on the **N1** and other parameter specifications is provided here only insofar as it relates to the description of automatic orientation.

Basically, the system has a "Ground" state, a "Ring" state, a "Chain" state, a "Library" state, which is entered when an object is stored for future use, and a "Retrieve" state, which is entered when requesting a user-defined object.

A state is entered by depressing a particular key. The nature of this key is immaterial; on keyboards provided with these, it is preferably a programmable function key. On the HP-2623A computer terminal, for which this system is implemented, such keys are not available, because all the available programmable function keys are used for the entry of bonds. On this machine, a particular state is entered by depressing a particular key, which then does not print—the "meaning" of the key is changed—but causes the system to enter the particular state. The Library state, for example, is entered by depressing the "underline" (_) key, and the Retrieve state is entered by depressing the colon (:) key. Actuating the carriage-return key returns the system to the Ground state.

The interpretation of meanings that the system of the present invention gives to the keys is defined by the "state" of the system. In the same state, the same keystrokes produce the same results. In different states, at least one, and possibly more than one key, is interpreted differently. Typing the digits 3 through 8 in the Ring state produces a display of rings of corresponding sizes; in the Chain state, typing the digits 1 through 9 produces chains of corresponding lengths. In neither case are these digits displayed.

User defined objects are retrieved in a similar manner, except that the user defines the designations that recall the objects

C3. Commands Specifying the Connecting Site

The system of the present invention allows the use of "cursor" keys, which are usually provided on graphic terminals, and which allow the user to move the cursor to the locations where an object is to be placed. The present inventive system provides additionally a method of using "markers" to move the cursor to such positions. Either way, selection of the desired connecting site is indicated on the display by the vicinity of the cursor.

The **N2** parameter must be specified for both the parent graph and the predefined objects. On the parent graph, this specification is made just before the object is requested; on the object, it is done prior to storage.

C4. Commands Specifying the Interface

The **N3** parameter specifies the nature or degree of the interface joining object to parent graph. As already mentioned and as summarized in TABLE I, this interface can consist of a bond or of one or more shared atoms.

The **N3** parameter is specified by means of a numerical code. With a value of "0" it specifies a bond or spiro attachment, with value "1" it specifies the fusion of one side, and with value "2" it specifies the fusion of at least two adjacent sides. FIGS. **7**, **8**, and **9** illustrate the use of these connection codes.

The **N3** parameter is always entered immediately preceding the object3 s **N1** specification, as shown in FIGS. **7**–**9**. If omitted, a default value takes effect. Default values for the **N3** parameter are 0 and 1, depending upon the **N4** command, which is addressed next.

An explanation is useful about the extension of the interface. If jointed or spiro, the interface has no extension, but if fused, it will encompass two or more atoms. In the first instance, the position of the cursor, set by the **N2** parameter, specifies the location of the interface adequately, but in the second instance, the cursor shows only one point along an interface with greater extension. This point, however, can be chosen so that it defines the entire interface. As also described in U.S. Pat. No. 4,476,462 to Feldman, the bonds in the present system have "direction". It is therein possible to distinguish the bonds leading into an atom, from those leading away from it. By placing the cursor next to the atom situated at the "base" of the interface—defined in the present system as the atom into which the interface bonds lead—the interface is specified. It may be specified ambiguously, as more than one bond may lead into the same atom. Such instance, however, are not too common. They can be resolved by using the retry command.

With an interface consisting of 3 atoms or more, the location of the interface is determined solely by the bond adjoining the base atom. The direction of the second bond is irrelevant. That again leaves room for ambiguity, as shown in FIG. **14**. But, as this figure further illustrates, this too can be resolved by using the retry command.

C5. Commands Specifying the Orientation of Requested Objects

Since the objects in the system of the present invention are oriented automatically, the commands used to specify **N4** parameters, in the main, serve not to orient objects, but to specify the degree of autonomy granted to the system. One command is used to flip objects. The following are the available **N4** commands.

TABLE II

Command	Operation
S1	Orient object without constraints.
S2	Orient object within the limits of certain constraints
S3	Retry. Orient object in accordance with last specifications, but avoid orientations already attempted.
S4	Flip. Transform object into its mirror image.

S1 and **S2** are implied commands. The "retry" command works through the "delete" key which, when depressed, erases the most recently entered object. The "delete" key is indicated throughout as the letter "DE". If next requested, that object will assume a different orientation. The flip command is made available when a user-defined object is requested. Use of the "flip" command is illustrated in FIG. **15**.

Unconstrained orientation means that no restrictions are being imposed by the user. The system, of course, is subject to the several constraints already discussed: those imposed by the N3 parameter, and those resulting from the limits of the available space.

The (implied) **S1** command is invoked by requesting an object while the cursor is either alone (i.e. located more than one space away from the nearest character or bond), or adjoins an atom of the parent graph.

Requesting an object with invocation of the **S1** command has the following effect. If the requested object does not possess a merging bond, then a hinged interface will result, specified by the value of the N3 parameter. The object will be oriented according to the preference criteria of the list for rotations (FIGS. **7**, **8**, and **9**). If the requested object has a merging bond, then that bond will participate in a jointed interface, and the object will be oriented according to the preference criteria of the list for angle-pairs (FIG. **10**.). If the cursor is alone, then the object is displayed in its standard orientation, not connected to the parent graph, if any. If it possesses a merging bond, this bond will be lost.

With unconstrained orientation, the default value of the N3 parameter is **1**. This means that typing **15**, for example, would produce the same display as typing **5**.

In the system of the present invention, automatic orientation can be partially or fully inhibited. This improves its versatility. In general, automatic systems are more flexible to the extent that their automatic features can be overridden.

Constrained orientation is invoked by means of the (implied) **S2** command. This is activated when an object is requested while the cursor adjoins the unattached end of a bond. This bond is called a "pointer" bond. It is the direction of this bond that restricts the orientation that objects may assume.

The pointer bond can be used to connect with objects that either have a merging bond, or that do not have one. The effects are as follows.

When connecting with objects possessing a merging bond, this bond and the pointer bond must overlap. That will force a corresponding orientation of the object. As an object, however, can be rotated only in increments of 90 degrees, an incompatibility will exist where one of the bonds is horizontal or vertical, and the other bond diagonal. As shown in FIG. **11**, this incompatibility is resolved in favor of the pointer bond, whose direction cannot change. The system rotates the merging bond, and the object attached to it, so as to minimize the difference with the pointer bond, discards the merging bond and connects the object to the pointer bond where the merging bond had been attached.

The object with the incompatible merging bond may be rotated so that this bond would have lain to one side or the other of the pointer bond. Consideration of fit will govern this choice which, otherwise, is resolved at the system's discretion.

If a connection needs to be made between a pointer bond and a merging bond whose lengths differ, the length of the pointer bond prevails; if their bond types differ (i.e. if the pointer bond is single, and the merging bond is double) then the merging bond type takes precedence. This is true whether the pointer bond overlaps the merging bond, or replaces it.

With constrained orientation, the default value of the N3 parameter is zero. The possession of a merging bond precludes objects from being connected to the parent graph except through a jointed interface. In the presence of a merging bond then, other N3 values are meaningless.

When a pointer bond connects with objects that do not possess a merging bond, and the value of the N3 parameter is zero, a jointed connected ensues, and the preference criteria of the list of angle-pairs govern the orientation of the object. FIG. **12** shows a number of examples. Other values of N3 produce a hinged interface, with the preference criteria of the list of rotations determining the orientation of the object.

As with overlapping pointer and merging bonds, the constraints imposed by such an interface are so severe, that it is meaningless to speak even of partially inhibited orientation. In fact, the hinged specification can be used to force an otherwise unattainable orientation, one, for example, that joins an object to the parent graph by a sharp angle, as illustrated in FIG. **13**.

Whether it was automatic or constrained, the user can override the orientation selected by the system. This is done by depressing the "delete" key, which causes the latest single entry—a single atom, or a bond, or an entire object—to be deleted. If the user then repeats the last command, the system will attempt to orient the last addition in a different manner, using the applicable order of preference. This is illustrated in FIG. **14**. After all alternatives have been exhausted, the system will issue an apologetic message. The user can then complete the graph in other ways.

The retry command is another instance of a **N4** parameter specification characteristic of automatic orientation, in that its purpose is not to orient objects, but to restrict or, in this case, to revise, the autonomy granted to the system.

In the system of the present invention, system-supplied objects, being symmetrical, need only to be rotated. User-defined objects, however, may have to be rotated, or flipped. The Flip command is made available as an option when requesting a predefined object—which is done by entering the Retrieve state. The option is specified by typing either the letter "A" (for axial symmetry) or the letter "P" (for point symmetry). If the user then enters the letter P, the system will rotate the object in attempting a fit. If the user enters the letter A, the object first is flipped, i.e. its mirror-image is used. An example of a flipped object is shown in FIG. **15**.

FIG. **4** illustrates the imaginary bond of spiro connections. FIG. **4**(*a*) illustrates an imaginary line at right angles to an imaginary bond between a parent graph and an object which has been added. FIG. **4**(*b*) shows an imaginary bond which overlaps one side of a parent graph, and a dotted line separating the parent graph from the object at the point of attachment and which is generally perpendicular to the imaginary bond line.

FIG. **11** illustrates constrained orientation with a bond-interfacing object. Here, the S2 command, while the system is in the chain state, uses the "pointer" bond. A number of examples are illustrated as FIGS. **11**(*a*-)-(*h*).

FIGS. **12**(*a*)-(*p*) illustrate constrained orientation with an atom-interfacing object with the connection code being Zero (default value). Here, the system is in a ring state. As can be seen, in each of the figures (a)(p), the "pointer" bond from the parent graph orients the object which has been called or retrieved. The result is a connected graph in a conventional form.

D. INTERACTIVE ADDRESSING OF TWO-DIMENSIONAL COMPUTER DISPLAYS

The steps just described are illustrated in FIGS. **16**, **17**, and **18**. FIG. **16** shows the diagram before the addition. The user, to specify the attachment site, depresses key 'b'. This causes the cursor to jump to marker 'b' (FIG. **17**). The user next specifies the entity to be attached, a four-atom chain, by depressing key '**4**'. This causes a four-atom chain to attach itself at marker 'b' (FIG. **18**).

In the context of chemical display encoding at least, all the operations that can be performed with the light pen, the drawing, the selecting, the dragging, can be performed by positioning the cursor in the above manner.

To draw an unusually placed or exceptional line, an instruction must be entered to indicate that, as the cursor jumps from one marker to another, a line (bond) is to be drawn. This function is not frequently necessary, as the system supplies bond lines where appropriate. This instruction is entered by typing of the character '%'. Thus, by typing 'e % a %', a line is drawn from marker 'e' (in FIGS. **18** and **19**) to marker 'a'. FIG. **19** shows the result. The second '%' is required to confirm the last marker, since that marker may appear more than once if more than one alphabet series or character is used.

In chemical diagrams encoded as above, a marker always indicates the location of an atom. The markers are preferably lower-case letters of the alphabet. There is no need to mark the location of a bond, as each bond is always attached to at least one atom. This arrangement limits the number of markers, so that they do not clutter the screen, nor interfere with the visual apprehension of the diagram. If a bond is entered, it attaches to a marker (or to an atom); if an atomic symbol is entered, it replaces a marker if there is one at that site. At an atom location, there is thus either a marker or an atom symbol, never both. It is good practice to make all attachments first, and to replace the markers (with element symbols) last. Generally, it is not necessary to replace all markers. Once the diagram has been completed, the program replaces all remaining markers with the symbol of the atom most commonly occurring in diagrams, namely carbon. The markers thus represent a temporary feature, characteristic of a diagram under construction. In the final diagram, they won't be present.

FIG. **20** shows the addition of a bond to a marker. The original diagram is that of FIG. **16** in which the cursor is located at marker 'c'. When depressing a special key that is programmed to enter a horizontal bond directed to the right, the bond appears at the marker location, which is shown in FIG. **20**. That bond can then either be lengthened, by again depressing the last key, or it can be followed by a marker or element symbol.

FIG. **21** shows the substitution of a marker by an atom. The original diagram again is tht of FIG. **16**, with the cursor at marker 'c'. The key bearing the letters P, @ and b are depressed, resulting in the display of the chemical symbol "Pb".

If this is the last alteration, the letter Q is typed, indicating that the structure has been completed. This causes all remaining markers to be changed to carbon atoms, and H's to be added as illustrated in FIG. **22**.

As markers, single lower case letters are used because, on a keyboard, there is a large number of keys bearing them, and because, in chemical diagrams, they are used rather infrequently. These letters need not be specified by the user. They are automatically assigned in sequence, as needed. After the end of the alphabet has been reached, the alphabet will repeat, the next letter being an 'a' again. The system resolves the ambiguity resulting from the presence of two or more alphabets by confining jumps to the last alphabet used. By actuating the same letter again, the preceding alphabet is accessed In this manner, all alphabets used are cycled through.

Until it is replaced, the operator may return to any marker as often as desired.

Although lower case characters have relatively little use in chemical structures, there are times when they must be printed. To preclude a lower case character from causing a jump when intending to let it print, such a character must be preceded by a specific code. This is the character @. It was typed, when obtaining the diagram in FIG. **21** above, to avoid jumping to marker 'b'.

The foregoing describes the use of markers. It remains now to indicate how they are created, and how they are placed into their strategic locations.

Entities that are entered on the screen, either as standalones or as attachments, are either primitives or composites. A primitive is a single, a double or a triple line (or bond), or the symbol of a chemical element. A composite, which may be a chain or a ring or a more complex fragment of a structure, is composed of a number of primitives. The operator may enter chemical symbols directly, or markers, which will be converted to chemical symbols later. To request a marker, the operator types a particular symbol, preferably the symbol '#'. The program will thereupon supply the next available marker, displaying it at the current cursor location. As already mentioned, markers are assigned by the program in alphabetical order. If the last assigned marker was an 'a', the marker next to be assigned will be a 'b'.

FIG. **23** shows the assignment of markers upon request. The user types a 'C', then depresses the key printing a horizontal right-oriented bond, whereupon the program inserts the necessary hydrogens. The user then types a '#' whereupon the program prints an 'a'. The user than types another bond then another 'C'. Wishing to return to the marker, the user then types an 'a'. This causes the necessary hydrogens to be added to the last C, and the cursor to jump to marker 'a'. The user can then either attach another bond at this site, or replace the marker, and go on.

If composites are used, the library, which supplies these, cannot predict where branch points may occur. Because of this, a composite, upon being displayed on the diagram, will have all its atoms represented by markers. That is illustrated in FIG. 18. (Exceptions—atoms represented as elements are, of course, readily accomodated). The same composite, requested a second time, will receive different markers. For example, if, in FIG. 18, the cursor is jumped to marker 'c' (by depressing key 'c'), and another four-atom chain is requested (by depressing key '4'), that chain will have the markers h through k, as shown in FIG. 24.

The flowchart of FIG. 25 shows the choices available to a user. Specification of required parameters permits automatic orientation of objects.

While preferred embodiments have been shown and discussed, it will be understood that the present invention is not limited thereto, but may otherwise be embodied within the scope of the following claims.

APPENDIX I

```
!       HPCHEM - VERSION 0.5 - DATE APRIL 6, 1986
!
$STORAGE:2
      BLOCK DATA
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*2 IELEM1(126,2),IELEM2(126,3)
      INTEGER*4 MM,IDTPIX
      REAL A
      CHARACTER*1 KAN
      COMMON /ELECHR/ IELEM(126,5)
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
      COMMON /CD/ MAXX,MAXY
        COMMON /ITERM/ITER
        COMMON /IOFFST/IOFF
        COMMON /HP/IHP  !IHP = 1 if terminal is HP else IHP = -1
      COMMON /SIZZE/ MULTX,MULTY
      COMMON /CHARS/IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /KEYS/ ICODE(8)
      COMMON /IPLUS/ IHIGH(14,2)
      COMMON /BONDS/ A(5,3,4,4),B(2,3,4)
      COMMON /XBOND/ GOODB(2,9)
      COMMON /RCAN/ CAN(10,10)
      COMMON /XRNG/ NORDRW(8,8,2),SOFAR
      EQUIVALENCE (IELEM(1,1),IELEM1),(IELEM(1,3),IELEM2)
      DATA IELEM1 /67,79,78,83,67,70,80,66,73,83,65,72,65,66,65,66,83,
     *   65,83,67,86,67,70,77,80,83,65,76,75,78,71,67,63,90,87,65,66,
     *   65,69,69,69,68,68,66,78,78,78,
     *   78,78,78,67,67,77,77,66,77,76,76,67,76,75,65,73,73,67,90,72,
     *   89,89,88,67,72,85,84,84,84,84,84,84,84,84,84,83,72,83,72,
     *   71,83,67,71,82,82,82,82,82,82,80,80,80,80,80,80,70,80,70,79,
     *   74,68,68,68,68,68,68,68,68,68,77,77,77,77,77,77,77,77,77,99,
     *   0,0,0,0,108,0,0,114,0,105,115,103,99,0,103,105,110,108,
     *   98,97,0,117,101,103,98,101,114,105,0,97,100,111,0,110,0,109,
     *   107,117,117,115,114,121,0,101,112,111,105,101,100,98,115,
     *   114,111,110,97,100,117,114,109,97,114,116,114,110,102,114,
     *   111,98,0,101,101,102,0,109,108,105,104,101,99,98,97,0,114,
     *   101,109,0,101,99,100,97,117,110,104,101,98,97,117,116,114,
     *   111,109,100,114,97,109,115,0,112,113,114,115,116,117,118,
     *   119,120,112,113,114,115,116,117,118,119,120,0/
      DATA IELEM2
     *   /4,2,3,2,1,1,3,1,1,4,3,1,3,3,1,3,2,3,3,2,5,1,2,2,2,
     *   2,1,1,1,1,3,2,1,2,6,3,3,3,2,3,3,3,1,2,3,2,2,0,3,3,1,2,6,4,2,
     *   2,3,3,3,3,0,1,3,3,3,4,3,2,3,0,3,4,4,3,1,4,4,2,4,3,5,1,2,0,2,
     *   1,2,3,2,3,3,0,3,4,1,2,4,2,3,2,3,2,1,4,3,8,1,
     *   1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,4,
     *   0,0,5,4,2,2,5,2,2,0,0,2,0,0,0,5,4,0,5,0,0,2,3,0,4,
     *   4,0,0,0,0,0,3,2,0,0,4,4,0,3,0,0,0,0,0,4,3,3,0,0,5,0,3,0,0,0,
     *   3,0,0,0,0,0,2,4,0,0,0,0,3,0,0,4,0,5,0,3,0,0,4,6,0,0,0,0,0,3,
     *   0,4,0,0,0,0,0,0,6,0,0,5,4,0,4,0,4,0,5,0,0,0,
     *   2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,2,0,
     *   0,0,0,6,7,7,0,7,7,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,
     *   6,0,0,0,0,0,0,3,0,0,5,0,0,0,0,0,0,0,0,5,0,0,0,0,0,0,6,0,0,0,
     *   0,0,0,0,0,0,7,0,0,0,0,0,0,0,0,0,0,6,0,0,0,0,6,7,0,0,0,0,0,0,
     *   0,0,0,0,0,0,0,0,7,0,0,6,0,0,0,0,0,0,0,0,0,0,
     *   3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,3,0/
      DATA IES/"33/
        DATA IHP/1/
      DATA IDOT/46/,ITAG/35/,JUMP/36/,LBOND/37/,KAN/'^'/,ISPACE/32/
```

```
      DATA MAXX,MAXY /73,38/
      DATA MULTX,MULTY /7,10/
        DATA ITER/1/
        DATA IOFF/0/      !Set IOFF to 0 to disable offset
                          !IOFF = 0 for HP
                          !IOFF = 1 FOR IBM
      DATA MM /3420*0/, IDTPIX /3420*0/
      DATA ICODE /22,23,24,25,31,30,29,28/
      DATA IHIGH /-2,-1,0,1,2,-2,-1,1,2,-2,-1,0,1,2,
     *   -1,-1,-1,-1,-1,0,0,0,0,1,1,1,1,1/
      DATA A /3.5,2.5,1.5,3.5,1.,0.,4.5,3.5,6.,6.,0.,0.,5.5,1.,3.5,0.,
     *   -1.,-2.,0.,2.,0.,8.,7.,9.,7.,0.,0.,2.,6.,-2.,0.,0.,
     *   0.,1.,0.,0.,7.,7.,6.,6.,0.,0.,0.,6.,0.,0.,-1.,-2.,
     *   0.,-2.,0.,8.,7.,9.,2.,0.,0.,2.,5.,7.,0.,0.,0.,0.,
     *   0.,0.,10.,10.,10.,0.,0.,0.,0.,10.,10.,0.,1.,2.,0.,-2.,
     *   0.,9.,10.,8.,10.,0.,0.,-2.,12.,2.,5.,4.,3.,5.,2.,0.,
     *   6.,5.,2.,5.,0.,0.,7.,8.,8.,10.,9.,8.,10.,8.,0.,1.,
     *   0.,2.,12.,0.,0.,12.,-2.,0.,3.5,2.5,1.5,6.,6.,0.,4.5,3.5,
     *   1.,3.5,0.,0.,5.5,3.5,1.,7.,6.,5.,9.,7.,0.,1.,0.,6.,
     *   -2.,0.,0.,9.,0.,2.,7.,7.,7.,6.,6.,0.,0.,0.,6.,0.,
     *   0.,0.,7.,1.,0.,7.,6.,5.,9.,2.,0.,1.,0.,5.,7.,0.,
     *   0.,9.,0.,-2.,10.,10.,10.,10.,0.,0.,0.,0.,10.,10.,0.,0.,
     *   10.,0.,0.,10.,11.,12.,8.,10.,0.,-1.,0.,12.,2.,0.,0.,8.,
     *   0.,-2.,5.,4.,3.,2.,5.,0.,6.,5.,8.,8.,0.,0.,7.,5.,
     *   2.,0.,-1.,-2.,2.,12.,0.,11.,10.,-2.,0.,0.,0.,2.,10.,8./
      DATA B /4,1,1,1,4,7,
     *         1,4,7,7,7,4,
     *         2,2,10,2,2,2,
     *         10,10,10,2,10,10/
      DATA GOODB /4,3,5,5,6,7,3,3,10,10,7,7,2,3,1,1,8,7/
      DATA CAN(1,3),CAN(2,3),CAN(3,3) /11,2,3/
      DATA CAN(1,4),CAN(2,4),CAN(3,4),CAN(4,4) /2,2,2,2/
      DATA CAN(1,5),CAN(2,5),CAN(3,5),CAN(4,5),CAN(5,5)/1,2,1,2,10/
      DATA CAN(1,6),CAN(2,6),CAN(3,6),CAN(4,6),CAN(5,6),CAN(6,6)
     *   /1,1,2,1,1,2/
      DATA CAN(1,7),CAN(2,7),CAN(3,7),CAN(4,7),CAN(5,7),CAN(6,7),
     *   CAN(7,7) /6,5,1,1,1,1,1/
      DATA CAN(1,8),CAN(2,8),CAN(3,8),CAN(4,8),CAN(5,8),CAN(6,8),
     *   CAN(7,8),CAN(8,8) /1,1,1,1,1,1,1,1/
      DATA CAN(1,9),CAN(2,9),CAN(3,9) /3,3,2/
      DATA CAN(1,10),CAN(2,10),CAN(3,10),CAN(4,10),CAN(5,10)
     *   /1,2,1,2,2/
      DATA NORDRW /128*0/,SOFAR /0/
      END
$STORAGE:2
C       MAIN ROUTINE OF XTCHEM
C
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,IDTPIX,DSKMEM
        REAL A
        LOGICAL*2 IEDIT,FIRST,EXIST,OPENED,OPSTD,OPED,DELAY,ALPHID
        CHARACTER*12 HLOID
        CHARACTER*10 ID,GETID,INID,FILE,STDFIL,INFILE,POUND,BLNK10,
     *     ZERO10
        CHARACTER*8 LIBRET
        CHARACTER*82 BLNK90
        CHARACTER*6 FNAME
        CHARACTER*20 DIRECT
        CHARACTER*1 KAN
        CHARACTER*1 AAA
        CHARACTER*1 AAAA
        CHARACTER*1 SSK
        CHARACTER*5 NSC(2),FSC
        CHARACTER*3 QUALIF
        CHARACTER*10 DIG10E
        CHARACTER*1 NAMSTR(10)
        CHARACTER*12 HALOE
        CHARACTER*4 HLOD2E
        CHARACTER*3 HLOE
        CHARACTER*1 NSC10(10),ID10(10),HALO(12),HLO(3),LIBR8(8,640),
     *     FNAM6(6),DIGIT(8),DIGI10(10),HLOD12(12),REPATM,HLOD2(4)
        EQUIVALENCE (NSC(1),FILE),(NSC(1),NSC10(1)),(ID10(1),GETID),
     *     (LIBRET,LIBR8),(FNAME,FNAM6),(DIGIT(1),DIGI10(2)),
     *     (GETID,HLOD12(2)),(HLOID,HLOD12(1))
        EQUIVALENCE (HLOE,HLO(1))
```

```
      EQUIVALENCE (HLOD2E,HLOD2(1))
      EQUIVALENCE (DIG10E,DIGI10(1))
      EQUIVALENCE (HALOE,HALO(1))

      COMMON /LIB/ LIBRET(640),NLIBS
      COMMON /ELECHR/ IELEM(126,5)
      COMMON /CD/ MAXX,MAXY
      COMMON /SIZZE/ MULTX,MULTY
      COMMON /HP/IHP
      COMMON /KEYS/ ICODE(8)
      COMMON /IPLUS/ IHIGH(14,2)
      COMMON /BONDS/ A(5,3,4,4),B(2,3,4)
      COMMON /XBOND/ GOODB(2,9)
      COMMON /RCAN/ CAN(10,10)
      COMMON /STRDEF/ NNODE,TABLE(255,43)
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /LABELS/ NR,NJLAST,NJNEXT
      COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
      COMMON /MODES/ JBTYPE,ICHR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
      COMMON /PROB/ IPROB,JPROB
      COMMON /IIDD/ IONDX,ID,FILE,INID(2500)
      COMMON /IIDD0/ INFILE(2500),PLACE
      COMMON /IIDD1/ RECNO(2500),NUMIDS,TOTIDS
      COMMON /BLANK/BLNK90
      COMMON /OLD/ IOX,IOY
      COMMON /H/ MOBILE(255,2)
      COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
      COMMON /M1/ MNUM,IMS(90,5)
      COMMON /NDE/ NODE(255,3),IATOM
      COMMON /CONNCT/ IBOND(255,16),KBOND(255,16)
      COMMON /KHARGE/ ICHRGE(50,4),NCHG
      COMMON /CUR/ ICUR
      COMMON /FUSE/ ITIMES
      COMMON /CHN/ CLARGE,CHBITS(65)
      COMMON /TRNS/ TRANS(200)
      COMMON /RANGE/ LOX,HIX,LOY,HIY
      COMMON /FROM/ LCHAR
      COMMON /XRNG/ NORDRW(8,8,2),SOFAR
      COMMON /QTVLNC/ OERR,CHER
      COMMON /ORECS/ OU,OREC
      COMMON /IRECS/ IU,IREC,TOPREC,BOTREC
      COMMON /ALPHID/ ALPHID
      COMMON /RET/ SYM,FSC(2)
      COMMON /DFAULT/ REPATM(2)
      COMMON /MOD/MODEL                    !VAA version
      COMMON /CINFO/ NDIRS(4),BDIRS(8,3)
      DIMENSION HPDIR(4),IBMDIR(4),BDHP(8,3),BDIBM(8,3)
      DATA HPDIR/3,7,1,5/
      DATA IBMDIR/3,7,5,1/
      DATA BDIBM/31,25,23,23,25,31,31,29,23,23,25,25,29,29,29,
     * 31,22,24,24,24,28,30,30,30/
      DATA BDHP/23,25,25,23,29,31,29,29,31,23,23,25,25,29,31,31,
     * 22,24,24,24,28,30,30,30/
      DATA POUND /'          '/, BLNK10 /'          '/,
     *    ZERO10 /'0000000000'/

!     This section does some HP terminal dependent chores
!     HNDOFF = Sets handshake type
!     DEVICE = Gets HP terminal model number  (2623A or 2647A)
!     DOWNLO = Loads the function keys

      CALL HNDOFF              !VAA version
      CALL DEVICE(MODEL)       !VAA version
      CALL DOWNLO              !VAA version

      BLNK90(1:1)='^'
      DO 919 I=2,81
      BLNK90(I:I)=' '
919   CONTINUE
      BLNK90(82:82)='^'
      IF (IHP .EQ. 1) THEN
      DO 456 I=1,4
```

```
156     NDIRS(I)=HPDIR(I)          !Set chain values for HP terminal
        DO 567 I=1,8
        DO 567 J=1,3
        BDIRS(I,J)=BDHP(I,J)
567     CONTINUE
        ELSE
        DO 678 I=1,4
678     NDIRS(I)=IBMDIR(I)         !Set chain values for IBM terminal
        DO 789  I=1,8
        DO 789 J=1,3
        BDIRS(I,J)=BDIBM(I,J)
789     CONTINUE
        ENDIF
C
C
C       The substructure library list file is read.
        NLIBS = 0
        LIO = 1
        INQUIRE(FILE='LIB.RET',EXIST=EXIST)
        IF (EXIST) THEN
           OPEN(LIO,FILE='LIB.RET',STATUS='OLD')
        IF (IHP .EQ. 1) THEN      !Handle DEC10 LIB.RET format here
                DO 505 I=1,645
                READ (LIO, 444,END=666) DIRECT
444             FORMAT(A20)
                J=INDEX(DIRECT,':')
                K=INDEX(DIRECT,'.')
                FNAME='      '
                FNAME=DIRECT(J+1:K-1)
                NLIBS = NLIBS+1
                LIBR8(1,NLIBS) = '^'
                DO 4040 J=1,6
                LIBR8(J+1,NLIBS)=FNAM6(J)
4040            CONTINUE
                LIBR8(8,NLIBS)='^'
505             CONTINUE
666             CONTINUE
                CLOSE(LIO)
        ELSE
           DO 50 I = 1,645
              READ(LIO,39,END=60) FNAME,QUALIF
39            FORMAT(A6,3X,A3)
              IF (QUALIF.EQ.'STR') THEN
                 NLIBS = NLIBS + 1
                 LIBR8(1,NLIBS) = '^'
                 DO 40 J = 1,6
                    LIBR8(J+1,NLIBS) = FNAM6(J)
40               CONTINUE
                 LIBR8(8,NLIBS) = '^'
              ENDIF
50         CONTINUE
60         CONTINUE
           CLOSE(LIO)
        ENDIF
        ELSE
           STOP 'TO EXECUTE PROGRAM ENTER COMMAND -RUN-'
        ENDIF
C
C       Initializations are made.
        FSC(1) = '      '
        FSC(2) = '      '
        OU = 30

        IU = 31
        OREC = 0
        IREC = 0
        TOPREC = 0
        BOTREC = 0
        IONDX = 32
        NUMIDS = 0
        TOTIDS = 0
        FILE = POUND
        STDFIL = POUND
        OPENED = .FALSE.
        OPSTD = .FALSE.
```

```
      OPED = .FALSE.
      HALO(1) = KAN
      HALO(12) = KAN
      HLOD2(1) = KAN
      HLOD2(4) = KAN
      HLO(1) = KAN
      HLO(3) = KAN
      HLOD12(1) = KAN
      HLOD12(12) = KAN
      CHER = 0
      FIRST = .TRUE.
      DELAY = .FALSE.
      ID = ZERO10
      The index file is read.
      INQUIRE(FILE='IDS.NDX',EXIST=EXIST)
      IF (EXIST) THEN
         OPEN(IONDX,FILE='IDS.NDX',STATUS='OLD',ACCESS='DIRECT',
     *      FORM='FORMATTED',RECL=80)
         DO 100 I = 1,2500
            NUMIDS = I - 1
            READ(IONDX,99,REC=I,END=110) INID(I),INFILE(I),RECNO(I)
            IF (INID(I).EQ.BLNK10) GO TO 110
100      CONTINUE
99       FORMAT(A10,A10,I6)
110      CONTINUE
         CLOSE(IONDX)
      ENDIF
      TOTIDS = NUMIDS
      FRSTID = NUMIDS
      CALL RESET(IX,IY,FIRST)
      CALL SETSCR(1)
      PAGE = 1
      CALL DISPLA(1)
C
      INQUIRE(FILE='XTCHEM.SPC',EXIST=EXIST)
      IF (EXIST) THEN
         OPEN(LIO,FILE='XTCHEM.SPC',STATUS='OLD')
         READ(LIO,149) AAA,SSK,(REPATM(I),I=1,2)
149      FORMAT(A1,1X,A1,1X,2A1)
         IF (AAA .EQ.'A') THEN
            ALPHID = .TRUE.
         ELSE
            ALPHID = .FALSE.
         ENDIF
         IF (SSK .EQ.'G') THEN
            ISKILL = 2
         ELSE
            ISKILL = 1
         ENDIF
         CLOSE(LIO)
      ELSE
         ALPHID = .FALSE.
         AAA = 'N'
         ISKILL = 2
         SSK = 'G'
         REPATM(1) = 'N'
         REPATM(2) = CHAR(0)
      ENDIF
61    CONTINUE
      CALL FTSIZE(2,18)
      CALL FTLOCA(6,22)
      CALL FTEXT('^Automatic chemical input generator...^')
      CALL FTLOCA(8,22)
      IF (ALPHID) THEN
         CALL FTEXT('^IDs are: ALPHANUMERIC^')
      ELSE
         CALL FTEXT('^IDs are: NUMERIC^')
      ENDIF
      CALL FTLOCA(9,22)
      IF (ISKILL.EQ.2) THEN
         CALL FTEXT('^Screen headers are: GUIDED^')
      ELSE
         CALL FTEXT('^Screen headers are: SOLO^')
```

```
      ENDIF
      CALL FTLOCA(10,22)
      CALL FTEXT('^The REPEAT STATE default replacement atom is: ^')
      HLOD2(2) = REPATM(1)
      HLOD2(3) = REPATM(2)
      CALL FTEXT(HLOD2E)
62    CONTINUE
      CALL FTLOCA(11,22)
      CALL FTEXT('^Do you want to change program parameters (Y/N)?^')
      CALL REDO(L,89,78,13,0,0,0)
      IF (L.EQ.89) THEN
88       CALL FTLOCA(8,23)
         CALL FTEXT('^Enter "A" for alphanumeric IDs -or-^')
         CALL FTLOCA(9,23)
         CALL FTEXT('^Enter "N" for numeric IDs with incremental defau
     *lts -or-^')
         CALL FTLOCA(10,23)
         HLO(2) = AAA
         CALL FTEXT('^Enter CR for current status of: ^')
         CALL FTEXT(HLOE)
         CALL REDO(AA,65,78,13,0,0,0)
         CALL FTLOCA(8,26)
         IF (AA.EQ.65) THEN
            CALL FTEXT('^IDs are ALPHANUMERIC.  Is this OK (Y/N)?^')
         ELSE IF (AA.EQ.78) THEN
            CALL FTEXT('^IDs are NUMERIC.  Is this OK (Y/N)?^')
         ENDIF
         IF (AA.NE.13) THEN
            L = GETCHR()
            CALL SETCOL(0)
            CALL CLR
            CALL SETCOL(1)
            IF ((L.NE.89).AND.(L.NE.121)) THEN
               CALL SETCOL(0)
               CALL CLR
               CALL SETCOL(1)
               GO TO 88
            ENDIF
            IF (AA.EQ.65) THEN
               ALPHID = .TRUE.
            ELSE
               ALPHID = .FALSE.
            ENDIF
         ELSE
            CALL SETCOL(0)
            CALL CLR
            CALL SETCOL(1)
            AA = ICHAR(AAA)
         ENDIF
         CALL FTLOCA(8,24)
         CALL FTEXT('^Enter "G" if you need HEADER guidance -or-^')
         CALL FTLOCA(9,24)
         CALL FTEXT('^Enter "S" if you wish to solo -or-^')
         CALL FTLOCA(10,24)
         CALL FTEXT('^Enter CR for current status of: ^')
         HLO(2) = SSK
         CALL FTEXT(HLOE)
         CALL REDO(SK,71,83,13,0,0,0)
         IF (SK.EQ.71) THEN
            ISKILL = 2
         ELSE IF (SK.EQ.83) THEN
            ISKILL = 1
         ELSE
            SK = ICHAR(SSK)
         ENDIF
63       CONTINUE
         CALL FTLOCA(8,22)
         CALL FTEXT('^Enter REPEAT STATE default replacement atom: ^')
         CALL FTLOCA(9,22)
         CALL FTEXT('^(CR for current: ^')
         CALL FTEXT(HLOD2E)
         CALL FTEXT('^)^')
         R1 = ICHAR(REPATM(1))
         R2 = ICHAR(REPATM(2))
      IF (IHP .EQ. 1) THEN
            CALL ALPCUR
```

```
            ACCEPT 695, REPATM(1),REPATM(2)
695      FORMAT(2A1)
         ELSE
            REPATM(1) = CHAR(GETCHR())
         ENDIF
            CALL FTLOCA(9,22)
            CALL FTEXT('^                                                   ^')
            CALL FTLOCA(1,1)
            CALL FTEXT('^                                                   ^')
            CALL FTLOCA(8,67)
            IF(ICHAR(REPATM(1)).EQ.13.OR. ICHAR(REPATM(1)) .EQ. 32) THEN
               REPATM(1) = CHAR(R1)
               REPATM(2) = CHAR(R2)
               HLO(2) = REPATM(1)
               CALL FTEXT(HLOE)
               HLO(2) = REPATM(2)
               CALL FTEXT(HLOE)
               GO TO 77
            ELSE
               HLO(2) = REPATM(1)
               CALL FTEXT(HLOE)
               HLO(2) = ' '
               CALL FTEXT(HLOE)
               IF ((ICHAR(REPATM(1)).LT.65).OR.(ICHAR(REPATM(1)).GT.
     *            90)) THEN
                  GO TO 73
               ENDIF
               IF (IHP .NE. 1) REPATM(2) = CHAR(GETCHR())
               IF ((ICHAR(REPATM(2)).EQ.13).OR.(ICHAR(REPATM(2)).EQ.32))
     *            THEN
                  REPATM(2) = CHAR(0)
               ELSE
                  CALL FTLOCA(8,68)
                  HLO(2) = REPATM(2)
                  CALL FTEXT(HLOE)
               ENDIF
            ENDIF
67          CONTINUE
            DO 72 I = 1,107
               IF ((ICHAR(REPATM(1)).EQ.IELEM(I,1)).AND.(ICHAR(REPATM(2))
     *            .EQ.IELEM(I,2))) GO TO 74
72          CONTINUE
73          CONTINUE
            CALL FTLOCA(1,1)
            CALL FTEXT('^ELEMENT DOES NOT EXIST IN THE ELEMENT TABLE^')
            REPATM(1) = CHAR(R1)
            REPATM(2) = CHAR(R2)
            GO TO 63
74          CONTINUE
            CALL FTLOCA(9,22)
            CALL FTEXT('^Is default replacement atom OK (Y/N)?^')
            CALL REDO(L,89,78,0,0,0,0)
            IF (L.NE.89) THEN
               REPATM(1) = CHAR(R1)
               REPATM(2) = CHAR(R2)
               GO TO 63
            ENDIF
77          OPEN(LIO,FILE='XTCHEM.SPC')
            AAAA=CHAR(AA)
            SSK=CHAR(SK)
            WRITE(LIO,149) AAAA,SSK,(REPATM(I),I=1,2)
            CLOSE(LIO)
            CALL SETCOL(0)
            CALL CLR
            CALL SETCOL(1)
         ENDIF
         GO TO 9
1        CONTINUE
C
C
C        The program is called.
         CALL STRINP(IX,IY,IEDIT,FIRST)
         FIRST = .FALSE.
         CALL SETSCR(1)
```

```
      PAGE = 1
      CALL DISPLA(1)
9     CALL FTSIZE(2,18)
      IF (IHP .NE. 1) THEN
      CALL MEMDSK(CLUSTS,CPDISK,BPSECT,SPCLUS)
      DSKMEM = CLUSTS * BPSECT * SPCLUS
      CALL FTLOCA(1,1)
      CALL REPNUM(DSKMEM,NDGT,DIGIT)
      CALL FTEXT('^Number of free bytes on disk: ^')
      DIGI10(1) = '^'
      DIGI10(10) = '^'
      CALL FTEXT(DIG10E)
      ENDIF
C
10    CONTINUE
C
C     The operator is prompted for next instruction.
      IEDIT = .FALSE.
      CHER = 0
      CALL FTSIZE(2,18)
      CALL FTLOCA(7,18)
      CALL FTEXT('^N TO ENTER NEXT COMPOUND - I TO EDIT NEXT COMPOUND
     *-^')
      CALL FTLOCA(8,15)
      CALL FTEXT('^P TO EDIT PREVIOUS COMPOUND - V TO VIEW PREVIOUS CO
     *MPOUND -^')
      CALL FTLOCA(9,20)
      CALL FTEXT('^'' TO VIEW LIST OF COMPOUNDS ON DISK - Q TO QUIT^')
      CALL REDO(L,78,73,80,81,86,39)
C

      IF (((L.EQ.86).OR.(L.EQ.80)).AND.(FIRST.OR.(NUMIDS.EQ.FRSTID)))
     *   GO TO 10
      IF (L.EQ.39) THEN
         IF (NUMIDS.GT.0) THEN
            CALL VIDNDX
         ELSE
            CALL FTLOCA(1,1)
            CALL FTEXT('^NO INDEX TABLE YET EXISTS^')
         ENDIF
         GO TO 10
      ENDIF
      IF (L.EQ.86) THEN
         CALL SETSCR(2)
         PAGE = 2
         CALL DISPLA(2)
         CALL FTSIZE(2,18)
         CALL FTLOCA(1,1)
         CALL FTEXT('^PRESS RETURN TO RETURN TO MENU^')
         AA = GETCHR()
         CALL SETSCR(1)
         PAGE = 1
         CALL DISPLA(1)
              IF (IHP .EQ. 1) THEN
              CALL FTLOCA(1,1)
              CALL FTEXT('^                                        ^')
              CALL GRAOFF
              ENDIF
         GO TO 10
      ENDIF
C
      IF (IHP .NE. 1) THEN
      IF (DSKMEM.LE.(36864+(80*TOTIDS))) THEN
         CALL FTLOCA(1,1)
         CALL FTEXT('^WARNING: Insufficient number of bytes on disk: ^
     *')
         CALL FTEXT(DIG10E)
         CALL FTEXT('^ PROGRAM TERMINATING^')
         L = 81
      ENDIF
      ENDIF
C
```

```
C       This section closes the program.
        IF (L.EQ.81) THEN
           OPEN(IONDX,FILE='IDS.NDX',ACCESS='DIRECT',
     *        FORM='FORMATTED',RECL=80)
           OCOUNT = 0
           DO 200 I = 1,NUMIDS
              IF (INFILE(I).NE.POUND) THEN
                 OCOUNT = OCOUNT + 1
                 WRITE(IONDX,99,REC=OCOUNT) INID(I),INFILE(I),RECNO(I)
              ENDIF
 200       CONTINUE
           DO 210 I = OCOUNT+1,OCOUNT+6
              WRITE(IONDX,289,REC=I) BLNK10
 210       CONTINUE
 289       FORMAT(A10)
           CLOSE(IONDX)
           IF (OPENED) THEN
              WRITE(OU,29,REC=1) OREC
              CLOSE(OU)

          ENDIF
          CALL CLOSEG
       IF (IHP .EQ. 1) CALL ALPCON      !Turn on alpha cursor
       IF (IHP .EQ. 1) STOP
          IF (DSKMEM.LE.(36864+(80*TOTIDS))) THEN
             STOP 'UPLOAD OR CLEAR DISK SPACE BEFORE USING XTCHEM'
          ELSE
             STOP
          ENDIF
C
C
C      THIS SECTION OPENS AN INPUT CONNECTION TABLE AND ITS FILE
C      FOR EDITING.
       ELSE IF ((L.EQ.73).OR.(L.EQ.80)) THEN
          IEDIT=.TRUE.
          IF (L.EQ.80) THEN
             OPED = .FALSE.
             IU = OU
             GETID = INID(NUMIDS)
             ID = GETID
             DO 554 I = 1,10
                HALO(I+1) = ID10(I)
 554         CONTINUE
             CALL FTLOCA(8,23)
             CALL FTEXT('^PREVIOUS STRUCTURE TO BE VIEWED: ^')
             CALL FTEXT(HALOE)
             FILE = INFILE(NUMIDS)
             IREC = RECNO(NUMIDS)
             PLACE = NUMIDS
             DO 555 I = 1,10
                HALO(I+1) = NSC10(I)
 555         CONTINUE
          ELSE
             FY = 10
             IF (FIRST) DELAY = .TRUE.
 565         CONTINUE
             IF (ALPHID) THEN
                GETID = BLNK10
             ELSE
                GETID = ZERO10
             ENDIF
             CALL FTLOCA(9,28)
             IF (ALPHID) THEN
                CALL FTEXT('^Enter (1-10) character ID^')
             ELSE
                CALL FTEXT('^Enter (1-10) digit ID^')
             ENDIF
C            Input structure ID
11445            J = 0
        IF (IHP .EQ. 1) THEN
              CALL ALPCUR
              ACCEPT 691, (NAMSTR(I),I=1,10)
 691          FORMAT(10A1)
              ENDIF
```

```
              DO 4445 I = 1,100
                 J = J + 1
                 FX = 27 + J
 1445            CONTINUE
           IF (IHP .EQ. 1) THEN
           AA=ICHAR(NAMSTR(J))

 ELSE
            AA = GETCHR()
 ENDIF
            IF (AA.EQ.13 .OR. AA .EQ. 32) THEN
               FIN = J - 1
               GO TO 4447
            ENDIF
            IF (AA.EQ.8) THEN
               IF (J.GT.1) J = J - 1
               FX = 27 + J
               CALL FTLOCA(FY,FX)
               CALL FTEXT('^ ^')
               IF (ALPHID) THEN
                  ID10(J) = ' '
               ELSE
                  ID10(J) = '0'
               ENDIF
               GO TO 1445
            ENDIF
            IF (((AA.GE.48).AND.(AA.LE.57)).OR.(AA.EQ.32)) THEN
               HLO(2) = CHAR(AA)
               IF (AA.EQ.32) AA = 48
           IF (IHP .NE. 1) THEN
               CALL FTLOCA(FY,FX)
               CALL FTEXT(HLOE)
           ENDIF
               ID10(J) = CHAR(AA)
            ELSE IF ((ALPHID).AND.(((AA.GE.65).AND.(AA.LE.90)).OR.
*              ((AA.GE.97).AND.(AA.LE.122)))) THEN
               IF (AA.GE.97) AA = AA - 32
               HLO(2) = CHAR(AA)
           IF (IHP .NE. 1) THEN
               CALL FTLOCA(FY,FX)
               CALL FTEXT(HLOE)
           ENDIF
               ID10(J) = CHAR(AA)
            ELSE
               HLO(2) = CHAR(AA)
               CALL FTLOCA(1,1)
               PAGE = 0
               CALL FTEXT(HLOE)
               CALL FTEXT('^ IS ILLEGAL INPUT. ENTER DIGITS OR SPAC
*ES AND CR^')
   IF (IHP .EQ. 1) THEN
   CALL FTLOCA(9,49)
   CALL FTEXT('^           ^')
   CALL FTLOCA(9,49)
   GO TO 11445
   ENDIF
               GO TO 1445
            ENDIF
            IF (J.EQ.10) THEN
               FIN = 10
               GO TO 4447
            ENDIF
4445       CONTINUE
4447       CONTINUE
           CALL SETCOL(0)
           CALL CLR
           CALL SETCOL(1)
           IF ((GETID.EQ.ZERO10).OR.(GETID.EQ.BLNK10)) THEN
              IF (FIRST) DELAY = .FALSE.
              GO TO 10
           ENDIF
           IF (FIN.LT.10) THEN
              J = 10 - FIN
              DO 8689 I = FIN,1,-1
```

```
            ID10(I+J) = ID10(I)
            IF (ALPHID) THEN
               ID10(I) = ' '
            ELSE
               ID10(I) = '0'
            ENDIF
8689     CONTINUE
      ENDIF
      DO 8334 I = 1,10
         HALO(I+1) = ID10(I)
8334  CONTINUE
      CALL FTLOCA(7,23)
      CALL FTEXT('^Seeking ID NUMBER: ^')
      CALL FTEXT(HALOE)
      DO 8335 I = 1,NUMIDS
         IF ((GETID.EQ.INID(I)).AND.(INFILE(I).NE.POUND)) THEN
            IF (FILE.NE.INFILE(I)) THEN
               IF (.NOT.FIRST) THEN
                  WRITE(OU,29,REC=1) OREC
                  CLOSE(OU)
                  OPENED = .FALSE.
               ENDIF
               OPED = .TRUE.
               OU = IU
            ELSE
               OPED = .FALSE.
               IU = OU
            ENDIF
            FILE = INFILE(I)
            IREC = RECNO(I)
            PLACE = I
            GO TO 8336
         ENDIF
8335  CONTINUE
      CALL FTLOCA(7,23)
      CALL FTEXT('^                                        ^')
      CALL FTLOCA(7,36)
      CALL FTEXT('^ID NUMBER: ^')
      CALL FTEXT(HALOE)
      CALL FTLOCA(1,1)
      CALL FTEXT('^ID NUMBER NOT FOUND IN DIRECTORY^')
      IF (FIRST) DELAY = .FALSE.
      GO TO 10
8336  CONTINUE
      CALL FTLOCA(8,23)
      CALL FTEXT('^Input from file: ^')
      DO 8837 I = 1,10
         HALO(I+1) = NSC10(I)
8837  CONTINUE
      CALL FTEXT(HALOE)
   ENDIF
   CALL FTLOCA(9,23)
   CALL FTEXT('^Edited structure will be appended to file: ^')
   CALL FTEXT(HALOE)
   CALL FTLOCA(10,23)
   CALL FTEXT('^Press RETURN to clear screen^')
   AA = GETCHR()
   CALL SETCOL(0)
   CALL CLR
   CALL SETCOL(1)
   IF (OPED) THEN
      INQUIRE(FILE=FILE,EXIST=EXIST)
   ELSE
      EXIST = .TRUE.
   ENDIF
   IF (.NOT.EXIST) THEN
      OPED = .FALSE.
      CALL FTLOCA(1,1)
      CALL FTEXT('^FILE IS NOT ON DISK^')
      IF (FIRST) DELAY = .FALSE.
      GO TO 10
   ELSE
```

```
            IF (OPED) THEN
               OPEN(IU,FILE=FILE,STATUS='OLD',ACCESS='DIRECT',
     *            FORM='FORMATTED',RECL=80)
               OPENED = .TRUE.
               READ(IU,29,REC=1) OREC
            ENDIF
            ID = GETID
         ENDIF
         GO TO 1
C
C
C     THIS SECTION OPENS THE STANDARD CONNECTION TABLE OUTPUT FILE.
      ELSE IF ((FIRST.AND.(.NOT.IEDIT)).OR.(DELAY.AND.(.NOT.IEDIT)
     *   .AND.(.NOT.FIRST))) THEN
         IF (DELAY) THEN
            WRITE(IU,29,REC=1) OREC
            CLOSE(IU)
            OPED = .FALSE.
            OPENED = .FALSE.
            OU = 30
            IU = 31
            DELAY = .FALSE.
         ENDIF
44       CONTINUE
         FILE = POUND
         TOPREC = 0
         BOTREC = 0
         CALL SETCOL(0)
         CALL CLR
         CALL SETCOL(1)
         CALL FTLOCA(9,20)
         CALL FTEXT('^Enter (1-6) character connection table output fi
     *le name^')
C        Request file name
C        Read file name
         J = 0
      IF (IHP .EQ. 1) THEN
              CALL ALPCUR
              ACCEPT 691,(NAMSTR(I),I=1,6)
      ENDIF
         DO 4444 I = 1,60
            J = J + 1
            FX = 19 + J
1444        CONTINUE
      IF (IHP .EQ. 1) THEN
      AA=ICHAR(NAMSTR(J))
      IF (AA .GT. 97) AA=AA-32
      ELSE
            AA = GETCHR()
      ENDIF
            IF (AA.EQ.13 .OR. AA .EQ. 32) GO TO 4446
            IF (AA.EQ.8) THEN
               IF (J.GT.1) J = J - 1
               FX = 19 + J
               CALL FTLOCA(10,FX)
               CALL FTEXT('^ ^')
               NSC10(J) = ' '
               GO TO 1444
            ENDIF
              IF (AA .GE. 97) AA = AA-32
            HLO(2) = CHAR(AA)
            CALL FTLOCA(10,FX)
            IF (((AA.GE.48).AND.(AA.LE.57)).OR.((AA.GE.65).AND.
     *         (AA.LE.90)).OR.((AA.GE.97).AND.(AA.LE.122))) THEN
               NSC10(J) = CHAR(AA)
            ELSE
               NSC10(J) = ' '
            ENDIF
            IF (IHP .NE. 1)CALL FTEXT(HLOE)
            IF (J.EQ.6) GO TO 4446
4444     CONTINUE
4446     CONTINUE
         CALL SETCOL(0)
         CALL CLR
         CALL SETCOL(1)
```

```
          IF (NSC(1) .EQ. '     ') GO TO 44
 443      FORMAT(2A5)
          NSC10(7) = '.'
          NSC10(8) = 'T'
          NSC10(9) = 'B'
          NSC10(10) = 'L'
          DO 8686 I = 1,10
             HALO(I+1) = NSC10(I)
 8686     CONTINUE
          CALL FTLOCA(8,21)
          CALL FTEXT('^All non-edited structures will output to file: ^
     *')
          CALL FTEXT(HALOE)
          CALL FTLOCA(9,21)
          CALL FTEXT('^All edited structures will be appended to their
     *input file^')
          CALL FTLOCA(10,21)
          CALL FTEXT('^Is file name OK (Y/N)?^')
          AA = GETCHR()
          CALL SETCOL(0)
          CALL CLR
          CALL SETCOL(1)
          IF ((AA.NE.89).AND.(AA.NE.121)) GO TO 44
          INQUIRE(FILE=FILE,EXIST=EXIST)
          IF (.NOT.EXIST) GO TO 404
          DO 8888 I = 1,NUMIDS
             IF (FILE.EQ.INFILE(I)) GO TO 466
 8888     CONTINUE
          GO TO 404
 C        File exists - Do you wish to append it (Y/N)?
 466      CONTINUE
          CALL FTLOCA(8,23)
          CALL FTEXT('^File exists - Do you wish to append it (Y/N)?^'
     *)
          IKAR = GETCHR()
          CALL SETCOL(0)
          CALL CLR
          CALL SETCOL(1)
          IF (IKAR.EQ.78 .OR. IKAR.EQ.110) GO TO 44
 C        If no - go get new file name
          IF (IKAR .EQ. 89 .OR. IKAR .EQ. 121) THEN
             OPEN(OU,FILE=FILE,STATUS='OLD',ACCESS='DIRECT',FORM=
     *           'FORMATTED',RECL=80)
             OPENED = .TRUE.
             OPSTD = .TRUE.
             STDFIL = FILE
             READ(OU,29,REC=1) OREC
             GO TO 55
          ENDIF
          CALL FTLOCA(10,23)
          CALL FTEXT('^Invalid response:^')
          HLO(2) = CHAR(IKAR)
          CALL FTEXT(HLOE)
 C        Invalid response - go try new entry
          GO TO 466
 404      OPEN(OU,FILE=FILE,STATUS='NEW',ACCESS='DIRECT',FORM=
     *       'FORMATTED',RECL=80)
          OPENED = .TRUE.
          OPSTD = .TRUE.
          STDFIL = FILE
          OREC = 1
          WRITE(OU,29,REC=OREC) OREC
 C
 C
 C     THIS SECTION REQUESTS THE STANDARD OUTPUT FILE TO RECEIVE ITS
 C     NEXT STRUCTURE.
       ELSE
          IEDIT = .FALSE.
          TOPREC = 0
          BOTREC = 0
          IF ((FILE.NE.STDFIL).OR.(OU.EQ.11)) THEN
             WRITE(IU,29,REC=1) OREC
 29          FORMAT(I5)
             CLOSE(IU)
             FILE = STDFIL
             OU = 30
```

```
              IU = 31
              OPEN(OU,FILE=FILE,STATUS='OLD',ACCESS='DIRECT',FORM=
     *          'FORMATTED',RECL=80)
              READ(OU,29,REC=1) OREC
              OPENED = .TRUE.
              OPED = .FALSE.
              OPSTD = .TRUE.
           ELSE
              CLOSE(OU)
              OPEN(OU,FILE=FILE,STATUS='OLD',ACCESS='DIRECT',FORM=
     *          'FORMATTED',RECL=80)
           ENDIF
        ENDIF
C
C
C       ENTER ID NUMBER OF NEXT INPUT STRUCTURE.
 55     CONTINUE
        CALL SETCOL(0)
        CALL CLR
        CALL SETCOL(1)
        IF (.NOT.IEDIT) THEN
           IF (ALPHID) THEN
              GETID = BLNK10
              MX = 32
              CALL FTLOCA(8,MX)
              CALL FTEXT('^Enter (1-10) character ID^')
           ELSE
              GETID = ZERO10
              MX = 28
              CALL FTLOCA(7,MX)
              CALL FTEXT('^Enter CR for default ID increment -or-^')
              CALL FTLOCA(8,MX)
              CALL FTEXT('^Enter (1-10) digit ID^')
           ENDIF
 11555          J = 0
          IF (IHP .EQ. 1) THEN
                CALL ALPCUR
                ACCEPT 691, (NAMSTR(I),I=1,10)
                ENDIF
           DO 5555 I = 1,100
              J = J + 1
              FX = MX + J - 1
 1555         CONTINUE
          IF (IHP .EQ. 1) THEN
          AA=ICHAR(NAMSTR(J))
          ELSE
              AA = GETCHR()
          ENDIF
              IF (AA.EQ.13 .OR. AA .EQ. 32) THEN

                IF ((GETID.EQ.ZERO10).OR.(GETID.EQ.BLNK10)) THEN
                   IF (ALPHID) GO TO 55
                   GETID = ID
                   IF ((NUMIDS.EQ.0).OR.((NUMIDS.GT.0).AND.
     *                (ID.EQ.INID(NUMIDS))).OR.(FIRST)) THEN
 5530                 DO 5535 K = 10,1,-1
                         ID10(K) = CHAR(ICHAR(ID10(K)) + 1)
                         IF (ID10(K).EQ.':') THEN
                            ID10(K) = '0'
                            IF (K.EQ.1) THEN
                               GETID = '0000000001'
                               GO TO 5536
                            ENDIF
                         ELSE
                            GO TO 5536
                         ENDIF
 5535                 CONTINUE
 5536                 CONTINUE
                      FIN = 10
                      DO 5566 K = 1,NUMIDS
                         IF (GETID.EQ.INID(K)) GO TO 5530
 5566                 CONTINUE
                        IF (IHP .NE. 1) THEN
                      CALL FTLOCA(9,28)
```

```
                    CALL FTEXT(HLOID)
                     ENDIF
                    GO TO 5556
                 ELSE
                    FIN = 10
                      IF (IHP .NE. 1) THEN
                    CALL FTLOCA(9,28)
                    CALL FTEXT(HLOID)
                      ENDIF
                    GO TO 6667
                 ENDIF
              ELSE
                 FIN = J - 1
                 GO TO 5556
              ENDIF
           ENDIF
           IF (AA.EQ.8) THEN
              IF (J.GT.1) J = J - 1
              FX = MX + J - 1
              CALL FTLOCA(9,FX)
              CALL FTEXT('^ ^')
              IF (ALPHID) THEN
                 ID10(J) = ' '
              ELSE
                 ID10(J) = '0'
              ENDIF
              GO TO 1555
           ENDIF
           IF (((AA.GE.48).AND.(AA.LE.57)).OR.(AA.EQ.32)) THEN
              HLO(2) = CHAR(AA)
              IF (AA.EQ.32) AA = 48
              IF (IHP .NE. 1) THEN
              CALL FTLOCA(9,FX)
              CALL FTEXT(HLOE)
              ENDIF
              ID10(J) = CHAR(AA)
           ELSE IF ((ALPHID).AND.(((AA.GE.65).AND.(AA.LE.90)).OR.
     *          ((AA.GE.97).AND.(AA.LE.122)))) THEN
              IF (AA.GE.97) AA = AA - 32
              HLO(2) = CHAR(AA)
              IF (IHP.NE.1)  THEN
              CALL FTLOCA(9,FX)
              CALL FTEXT(HLOE)
              ENDIF
              ID10(J) = CHAR(AA)
           ELSE
              HLO(2) = CHAR(AA)
              CALL FTLOCA(1,1)
              PAGE = 0
              CALL FTEXT(HLOE)
              CALL FTEXT('^ IS ILLEGAL INPUT. ENTER DIGITS OR SPAC
     *ES AND CR^')
        IF (IHP .EQ. 1) THEN
        CALL FTLOCA(9,49)
        CALL FTEXT('^              ^')
        CALL FTLOCA(9,49)
        GO TO 11555
        ENDIF
              GO TO 1555
           ENDIF
           IF (J.EQ.10) THEN
              FIN = 10
              GO TO 5556
           ENDIF
5555     CONTINUE
5556     CONTINUE
         IF ((GETID.EQ.ZERO10).OR.(GETID.EQ.BLNK10)) GO TO 55
         IF (FIN.LT.10) THEN
            J = 10 - FIN
            DO 6663 I = FIN,1,-1
               ID10(I+J) = ID10(I)
               IF (ALPHID) THEN
                  ID10(I) = ' '
               ELSE
                  ID10(I) =  '0'
               ENDIF
```

```
6663          CONTINUE
           ENDIF
           DO 6666 I = 1,NUMIDS
              IF (GETID.EQ.INID(I)) THEN
                 CALL FTLOCA(10,MX)
                 CALL FTEXT('^WARNING - ID already exists on current file
     *s - ^')
                 CALL FTLOCA(11,MX)
                 CALL FTEXT('^Upload existing structure prior to new entr
     *y^')
                 CALL FTLOCA(12,MX)
                 CALL FTEXT('^Press RETURN to continue^')
                 AA = GETCHR()
                 GO TO 55
              ENDIF
6666       CONTINUE
6667       CONTINUE
           CALL FTLOCA(10,MX)
           CALL FTEXT('^Output ID: ^')
           CALL FTEXT(HLOID)
           CALL FTLOCA(11,MX)
           CALL FTEXT('^Is ID OK (Y/N)?^')
           IKAR = GETCHR()
C          If no - go get new ID
           IF (IKAR.NE.89 .AND. IKAR.NE.121) GO TO 55
           ID = GETID
           CALL SETCOL(0)
           CALL CLR
           CALL SETCOL(1)
        ENDIF
C
        GO TO 1
        END
C
C
C     SUBROUTINE VCONTB writes the file format image of the input for
C     edit connection table to the screen.
C
C     ORI   Paul Broderick   April, 1985
      SUBROUTINE VCONTB
      IMPLICIT INTEGER*2(A-Z)
      CHARACTER*82 LINE
      CHARACTER*12 IDHLO
      CHARACTER*10 ID,FILE,INID,PASSID
      CHARACTER*1 CONTBL,LINE82(82),ID12(12)
      EQUIVALENCE (LINE;LINE82),(ID,ID12(2)),(IDHLO,ID12(1))
      COMMON /CONTBL/ CONTBL(80,258),LTBL
      COMMON /IIDD/ IONDX,PASSID,FILE,INID(2500)
C
      ID = PASSID
      CALL SETSCR(1)
      PAGE = 1
      CALL DISPLA(1)
      LINE82(1) = '^'
      LINE82(82) = '^'
      ID12(1) ='^'
      ID12(12) = '^'
      LOW = 1
      PASSES = LTBL / 32
      IF (MOD(LTBL,32).GT.0) PASSES = PASSES + 1
      IF (LTBL.GT.32) THEN
         HIGH = 32
      ELSE
         HIGH = LTBL
      ENDIF
C
      DO 300 I = 1,PASSES
         CALL FTSIZE(1,10)
         FY = 1
         CALL FTLOCA(FY,1)
         CALL FTEXT(IDHLO)
         DO 200 J = LOW,HIGH
            DO 100 K = 1,80
               LINE82(K+1) = CONTBL(K,J)
100         CONTINUE
```

```
         FY = FY + 1
         CALL FTLOCA(FY,1)
         CALL FTEXT(LINE)
200      CONTINUE
      FY = FY + 1
      CALL FTLOCA(FY,1)
      CALL FTSIZE(2,18)
      CALL FTEXT('^Press RETURN to continue^')
      KHAR = GETCHR()
      LOW = LOW + 32
      IF (PASSES.EQ.(I+1)) THEN
         HIGH = HIGH + LTBL - (I * 32)
      ELSE IF (PASSES.GT.1) THEN
         HIGH = HIGH + 32
      ENDIF
      CALL SETCOL(0)
      CALL CLR
      CALL SETCOL(1)
300   CONTINUE
C
      CALL SETSCR(2)
      PAGE = 2
      CALL DISPLA(2)
      CALL FTSIZE(1,10)
      RETURN
      END
C
C
C     SUBROUTINE VIDNDX
C
C     ORI   Paul Broderick   April, 1985
C
      SUBROUTINE VIDNDX
      IMPLICIT INTEGER*2(A-Z)
      INTEGER*4 VAL
      CHARACTER*12 OID,OFILE
        CHARACTER*9 DIGT9E
        EQUIVALENCE (DIGT9E,DIGIT9(1))
      CHARACTER*10 INID,INFILE,ID,FILE,PID,PFILE
      CHARACTER*1 ID12(12),FILE12(12),DIGIT(7),DIGIT9(9)
      EQUIVALENCE (PID,ID12(2)),(OID,ID12(1)),(PFILE,FILE12(2)),
     *   (OFILE,FILE12(1)),(DIGIT(1),DIGIT9(2))
      COMMON /IIDD/ IONDX,ID,FILE,INID(2500)
        COMMON /HP/IHP
      COMMON /IIDD0/ INFILE(2500),PLACE
      COMMON /IIDD1/ RECNO(2500),NUMIDS,TOTIDS
C
      ID12(1) = '^'
      ID12(12) = '^'
      FILE12(1) = '^'
      FILE12(12) = '^'
      NUMCNT = 0
        IF (IHP .EQ. 1) THEN              !Set ID's/line to 3 for HP
                ILINE=3
        ELSE
                ILINE=4                   !Set ID's/line to 4 for IBM PC
        ENDIF
      PASSES = NUMIDS / 128
      IF (MOD(NUMIDS,128).GT.0) PASSES = PASSES + 1
      LOW = 1
      IF (NUMIDS.GT.128) THEN
         HIGH = 32
      ELSE
         HIGH = NUMIDS / ILINE
         IF (MOD(NUMIDS,ILINE).GT.0) HIGH = HIGH + 1
      ENDIF
      VAL = TOTIDS
      CALL REPNUM(VAL,NDGT,DIGIT)
      DIGIT9(1) = '^'
      DIGIT9(9) = '^'
      FY = 1
      CALL FTSIZE(1,10)
      CALL FTLOCA(FY,1)
      CALL FTEXT('^Number of structures in index: ^')
      CALL FTEXT(DIGT9E)
```

```
      DO 300 I = 1,PASSES
         DO 200 J = LOW,HIGH
            FY = FY + 1
            FX = 1
            DO 100 K = 1,ILINE
               NUMCNT = NUMCNT + 1
               IF (NUMCNT.GT.NUMIDS) GO TO 201
               PID = INID(NUMCNT)
               PFILE = INFILE(NUMCNT)
               DO 50 L = 2,7
                  IF ((FILE12(L).GE.'a').AND.(FILE12(L).LE.'z'))
     *               FILE12(L) = CHAR(ICHAR(FILE12(L)) - 32)
50             CONTINUE
               CALL FTLOCA(FY,FX)
               CALL FTEXT(OID)
               CALL FTEXT('^ ^')
               CALL FTEXT(OFILE)
               FX = FX + 23
100         CONTINUE
200      CONTINUE
201      CONTINUE
         FY = FY + 1
         CALL FTLOCA(FY,1)
         CALL FTSIZE(2,18)
         CALL FTEXT('^Enter CR to break or C and CR to continue^')
         KHAR = GETCHR()
         IF (KHAR.NE.13 .AND. KHAR .NE. 32) THEN
            LOW = LOW + 32
            IF (PASSES.EQ.I+1) THEN
               HIGH = HIGH + (NUMIDS / ILINE) - (I * 32)
               IF (MOD(NUMIDS,ILINE).GT.0) HIGH = HIGH + 1
            ELSE IF (PASSES.GT.1) THEN
               HIGH = HIGH + 32
            ENDIF
            CALL SETCOL(0)
            CALL CLR
            CALL SETCOL(1)
         ELSE
            CALL SETCOL(0)
            CALL CLR
            CALL SETCOL(1)
            RETURN
         ENDIF
         CALL FTSIZE(1,10)
         FY = 0
300   CONTINUE
      RETURN
      END
C
       SUBROUTINE QUIT(IRESET,KAR,KX,KY)
       IMPLICIT INTEGER*2 (A-Z)
       INTEGER*4 MM,IDTPIX,VAL
       LOGICAL*2 RTNMSG
       CHARACTER*82 BLNK90
       CHARACTER*10 ID,INID,FILE,INFILE
       CHARACTER*12 HALOE
       CHARACTER*1 NSC10(10),HALO(12),HLO(3),RET(7),DIGIT(9)
       CHARACTER*1 KAN
       EQUIVALENCE (ID,NSC10),(RET(1),DIGIT(2))
       EQUIVALENCE (HALOE,HALO(1))
       COMMON /STRDEF/ NNODE,TABLE(255,43)
       COMMON /CD/ MAXX,MAXY
       COMMON /SIZZE/ MULTX,MULTY
       COMMON /RANGE/ LOX,HIX,LOY,HIY
       COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
       COMMON /HP/IHP
       COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
       COMMON /MODES/ JBTYPE,ICHR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
       COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
       COMMON/BLANK/BLNK90
       COMMON /HEAD/ MW(12),ISTATE,PAGE
       COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
       COMMON /LABELS/ NR,NJLAST,NJNEXT
       COMMON /PROB/ IPROB,JPROB
       COMMON /CUR/ ICUR
```

```
      COMMON /QTVLNC/ OERR,CHER
      COMMON /WARN/ ERR
      COMMON /DARK/ OCUR
      COMMON /IRECS/ INU,IREC,TOPREC,BOTREC
      COMMON /IIDD/ IONDX,ID,FILE,INID(2500)
      COMMON /IIDD0/ INFILE(2500),PLACE
      COMMON /IIDD1/ RECNO(2500),NUMIDS,TOTIDS
      COMMON /M1/ MNUM,IMS(90,5)
      COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
      COMMON /LNGOUT/ LNGNDE(100,2)
      COMMON /DTDS/ DTN,DTX(30),DTY(30),DTN1(30),DTN2(30)
      COMMON /GPRNT/ KHAR
      IBLANK='    '
C If IRESET=1, arrays are to be reset in subrout RESET.
      HALO(1) = KAN
      DO 7 I = 1,10
         HALO(I+1) = NSC10(I)
7     CONTINUE
      HALO(12) = KAN
      HLO(1) = KAN
      HLO(3) = KAN
      NLARGE = 1
      OCUR = 1
      IRESET=0
      KAR=13
      CALL SETSCR(1)
      CALL DISPLA(1)
      IF (IHP .EQ. 1) CALL GRAOFF
      CALL SETCOL(0)
      CALL CLR
      CALL SETCOL(1)
      IF (PAGE.EQ.0) THEN
         RTNMSG = .TRUE.
         RR = ERR
         CHER = 2
         CALL MYERR(RR,32,32)
         CHER = 0
      ELSE
         RTNMSG = .FALSE.
      ENDIF
11    CONTINUE
      CALL FTSIZE(2,18)
      PAGE = 1
C
C Short menu only
824   IF (ISKILL.EQ.1) GOTO 10
C
      CALL FTLOCA(6,18)
      CALL FTEXT('^You are now in END OF STRUCTURE MODE^')
      CALL FTLOCA(7,18)
      CALL FTEXT('^C--Allows you to continue building current structure^
     *')
      CALL FTLOCA(8,18)
      CALL FTEXT('^H--Makes hard copy & returns to this menu^')
      CALL FTLOCA(9,18)
      CALL FTEXT('^X--Cancels current structure & prepares for re-entry^
     *')
      CALL FTLOCA(10,18)
      CALL FTEXT('^S--Generates connection table and exits^')
      CALL FTLOCA(11,18)
      CALL FTEXT('^G--Makes hard copy, generates connection table and ex
     *its^')
      CALL FTLOCA(12,18)
      CALL FTEXT('^D--Deletes the existing connection table on file^')
      CALL FTLOCA(13,18)
      CALL FTEXT('^Q--Exits with no output^')
10    CONTINUE
      IF (ISKILL.EQ.1) THEN
         CALL FTLOCA(8,30)
      ELSE
         CALL FTLOCA(14,18)
      ENDIF
      CALL FTEXT('^Enter C, H, X, S, G, D, or Q: ^')
      KHAR = GETCHR()
C
```

```
C Convert lc to cap
      IF ((KHAR.GE.97).AND.(KHAR.LE.122)) KHAR=KHAR-32
C
C C=continue same structure
      IF (KHAR.EQ.67) GOTO 67
C H=hard copy
      IF (KHAR.EQ.72) GOTO 72
C X=kill this structure
      IF (KHAR.EQ.88) GOTO 88
      IF(KHAR .EQ. 81) GO TO 81
C S=make connection table
      IF (KHAR.EQ.83) GOTO 83
C G=make hard copy and connection table
      IF (KHAR.EQ.71) GO TO 83
C D=delete existing structure on file
      IF (KHAR.EQ.68) GO TO 68
C If KHAR is not in above list.
      CALL SETCOL(0)
      CALL CLR
      CALL SETCOL(1)
      CALL ERRMSG(KHAR)
      CALL FTSIZE(2,18)
      GO TO 824
C
C Return to same structure
68    CONTINUE
      CALL FTLOCA(16,18)
      CALL FTEXT('^Are you sure you want structure on file deleted (Y/
     *N)?^')
      KHAR = GETCHR()
      CALL SETCOL(0)
      CALL CLR
      CALL SETCOL(1)
      IF ((KHAR.NE.89).AND.(KHAR.NE.121)) GO TO 824
      IF (TOPREC.GT.0) THEN
         INFILE(PLACE) = '          '
         DO 5 I = TOPREC,BOTREC
            WRITE(INU,9,REC=I) BLANK
9           FORMAT(A1)
5        CONTINUE
         TOPREC = 0
         TOTIDS = TOTIDS - 1
      ELSE
         CALL FTLOCA(1,1)
         CALL FTEXT('^NO INPUT STRUCTURE IS ON DISK - NO DELETION POSS
     *IBLE^')
      ENDIF
      GO TO 824
67    CONTINUE
      CALL SETCOL(0)
      CALL CLR
      CALL SETCOL(1)
6677  CONTINUE
      MODE=1
C return to ground state
      LASTN=0
C Allows us to rewrite header
      DO 999 I=1,12
         MW(I)=999
999   CONTINUE
C Graphic display on
      CALL SETSCR(2)
      PAGE = 2
      CALL DISPLA(2)
      CALL FTSIZE(1,10)
      CALL HEADER
      RETURN
C
C     HARD COPY OPTION
C
72    CONTINUE
      CALL SETCOL(0)
      CALL CLR
      CALL SETCOL(1)
      CALL SETSCR(2)
```

```
        PAGE = 2
        CALL FTSIZE(1,10)
        CALL FTLOCA(1,1)
        CALL FTEXT(BLNK90)
        CALL FTLOCA(2,1)
        CALL FTEXT(BLNK90)
        CALL FTLOCA(3,1)
        CALL FTEXT(BLNK90)
        IF (IHP .NE. 1) THEN
        CALL FTLOCA(2,1)
        CALL FTEXT('^Structure ID: ^')
        CALL FTEXT(HALOE)
        ENDIF
        ICUR = 0
        IF (IHP .NE. 1)       CALL CURSOR(IX,IY)
        CALL DISPLA(2)
        CALL GPRINT
        IF (IHP .EQ. 1) THEN
        CALL FTLOCA(1,1)
        CALL FTEXT('^     ^')
        ENDIF
        CALL SETSCR(1)
        CALL GRAOFF
        PAGE = 1
        CALL DISPLA(1)
        CALL FTSIZE(2,18)
        DO 9331 I = 1,12
           MW(I) = 999
9331    CONTINUE
C       Return to menu
        GOTO 11
C
C CLEAR SCREEN
83      CONTINUE
        CHER = 1
        CALL SETCOL(0)
        CALL CLR
        CALL SETCOL(1)
        CALL SETSCR(2)
        CALL FTSIZE(1,10)
        PAGE = 2
        CALL DISPLA(2)
        CALL FTLOCA(1,1)
        CALL FTEXT(BLNK90)
        CALL FTLOCA(2,1)
        CALL FTEXT(BLNK90)
        CALL FTLOCA(3,1)
        CALL FTEXT(BLNK90)
        CALL FTLOCA(2,1)
        CALL FTEXT('^Structure ID: ^')
        CALL FTEXT(HALOE)
        CALL FTSIZE(2,18)
        CALL FTLOCA(3,1)
        CALL FTEXT('^CONNECTION TABLE IS BEING PROCESSED^')
        CALL FTSIZE(1,10)
        IF (RTNMSG) CALL MYERR(RR,32,32)
C
C Following code writes out MM array & Text common to files:
C
C       GO MAKE CONNECTION TABLE
C
        CALL FTSIZE(1,10)
        DO 603 I = 1,NJNEXT+1
        OERR = 0
605     CONTINUE
        IF ((LABL(I,1).LE.0).OR.(LABL(I,1).GT.MAXX).OR.(LABL(I,2).LE.0)
     *      .OR.(LABL(I,2).GT.MAXY)) GO TO 603
        IF (MM(LABL(I,1),LABL(I,2)).NE.46) GOTO 603
C If no chain marker go to 607
        IF (MRKCHN(I) .EQ. 0) GO TO 607
C ASCII 'C'
        IX = LABL(I,1)
        IY = LABL(I,2)
        FX = IX + 1
        FY = IY
```

```
      JCHAR = 2
      CALL DEL(46,FX,FY,0,0,0)
      HLO(2) = 'C'
      CALL CURSOR(IX,IY)
      CALL TEXT(HLO)
      MM(IX,IY) = 67
      LABL(I,1) = -999
      LABL(I,2) = -999
      GO TO 603
607   CONTINUE
C Blank out marker with space
      IX = LABL(I,1)
      IY = LABL(I,2)
      FX = IX + 1
      FY = IY
      JCHAR = 2
      CALL DEL(46,FX,FY,0,0,0)
      MM(IX,IY) = 46
      JX = IX * MULTX - 6
      JY = IY * MULTY - 4
      J3X = JX + 3
      J3Y = JY - 3
      CALL BAR(JX,JY,J3X,J3Y)
      LABL(I,1)=-999
      LABL(I,2)=-999
C Undoes cursor move done in DOT
C     CHECK VALENCE
603   CONTINUE
C
      IF (KHAR.EQ.71) THEN
         CALL FTSIZE(2,18)
         IF ((RTNMSG).OR.(PAGE.EQ.0)) THEN
            CALL FTLOCA(1,1)
            CALL FTEXT(BLNK90)
            IF (LOY.LE.2) THEN
               DO 1153 I = LOX,HIX+6,6
                  LX = MIN0(I,MAXX)
                  CALL REPLCE(LX,1,1,1,0,0,2)
 53            CONTINUE
               CALL RELONG
            ENDIF
         ENDIF
         CALL FTLOCA(3,1)
         ALL FTEXT(BLNK90)

            E.EQ.1) THEN
             SETSCR(2)
              SPLA(2)


     PAGE = 2
     IF (RTNMSG) CALL MYERR(RR,32,32)
     CHER = 2


     CALL BOND(IERR,KX,KY)

     CALL FTSIZE(2,18)
     CALL FTLOCA(3,1)
     CALL FTEXT(BLNK90)
     CALL FTSIZE(1,10)
     IF (IERR.EQ.0) GO TO 5353
        IF (IERR.EQ.100) THEN
           CALL SETSCR(1)
           PAGE = 1
           CALL DISPLA(1)
           CALL FTSIZE(2,18)
           CALL FTLOCA(1,1)
           CALL FTEXT('^INSUFFICIENT DISK SPACE FOR STRUCTURE^')
           IERR = 18
           CALL MYERR(IERR,KAR,KAR)
           CHER = 0
           PAGE = 0
```

```
      IRESET = 3
      RETURN
   ENDIF
   DO 50 L1 = 1,DTN
      MM(DTX(L1),DTY(L1)) = 42
      DTX(L1) = 0
      DTY(L1) = 0
      DTN1(L1) = 0
      DTN2(L1) = 0
50 CONTINUE
   DO 55 L1 = 1,2
      DO 55 L2 = 1,LBLEN
         LNGNDE(L2,L1) = 0
55 CONTINUE
   DO 66 L2 = 1,NBD1
      DSCNC(1,L2) = 0
66 CONTINUE
   DO 86 L2 = 1,MNUM
      IF (IMS(7,L2).GT.0) THEN
         VAL = IMS(7,L2)
         CALL REPNUM(VAL,NDGT,RET)
         DO 74 L0 =  NDGT,1,-1
            MM(IMS(3,L2)-L0,IMS(4,L2)) = ICHAR(RET(NDGT+1-L0))
74       CONTINUE
         L1 = NDGT + 1
         MM(IMS(3,L2)-L1,IMS(4,L2)) = 47
      ELSE
         L1 = 0
      ENDIF
      IF (IMS(1,L2).GT.1) THEN
         VAL = IMS(1,L2)
         CALL REPNUM(VAL,NDGT,RET)
         DO 76 L0 =  NDGT,1,-1
            MM(IMS(3,L2)-L0-L1,IMS(4,L2)) =
     *        ICHAR(RET(NDGT+1-L0))
76       CONTINUE
         MM(IMS(3,L2)-(NDGT+1+L1),IMS(4,L2)) = 42
         MM(IMS(3,L2),IMS(4,L2)) = 77
         MM(IMS(3,L2)+1,IMS(4,L2)) = IMS(2,L2)
      ELSE
         MM(IMS(3,L2)-1,IMS(4,L2)) = 42
         MM(IMS(3,L2),IMS(4,L2)) = 77
         MM(IMS(3,L2)+1,IMS(4,L2)) = IMS(2,L2)
      ENDIF
      DO 80 L1 = 0,IMS(6,L2)
         IF ((IMS(8+L1,L2).EQ.43).OR.(IMS(8+L1,L2).EQ.45)) THEN
            MM(IMS(3,L2)+2+L1,IMS(4,L2)) = (8 * 2**13) +
     *         IMS(8+L1,L2)
         ELSE
            MM(IMS(3,L2)+2+L1,IMS(4,L2)) = IMS(8+L1,L2)
         ENDIF
         IMS(8+L1,L2) = 0
80    CONTINUE
      DO 84 L1 = 1,7
         IMS(L1,L2) = 0
84    CONTINUE
86 CONTINUE
   DO 1066 I = 1,12
      MW(I) = 999
1066 CONTINUE
   IF (IERR.EQ.12) THEN
      MODE=1
C     Return to ground state
C     Allows us to rewrite header
      CALL HEADER
      MCHAR = 0
      JCHAR = 2
      RETURN
   ENDIF
   CALL SETSCR(1)
   PAGE = 1
   CALL DISPLA(1)
   IF (IERR.EQ.41) THEN
      JCHAR = 1
   ELSE
```

```
            JCHAR = 2
         ENDIF
         IERR = 18
         CALL MYERR(IERR,IERR,IERR)
C        SET ERR = BAD DATA
         JPROB = 1
         CHER = 0
         OERR = -1
         MCHAR = 0
      IF (IHP .EQ. 1) CALL CLEAR
      RETURN
5353  CONTINUE
      IF (IHP .EQ. 1) CALL CLEAR

      CALL GRAOFF
      CHER = 0
      PAGE = 2
      IRESET = 3
      RETURN
C
C Kill structure & reset
88    IRESET=1
      RETURN
1     IRESET=3
      RETURN
      END
```

SUBROUTINE REPNUM assigns the ASCII representation of a passed decimal integer value of 1 - 7 digits.

ORI Paul Broderick April, 1985

```
      SUBROUTINE REPNUM(VALUE,NDGT,RET)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 VALUE,VAL
      CHARACTER*1 DIGIT(8),RET(8)
C
      IF ((VALUE.GT.99999999).OR.(VALUE.LT.-9999999)) RETURN
      VAL = IABS(VALUE)
      DO 100 I = 1,8
         DIVD = MOD(VAL,10)
         VAL = VAL / 10
         DIGIT(I) = CHAR(DIVD + 48)
         NDGT = I
         IF (VAL.EQ.0) GO TO 110
100   CONTINUE
110   CONTINUE
C
      IF (VALUE.LT.0) THEN
         NDGT = NDGT + 1
         DIGIT(NDGT) = '-'
      ENDIF
      N = 0
      DO 200 I = NDGT,1,-1
         N = N + 1
         RET(N) = DIGIT(I)
200   CONTINUE
      N = N + 1
      DO 300 I = N,8
         RET(I) = ' '
300   CONTINUE
C
      RETURN
      END
C
      SUBROUTINE HEADER
      IMPLICIT INTEGER*2 (A-Z)
      LOGICAL*2 FIRST
      CHARACTER*1 RET(3),HALO(3),MWB1(16),MWB2(36),MWB3(36),MWB4(13),
     *   MWB6(13),MWB7(90),MWB9(90),MWB107(90),MWB109(90),
     *   MWB11(90),MWB13(90),MWB14(90),MWB15(90),MWB16(90),
     *   MWB17(90),MWB18(90),IDHLO(12),ID10(10),MWB19(18),MWB20(6),
     *   KSC10(10),HCMD,HLO(4),MWB21(90),MWB111(90),
     *   MWB113(90),MWB115(90),MWB116(90),MWB117(90),MWB118(90)
```

```
      CHARACTER*1 KAN
      CHARACTER*3 HALOE
      CHARACTER*4 HLOE
      CHARACTER*1 ISTAT
      CHARACTER*5 KSC
      CHARACTER*6 MW20
      CHARACTER*7 IPNT,IAXE
      CHARACTER*10 ID2,FILE,INID
      CHARACTER*12 IDH12
      CHARACTER*13 MW4,MW6
      CHARACTER*16 MW1
      CHARACTER*36 MW2,MW3
      CHARACTER*18 MW19
      CHARACTER*90 MW7,MW9,MW11,MW13,MW14,MW15,MW16,MW17,
     *    MW18,MW21,MW107,MW109,MW111,MW113,MW115,MW116,MW117,MW118
      COMMON /IIDD/ IONDX,ID2,FILE,INID(2500)
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /ISTATE/ ISTAT
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
      COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
      COMMON /RET/ SYM,KSC(2)
      COMMON /QTVLNC/ OERR,CHER
      COMMON /REP/ HCMD(2)
      EQUIVALENCE (ID2,ID10),(KSC,KSC10),(MW1,MWB1),(MW2,MWB2),
     *    (MW3,MWB3),(MW4,MWB4),(MW6,MWB6),(MW7,MWB7),(MW9,MWB9),
     *    (MW11,MWB11),(MW13,MWB13),(MW14,MWB14),(MW15,MWB15),
     *    (MW16,MWB16),(MW17,MWB17),(MW18,MWB18),(MW19,MWB19),
     *    (MW20,MWB20),(MW21,MWB21),(MWB107,MW107),(MWB109,MW109),
     *    (MWB111,MW111),(MWB113,MW113),(MWB115,MW115),(MWB116,MW116),
     *    (MWB117,MW117),(MWB118,MW118),(IDHLO,IDH12)
      EQUIVALENCE (HALOE,HALO(1))
      EQUIVALENCE (HLOE,HLO(1))
     DATA MW1 /'^Structure ID: ^'/
     DATA MW2 /'^Terminal is DUMB                       ^'/
     DATA MW3 /'^Terminal is SMART                      ^'/
     DATA MW7  /'?GND:UC lc  Bd  No  -+ sp/bksp  &   !   ^   _   :
    * #   %   @   *    DEL  Q    ?'/
     DATA MW107/'^    el jmp bd bdtp chg dumb  nlrg chn rng lib ret
    * mrk lgbd rep dotdis del quit  ^'/
     DATA MW11 /'^RING:No UC  lc Bd sp/bksp ESC  &    !   _   :   #
    *%  @   |  -+  DEL  Q   CR ^'/
     DATA MW111/'^   size el jmp bnd  dumb  rec nlrg chn lib ret
    * mrk lgbd rep num chg del quit rtn ^'/
     DATA MW9 /'?CHAIN:No UC lc  Bd sp/bksp &   ESC  ^   _   :
    *  #   %   @   |  -+  DEL  Q   CR  ?'/
     DATA MW109/'^    size el jmp bd  dumb  nlrg rec rng lib ret
    * mrk lbnd rep num chg del quit rtn ^'/
     DATA MW4 /'^Bond=       ^'/
     DATA MW6 /'^Enlrge=     ^'/
     DATA MW13 /'^LONG BOND:  lc    #     No       %     CR   Q
    *                                 ^'/
     DATA MW113/'^               jmp  mrkr  bndtype  draw  rtn  quit
    *                                 ^'/
     DATA MW14 /'^DUMB MODE:  Bd to return to SMART MODE
    *                                 ^'/
     DATA MW15 /'^REPEAT:  No      UC     lc     ''     UC$lc    Bd    CR
    *                                 ^'/
     DATA MW115/'^             bndtyp  elem  jump  draw  setelem  bond  rtn
    *                                 ^'/
     DATA MW16 /'^DOT DISCONNECT: No  /    UC/lc -+  sp  Q    HCl   Na
    *  Na+  Cl  Cl-  H+  Mx:          ^'/
     DATA MW116/'^                    mult frac elem  chg rtn quit
    *                                 ^'/
     DATA MW17 /'^LIBRARY: lc    Bd     No      DEL E      S      ESC
    *   CR                            ^'/
     DATA MW117/'^            jump bond  bndtyp del attach cursor rec
    *    rtn                           ^'/
     DATA MW18 /'^RETRIEVE:sp/bksp  ''  ESC  #  DEL  Bd   lc    L    F
    *   V     A     P    CR    Q       ^'/
     DATA MW118/'^            dumb  draw rec mrk del bond jump list file
    * view axial point rtn quit         ^'/
     DATA MW19 /'^ File name=          ^'/
     DATA MW20 /'^Sym=^'/
     DATA MW21 /'^ENLARGE: num(set bond enlargement factor), &(exit)
    *                                 ^'/
```

```
      DATA IOST /71/
      DATA IPNT /'^Point^'/
      DATA IAXE /'^Axial^'/
      DATA FIRST /.TRUE./
C
        IF (CHER.GT.0) RETURN
        IF (PAGE.NE.2) THEN
           CALL SETSCR(2)
           PAGE = 0
           CALL FTSIZE(1,10)
        ENDIF
        IF (FIRST) THEN
           HALO(1) = KAN
           HALO(3) = KAN
           IDHLO(1) = KAN
           IDHLO(12) = KAN
           HLO(1) = KAN
           HLO(4) = KAN
           FIRST = .FALSE.
        ENDIF
        IF (ISTATE.EQ.0) THEN
           IF (MODE.EQ.1) THEN
              ISTTT = 71
           ELSE IF (MODE.EQ.2) THEN
              ISTTT = 78
           ENDIF
        ELSE IF (ISTATE.NE.0) THEN
           ISTTT=ICHAR(ISTAT)
        ENDIF
C       SOLO, NO CHANGE
      IF ((MW(1).NE.999).AND.(ISKILL.EQ.1).AND.(ISTTT.EQ.IOST)) RETURN
C ISTAT = SINGLE CHAR CODE FOR STATE - USED IN SOLO MODE
        IOST=ISTTT
        CALL MEMOFF      !HP code - unlock memory
        CALL HOME        !HP code - move alpha cursor home
C
C      MW(1)= displayed ID(structure number)
C      2              terminal smartness; 1=smart
C      3              ISTATE OR (MODE IF ISTATE= 0)
C      4              last numeral entered
C      5              last bond type
C      6              Enlargement factor (NLARGE)
C
C      ISTATE=1   Don't use--USE MODE=1 instead
C              2    "    "    "   " =2    "
C              3  Chain state
C              4  Chain/number entry
C              5  Ring
C              6  Ring/number entry
C              7  Long bond
C              8  Dumb mode
C              9  Repeat state
C             10  Dot disconnect mode
C             11  Library
C             12  Retrieve
C             13  Enlarge
C     Following only displays changed infor on screen:
        IF (MW(1).EQ.999) THEN
           DO 2 I = 1,10
              IDHLO(I+1) = ID10(I)
2          CONTINUE
           MW(1) = 0
           IF (ISKILL.EQ.2) THEN
              CALL FTLOCA(1,1)
              CALL FTEXT(MW1)
           ELSE
              CALL FTLOCA(2,1)
           ENDIF
           CALL FTEXT(IDH12)
           CALL FTEXT('^      ^')
        ENDIF
        IF (ISKILL.EQ.1) GOTO 19
        IF (ISTATE.EQ.9) THEN
           IF (MW(3).NE.9) THEN
              CALL FTLOCA(2,1)
```

```
            CALL FTEXT(MW15)
            CALL FTLOCA(3,1)
            CALL FTEXT(MW115)
         ENDIF
         CALL FTLOCA(1,54)
         DO 140 I = 1,2
            HLO(I+1) = HCMD(I)
140      CONTINUE
      IF (HLO(3) .EQ. '0') HLO(3)=' '
         CALL FTEXT('^ATOM ACTIVE=^')
         CALL FTEXT(HLOE)
         CALL FTEXT('^   ^')
         MW(3) = 9
      ELSE IF (ISTATE.EQ.12) THEN
         IF (MW(3).NE.12) THEN
            CALL FTLOCA(2,1)
            CALL FTEXT(MW18)
            CALL FTLOCA(3,1)
            CALL FTEXT(MW118)
         ENDIF
         MW(6) = 999
         MW(9) = SYM
         CALL FTLOCA(1,52)
         CALL FTEXT(MW20)
         IF (SYM.EQ.2) THEN
            CALL FTEXT(IPNT)
         ELSE IF (SYM.EQ.1) THEN
            CALL FTEXT(IAXE)
         ENDIF
         CALL FTEXT('^  ^')
         DO 292 I = 1,6
            MWB19(12+I) = KSC10(I)
292      CONTINUE
         CALL FTEXT(MW19)
         MW(3) = 12
         GO TO 17
   ENDIF
   IF (ISMART.NE.MW(2)) THEN
      MW(2)=ISMART
      IF (ISMART.EQ.1) THEN
         CALL FTLOCA(1,52)
         CALL FTEXT('^  ^')
         CALL FTEXT(MW3)
      ELSE
         IF (MW(3).NE.ISTATE) THEN
            MW(5) = 999
            MW(6) = 999
            CALL FTLOCA(1,30)
            CALL FTEXT('^
            CALL FTEXT('^                                  ^')
            CALL FTLOCA(1,54)
            CALL FTEXT(MW2)
            CALL FTLOCA(2,1)
            CALL FTEXT(MW14)
            CALL FTLOCA(3,1)
      CALL FTEXT('^
      CALL FTEXT('^
            MW(3) = ISTATE
            GO TO 190
         ELSE
            GO TO 190
         ENDIF
      ENDIF
   ENDIF
   IF (ISTATE.NE.MW(3)) THEN
      CALL FTLOCA(2,1)
      IF ((ISTATE.EQ.1).OR.(ISTATE.EQ.0)) THEN
         CALL FTEXT(MW7)
         CALL FTLOCA(3,1)
         CALL FTEXT(MW107)
      ELSE IF (ISTATE.EQ.3) THEN
         CALL FTEXT(MW9)
         CALL FTLOCA(3,1)
         CALL FTEXT(MW109)
      ELSE IF (ISTATE.EQ.5) THEN
```

```
            CALL FTEXT(MW11)
            CALL FTLOCA(3,1)
            CALL FTEXT(MW111)
         ELSE IF (ISTATE.EQ.7) THEN
            CALL FTEXT(MW13)
            CALL FTLOCA(3,1)
            CALL FTEXT(MW113)
         ELSE IF (ISTATE.EQ.10) THEN
            CALL FTEXT(MW16)
            CALL FTLOCA(3,1)
            CALL FTEXT(MW116)
         ELSE IF (ISTATE.EQ.11) THEN
            CALL FTEXT(MW17)
            CALL FTLOCA(3,1)
            CALL FTEXT(MW117)
         ELSE IF (ISTATE.EQ.13) THEN
            CALL FTEXT(MW21)
            CALL FTLOCA(3,1)
         CALL FTEXT('^
         CALL FTEXT('^
         ENDIF
         MW(3) = ISTATE
      ENDIF
 17   CONTINUE
      IF (NLARGE.NE.MW(6)) THEN
         DO 310 I = 9;11
            MWB6(I) = ' '
 310     CONTINUE
         PAS = NLARGE
         CALL NUMCHR(PAS,RET,NDGT)
         DO 300 I = 1,NDGT
            MWB6(I+8) = RET(I)
 300     CONTINUE
         MW(6)=NLARGE
         CALL FTLOCA(1,41)
         CALL FTEXT(MW6)
      ENDIF
      IF (IBTYPE.EQ.MW(5)) GO TO 190
         I = IBTYPE + 48
         MWB4(7) = CHAR(I)
         CALL FTLOCA(1,30)
         CALL FTEXT(MW4)
         MW(5) = IBTYPE
C
C     THIS NEXT CODE FOOLS THE HEADER ROUTINE INTO THINKING
C     THAT IBTYPE HAS BEEN SWITCHED FROM NON-PERMANENT TO 1
C     BEFORE IT HAS ACTUALLY HAPPENED.
C     I DIDN'T WANT TO ACTUALLY RESET IBTYPE BECAUSE IT HAS
C     TOO MANY REPERCUSSIONS.
C
 19   IF (ISKILL .EQ. 2) GO TO 190
         HALO(2) = CHAR(ISTTT)
         CALL FTLOCA(3,1)
         IF (ISTATE.EQ.5) THEN
            HALO(1) = ';'
            HALO(3) = ';'
            CALL FTEXT(HALOE)
            HALO(1) = '^'
            HALO(3) = '^'
         ELSE
           CALL FTEXT(HALOE)
        ENDIF
     GO TO 119
190  IF ((ISTATE.EQ.9).OR.(ISTATE.EQ.13)) GO TO 119
     IF (.NOT.(ICHAR.EQ.1 .AND.
    1 (IBTYPE.EQ.2 .OR. IBTYPE.EQ.3 .OR. IBTYPE.EQ.5
    2 .OR. IBTYPE.EQ.6 .OR. IBTYPE.EQ.7))) GO TO 119
        IFOOL=1
        MW(5) = 999
        MWB4(7) = '1'
119  CONTINUE
     CALL LINE4       !HP code - move to line 4
     CALL MEMON       !HP code - lock memory
     RETURN
     END
```

```
$STORAGE:2
C
C       THIS SUBROUTINE WILL MAKE A LIBRARY ENTRY
C
        SUBROUTINE LIBRA(IX,IY,KAR)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,IDTPIX,IFIRST,ONE,DSKMEM
        INTEGER*2 CGINFO(10,4)
        LOGICAL*2 EXIST,OVRWRT
        CHARACTER*10 FILE,LFILE,LSC
        CHARACTER*8 LIBRET
        CHARACTER*5 NSC
        CHARACTER*1 KAN
        CHARACTER*1 NAMSTR(6)
        CHARACTER*1 ISTAT
        CHARACTER*1 NSC10(10),HALO(12),HLO(3),LIBR8(8,640)
        CHARACTER*12 HALOE
        CHARACTER*3 HLOE
        EQUIVALENCE (HALOE,HALO(1))
        EQUIVALENCE (HLOE,HLO(1))
        EQUIVALENCE (NSC,FILE),(NSC,NSC10),(LIBRET,LIBR8)
        COMMON /RET/ SYM,NSC(2)
        COMMON /BAKLIB/ LSC
        COMMON /LIB/ LIBRET(640),NLIBS
        COMMON /CD/ MAXX,MAXY
        COMMON /IPLUS/ IHIGH(14,2)
        COMMON /MKSKP/ ISKIP
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /ISTATE/ ISTAT
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
        COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /HEAD/ MW(12),ISTATE,PAGE
        COMMON /CUR/ ICUR
        COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /FROM/ LCHAR
        COMMON /IIDD1/ RECNO(2500),NUMIDS,TOTIDS
        COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
        COMMON /HP/IHP
        COMMON /RETLIB/OVRWRT
:       DATA OU /35/
C***********************************************************************
C This section initializes some parameters and calls HEADER
C***********************************************************************
        IF (IHP .NE. 1) THEN
        CALL MEMDSK(CLUSTS,CPDISK,BPSECT,SPCLUS)
        DSKMEM = CLUSTS * BPSECT * SPCLUS
        IF (DSKMEM.LE.(36864+(80*TOTIDS))) THEN
           PAGE = 0
           CALL FTSIZE(2,18)
           CALL FTLOCA(1,1)
           CALL FTEXT('^INSUFFICIENT DISK SPACE FOR ADDITIONAL SUBSTRUCT
     *URES-MAY ATTEMPT CONNECTION TABLE^')
           CALL FTSIZE(1,10)
           GO TO 409
        ENDIF
        ENDIF
        HLO(1) = KAN
        HLO(3) = KAN
        HALO(1) = KAN
        LFILE = FILE
1       CONTINUE
        OVRWRT = .FALSE.
        DOT = 0
        ISKIP = 1
        ISTAT = '_'
        MODE=1
        ISTATE=11
        KAR=13
        DBONDX=0
        DBONDY=0
C       Set attaching bond coordinates to 0
C       They will remain 0 if we have a stand alone structure
        DO 786 I = 1,10
```

```
        DO 786 J = 1,4
           CGINFO(I,J) = 0
786     CONTINUE
        DVAL=0
        BLEN=0
C       Set attaching bond length and bond direction to 0
C       They will remain 0 if we have a stand alone structure
        CALL HEADER
61      CONTINUE
C       Abort if input=A
        ONE = MM(IX,IY)
C Picture value at cursor when LIBRA was entered
        IF (ONE .EQ. 42) GO TO 5050
C If we are at a * don't call valence or clear hydrogen
        CALL CLRHYD(IX-1,IY)
        CALL VALNCE(2,IX-1,IY,0,0)
C Clear valence hydrogens and replace as needed
        ICUR = 1
        CALL CURSOR(IX,IY)
C*************************************************************************
C This section looks for a Dot Disconnected structure - If a pure dot disconnec
C detected then "merging and exit bond" prompts are ignored and the
C final cursor position is set to the *
C A dot dis is stored with DOT = 1 - Charges are not stored separately
C and valence hydrogens are not removed
C If a mixture of dotdis and regular structure is found - the structure
C is disallowed and the command is rejected
C*************************************************************************
5050    IFIRST=0
        DO 345 I = LOX,HIX
        DO 345 J = LOY,HIY
        IF (IFIRST .NE. 0) GO TO 42
        IF (MM(I,J) .NE. 0) IFIRST=MM(I,J)
 2      IF (MM(I,J) .NE. 42) GO TO 345
        DOT = 1
        LBONDX=I
        LBONDY=J
        IF (IFIRST .EQ. 42 .AND. ONE .EQ. 42) GO TO 731
: Test for unmixed DOT DIS
        IERR = 52
        CALL MYERR(IERR,KAR,KAR)
        ICNT=ICNT+1
        GO TO 409
'31     CONTINUE
        CALL FTSIZE(2,18)
        CALL FTLOCA(6,1)
        CALL FTEXT('^DOTDIS structure detected^')
        CALL DELAY
        CALL FTSIZE(1,10)
        PAGE = 0
        ICNT=ICNT+1
        GO TO 800
345     CONTINUE
:*************************************************************************
: This section obtains the connecting site
: Make sure connecting site is a marker or bond
:*************************************************************************
56      CONTINUE
        CALL FTSIZE(2,18)
        CALL FTLOCA(6,1)
        CALL FTEXT('^Move cursor to connecting site - Type E to finalize
     * position      ^')
        PAGE = 0
        AKAR=69
: Primary terminator character = E
        BKAR=83
        REST = 1
: Alternate terminator character = S
        CALL SITE(IX,IY,AKAR,BKAR,TER,ICNT,REST)
        IF (REST.EQ.131) GO TO 1
: Get connecting site
        IF (TER .EQ. 13) GO TO 409
: Abort if return from SITE was CR
: Cursor should be at a marker or bond - Find out which
        KIX=IX
```

```
      KIY=IY
      IVAL=LMM(IX,IY)
      IF (IVAL .NE. 46) GO TO 2002
      IX=IX+1
C Cursor right on marker - placed there by moving the cursor
C Save DBONDX AND DBONDY and call CURSOR
      ICUR = 1
      CALL CURSOR(IX,IY)
      GO TO 2003
2002  IF (LMM(IX-1,IY) .NE. 46) GO TO 2001
2003  DBONDX=IX
C We are at a marker
      DBONDY=IY
      BLEN=0
      DVAL=0
      GO TO 2000
2001  IF (IVAL .EQ. 0) GO TO 47
C     Spot is empty - Are we at the end of a bond?
      IF (IVAL .LT. 256 .OR. IVAL .GT. 2**13)  GOTO 64
      GO TO 480
47    CALL FINDB(IBDIR,KBDIR,IX,IY)
C     See if we are at the end of a bond
      IF (IBDIR .EQ. -1) GO TO 64
C     -1 means we are not at the end of a bond
      DVAL = KBDIR
C     Find end of bond
      CALL DELTA(DVAL,KNCX,KNCY)
      INCX=KNCX
      INCY=KNCY
      KIX=KIX-INCX
      KIY=KIY-INCY
      IVAL=MM(KIX,KIY)
      GO TO 53
480   DVAL=IVAL/256
      DVAL=IVAL-DVAL*256
      CALL DELTA(DVAL,INCX,INCY)
53    DO 73   K=1,2
      DO 72   I=1,20
      KIX=KIX+INCX
      KIY=KIY+INCY
      LVAL=LMM(KIX,KIY)
      IF (LVAL .EQ. 0) GO TO 71
      IF (LVAL .NE. IVAL) GO TO 75
72    CONTINUE
75    INCX=-INCX
      INCY=-INCY
      KIX=IX
      KIY=IY
73    CONTINUE
64    CONTINUE
      CALL FTSIZE(2,18)
      CALL FTLOCA(4,1)
      CALL FTEXT('^Cursor not at a bond or a marker^')
      PAGE = 0
      CALL FTSIZE(1,10)
      GO TO 66
71    DBONDX=KIX-INCX
      DBONDY=KIY-INCY
C     Get length of attaching bond
      KIX=DBONDX
      KIY=DBONDY
      DO 67 I=1,20
         II = I
         KIX=KIX-KNCX
         KIY=KIY-KNCY
         IF (LMM(KIX,KIY) .NE. IVAL) GO TO 68
67    CONTINUE
      GO TO 64
C     Something funny with bond length - issue error message and try again
68    BLEN=II
C***********************************************************************
C This section assigns an output channel, gets the file name, checks
C to see if the name already exists, asks if an existing file is to
C be overwritten, aborts the command if the file is not to be over-
C written, opens the file, writes the file, closes the file and releases
```

```
C the output channel
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
        IX=DBONDX+KNCX
        IY=DBONDY+KNCY
        ICUR = 1
        CALL CURSOR(IX,IY)
C Set X and Y and call CURSOR
2000    CONTINUE
        IF (TER .NE. BKAR) GO TO 777
        LBONDX=IX
        IF (MM(IX,IY).EQ.0 .AND. MM(IX-1,IY).EQ.46) LBONDX = LBONDX - 1
C If TER = S then skip entry of exit site data
        LBONDY=IY
C and use connecting site data for exit data
        GO TO 800
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
C This section obtains the exit site
C Make sure exit site is a marker or bond
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
777     AKAR=83
C Set terminator to S
77      ICNT=ICNT+1
        CALL FTSIZE(2,18)
        CALL FTLOCA(6,1)
        CALL FTEXT('^Move cursor to exit site - Type S to finalize posit
     *ion      ^')
        PAGE = 0
        REST = 2
        CALL SITE(IX,IY,AKAR,BKAR,TER,ICNT,REST)
        IF (REST.EQ.131) GO TO 1
C Get exit site
        IF (TER .EQ. 13) GO TO 409
C Terminator was CR - bail out
        IBDIR=0
        IVAL=LMM(IX,IY)
        IF (IVAL .NE.46) GO TO 6002
        IX=IX+1
C Cursor is right on marker - Adjust X and go on
        GO TO 6003
6002    IF (LMM(IX-1,IY) .EQ. 46) GO TO 6003
C We are at a marker - go on
        IF (IVAL .EQ. 0) CALL FINDB(IBDIR,KBDIR,IX,IY)
C We are at an empty spot - See if we are at the end of a bond
        IF ((IBDIR .NE. -1 .AND. IVAL .EQ. 0) .OR. IVAL .GE. 256)
     1  GO TO 6003
C We are at a bond - go to 6003
        ICNT=ICNT+1
C Not at a bond or marker - try again
        GO TO 77
        ICUR = 1
6003    CALL CURSOR(IX,IY)
        LBONDX=IX
        IF (MM(IX,IY).EQ.0 .AND. MM(IX-1,IY).EQ.46) LBONDX = LBONDX - 1
C Set final cursor postion
        LBONDY=IY
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
C This section deletes all valence hydrogens before the file is stored on disk
C MM is copied to IDTPIX - Valence H's are removed from IDTPIX
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
800     CONTINUE
!         Trap for " on 2 letter element - Bail out if you find one
!
         IF (NBD1 .EQ. 0) GO TO 962
         DO 963 I=1,NBD1
         LX=DSCNC(3,I)
         LY=DSCNC(4,I)
         MX=DSCNC(5,I)
         MY=DSCNC(6,I)
         IF (MM(MX,MY) .NE. 34) GO TO 963
         M1=MM(LX,LY)
         M2=MM(LX+1,LY)
         IF ((M1 .GE. 65 .AND. M1 .LE. 90) .AND.
     *   (M2 .GE. 97 .AND. M2 .LE. 122)) THEN
         IERR=61
         CALL MYERR(IERR,IERR,IERR)
```

```
      GO TO 409
      ENDIF
963   CONTINUE
962   CONTINUE
!
!     Trap for charges on 2 letter elements
!
      IF (DOT .EQ. 1) GO TO 842       !Skip if DOTDIS
      DO 617 I=LOX,HIX
      DO 617 J=LOY,HIY
      IF (LMM(I,J) .NE. 43 .AND. LMM(I,J).NE.45) GO TO 617
      LOC = IHMM(I,J)
      IF (LOC .EQ. 0) GO TO 617
      ITX=I-IHIGH(LOC,1)
      ITY=J+IHP*IHIGH(LOC,2)
      M1=LMM(ITX,ITY)
      M2=LMM(ITX+1,ITY)
      IF ((M1 .GE. 65 .AND. M1 .LE.90) .AND. (M2 .GE. 97
     * .AND. M2 .LE. 122)) THEN
      IERR=61
      CALL MYERR(IERR,IERR,IERR)
      GO TO 409
      ENDIF
617   CONTINUE
842   DO 81 I = LOX,HIX
      DO 81 J = LOY,HIY
      IDTPIX(I,J)=MM(I,J)
81    CONTINUE
      IF (DOT .EQ. 1) GO TO 589
C Skip CLEARH if this is a DOTDIS
      DO 80 I = LOX,HIX
      DO 80 J = LOY,HIY
      II = I
      JJ = J
      IF (IDTPIX(I,J).GE.65 .AND. IDTPIX(I,J) .LE. 97
     1 .AND. (IDTPIX(I,J) .NE. 72 .OR. (IDTPIX(I,J) .EQ. 72
     2 .AND. IDTPIX(I+1,J) .GE. 97 .AND. IDTPIX(I+1,J) .LE. 122)))
     3 CALL CLEARH(2,II,JJ)
80    CONTINUE
589   CONTINUE
44    ICNT = ICNT +1
      IF (PAGE.NE.1) THEN
         CALL SETSCR(1)
         PAGE = 1
        CALL DISPLA(1)
        CALL FTSIZE(2,18)
      ENDIF
      IF (IHP .EQ. 1) THEN
      CALL LINE4          !Partial clear for HP
      CALL ACLEAR
      ELSE
      CALL SETCOL(0)
      CALL CLR
      CALL SETCOL(1)
      ENDIF
      FILE = '          '

      CALL FTLOCA(7,20)
      CALL FTEXT('^Enter designation for structure (1-6 alphanumerics)
     * ^')
444   CONTINUE
      J = 0
      IF (IHP .EQ. 1) THEN
      CALL ALPCUR
      ACCEPT 691, (NAMSTR(I),I=1,6)
691   FORMAT(6A1)
      ENDIF
      DO 4444 I = 1,60
         J = J + 1
         FX = 19 + J
4444     CONTINUE
      IF (IHP .EQ. 1) THEN
      A=ICHAR(NAMSTR(J))
      IF (A .GE. 97) A=A-32
      ELSE
```

```
            A = GETCHR()
          ENDIF
            IF (A.EQ.13 .OR. A .EQ. 32) GO TO 4446
            IF (A.EQ.8) THEN
              IF (J.GT.1) J = J - 1
              FX = 19 + J
              CALL FTLOCA(8,FX)
              CALL FTEXT('^ ^')
              NSC10(J) = ' '
              GO TO 1444
            ENDIF
            HLO(2) = CHAR(A)
          IF (IHP .NE. 1) THEN
            CALL FTLOCA(8,FX)
            CALL FTEXT(HLOE)
          ENDIF
            IF (((A.GE.48).AND.(A.LE.57)).OR.((A.GE.65).AND.
     *        (A.LE.90)).OR.((A.GE.97).AND.(A.LE.122))) THEN
              NSC10(J) = CHAR(A)
            ELSE
              NSC10(J) = ' '
            ENDIF
            IF (J.EQ.6) GO TO 4446
4444      CONTINUE
4446      CONTINUE
          IF (IHP .EQ. 1) THEN
          CALL LINE4
          CALL ACLEAR     !Partial clear for HP
          ELSE
          CALL SETCOL(0)
          CALL CLR
          CALL SETCOL(1)
          ENDIF
C         NULL FILE NAME IMPLIES ABORT COMMAND.
          IF (NSC(1) .EQ. '      ') GO TO 409
C         CONCATENATE .STR EXTENSION TO FILE NAME
          NSC10(7) = '.'
          NSC10(8) = 'S'
          NSC10(9) = 'T'
          NSC10(10) = 'R'
          DO 8686 I = 1,10
            HALO(I+1) = NSC10(I)
8686      CONTINUE
          HALO(12) = KAN
          CALL FTLOCA(7,26)
          CALL FTEXT('^Output to file: ^')
          CALL FTEXT(HALOE)
          CALL FTLOCA(8,26)
          CALL FTEXT('^Press RETURN to clear screen^')
          A = GETCHR()
          IF (IHP .EQ. 1) THEN
          CALL LINE4
          CALL ACLEAR     !Partial clear for HP
          ELSE
          CALL SETCOL(0)
          CALL CLR
          CALL SETCOL(1)
          ENDIF
          INQUIRE(FILE=FILE,EXIST=EXIST)
          IF (.NOT.EXIST) GO TO 404
C
C File exists - Do you wish to replace it (Y/N)?
        CALL FTLOCA(7,23)
        CALL FTEXT('^File exists - Do you wish to replace it (Y/N)?^')
460     CONTINUE
        IKAR = GETCHR()
         IF (IHP .EQ. 1) THEN
         CALL LINE4      !Partial clear for HP
         CALL ACLEAR
         ELSE
        CALL SETCOL(0)
        CALL CLR
        CALL SETCOL(1)
         ENDIF
```

```
      IF (IKAR.EQ.95) THEN
         IERR = 39
         CALL MYERR(IERR,IERR,IERR)
         GO TO 460
      ELSE IF (IKAR.EQ.13 .OR. IKAR.EQ.78 .OR. IKAR.EQ.110) THEN
         GO TO 44
C If no - go get new file name
      ELSE IF (IKAR .EQ. 89 .OR. IKAR .EQ. 121) THEN
         OVRWRT = .TRUE.
         GO TO 404
      ENDIF
        CALL FTLOCA(8,23)
        CALL FTEXT('^Invalid response: ^')
        HLO(2) = CHAR(IKAR)
        CALL FTEXT(HLOE)
C Invalid response - go try new entry
        GO TO 460
404     OPEN(OU,FILE=FILE)
        IF (DOT .EQ. 1) GO TO 912
C Skip charge processing for DOTDIS
C       Get charges
        LENC = 0
        DO 85 I = LOX,HIX
        DO 85 J = LOY,HIY
        IF(LMM(I,J) .NE. 43 .AND. LMM(I,J) .NE. 45) GO TO 85
        LENC=LENC+1
        IF (LENC .GT. 10) GO TO 1234
C Too many charges - bail out
        LOC = IHMM(I,J)
C Get index if IHIGH so we can determine the
C coordinates of the associated node
        IF (LOC .NE. 0) GO TO 86
        CGINFO(LENC,1)=I
C Delocalized charge - X value
        CGINFO(LENC,2)=J
C Delocalized charge - y value
        GO TO 87
86      CGINFO(LENC,1)=I-IHIGH(LOC,1)
C X value
        CGINFO(LENC,2)=J+IHP*IHIGH(LOC,2)
C Y value
87      CGINFO(LENC,3)=LMM(I,J)
C + OR -
        IDTPIX(I,J)=0
        CGINFO(LENC,4)=0
        IF(MM(I+1,J).GE.50.AND.MM(I+1,J).LE.57) CGINFO(LENC,4)=MM(I+1,J)
C Digit following sign
        IF (CGINFO(LENC,4) .NE. 0) IDTPIX(I+1,J)=0
85      CONTINUE
C
C       D1 data is prepared for output.
        LEND = 0
        DO 300 I = 1,NBD1
           MX = DSCNC(5,I)
           MY = DSCNC(6,I)
           IF (MM(MX,MY).NE.34) GO TO 300
           LEND = LEND + 1
           IDTPIX(MX,MY) = 0
300     CONTINUE
C
C       THE FOLLOWING CODE GETS THE LENGTHS OF THE ARRAYS
C       MM - LABL - MRKCHN - AND LNGBND
C       SO THAT WE CAN COMPRESS THE DISK FILES
        LOX = MAX0(LOX,1)
        LOY = MAX0(LOY,1)
        HIX = MIN0(HIX,MAXX)
        HIY = MIN0(HIY,MAXY)
912     LENP=0
        DO 45 I= LOX,HIX
        DO 45 J= LOY,HIY
        IF (IDTPIX(I,J) .NE. 0) LENP=LENP+1
45      CONTINUE
        LENM=0
        FLENM = 0
        DO 46 I=1,260
```

```
      IF ((LABL(I,1).NE.0).AND.(LABL(I,2).NE.0)) THEN
         FLENM = FLENM + 1
         IF ((LABL(I,1).GT.0).AND.(LABL(I,2).GT.0)) LENM = LENM + 1
      ELSE
         GO TO 4466
      ENDIF
46    CONTINUE
4466  CONTINUE
C
      LENL = LBLEN
C
100   FORMAT(7I4)
      WRITE(OU,100) DBONDX,DBONDY,DVAL,BLEN,DOT,LBONDX,LBONDY
      WRITE(OU,100) LENP
      DO 49 I= LOX,HIX
      DO 49 J= LOY,HIY
      IF (IDTPIX(I,J) .NE. 0) WRITE (OU,400) I,J,IDTPIX(I,J)
49    CONTINUE
400   FORMAT(2I4,I10)
C
      WRITE(OU,100) LENM
      IF (LENM .EQ. 0) GO TO 406
      DO 401 I=1,FLENM
      IF ((LABL(I,1).GT.0).AND.(LABL(I,2).GT.0))
     *   WRITE(OU,100) LABL(I,1),LABL(I,2), MRKCHN(I)
401   CONTINUE
C
406   WRITE (OU,100) LENL
      IF (LENL .EQ. 0) GO TO 4077
      DO 403 I=1,LENL
         WRITE(OU,100) (LNGBND(I,J),J=1,5)
403   CONTINUE
C
4077  WRITE(OU,100) LENC
      DO 4033 I = 1,LENC
         WRITE(OU,100) (CGINFO(I,J),J=1,4)
4033  CONTINUE
      WRITE(OU,100) LEND
      DO 310 I = 1,NBD1
         MX = DSCNC(5,I)
         MY = DSCNC(6,I)
         IF (MM(MX,MY).EQ.34) WRITE(OU,100) (DSCNC(J,I),J=3,4)
310   CONTINUE
      IF (.NOT.OVRWRT) THEN
         NLIBS = NLIBS + 1
         IF (NLIBS.GT.640) THEN
            CALL FTLOCA(4,1)
            CALL FTEXT('^WARNING-MORE THAN 640 SUBSTRUCTURE FILES EXIS
     *T-NOT ALL NAMES CAN BE LISTED IN RETRIEVE^')
            PAGE = 0
            GO TO 407
         ENDIF
         LIBR8(1,NLIBS) = '^'
         DO 4088 I = 1,6
            LIBR8(I+1,NLIBS) = NSC10(I)
4088     CONTINUE
         LIBR8(8,NLIBS) = '^'
      ENDIF
407   CLOSE (OU)
C     RELEASE CHANNEL
C*********************************************************************
C This section clears the dialog from the screen, positions the cursor,
C sets some return variables, calls HEADER and returns
C*********************************************************************
409   CONTINUE
      IF (IHP .EQ. 1) THEN
      CALL LINE4
      CALL ACLEAR     !Do partial clear for HP
      ENDIF
      IF (PAGE.EQ.1) THEN
         CALL SETCOL(0)

      IF (IHP .NE. 1)    CALL CLR
         CALL SETCOL(1)
         CALL SETSCR(2)
```

```
         PAGE = 2
         CALL DISPLA(2)
         CALL FTSIZE(1,10)
      ENDIF
      ICUR = 1
      CALL CURSOR(IX,IY)
C     Position cursor correctly and set parameters accordingly
      ISTATE=0
      IF (FILE.EQ.'           ') THEN
         FILE = LFILE
      ELSE
         LSC = LFILE
      ENDIF
      IF ((LCHAR.EQ.12).OR.(LCHAR.EQ.13)) GO TO 3000
      LEVEL=0
      CALL HEADER
      ISKIP = 0
C     SET LEVEL AND ISTATE TO GROUND AND CALL HEADER
      RETURN
3000  CONTINUE
      LFLAG = 1
      LEVEL = 1
      ICHAR = LCHAR
      IF (ICHAR.EQ.12) KAR = 94
      IF (ICHAR.EQ.13) KAR = 33
      ISKIP = 0
      CALL HEADER
      RETURN
1234  IERR = 51
      CALL MYERR(IERR,KAR,KAR)
      GO TO 407
      END
C
C     SUBROUTINE REFORM creates from connection table input the graphics
C     image in arrays MM and LNGBND.  SUBROUTINE GETLIN is called to
C     return a record of connection table input and SUBROUTINE CHRNUM is
C     called to convert strings of numeric digits to integer values.
C
C     ORI   Paul Broderick   December, 1984
C
      SUBROUTINE REFORM(STATUS)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM
      DIMENSION NODE(2),MULT(2),BOND(255,16),BTYPE(255,16),X(255),
     *   Y(255),NCON(255)
      CHARACTER*1 LINE,COMMA,APOST,STAR,BLANK,CONTBL,SLASH
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /TRANS/ LINE(160)
      COMMON /CD/ MAXX,MAXY
      COMMON /RANGE/ LOX,HIX,LOY,HIY
      COMMON /QTVLNC/ OERR,CHER
      COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
      COMMON /IRECS/ IU,IREC,TOPREC,BOTREC
      COMMON /CONTBL/ CONTBL(80,258),LTBL
        COMMON /HP/IHP
      DATA COMMA /','/,APOST /'"'/,STAR /'*'/,CANCEL /24/,
     *   BLANK/' '/,SLASH /'/'/
C
      STATUS = 0
      TOPREC = IREC
      LTBL = 0
      LONODE = 1
      HINODE = 0
C
C     The header record is input.
10    CONTINUE
      CALL TTYGET(LENGTH,STATUS)
      POS = 1
      CALL CHRNUM(RECNO,BEG,POS)
      IF ((RECNO.NE.0).OR.(STATUS.NE.0)) THEN
         CHER = 2
         CALL MYERR(37,37,37)
         CALL FTSIZE(2,18)
         CALL FTLOCA(1,35)
         CALL FTEXT('^-OR-IN FILE VERSION-INPUT RECORD OUT OF ORDER^')
```

```
         STATUS = 1
         RETURN
      ENDIF
      PRVREC = RECNO
C
C     The number of records to follow is identified.
      POS = 3
      CALL CHRNUM(NRECS,BEG,POS)
C
C     Each node is processed into the picture array.
      DO 1000 I = 1,NRECS
         CALL TTYGET(LENGTH,STATUS)
C
C        The record number is identified.
         POS = 1
         CALL CHRNUM(RECNO,BEG,POS)
         IF ((RECNO.NE.PRVREC+1).OR.(STATUS.NE.0)) THEN
            CHER = 2
            CALL MYERR(37,37,37)
            CALL FTSIZE(2,18)
            CALL FTLOCA(1,35)
            CALL FTEXT('^-OR-IN FILE VERSION-INPUT RECORD OUT OF ORDER^'
     *)
            STATUS = 1
            RETURN
         ENDIF
         PRVREC = RECNO
C
C        The chemical symbol is identified.
         POS = POS + 1
         IF (LINE(POS).NE.'c') THEN
            NODE(1) = ICHAR(LINE(POS))
         ELSE
            NODE(1) = 46
         ENDIF
         NOD = 1
         POS = POS + 1
         IF (LINE(POS).NE.BLANK) THEN
            NODE(2) = ICHAR(LINE(POS))
            NOD = 2
         ENDIF
C
C        The x and y coordinates are identified.
         POS = POS + 2
         CALL CHRNUM(VAL,BEG,POS)
         X(I) = VAL
         IF (X(I).LT.LOX) THEN
            LOX = X(I)
         ELSE IF (X(I).GT.HIX) THEN
            HIX = X(I)
         ENDIF
         POS = POS + 1
         CALL CHRNUM(VAL,BEG,POS)
         Y(I) = VAL
         IF (Y(I).LT.LOY) THEN
            LOY = Y(I)
         ELSE IF (Y(I).GT.HIY) THEN
            HIY = Y(I)
         ENDIF
C
         POS = POS + 1
C        If the node is a dot-disconnect marker, it is processed.
         IF (NODE(1).EQ.42) THEN
            MM(X(I),Y(I)) = NODE(1)
    IF ((ICHAR(LINE(POS)).GE.49).AND.(ICHAR(LINE(POS)).LE.57)) THEN
               KNT = 0
 20            CALL CHRNUM(VAL,BEG,POS)
               DO 30 RNT = BEG,POS-1
                  KNT = KNT + 1
                  MM(X(I)+KNT,Y(I)) = ICHAR(LINE(RNT))
 30            CONTINUE
               KNT = KNT + 1
               POS = POS + 1
```

```
      IF ((ICHAR(LINE(POS)).GT.48).AND.(ICHAR(LINE(POS)).LE.57)) THEN
               MM(X(I)+KNT,Y(I)) = ICHAR(SLASH)
               GO TO 20
            ENDIF
         ENDIF
         LONODE = LONODE + 1
C
C     If the node is a non-localized charge, it is processed.
      ELSE IF ((NODE(1).EQ.43).OR.(NODE(1).EQ.45)) THEN
         DO 50 J = 1,NOD
            IF (NODE(J).NE.49) MM(X(I)-1+J,Y(I)) = NODE(J)
50       CONTINUE
         HINODE = 1
C
C     If the node is a D structure, it is processed.
      ELSE
         IF ((NODE(1).EQ.68).AND.(NODE(2).GE.49).AND.(NODE(2).LE.
     *   57)) THEN
         NODE(2) = NODE(2) + 63
         MUL = 1
         MULT(1) = ICHAR(LINE(POS))
         POS = POS + 1
      IF ((ICHAR(LINE(POS)).GE.48).AND.(ICHAR(LINE(POS)).LE.57)) THEN
            MULT(2) = ICHAR(LINE(POS))
            MUL = 2
            POS = POS + 1
         ENDIF
         POS = POS + 1
         IF ((MULT(1).GE.50).OR.(MUL.EQ.2)) THEN
            K = 1
            DO 100 J = MUL,1,-1
               MM(X(I)-J,Y(I)) = MULT(K)
               K = MUL
100         CONTINUE
         ELSE
            MUL = 0
         ENDIF
         DO 200 J = 1,NOD
            MM(X(I)-1+J,Y(I)) = NODE(J)
200      CONTINUE
C
C     If the node is an *M structure, it is processed.
      ELSE IF ((NODE(1).EQ.77).AND.(NODE(2).GE.49).AND.(NODE(2)
     *   .LE.57)) THEN
         NODE(2) = NODE(2) + 63
         DO 300 J = 1,NOD
            MM(X(I)-1+J,Y(I)) = NODE(J)
300      CONTINUE
C
C     If the node is an atom node, it is processed.
      ELSE
         IF ((NODE(1).EQ.72).AND.(NOD.EQ.1)) NODE(1) = 74
         DO 400 J = 1,NOD
            MM(X(I)-1+J,Y(I)) = NODE(J)
400      CONTINUE
C
C        The charge or possible D1 bond site is identified.
         CALL CHRNUM(CHG,BEG,POS)
         LOW = BEG
         HIGH = POS - 1
C
C        The relative charge or bond site position is identified.
         POS = POS + 1
         CALL CHRNUM(RELCGP,BEG,POS)
         IF (CHG.NE.0) THEN
            IF (RELCGP.EQ.1) THEN
               IGH = 3
               INKX = 0
               INKY = IHP
            ELSE IF (RELCGP.EQ.2) THEN
               IGH = 4
               INKX = 1
               INKY = IHP
            ELSE IF (RELCGP.EQ.12) THEN
               IGH = 5
               INKX = 2
               INKY = IHP
```

```
      ELSE IF (RELCGP.EQ.3) THEN
         IGH = 8
         INKX = 1
         INKY = 0
      ELSE IF (RELCGP.EQ.13) THEN
         IGH = 9
         INKX = 2
         INKY = 0
      ELSE IF (RELCGP.EQ.4) THEN
         IGH = 13
         INKX = 1
         INKY = -IHP
      ELSE IF (RELCGP.EQ.14) THEN
         IGH = 14
         INKX = 2
         INKY = -IHP
      ELSE IF (RELCGP.EQ.5) THEN
         IGH = 12
         INKX = 0
         INKY = -IHP
      ELSE IF (RELCGP.EQ.6) THEN
         IGH = 11
         INKX = -1
         INKY = -IHP
      ELSE IF (RELCGP.EQ.16) THEN
         IGH = 10
         INKX = -2
         INKY = -IHP
      ELSE IF (RELCGP.EQ.7) THEN
         IGH = 7
         INKX = -1
         INKY = 0
      ELSE IF (RELCGP.EQ.17) THEN
         IGH = 6
         INKX = -2
         INKY = 0
      ELSE IF (RELCGP.EQ.8) THEN
         IGH = 2
         INKX = -1
         INKY = IHP
      ELSE IF (RELCGP.EQ.18) THEN
         IGH = 1
         INKX = -2
         INKY = IHP
      ENDIF
      IF (CHG.LT.100) THEN
        IMPLUS = 0
        IF ((CHG.GT.0).AND.(ICHAR(LINE(J)).NE.43)) THEN
           MM(X(I)+INKX,Y(I)+INKY) = 43
           IMPLUS = 1
         ENDIF
         DO 600 J = LOW,HIGH
            L = J - LOW + IMPLUS
            IF (ICHAR(LINE(J)).NE.49)
               MM(X(I)+INKX+L,Y(I)+INKY) = ICHAR(LINE(J))
         CONTINUE
         MM(X(I)+INKX,Y(I)+INKY) = MM(X(I)+INKX,Y(I)+INKY)
            + IGH * 2**13
      ELSE
         NBD1 = NBD1 + 1
           MM(X(I)+INKX,Y(I)+INKY) = ICHAR(APOST)
           DSCNC(2,NBD1) = RELCGP
           DSCNC(3,NBD1) = X(I)
           DSCNC(4,NBD1) = Y(I)
           DSCNC(5,NBD1) = X(I) + INKX
           DSCNC(6,NBD1) = Y(I) + INKY
         ENDIF
      ENDIF
C
C     The number of attached hydrogens is identified.
      POS = POS + 1
      CALL CHRNUM(HYDS,BEG,POS)
      LOW = BEG
      HIGH = POS - 1
C
```

```
C               The relative hydrogen position is identified.
                POS = POS + 1
                CALL CHRNUM(RLHYDP,BEG,POS)
                IF (HYDS.GT.0) THEN
                   IF ((RLHYDP.GE.2).AND.(RLHYDP.LE.4)) THEN
                      INKX = NOD
                   ELSE IF ((RLHYDP.EQ.1).OR.(RLHYDP.EQ.5)) THEN
                      INKX = 0
                   ELSE
                      IF (HYDS.EQ.1) THEN
                         INKX = -1
                       ELSE
                         INKX = -2
                       ENDIF
                   ENDIF
                   IF ((RLHYDP.EQ.3).OR.(RLHYDP.EQ.7)) THEN
                      INKY = 0
                   ELSE IF ((RLHYDP.EQ.8).OR.(RLHYDP.LE.2)) THEN
                      INKY = - 1
                   ELSE
                      INKY = 1
                   ENDIF
                   MM(X(I)+INKX,Y(I)+INKY) = 72
                   IF (HYDS.GT.1) THEN
                      DO 700 J = LOW,HIGH
                         L = J - LOW + 1
                         MM(X(I)+INKX+L,Y(I)+INKY) = ICHAR(LINE(J))
 700                  CONTINUE
                   ENDIF
                ENDIF
C
C               The abnormal mass is identified.
                POS = POS + 1
                CALL CHRNUM(MS,BEG,POS)
                POS = POS + 1
             ENDIF
C
C            The number of connections from the node is identified.
             CALL CHRNUM(VAL,BEG,POS)
             NCON(I) = VAL
C
C            Each connection and bond type is stored for bond tracing.
             DO 800 J = 1,NCON(I)
                POS = POS + 1
                CALL CHRNUM(VAL,BEG,POS)
                BOND(I,J) = VAL
                POS = POS + 1
                CALL CHRNUM(VAL,BEG,POS)
                IF (VAL.LE.3) THEN
                   BTYPE(I,J) = VAL
                ELSE
                   BTYPE(I,J) = VAL + 1
                ENDIF
 800         CONTINUE
          ENDIF
 1000  CONTINUE
C
C      Bonds are drawn.
       DO 2000 I = LONODE,NRECS-HINODE
          DO 1500 J = 1,NCON(I)
             DX = X(BOND(I,J)) - X(I)
             DY = Y(BOND(I,J)) - Y(I)
C
C            If a bond does not fit a normal bond direction, it is
C            assumed to be a long bond.

             IF ((IABS(DX).NE.IABS(DY)).AND.(DX.NE.0).AND.(DY.NE.0)) THEN
                LBLEN = LBLEN + 1
                LNGBND(LBLEN,1) = X(I)
                LNGBND(LBLEN,2) = Y(I)
                LNGBND(LBLEN,3) = X(BOND(I,J))
                LNGBND(LBLEN,4) = Y(BOND(I,J))
                LNGBND(LBLEN,5) = BTYPE(I,J)
C
```

```
C             The bonds directional increments and directional code are
C             computed
              ELSE
                 IF (DX.NE.0) THEN
                    INKX = DX / IABS(DX)
                 ELSE
                    INKX = 0
                 ENDIF
                 IF (DY.NE.0) THEN
                    INKY = DY / IABS(DY)
                 ELSE
                    INKY = 0
                 ENDIF
                 IF (INKX.EQ.0) THEN
                    LOW = 1
                    HIGH = IABS(Y(BOND(I,J)) - Y(I)) - 1
                    INK = INKY
                    IF (INKY.EQ.1) THEN
                       BIDIR = 5
                    ELSE
                       BIDIR = 1
                    ENDIF
                 ELSE IF (INKX.EQ.1) THEN
                    LOW = 1
                    HIGH = IABS(X(BOND(I,J)) - X(I)) - 1
                    INK = INKX
                    IF (INKY.EQ.1) THEN
                       BIDIR = 4
                    ELSE IF (INKY.EQ.0) THEN
                       BIDIR = 3
                    ELSE IF (INKY.EQ.-1) THEN
                       BIDIR = 2
                    ENDIF
                 ELSE
                    LOW = 1
                    HIGH = IABS(X(BOND(I,J)) - X(I)) - 1
                    INK = INKX
                    IF (INKY.EQ.-1) THEN
                       BIDIR = 8
                    ELSE IF (INKY.EQ.0) THEN
                       BIDIR = 7
                       IF (NOD.EQ.2) HIGH = HIGH - 1
                    ELSE
                       BIDIR = 6
                    ENDIF
                 ENDIF
C
C                Normal bonds are traced into the picture array.
                 DO 1100 K = LOW,HIGH,INK
                    LO = K
                    AX = X(I) + (K * INKX)
                    AY = Y(I) + (K * INKY)
                    IF ((MM(AX,AY).EQ.0).OR.(MM(AX,AY).GE.256)) GO TO 115
1100             CONTINUE
1150             CONTINUE
                 DO 1300  K = LO,HIGH,INK
                    KX = K * INKX + X(I)
                    KY = K * INKY + Y(I)
                    IF (MM(KX,KY).GT.0) THEN
C
C                      If the bond crosses a node or other bond, it is
C                      reassessed as a long bond.
                       IF ((LMM(KX,KY).LT.48).OR.
     *                    ((MM(KX,KY).GT.57).AND.(MM(KX,KY).NE.72).AND.
     *                    (MM(KX,KY).LE.96)).OR.(LMM(KX,KY).GE.256))
     *                    GO TO 1175
                       IF (((MM(LX,LY).EQ.46).OR.(MM(LX,LY).EQ.63).OR.
     *                    ((MM(LX,LY).GE.65).AND.(MM(LX,LY).LE.90))).AND.
     *                    ((X(BOND(I,J)).NE.LX).OR.(Y(BOND(I,J)).NE.LY)))
     *                    GO TO 1175
                       IF (((MM(LX,LY).GE.97).AND.(MM(LX,LY).LE.122).AND.
     *                    ((X(BOND(I,J)).NE.LX+INKX).OR.(Y(BOND(I,J))
     *                    .NE.LY))) GO TO 1175
                          GO TO 1400
```

```
1175                CONTINUE
                    DO 1200 L = LO,K-1
                       KX = L * INKX
                       KY = L * INKY
                       MM(X(I)+KX,Y(I)+KY) = 0
1200                CONTINUE
                    LBLEN = LBLEN + 1
                    LNGBND(LBLEN,1) = X(I)
                    LNGBND(LBLEN,2) = Y(I)
                    LNGBND(LBLEN,3) = X(BOND(I,J))
                    LNGBND(LBLEN,4) = Y(BOND(I,J))
                    LNGBND(LBLEN,5) = BTYPE(I,J)
                    GO TO 1400
C                   If a bond stumbles across an attached hydrogen or
C                   charge bond extension ceases.
                 ELSE
                    MM(KX,KY) = (BTYPE(I,J) * 256) + BIDIR
                 ENDIF
1300          CONTINUE
1400          CONTINUE
           ENDIF
1500    CONTINUE
2000  CONTINUE
C
C     The trailer record is processed.
      CALL TTYGET(LENGTH,STATUS)
      POS = 1
      CALL CHRNUM(RECNO,BEG,POS)
      IF ((RECNO.NE.-1).OR.(STATUS.GT.0)) THEN
         CHER = 2
         CALL MYERR(37,37,37)
         CALL FTSIZE(2,18)
         CALL FTLOCA(1,35)
         CALL FTEXT('^-OR-IN FILE VERSION-INPUT RECORD OUT OF ORDER^')
         STATUS = 1
         RETURN
      ENDIF
      DELEMS = 0
      POS = 3
2100  CONTINUE
      IF (LINE(POS).EQ.COMMA) DELEMS = DELEMS + 1
      POS = POS + 1
      IF ((DELEMS.GE.11).OR.(ICHAR(LINE(POS)).EQ.48))   GO TO 3100
         IF ((ICHAR(LINE(POS)).GE.49).AND.(ICHAR(LINE(POS)).LE.57)) THEN
            CALL CHRNUM(NOD,BEG,POS)
            POS = POS + 1
            CALL CHRNUM(XM,BEG,POS)
            IF (XM.LT.LOX) THEN
               LOX = XM
            ELSE IF (XM+NOD.GT.HIX) THEN
               HIX = XM + NOD
            ENDIF
            POS = POS + 1
            CALL CHRNUM(YM,BEG,POS)
            IF (YM.LT.LOY) THEN
               LOY = YM
            ELSE IF (YM.GT.HIY) THEN
               HIY = YM
            ENDIF
            POS = POS + 1
            IF (ICHAR(LINE(POS)).NE.77) THEN
               CALL CHRNUM(MUL,BEG,POS)
               IF (LINE(POS).EQ.SLASH) THEN
                  POS = POS + 1
                  CALL CHRNUM(MUL,DUM,POS)
               ENDIF
               LSHFT = POS - BEG
               K = 0
               DO 2200 J = LSHFT,1,-1
                  MM(XM-J,YM) = ICHAR(LINE(BEG+K))
                  K = K + 1
2200           CONTINUE
               POS = POS + 1
            ELSE
               LSHFT = 0
```

```
      ENDIF
      MM(XM,YM) = ICHAR(LINE(POS))
      POS = POS + 1
      MM(XM+1,YM) = ICHAR(LINE(POS)) + 63
      POS = POS + 1
      MM(XM-(LSHFT+1),YM) = ICHAR(STAR)
      PLACE = POS
      DO 2500 J = PLACE,LENGTH
         POS = J
         IF (LINE(POS).EQ.COMMA) THEN
            DELEMS = DELEMS + 1
            IF (ICHAR(LINE(POS+1)).EQ.48) THEN
               GO TO 3100
            ELSE
               POS = POS + 1
               GO TO 2100
            ENDIF
         ENDIF
         K = J + 2 - PLACE
         IF (XM+K.GT.HIX) HIX = XM + K
         IF ((ICHAR(LINE(POS)).EQ.43).OR.(ICHAR(LINE(POS)).EQ.45))
*           THEN
            MM(XM+K,YM) = (8 * 2**13) + ICHAR(LINE(POS))
               ELSE
                  MM(XM+K,YM) = ICHAR(LINE(POS))
               ENDIF
 2500       CONTINUE
         ENDIF
      IF (POS.GE.LENGTH) GO TO 3100
      GO TO 2100
 3100 CONTINUE
      LOX = MAX0(LOX-2,1)
      HIX = MIN0(HIX+3,MAXX)
      LOY = MAX0(LOY-1,1)
      HIY = MIN0(HIY+1,MAXY)
      RETURN
      END
C
C     SUBROUTINE CHRNUM returns the integer value that is represented
C     by a string of digits that is delimited by either commas or
C     horizontal bars.
C
C     ORI   Paul Broderick   December, 1984
      SUBROUTINE CHRNUM(VAL,BEG,POS)
      IMPLICIT INTEGER*2 (A-Z)
      CHARACTER*1 LINE,COMMA,BAR,NEGA,POSI,SLASH
      COMMON /TRANS/ LINE(160)
      DATA COMMA /','/, BAR /'|'/, NEGA /'-'/, POSI /'+'/, SLASH /'/'/
C
      BEG = POS
      VAL = 0
      POW = 1
C
      IF (LINE(POS).EQ.NEGA) THEN
         SIGN = -1
         POS = POS + 1
      ELSE IF (LINE(POS).EQ.POSI) THEN
         SIGN = 1
         POS = POS + 1
      ELSE
         SIGN = 1
      ENDIF
 10   CONTINUE
      IF ((LINE(POS).NE.COMMA).AND.(LINE(POS).NE.BAR).AND.
     *    LINE(POS).NE.SLASH) THEN
         VAL = (VAL * POW) + (ICHAR(LINE(POS)) - 48)
         POW =  10
         POS = POS + 1
         GO TO 10
      ENDIF
C
      VAL = VAL * SIGN
      RETURN
      END
C
```

```
C     SUBROUTINE TTYGET is used to input a line of the connection table.
      SUBROUTINE TTYGET(LENGTH,STATUS)
      IMPLICIT INTEGER*2(A-Z)
      LOGICAL*2 TERMN
      CHARACTER*1 LINE,CONTBL
      COMMON /TRANS/ LINE(160)
      COMMON /IRECS/ IU,IREC,TOPREC,BOTREC
      COMMON /CONTBL/ CONTBL(80,258),LTBL
      DATA POS /80/
C
      STATUS = 0
      DO 10 I = 1,POS
         LINE(I) = CHAR(0)
10    CONTINUE
      IREC = IREC + 1
      READ(IU,999,REC=IREC,END=40) (LINE(L),L=1,80)
40    CONTINUE
      LMAX = 80
      BOTREC = IREC
      LTBL = LTBL + 1
      TERMN = .FALSE.
      DO 400 I = 1,80
         CONTBL(I,LTBL) = LINE(I)
         IF ((((ICHAR(LINE(I)).EQ.32).AND.((I.GT.6).OR.(LINE(1)
     *      .EQ.'0'))).OR.(I.EQ.80)).AND.(.NOT.TERMN)) THEN
            IF (I.EQ.80) THEN
               LENGTH = I
               IF ((ICHAR(LINE(1)).EQ.45).AND.(ICHAR(LINE(2)).EQ.49))
     *            THEN
                  IREC = IREC + 1
                  DO 100 L = 81,160
                     LINE(L) = CHAR(0)
100               CONTINUE
                  READ(IU,999,REC=IREC,END=110) (LINE(L),L=81,160)
110               LTBL = LTBL + 1
                  LMAX = 160
                  BOTREC = IREC
                  DO 200 L = 81,160
                     CONTBL(L-80,LTBL) = LINE(L)
                     LENGTH = L
                     IF (ICHAR(LINE(L)).EQ.32) GO TO 410
200               CONTINUE
               ENDIF
            ELSE
               LENGTH = I - 1
            ENDIF
            TERMN = .TRUE.
         ENDIF
400   CONTINUE
410   IF (LENGTH.LT.LMAX) POS = LENGTH + 1
999   FORMAT(80A1)
      RETURN
      END
C
C    SUBROUTINE TBLCHR prepares connection table data for transmission by
C    transforming the numeric elements of the connection table to
C    character representation, inserts commas between the elements,
C    and heads each record string with SOH and appends the string with
C    its computed check digit and CR, LF.
C
C    ORI   Paul Broderick   July, 1984
      SUBROUTINE TBLCHR(IERR)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 DSKMEM
      LOGICAL*2 EXIST,NEWNME,ALPHID
      CHARACTER*10 ID,FILE,INID,INFILE,BLNK10,GETID,ZERO10
       CHARACTER*1 NAMSTR(10)
      CHARACTER*12 HLOID
      CHARACTER*1 ID10(10),HLOD12(12),HLO(3)
       CHARACTER*3 HLOE
       EQUIVALENCE (HLOE,HLO(1))
      EQUIVALENCE (ID10(1),GETID),(GETID,HLOD12(2)),(HLOID,HLOD12(1))
      CHARACTER*1 TRANS,CHK,RET(3),BLANK
       CHARACTER*1 COMMA
      COMMON /STRDEF/ NNODE,TABLE(255,43)
```

```
      COMMON /IRNS/ TRANS(80)
       COMMON /HP/IHP
      COMMON /ORECS/ OU,OUTREC
      COMMON /IRECS/ IU,INREC,TOPREC,BOTREC
      COMMON /IIDD/ IONDX,ID,FILE,INID(2500)
      COMMON /IIDD0/ INFILE(2500),PLACE
      COMMON /IIDD1/ RECNO(2500),NUMIDS,TOTIDS
C
C     Variable MNUM the number of *M structures and array
C     IMS contains the following items for each *M structure:
C        1 - Multiplier of the structure.
C        2 - *M identifying ordinal value.
C        3,4 - X and Y coordinates of the M.
C        5 - Length of connection table entry for the *M structure.
C        6 - Length of the formula to follow.
C        7 - Divisor of multiplier.
C        8 thru 90 - The molecular formula of the *M structure.
      COMMON /M1/ MNUM,IMS(90,5)
      COMMON /ALPHID/ ALPHID
      COMMON /DTDS/ DTN,DTX(30),DTY(30),DTN1(30),DTN2(30)
      DATA COMMA /','/, BLANK /' '/, BLNK10/'          '/
      DATA ZERO10 /'0000000000'/
C
       IF (IHP .NE.1) THEN
      CALL MEMDSK(CLUSTS,CPDISK,BPSECT,SPCLUS)
      DSKMEM = CLUSTS * BPSECT * SPCLUS
      IF ((DSKMEM.LE.((TOTIDS+NNODE+80)*80))) THEN
         IERR = 100
         WRITE(OU,89,REC=1) OUTREC
89       FORMAT(I6)
         CLOSE(OU)
         OPEN(IONDX,FILE='IDS.NDX',STATUS='NEW',ACCESS='DIRECT',
     *      FORM='FORMATTED',RECL=80)
         DO 13 I = 1,NUMIDS
            IF (INFILE(I).NE.'            ') WRITE(IONDX,79,REC=I)
     *      INID(I),INFILE(I),RECNO(I)
13       CONTINUE
         CLOSE(IONDX)
         CALL CLOSEG
      ENDIF
       ENDIF
C
C     The original copy of the edited structure is deleted from the
C     file.
      IF (TOPREC.GT.0) THEN
         CALL SETSCR(1)
         PAGE = 1
         CALL DISPLA(1)
55       CONTINUE
         CALL SETCOL(0)
         CALL CLR
         CALL SETCOL(1)
         CALL FTSIZE(2,18)
         CALL FTLOCA(8,24)
         CALL FTEXT('^Do you want to replace edited version (Y/N)?^')
         AA = GETCHR()
         CALL FTLOCA(8,24)
         CALL FTEXT('^                                             ^')
         IF ((AA.NE.89).AND.(AA.NE.121)) THEN
            IF (ALPHID) THEN
               GETID = BLNK10
               MX = 32
               CALL FTLOCA(8,MX)
               CALL FTEXT('^Enter (1-10) character ID^')
            ELSE
               GETID = ZERO10
               MX = 28
               CALL FTLOCA(7,MX)
               CALL FTEXT('^Enter CR for default ID increment -or-^')
               CALL FTLOCA(8,MX)
               CALL FTEXT('^Enter (1-10) digit ID ^')
            ENDIF
```

```
11555          J = 0
          IF (NUMIDS+1.LE.2500) INID(NUMIDS+1) = ID
             IF (IHP .EQ. 1) THEN
             CALL ALPCUR
             ACCEPT 691,(NAMSTR(I),I=1,10)
691          FORMAT(10A1)
             ENDIF
          DO 5555 I = 1,100
             J = J + 1
             FX = MX + J - 1
1555         CONTINUE
             IF (IHP .EQ. 1) THEN
             AA=ICHAR(NAMSTR(J))
             ELSE
             AA = GETCHR()
             ENDIF
             IF (AA.EQ.13 .OR. AA .EQ. 32) THEN
                IF ((GETID.EQ.ZERO10).OR.(GETID.EQ.BLNK10)) THEN
                   IF (ALPHID) GO TO 55
                   GETID = ID
                   IF (NUMIDS.GT.0) THEN
5530                  DO 5535 K = 10,1,-1
                         ID10(K) = CHAR(ICHAR(ID10(K)) + 1)
                         IF (ID10(K).EQ.':') THEN
                            ID10(K) = '0'
                            IF (K.EQ.1) THEN
                               GETID = '0000000001'
                               GO TO 5536
                            ENDIF
                         ELSE
                            GO TO 5536
                         ENDIF
5535                  CONTINUE
5536                  CONTINUE
                      FIN = 10
                      DO 5566 K = 1,NUMIDS+1
                         IF (GETID.EQ.INID(K)) GO TO 5530
5566                  CONTINUE
                     IF (IHP .NE.1) THEN
                      CALL FTLOCA(9,28)
                      CALL FTEXT(HLOID)
                     ENDIF
                      GO TO 5556
                   ELSE
                     IF (IHP .NE. 1) THEN
                      CALL FTLOCA(9,28)
                      CALL FTEXT(HLOID)
                     ENDIF
                      FIN = 10
                      GO TO 6667
                   ENDIF
                ELSE
                   FIN = J - 1
                   GO TO 5556
                ENDIF
             ENDIF
             IF (AA.EQ.8) THEN
                IF (J.GT.1) J = J - 1
                FX = MX + J - 1
                CALL FTLOCA(9,FX)
                IF (ALPHID) THEN
                   CALL FTEXT('^ ^')
                   ID10(J) = ' '
                ELSE
                   CALL FTEXT('^0^')
                   ID10(J) = '0'
                ENDIF
                GO TO 1555
             ENDIF
             IF (((AA.GE.48).AND.(AA.LE.57)).OR.(AA.EQ.32)) THEN
                 HLO(2) = CHAR(AA)
                 IF (AA.EQ.32) AA = 48
                     IF (IHP .NE. 1) THEN
```

```
                CALL FTLOCA(9,FX)
                CALL FTEXT(HLOE)
                    ENDIF
                ID10(J) = CHAR(AA)
             ELSE IF ((ALPHID).AND.(((AA.GE.65).AND.(AA.LE.90)).OR.
     *          ((AA.GE.97).AND.(AA.LE.122)))) THEN
                IF (AA.GE.97) AA = AA - 32
                HLO(2) = CHAR(AA)
                    IF (IHP .NE. 1) THEN
                CALL FTLOCA(9,FX)
                CALL FTEXT(HLOE)
                    ENDIF
                ID10(J) = CHAR(AA)
             ELSE
                HLO(2) = CHAR(AA)
                CALL FTLOCA(1,1)
                PAGE = 0
                CALL FTEXT(HLOE)
                CALL FTEXT('^ IS ILLEGAL INPUT. ENTER DIGITS OR SPA(
     *E AND CR^')
            IF (IHP .EQ. 1) THEN
            CALL FTLOCA(8,49)
            CALL FTEXT('^             ^')
            CALL FTLOCA(8,49)
               GO TO 11555
            ENDIF
            ENDIF
            IF (J.EQ.10) THEN
               FIN = J
               GO TO 5556
            ENDIF
 5555    CONTINUE
 5556    CONTINUE
         IF ((GETID.EQ.ZERO10).OR.(GETID.EQ.BLNK10)) GO TO 55
         IF (FIN.LT.10) THEN
            J = 10 - FIN
            DO 6664 I = FIN,1,-1
               ID10(I+J) = ID10(I)
               IF (ALPHID) THEN
                  ID10(I) = ' '
               ELSE
                  ID10(I) = '0'
               ENDIF
 6664       CONTINUE
         ENDIF
         DO 6666 I = 1,NUMIDS+1
            IF (GETID.EQ.INID(I)) THEN
               CALL FTLOCA(10,MX)
               CALL FTEXT('^WARNING - ID already exists on current
     *iles - ^')
               CALL FTLOCA(11,MX)
               CALL FTEXT('^Upload existing structure prior to new
     *ntry^')
               CALL FTLOCA(12,MX)
               CALL FTEXT('^Press RETURN to continue^')
               AA = GETCHR()
               GO TO 55
            ENDIF
 6666    CONTINUE
 6667    IF (NUMIDS+1.LE.2500) INID(NUMIDS+1) = ZERO10
         NEWNME = .TRUE.
      ELSE
         GETID = ID
         NEWNME = .FALSE.
         MX = 32
      ENDIF
      CALL FTLOCA(9,MX)
      CALL FTEXT('^Output ID: ^')
      CALL FTEXT(HLOID)
      CALL FTLOCA(10,MX)
      CALL FTEXT('^Is ID OK (Y/N)?^')
      IKAR = GETCHR()
```

```
C         If no - go get new ID
          IF (IKAR.NE.89 .AND. IKAR.NE.121) GO TO 55
          CALL SETCOL(0)
          CALL CLR
          CALL SETCOL(1)
          CALL SETSCR(2)
          PAGE = 2
          CALL DISPLA(2)
          CALL FTSIZE(1,10)
          IF (NEWNME) THEN
             ID = GETID
             TOPREC = 0
                IF (IHP .NE. 1) THEN
             CALL FTLOCA(331)
             CALL FTEXT('^Structure ID: ^')
             CALL FTEXT(HLOID)
                ENDIF
          ENDIF
       ENDIF
C
       IF (TOPREC.GT.0) THEN
          INFILE(PLACE) = '          '
          DO 2 I = TOPREC,BOTREC
             WRITE(IU,9,REC=I) BLANK
2         CONTINUE
       ELSE
          TOTIDS = TOTIDS + 1
          IF (TOTIDS.GT.2500) THEN
             WRITE(OU,89,REC=1) OUTREC
             OPEN(IONDX,FILE='IDS.NDX',STATUS='NEW',ACCESS='DIRECT',
     *          FORM='FORMATTED',RECL=80)
             DO 3 I = 1,NUMIDS
                IF (INFILE(I).NE.'          ') WRITE(IONDX,79,REC=I)
     *             INID(I),INFILE(I),RECNO(I)
79              FORMAT(A10,A10,I6)
3            CONTINUE
             CLOSE(IONDX)
             CALL CLOSEG
          STOP 'CANNOT EXCEED 2500 STRUCTURES. NULL CONNECTION TABLE.'
          ENDIF
       ENDIF
C
C      The structure id number is output to the output file.
       OUTREC = OUTREC + 1
       WRITE(OU,999,REC=OUTREC) ID,OUTREC
999    FORMAT(A10,1X,I10)
C      The structure id number, file name, and record number are output
C      to the index file.
       NUMIDS = NUMIDS + 1
       PLNTID = NUMIDS
       IF (NUMIDS.GT.2500) THEN
          DO 6 I = 1,2500
             IF (INFILE(I).EQ.'          ') THEN
                PLNTID = I
                IF (I.LT.2500) THEN
                   DO 4 J = I,2499
                      INID(J) = INID(J+1)
                      INFILE(J) = INFILE(J+1)
                      RECNO(J) = RECNO(J+1)
4                  CONTINUE
                ENDIF
                NUMIDS = NUMIDS - 1
                GO TO 7
             ENDIF
6         CONTINUE
       ENDIF
7      CONTINUE
       INID(PLNTID) = ID
       INFILE(PLNTID) = FILE
       RECNO(PLNTID) = OUTREC
C
C      The header transmission record string is prepared.
       POS = 1
```

```
      OREC = 1
      TRANS(POS) = '0'
      POS = POS + 1
      TRANS(POS) = COMMA
C
C     The number of node records to follow is assigned.
      VAL = NNODE
      CALL NUMCHR(VAL,RET,NDGT)
      DO 10 I = 1,NDGT
         POS = POS + 1
         TRANS(POS) = RET(I)
10    CONTINUE
      POS = POS + 1
      TRANS(POS) = COMMA
C
C     The header string's check character is computed and assigned.
      CALL CHKGEN(POS,CHK)
      POS = POS + 1
      TRANS(POS) = CHK
C
C     The number of header characters is assigned to define the length
C     of header transmission.
      OUTN = POS
C
C     The string is uploaded.
      RESULT = SEND(TRANS,OUTN)
C
C     A transmission string for each node in the structure is prepared.
      DO 500 IREC = 1,NNODE
         OREC = IREC + 1
C
C        The number of items in the connection table record is
C        assessed.
         IF (TABLE(IREC,2).EQ.42) THEN
            LNG = 7
         ELSE IF ((TABLE(IREC,2).EQ.43).OR.(TABLE(IREC,2).EQ.45)) THEN
            LNG = 5
         ELSE IF ((TABLE(IREC,2).EQ.68).AND.((TABLE(IREC,3).GE.112)
     *      .AND.(TABLE(IREC,3).LE.120))) THEN
            LNG = 7 + (TABLE(IREC,7) * 2)
         ELSE IF ((TABLE(IREC,2).EQ.77).AND.((TABLE(IREC,3).GE.112)
     *      .AND.(TABLE(IREC,3).LE.120))) THEN
            LNG = 6 + (TABLE(IREC,6)*2)
         ELSE
            LNG = 11 + (TABLE(IREC,11) * 2)
         ENDIF
C
         POS = 0
C        The record node number is assigned.
         VAL = TABLE(IREC,1)
         CALL NUMCHR(VAL,RET,NDGT)
         DO 100 I = 1,NDGT
            POS = POS + 1
            TRANS(POS) = RET(I)
100      CONTINUE
         POS = POS + 1
         TRANS(POS) = COMMA
C
C        The element symbol is assigned.
         POS = POS + 1
         TRANS(POS) = CHAR(TABLE(IREC,2))
         POS = POS + 1
         TRANS(POS) = CHAR(TABLE(IREC,3))
```

```
C        Any *D or *M identifying ordinal value is converted from
C        letter to digit.
         IF (((TABLE(IREC,2).EQ.68).OR.(TABLE(IREC,2).EQ.77))
     *      .AND.((TABLE(IREC,3).GE.112).AND.(TABLE(IREC,3).LE.
     *      120))) TRANS(POS) = CHAR(TABLE(IREC,3) - 63)
         POS = POS + 1
         TRANS(POS) = COMMA
C
C        The x-coordinate, the y-coordinate, the charge value,
C        the relative charge position, the number of hydrogens,
C        the hydrogen's relative graphic position, the abnormal
C        mass, the number of the node's connections, the connected
C        node's numbers and the connection's bond types are assigned
C        to the string.
         DO 200 I = 4,LNG
            VAL = TABLE(IREC,I)
            CALL NUMCHR(VAL,RET,NDGT)
            DO 110 J = 1,NDGT
               POS = POS + 1
               TRANS(POS) = RET(J)
110         CONTINUE
            POS = POS + 1
            TRANS(POS) = COMMA
200      CONTINUE
C
C        The transmission string's check character is computed and
C        assigned.
         CALL CHKGEN(POS,CHK)
         POS = POS + 1
         TRANS(POS) = CHK
C
C        The number of transmission string characters is passed to
C        define the length of record transmission.
         OUTN = POS
C
         RESULT = SEND(TRANS,OUTN)
500   CONTINUE
C
C     The trailer record is assembled.
      TRANS(1) = '-'
      TRANS(2) = '1'
      TRANS(3) = COMMA
      POS = 3
C
C     Any of up to 5 *M structure formulas along with multipliers and x,y
C     coordinates of the formula definition is positionally inserted into
C     the trailer.
      DO 900 IMSPOS = 1,MNUM
C
         VAL = IMS(5,IMSPOS)
         CALL NUMCHR(VAL,RET,NDGT)
         DO 730 I = 1,NDGT
            POS = POS + 1
            IF (POS.EQ.81) CALL MCONT(POS,TRANS)
            TRANS(POS) = RET(I)
730      CONTINUE
         POS = POS + 1
         IF (POS.EQ.81) CALL MCONT(POS,TRANS)
         TRANS(POS) = COMMA
C
C        X and Y coordinates are assigned.
         VAL = IMS(3,IMSPOS)
         CALL NUMCHR(VAL,RET,NDGT)
         DO 770 I = 1,NDGT
            POS = POS + 1
            IF (POS.EQ.81) CALL MCONT(POS,TRANS)
            TRANS(POS) = RET(I)
770      CONTINUE
         POS = POS + 1
         IF (POS.EQ.81) CALL MCONT(POS,TRANS)
         TRANS(POS) = '|'
         VAL = IMS(4,IMSPOS)
         CALL NUMCHR(VAL,RET,NDGT)
         DO 790 I = 1,NDGT
            POS = POS + 1
```

```
            IF (POS.EQ.81) CALL MCONT(POS,TRANS)
            TRANS(POS) = RET(I)
 790      CONTINUE
          POS = POS + 1
          IF (POS.EQ.81) CALL MCONT(POS,TRANS)
          TRANS(POS) = '|'
 C
 C        The multiplier of the *M structure is assigned.
          IF (IMS(1,IMSPOS).GT.1) THEN
            VAL = IMS(1;IMSPOS)
 810        CALL NUMCHR(VAL,RET,NDGT)
            DO 840 I = 1,NDGT
               POS = POS + 1
               IF (POS.EQ.81) CALL MCONT(POS,TRANS)
               TRANS(POS) = RET(I)
 840        CONTINUE
            POS = POS + 1
            IF (POS.EQ.81) CALL MCONT(POS,TRANS)
            IF (IMS(7,IMSPOS).GT.0) THEN
               TRANS(POS) = '/'
               VAL = IMS(7,IMSPOS)
               IMS(7,IMSPOS) = 0
               GO TO 810
            ENDIF
            TRANS(POS) = '|'
          ENDIF
 C
          POS = POS + 1
          IF (POS.EQ.81) CALL MCONT(POS,TRANS)
          TRANS(POS)  = 'M'
          POS = POS + 1
          IF (POS.EQ.81) CALL MCONT(POS,TRANS)
          TRANS(POS) = CHAR(IMS(2,IMSPOS) - 63)
 C
 C        Molecular formula of *M structure.
          DO 850 I = 1,IMS(6,IMSPOS)
             POS = POS + 1
             IF (POS.EQ.81) CALL MCONT(POS,TRANS)
             TRANS(POS) = CHAR(IMS(7+I,IMSPOS))
 850      CONTINUE
          POS = POS + 1
          IF (POS.EQ.81) CALL MCONT(POS,TRANS)
          TRANS(POS) = COMMA
 C
 900   CONTINUE
 C
 C     The trailer's positional fillers rather than *M structure formula
 C     strings are assigned.
       DO 1000 I = MNUM+1,5
          POS = POS + 1
          IF (POS.EQ.81) CALL MCONT(POS,TRANS)
          TRANS(POS) = '0'
          POS = POS + 1
          IF (POS.EQ.81) CALL MCONT(POS,TRANS)
          TRANS(POS) = COMMA
          POS = POS + 1
          IF (POS.EQ.81) CALL MCONT(POS,TRANS)
          TRANS(POS) = COMMA
 1000   CONTINUE
 C
 C     The trailer's check digit is computed and assigned.
       CALL CHKGEN(POS,CHK)
       POS = POS + 1
       IF (POS.EQ.81) CALL MCONT(POS,TRANS)
       TRANS(POS) = CHK
 C
 C     The number of trailer string characters is assigned to define
 C     length of trailer transmission.
       OUTN = POS
 C
 C     The molecular strucure is passed for transmission.
       ONODES = NNODE + 2
       RESULT = SEND(TRANS,OUTN)
 C
```

```
      DO 2000 I = OUTREC+1,OUTREC+6
         WRITE(OU,9,REC=I) BLANK
 2000 CONTINUE
      INQUIRE(FILE='IDS.NDX',EXIST=EXIST)
      IF (EXIST) THEN
         OPEN(IONDX,FILE='IDS.NDX',STATUS='OLD',ACCESS='DIRECT',
     *       FORM='FORMATTED',RECL=80)
      ELSE
         OPEN(IONDX,FILE='IDS.NDX',STATUS='NEW',ACCESS='DIRECT',
     *       FORM='FORMATTED',RECL=80)
      ENDIF
      WRITE(IONDX,79,REC=PLNTID) ID,FILE,OUTREC
      DO 2010 I = NUMIDS+1,NUMIDS+6
         WRITE(IONDX,189,REC=I) BLNK10
 2010 CONTINUE
      CLOSE(IONDX)
 9    FORMAT(A1)
 189  FORMAT(A10)
      RETURN
      END
C
C    FUNCTION SEND outputs the transmission strings of each molecular
C    structure.
C
C    ORI   Paul Broderick   July, 1984
C
       INTEGER*2 FUNCTION SEND(TRANS,OUTN)
       IMPLICIT INTEGER*2 (A-Z)
       CHARACTER*1 TRANS(80)
       COMMON /ORECS/ OU,OREC
C
      IF (OUTN.NE.80) THEN
         OUTN = OUTN + 1
         TRANS(OUTN) = CHAR(32)
      ENDIF
C
C     Output transmission string.
      OREC = OREC + 1
      WRITE(OU,999,REC=OREC) (TRANS(L),L=1,OUTN)
C
      SEND = 1
      RETURN
999   FORMAT(80A1)
      END
C
C
      SUBROUTINE MCONT(POS,TRANS)
      IMPLICIT INTEGER*2 (A-Z)
      CHARACTER*1 TRANS(80)
C
      OUTN = POS -1
      RESULT = SEND(TRANS,OUTN)
      POS = 1
      RETURN
      END
$STORAGE:2
C
C       XTCHEM: VERSION 1 - MARCH, 1984
C
C       ADAPTED FROM HPCHEM: VERSION 5 - APRIL 25,1984
C            through HPCHEM: VERSION 8 - FEB 5, 1985
C
        SUBROUTINE STRINP(IX,IY,IEDIT,FIRST)
        IMPLICIT INTEGER*2 (A-Z)
        REAL A
        INTEGER*4 MM,IDTPIX
        LOGICAL*2 FIRST,IEDIT
        CHARACTER*1 ISTAT
        COMMON /ELECHR/ IELEM(126,5)
        COMMON /STRDEF/ NNODE,TABLE(255,43)
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
C Input program for chem structures. Version 4Apr83. Includes setting
C setting markers with'#',jump to marker by typing lowercase letter,
C typing second letter of 2-letter element with '$' precedence code.
C No changing of previously-entered markers. GMK
        COMMON /KEYS/ ICODE(8)
```

```
        COMMON /CD/ MAXX,MAXY
        COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
        COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
        COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /HEAD/ MW(12),ISTATE,PAGE
        COMMON /PROB/ IPROB,JPROB
C Line segments to draw bonds(see SUB DRAW)
        COMMON /BONDS/ A(5,3,4,4),B(2,3,4)
C X,Y  of up to 10
        COMMON /LABELS/ NR,NJLAST,NJNEXT
C               alphabets of lowercase label locations (0 if unused,
C               -999 if used but erased). NR is the last line of LABL
C               which has been jumped to, NJLAST is the last lowercase
C               label which has been jumped to minus 96, and NJNEXT is
C               the last line number where XY coordinates were added to
C               the list in LABL by subroutine MARK.
        COMMON /SIZZE/ MULTX,MULTY
        COMMON /ISTATE/ ISTAT
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /CUR/ ICUR
C       Subroutine CHAIN; includes some which may have been already changed
        COMMON /IPLUS/ IHIGH(14,2)
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /MKSKP/ ISKIP
        COMMON /WARN/ ERR
        COMMON /QTVLNC/ OERR,CHER
        COMMON /FROM/ LCHAR

C
C THIS PROGRAM GENERATES A CHARACTER MATRIX FOR CHEMICAL STRUCTURES.
C THE PROGRAM FACILITATES TYPING BY GENERATING ATOMIC SYMBOLS WHERE
C THESE ARE MANDATORY.
C
C       MCHAR is last character entered.
C       LASTN is last numeral entered.
C SET RETURN = OK UNTIL OTHERWISE KNOWN
        LFLAG = 0
        ISKIP = 0
        LPIX = MAXX * MAXY
        ISTAT = ' '
        IPROB=0
        JPROB=0
        IRESET = 0
        INCX = 0
        INCY = 0
        IF (FIRST) THEN
           LOX = 26
           HIX = 26
           LOY = 15
           HIY = 15
        ELSE
           CALL RESET(IX,IY,FIRST)
        ENDIF
C
100     IF (IRESET.EQ.1) CALL RESET(IX,IY,FIRST)
        CALL SETSCR(2)
        PAGE = 2
        CALL DISPLA(2)
        CALL FTSIZE(1,10)
        CALL INITHC(3,3,1)
        ICUR = 1
        CALL CURSOR(IX,IY)
C
C Go on if we are not in EDIT mode
        IF (.NOT.IEDIT) GO TO 50
           CALL REFORM(STATUS)
           IF (STATUS.NE.0) RETURN
           CALL REMARK(IERR)
C          Call STRDRW with markers displayed as markers
           ISWIT=1
C          Display old picture
           CALL STRDRW(ISWIT)
C       Sense cursor position after displaying picture
        DO 61 J = LOY,HIY
```

```
              DO 60 I = LOX,HIX
                 II = I
                 JJ = J
                 M = LMM(I,J)
                 IF (M.EQ.42) GO TO 61
                 IF ((M.EQ.46).OR.((M.GE.65).AND.(M.LE.90)
     *              .AND.(.NOT.((M.EQ.72).AND.((MM(IX+1,J).LT.97).OR.
     *              (MM(IX+1,J).GT.122)))))) GO TO 65
60            CONTINUE
61          CONTINUE
            IX = 26
            IY = 15
            GO TO 66
65          IX = II+1
C Set cursor position
            IY = JJ
            ICHAR = 2
            JCHAR = 2
            KAR = M
            MCHAR = KAR
66          CALL CURSOR(IX,IY)
C
50          IEDIT=.FALSE.
C When IRESET=1, done with a structure; recycle to 100
            IRESET=0
C Display status info on top of screen
            ICUR = 1
            CALL HEADER
1           CONTINUE
            LEVEL = 0
            LCHAR = 0
            CALL INPUTX(KAR,IX,IY)
3           CALL IDENT(KAR,IX,IY,INCX,INCY,IRESET)
            IF ((KAR.EQ.13).OR.(KAR.EQ.127)) THEN
               ICUR = 1
               CALL CURSOR(IX,IY)
            ENDIF
          IF (LEVEL.EQ.1) THEN
             IF (ICHAR.EQ.33) THEN
             CALL LIBRA(IX,IY,KAR)
          ELSE IF (ICHAR.EQ.12) THEN
             CALL RING(KAR,IX,IY,INCX,INCY,IRESET,LFLAG)
             IF ((LCHAR.EQ.13).AND.(LFLAG.EQ.0).AND.(JPROB.EQ.0)) THEN
                KAR = 33
                LCHAR = 0
                GO TO 3
             ENDIF
          ELSE IF (ICHAR.EQ.13) THEN
             CALL CHAIN(KAR,IX,IY,INCX,INCY,IRESET,LFLAG)
             IF ((LCHAR.EQ.12).AND.(LFLAG.EQ.0).AND.(JPROB.EQ.0)) THEN
                KAR = 94
                LCHAR = 0
                GO TO 3
             ENDIF
          ELSE IF (ICHAR.EQ.14) THEN
             CALL REPEAT(KAR,IX,IY,INCX,INCY,IRESET,LFLAG)
          ELSE IF (ICHAR.EQ.16) THEN
             CALL DOTDIS(KAR,IX,IY,IRESET,LFLAG)
          ELSE IF (ICHAR.EQ.21) THEN
             CALL GETIT(IX,IY,LFLAG,KAR)
          ENDIF
          ICUR = 1
          CALL CURSOR(IX,IY)
        ENDIF
C EXIT TO DIS WITH GOOD OR BAD RETURN
        IF ((KAR.EQ.17).OR.(KAR.EQ.18)) GO TO 850
        IF (JPROB .NE. 0) GO TO 70
        IF (LFLAG .NE. 1) GO TO 2
        LFLAG=0
        GO TO 3
2       IF (IRESET.EQ.1) THEN
           FIRST = .FALSE.
           GO TO 100
         ENDIF
         IF (IRESET .EQ. 3) RETURN
         GO TO 1
```

```
 70       IF(JPROB .EQ. 1) GO TO 72
           CALL FTSIZE(2,18)
             IF (PAGE.NE.1) THEN
                CALL SETSCR(1)
                PAGE = 1
                CALL DISPLA(1)
             ENDIF
             CALL FTLOCA(8,20)
             CALL FTEXT('^ Do you wish to^')
             CALL FTLOCA(9,20)
             CALL FTEXT('^ (R)enter new structure or (E)xit - (data will b
     *e lost)^')
             CALL FTLOCA(10,20)
             CALL FTEXT('^ Type R or E: ^')
 799         CONTINUE
             ERR = 100
             CALL INPUTX(L,IX,IY)
             ERR = 0
             JCHAR = 2
C         HE WANTS TO REENTER
          IF (L.EQ. 82 .OR. L .EQ. 114) GO TO 800
C         HE WANTS TO ABORT
          IF(L.EQ. 69 .OR. L .EQ.101) GO TO 850
          CALL SETCOL(0)
          CALL CLR
          CALL SETCOL(1)
          CALL FTLOCA(8,20)
          CALL FTEXT('^ You should have typed R or E - Please try again:^'
     *    )
          GO TO 799
 800      IRESET=1
          JPROB=0
          GO TO 100
 850      CONTINUE
          CALL SETCOL(0)
          CALL CLR
          CALL SETCOL(1)
          RETURN
 72       CONTINUE
          CALL SETSCR(1)
          PAGE = 1
          CALL FTSIZE(2,18)
          CALL DISPLA(1)
          CALL FTLOCA(8,20)
          CALL FTEXT('^ Do you wish to^')
          CALL FTLOCA(9,20)
          CALL FTEXT('^ (C)ontinue structure or (E)xit - (data will be los
     *t)^')
          CALL FTLOCA(10,20)
          CALL FTEXT('^ Type C or E: ^')
 888      CONTINUE
          ERR = 100
          CALL INPUTX(L,IX,IY)
          ERR = 0
          IF (L.EQ.67 .OR. L.EQ.99) GO TO 805
          IF (L.EQ.69 .OR. L .EQ.101) GO TO 850
          CALL SETCOL(0)
          CALL CLR
          CALL SETCOL(1)
          CALL FTLOCA(8,20)
          CALL FTEXT('^ You should have typed C or E - Please try again:^'
     *    )
          GO TO 888
 805      CONTINUE
          JPROB=0
          CALL SETCOL(0)
          CALL CLR
          CALL SETCOL(1)
          MODE=1
          LASTN=0
          DO 999 I=1,12
             MW(I)=999
 999      CONTINUE
```

```
      IF (OERR.EQ.-1) THEN
         OERR = 0
         CALL SETSCR(2)
         CALL SETCOL(0)
         CALL CLR
         CALL SETCOL(1)
         PAGE = 2
         CALL DISPLA(2)
      CALL CLR
         CALL REMARK(IERR)
         ISWIT = 1
         CALL STRDRW(ISWIT)
      ELSE
         CALL SETSCR(2)
         PAGE = 2
         CALL DISPLA(2)
      ENDIF
      CALL FTSIZE(1,10)
      CALL HEADER
      ICUR = 1
      CALL CURSOR(IX,IY)
      GO TO 1
      END
C
      SUBROUTINE REDO(L,I1,I2,I3,I4,I5,I6)
      IMPLICIT INTEGER*2 (A-Z)
      CHARACTER*1 HALO(3)
      CHARACTER*1 KAN
      CHARACTER*3 HALOE
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      EQUIVALENCE (HALOE,HALO(1))
C
C SUBROUTINE MONITORS FOR CORRECTNESS OF SPECIFIED INPUT CHARACTER.
C
      HALO(1) = KAN
      HALO(3) = KAN
5     CONTINUE
C
      L = GETCHR()
      HALO(2) = CHAR(L)
C
C Lower case ok too.
      IF (L.GT.95) L=L-32
      CALL SETCOL(0)
      CALL CLR
      CALL SETCOL(1)
      IF ((L.EQ.I1).OR.(L.EQ.I2).OR.(L.EQ.I3).OR.(L.EQ.I4).OR.
     *   (L.EQ.I5).OR.(L.EQ.I6)) RETURN
C
      CALL FTLOCA(7,26)
      CALL FTEXT('^ NO! YOU TYPED: ^')
      CALL FTEXT(HALOE)
      CALL FTLOCA(8,26)
      HALO(2) = CHAR(I1)
      CALL FTEXT('^ YOU SHOULD HAVE TYPED: ^')
      CALL FTEXT(HALOE)
      FY = 9
      IF (I2.EQ.0) GO TO 900
         HALO(2) = CHAR(I2)
         CALL FTLOCA(9,45)
         CALL FTEXT('^ OR: ^')
         CALL FTEXT(HALOE)
         FY = 10
      IF (I3.EQ.0) GO TO 900
         HALO(2) = CHAR(I3)
         CALL FTLOCA(10,45)
         CALL FTEXT('^ OR: ^')
         CALL FTEXT(HALOE)
         FY = 11
      IF (I4.EQ.0) GO TO 900
         HALO(2) = CHAR(I4)
         CALL FTLOCA(11,45)
         CALL FTEXT('^ OR: ^')
         CALL FTEXT(HALOE)
         FY = 12
```

```
      IF (I5.EQ.0) GO TO 900
         HALO(2) = CHAR(I5)
         CALL FTLOCA(12,45)
         CALL FTEXT('^ OR: ^')
         CALL FTEXT(HALOE)
         FY = 13
      IF (I6.EQ.0) GO TO 900
         HALO(2) = CHAR(I6)
         CALL FTLOCA(13,45)
         CALL FTEXT('^ OR: ^')
         CALL FTEXT(HALOE)
         FY = 14
900   CONTINUE
C
      CALL FTLOCA(FY,26)
      CALL FTEXT('^ PLEASE TRY AGAIN. ^')
      GO TO 5
      END
C
      SUBROUTINE RESET(IX,IY,FIRST)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM,IDTPIX
      LOGICAL*2 FIRST,NOMSG,BONDEL,BAR,CNTX
      CHARACTER*1 ISTAT
      COMMON /CD/ MAXX,MAXY
      COMMON /RANGE/ LOX,HIX,LOY,HIY
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
      COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /ISTATE/ ISTAT
      COMMON /LABELS/ NR,NJLAST,NJNEXT
      COMMON /STRDEF/ NNODE,TABLE(255,43)
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
      COMMON /RETLIB/OVRWRT
      COMMON /H/ MOBILE(255,2)
      COMMON /CUR/ ICUR
      COMMON /DARK/ OCUR
      COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
      COMMON /M1/ MNUM,IMS(90,5)
      COMMON /KHARGE/ ICHRGE(50,4),NCHG
      COMMON /CONNCT/ IBOND(255,16),KBOND(255,16)
      COMMON /TEMP/ LLBOND(100,5),LLABL(260,2),MCHN(260)
      COMMON /FROM/ LCHAR
      COMMON /QTVLNC/ OERR,CHER
      COMMON /LNGOUT/ LNGNDE(100,2)
      COMMON /VLNPRV/ MLARGE
      COMMON /LEAPER/ NOMSG
      COMMON /DELBND/ BONDEL
      COMMON /BTPDIR/ BAR
      COMMON /CNTX/ CNTX
      COMMON /DTDS/ DTN,DTX(30),DTY(30),DTN1(30),DTN2(30)
      DATA OVRWRT/.FALSE./
C
C CURSOR HOME
C     (ERASE GRAPHICS MEMORY, TURN ON ALPHA DISPLAY, TURN ON
C      GRAPHICS DISPLAY, TURN OFF GRAPHICS TEXT MODE)
      IF (.NOT.FIRST) CALL CLOSEG
      CALL INITGR(0)
C
      CALL SETSCR(1)
      CALL SETGPR(1)
      CALL SETCOL(1)
      CALL FTINIT
      CALL FTSIZE(2,18)
      CALL FTCOLO(0,1)
C
      CALL SETSCR(2)
      CALL SETCOL(1)
      PAGE = 2
      CALL DISPLA(2)
      CALL STARTG(0)
      CALL SETGPR(1)
      CALL SETIEE(1)
      CALL SETDEG(1)
```

```
      CALL INITTC(0,0,0)
      CALL SETTEX(1,1,0,0)
      CALL SETTCL(1,0)
C
      IX = 26
      IY = 15
      NOMSG = .FALSE.
      BAR = .FALSE.
      BONDEL = .FALSE.
      CNTX = .FALSE.
      ISTAT=' '
      ICUR = 0
      OCUR = 1
      CALL CURSOR(IX,IY)
C     (INITIALIZE CURSOR)
      MCHAR=0
      JCHAR=0
      LASTN=0
C ISP = 0 IMPLIES WE HAVE NOT JUST RETURNED FROM SPACE
      ISP=0
C THIS VARIABLE IS USED TO KEEP US FROM CALLING VALNCE
C AFTER RETURN FROM SPACE AND JUST BEFORE CALL TO LEAP
C TERMINAL SMART=1, DUMB=0
      ISMART=1
      IBDIR=3
      IBTYPE=1
C 1 means chain or ring state
      LEVEL=0
      MODE=1
      NLARGE=1
      MLARGE = NLARGE
      CHER = 0
      NR=1
      NBD1 = 0
      LBLEN = 0
      IDNUM = 0
      NJNEXT = 0
      NJLAST=0
      ISTATE = 0
      LCHAR = 0
      DO 200 I=1,9
         DO 100 J = 1,6
            IDS(I,J) = 0
100      CONTINUE
         MW(I)=999
200   CONTINUE
      DO 400 I = 10,12
         DO 300 J = 1,6
            IDS(I,J) = 0
300      CONTINUE
400   CONTINUE
      DO 500 I = LOX,HIX
      DO 500 J = LOY,HIY
         MM(I,J)=0
         IDTPIX(I,J)=0
500   CONTINUE
      LOX = IX
      HIX = IX
      LOY = IY
      HIY = IY
      DO 2000 I = 1,50
         DO 1100 J = 1,2
            MOBILE(I,J) = 0
            IBOND(I,J) = 10000
            KBOND(I,J) = 10000
            DSCNC(J,I) = 0
            IMS(I,J) = 0
            ICHRGE(I,J) = 10000
            LNGBND(I,J) = 0
            LLBOND(I,J) = 0
            LNGNDE(I,J) = 0
            LABL(I,J) = 0
            LLABL(I,J) = 0
1100     CONTINUE
         DO 1500 J = 3,4
```

```
          IBOND(I,J) = 10000
          KBOND(I,J) = 10000
          IMS(I,J) = 0
          ICHRGE(I,J) = 10000
          LNGBND(I,J) = 0
          LLBOND(I,J) = 0
          DSCNC(J,I) = 0
1500    CONTINUE
        DSCNC(5,I) = 0
        DSCNC(6,I) = 0
        IMS(I,5) = 0
        MRKCHN(I)=0
        MCHN(I) = 0
        IBOND(I,5) = 10000
        KBOND(I,5) = 10000
        LNGBND(I,5)=0
        LLBOND(I,5) = 0
        DO 1800 J = 6,16
          IBOND(I,J) = 10000
          KBOND(I,J) = 10000
1800    CONTINUE
        IF (I.LE.30) THEN
          DTX(I) = 0
          DTY(I) = 0
          DTN1(I) = 0
          DTN2(I) = 0
        ENDIF
2000  CONTINUE
C
      DO 3000 I=51,90
        MRKCHN(I)=0
        MCHN(I) = 0
        DO 2200 J=1,2
          MOBILE(I,J) = 0
          IBOND(I,J) = 10000
          KBOND(I,J) = 10000
          LNGBND(I,J)=0
          LLBOND(I,J) = 0
          LNGNDE(I,J) = 0
          LABL(I,J) = 0
          LLABL(I,J) = 0
          IMS(I,J) = 0
2200    CONTINUE
        DO 2300 J = 3,5
          IBOND(I,J) = 10000
          KBOND(I,J) = 10000
          LNGBND(I,J)=0
          LLBOND(I,J) = 0
          IMS(I,J) = 0
2300    CONTINUE
        DO 2400 J = 6,16
          IBOND(I,J) = 10000
          KBOND(I,J) = 10000
2400    CONTINUE
3000  CONTINUE
      DO 4000 I = 91,100
        MRKCHN(I)=0
        MCHN(I) = 0
        DO 3100 J=1,2
          MOBILE(I,J) = 0
          IBOND(I,J) = 10000
          KBOND(I,J) = 10000
          LNGBND(I,J)=0
          LLBOND(I,J) = 0
          LNGNDE(I,J) = 0
          LABL(I,J)=0
          LLABL(I,J)=0
3100    CONTINUE
        DO 3200 J = 3,5
          IBOND(I,J) = 10000
          KBOND(I,J) = 10000
          LNGBND(I,J)=0
          LLBOND(I,J) = 0
3200    CONTINUE
        DO 3300 J = 6,16
          IBOND(I,J) = 10000
          KBOND(I,J) = 10000
```

```
 3300          CONTINUE
 4000       CONTINUE
            DO 5000 I=101,255
               MRKCHN(I)=0
               MCHN(I) = 0
               DO 4100 J=1,2
               MOBILE(I,J) = 0
               IBOND(I,J) = 10000
               KBOND(I,J) = 10000
               LABL(I,J) = 0
               LLABL(I,J) = 0
4100        CONTINUE
            DO 4200 J = 3,16
               IBOND(I,J) = 10000
               KBOND(I,J) = 10000
4200        CONTINUE
5000     CONTINUE
         DO 5500 I=256,260
            MRKCHN(I)=0
            MCHN(I) = 0
            DO 5100 J=1,2
               LABL(I,J) = 0
               LLABL(I,J) = 0
5100        CONTINUE
5500     CONTINUE
7000     CONTINUE
         RETURN
         END
C
         SUBROUTINE IDENT(KAR,IX,IY,INCX,INCY,IRESET)
         IMPLICIT INTEGER*2 (A-Z)
         INTEGER*4 MM
         LOGICAL*2 BONDEL,DELTED,BAR
         CHARACTER*1 ISTAT
         COMMON /CD/ MAXX,MAXY
         COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
         COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
         COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
         COMMON /OLD/ IOX,IOY
         COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
         COMMON /ISTATE/ ISTAT
         COMMON /HEAD/ MW(12),ISTATE,PAGE
         COMMON /PROB/ IPROB,JPROB
         COMMON /FROM/ LCHAR
         COMMON /WARN/ ERR
         COMMON /IRECS/ IU,IREC,TOPREC,BOTREC
CXT      BONDEL = TRUE indicates that a bond has been drawn between 2
CXT      nodes so subsequent deletion should delete the bond, not a node.
         COMMON /DELBND/ BONDEL
CXT      BAR is used in conjunction with NOCHG and LASTN to control
CXT      bond type determination in relation to default bond types.
         COMMON /BTPDIR/ BAR
C
C  This subroutine identifies input characters and sets modes and states
C  accordingly.
C  Previous mode(state)
CXT DELTED = TRUE after SUBROUTINE DEL is called.
         DELTED = .FALSE.
16       JMODE=MODE
C Assume reset to bondtype 1
         IF ((KAR.NE.58).AND.(ISTATE.NE.12).AND.(ISTATE.NE.3).AND.
     *      (ISTATE.NE.5).AND.(KAR.NE.94).AND.(KAR.NE.33)) THEN
            IF ((LASTN.NE.IBTYPE).AND.(ISTATE.NE.9)) NOCHG = 0
         ELSE IF ((KAR.EQ.58).OR.(KAR.EQ.33).OR.(KAR.EQ.94)) THEN
            BAR = .TRUE.
         ENDIF
         LASTN = 0
         ITEMP=0
         IF (KAR.NE.127) BONDEL = .FALSE.
         IF (ICHAR.EQ.30) ITEMP=30
         IF ((ICHAR.EQ.18).OR.(ICHAR.EQ.25)) ITEMP=18
C character type
         ICHAR=0
         JJJ=IX
```

```
         DO 428 I=0,-3,-1
         IF (((MM(IX+I,IY).GE.65).AND.(MM(IX+I,IY).LE.90).AND.
     2      (MM(IX+I,IY).NE.72)).OR.((MM(IX+I,IY).EQ.72).AND.
     3      (MM(IX+I+1,IY).GE.97).AND.(MM(IX+I+1,IY).LE.122))) THEN
            JJJ=IX+I
            GO TO 427
         ENDIF
428      CONTINUE
427      IF(KAR .EQ. 81) GO TO 966
C GOTO if not ground state
         IF (KAR.EQ.21) THEN
            ISMART = 0
            CALL SPACE(IX,IY)
            MCHAR = 0
            JCHAR = 2
            RETURN
         ENDIF
CXT      IF (MODE.GT.1) GOTO 20
         IF ((KAR.GE.48).AND.(KAR.LE.57).AND.(ITEMP.NE.30)) THEN
            ICHAR = 29
            CALL NUMBER(KAR,IX,IY)
            MCHAR = KAR
            RETURN
         ENDIF
C
C                Ground state:
C
C Select bonds
         IF (KAR.EQ.124) RETURN
         IF ((KAR.LT.22) .OR. (KAR.GT.31)) GOTO 1
C bonds
18       ICHAR=1
C set bond direction
         IBDIR = KAR-21
         IF (IBDIR.GT.4) IBDIR=IBDIR-2
         GOTO 4400
C 81=Q--quit
1        IF (KAR.NE.81) GOTO 2
966      ICHAR=20
         IF (ITEMP.NE.18) CALL CLRHYD(JJJ,IY)
         IF (ITEMP.NE.18) CALL VALNCE(2,JJJ,IY,0,0)
         IF (JPROB.NE.0) RETURN
         CALL QUIT(IRESET,KAR,IX,IY)
         IF ((MM(JJJ,IY).NE.0).AND.(ERR.NE.18).AND.(ERR.NE.12)) JCHAR = 2
         IF ((PAGE.EQ.2).AND.(IRESET.EQ.0)) THEN
            ICUR = 1
            CALL CURSOR(IX,IY)
         ENDIF
         IF ((PAGE.NE.2).AND.(JPROB.NE.1)) THEN
            CALL SETCOL(0)
            CALL CLR
            CALL SETCOL(1)
         ENDIF
         IF ((IRESET.NE.3).OR.(IRESET.EQ.1)) THEN
            CALL SETSCR(2)
            PAGE = 0
            CALL FTSIZE(1,10)
         ENDIF
C WE ARE DONE - EXIT
         IF ((IRESET.EQ.1).OR.(IRESET.EQ.3)) RETURN
         MODE = 1
         RETURN
C        GO TO 4400
C        Seperate UC; '?'; and '.'
2        IF (((KAR.LT.65) .OR. (KAR.GT.90)) .AND. (KAR.NE.63) .AND.
     2    (KAR.NE.46))  GOTO 3
C UC after '$'--2nd letter of elem symb
         IF (ITEMP.NE.30) GOTO 35
C        Convert UC to LC
         KAR=KAR+32
         GOTO 3
35       ICHAR = 2
         GOTO 4400
C separate lowercase
C LINE FOOLS PROGRAM INTO ACCEPTING D1'S AND M1'S.
```

```
3       IF ((KAR.GT.48).AND.(KAR.LT.58).AND.(ITEMP.EQ.30))
     *     GO TO 44
        IF ((KAR.LT.97).OR.(KAR.GT.122)) GO TO 4
C       If lc is second letter of element
44      IF (ITEMP.EQ.30) ICHAR = 4
        ITEMP=0
C jump to marker
        IF (ICHAR.NE.4)  ICHAR=31
        IF (ICHAR.EQ.31) CALL CLRHYD(JJJ,IY)
        GOTO 4400
C sign+-
4       CONTINUE
C % ring mode
5       IF (KAR.NE.94) GOTO 6
        ICHAR=12
        LEVEL=1
        GOTO 4400
C chain mode
6       IF (KAR.NE.33) GOTO 7
        ICHAR=13
        LEVEL=1
        GOTO 4400
C @ repeat mode
7       IF (KAR.NE.64) GOTO 88
        ICHAR=14
        LEVEL=1
        GOTO 4400
88      IF(KAR.NE.42) GO TO 8
        ICHAR=16
        LEVEL=1
        GO TO 4400
C % long bond
8       IF (KAR.NE.LBOND) GOTO 11
        ICHAR=17
        GOTO 4400
C & enlarge state
11      IF (KAR.NE.38) GOTO 12
        ICHAR=15
        GOTO 4400
C delete state
12      IF (KAR.NE.127) GOTO 13
        ICHAR=19
        GOTO 4400
C backspace
13      IF (KAR.NE.8) GOTO 14
        ICHAR=18
        ISMART=0
        GOTO 4400
C space
14      IF (KAR.NE.ISPACE) GOTO 15
        ICHAR=25
        GOTO 4400
C Carriage return--return to gnd state
15      IF (KAR.NE.13) GOTO 19
        ICHAR=26
        MODE=1
        GOTO 4400
C '$':2nd letter of element symbol next
19      IF (KAR.NE.JUMP) GOTO 33
C WE MISTAKENLY CHANGED A H
        IF(MCHAR .NE. 74) GO TO 1119
C TO A J - NOW CHANGE IT BACK
        MM(IX-1,IY)=72
1119    ICHAR=30
        GOTO 4400
C '#'set a marker
33      IF (KAR.NE.ITAG) GOTO 341
        ICHAR=28
        GOTO 4400
```

```
C _ Library
341     IF (KAR.NE.95) GO TO 3004
           ICHAR = 33
           LEVEL = 1
           GO TO 4400
C : Retrieve
3004    IF (KAR.NE.58) GO TO 3404
           ICHAR = 21
           LEVEL = 1
           GO TO 4400
C D1 " indeterminant bond site marker
3404    IF (KAR.NE.34) GO TO 34
           ICHAR = 9
           GO TO 4400
C Chg+-=
34      IF ((KAR.NE.43).AND.(KAR.NE.45)) GOTO 4455
           ICHAR = 6
           IF (JCHAR.NE.6) THEN
              HCHAR = JCHAR
              NCHRG = 1
           ELSE IF ((KAR.EQ.MCHAR).AND.(NCHRG.LT.9)) THEN
              NCHRG = NCHRG + 1
           ELSE
              CALL MYERR(55,55,55)
              CALL DEL(KAR,IX,IY,INCX,INCY,0)
        IF (JCHAR .EQ. 6) JCHAR=2
              DELTED = .TRUE.
              JCHAR = HCHAR
              GO TO 4444
           ENDIF
           GO TO 4400
C Types the connection table of input structure to screen from GND
4455    IF ((KAR.NE.39).OR.(TOPREC.EQ.0)) GO TO 45
           CALL VCONTB
           ICUR = 1
           CALL CURSOR(IX,IY)
           RETURN
C Unrecognized character for this mode
45      CALL ERRMSG(KAR)
        RETURN
C draw printable char
4400    IF (ICHAR.LT.10) THEN
CXT        IF (ERR.EQ.45) ERR = 0
           IF (ICHAR.EQ.6) THEN
              CALL CHARGE(KAR,IX,IY,NCHRG)
           ELSE IF (ICHAR.EQ.9) THEN
              IDRAW = 0
              CALL IND1(KAR,IX,IY,IDRAW,IERR)
           ELSE
              CALL DRAW (KAR,IX,IY,INCX,INCY)
           ENDIF
C backspace
        ELSE IF (ICHAR.EQ.18) THEN
           CALL BKSPCE(IX,IY)
           JCHAR = 2
           MCHAR = 0
C delete
        ELSE IF (ICHAR.EQ.19) THEN
           CALL DEL(KAR,IX,IY,INCX,INCY,0)
           DELTED = .TRUE.
        ENDIF
        CALL HEADER
C save last printable character
        ISP = 0
        IF (ICHAR.LE.10) THEN
           MCHAR=KAR
C save last char type
           JCHAR=ICHAR
        ELSE IF (ICHAR.EQ.28) THEN
           CALL MARK(KAR,IX,IY,IERR)
        ELSE IF (ICHAR.EQ.25) THEN
           IX = IX - 1
           CALL CURSOR(IX,IY)
           CALL CLRHYD(IX,IY)
           CALL VALNCE(2,IX,IY,0,0)
```

```
      IF (JPROB.EQ.1) RETURN
      IX = JJJ
      CALL SPACE(IX,IY)
      JCHAR = 2
      MCHAR = 0
   ELSE IF (ICHAR.EQ.15) THEN
      CALL SETLRG
   ELSE IF (ICHAR.EQ.16) THEN
      IF (JCHAR.EQ.2.OR.JCHAR.EQ.4) THEN
         CALL CLRHYD(IOX-1,IOY)
C        CALL VALENCE BEFORE DOTDIS
         CALL VALNCE(2,IOX-1,IOY,0,0)
      ENDIF
   ELSE IF (ICHAR.EQ.31) THEN
      IF ((MM(JJJ,IY).NE.46).AND.(MM(JJJ-1,IY).NE.46))
   *     CALL VALNCE(2,JJJ,IY,0,0)
      CALL LEAP(KAR,IX,IY)
C  LEAP to label KAR
   ELSE IF (ICHAR.EQ.17) THEN
      CALL LONG(KAR,IX,IY)
      IF (KAR.EQ.81) GO TO 966
   ENDIF
C  RETURNED FROM LONG BOND WITH Q - GO TO QUIT
   IF ((DELTED).OR.(ICHAR.EQ.18).OR.(ICHAR.EQ.25)) GO TO 4444
   JBTYPE=IBTYPE
   JBDIR=IBDIR
4444 CONTINUE
   IF (LEVEL.NE.1) LCHAR = 0
   RETURN
   END
C
C
C     This subroutine replaces most of the number entry section of IDENT.
C     This subroutine sets bondtype and draws a bond of the new type
C                                                    or
C     sets  charge value and displays the charge.
C
      SUBROUTINE NUMBER(KAR,IX,IY)
      IMPLICIT INTEGER*2 (A-Z)
      LOGICAL*2 BAR
        CHARACTER*1 ISTAT
      COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
      COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
      COMMON /OLD/ IOX,IOY
      COMMON /ISTATE/ ISTAT
      COMMON /HEAD/ MW(12),ISTATE,PAGE
CXT   BAR is used in conjunction with NOCHG and LASTN to control
CXT   bond type determination in relation to default bond types.
      COMMON /BTPDIR/ BAR
      LASTN = 0
C
C     If KAR = | discard it.
      IF ((KAR.GE.48).AND.(KAR.LE.57)) THEN
         BAR = .FALSE.
         GO TO 100
      ENDIF
      BAR = .TRUE.
 50   CALL INPUTX(KAR,IX,IY)
      IF ((KAR.GE.48).AND.(KAR.LE.57)) THEN
         GO TO 100
      ELSE IF (KAR.EQ.124) THEN
         GO TO 400
      ELSE IF (KAR.EQ.13) THEN
         GO TO 600
      ELSE IF (KAR.EQ.81) THEN
         GO TO 700
      ELSE
         GO TO 800
      ENDIF
C
C     Digit processing
 100  LASTN = KAR - 48
      IBTYPE = LASTN
```

```
      CALL HEADER
      IF (IBTYPE.EQ.9) GO TO 500
      NOCHG = 1
      RETURN
C
C     Already in current state
400   IERR = 39
      CALL MYERR(IERR,IERR,IERR)
      GO TO 50
C
C     Bad bond type or charge value - cmd rejected - get new cmd
500   IERR = 55
      CALL MYERR(IERR,IERR,IERR)
      IBTYPE = 1
      LASTN = 0
      CALL HEADER
      RETURN
C
C     Return with CR or Q
600   ICHAR = 26
700   MODE = 1
      NOCHG = 0
      LASTN = 0
      IBTYPE = 1
      CALL HEADER
      RETURN
800   IERR = 5
      CALL MYERR(IERR,IERR,IERR)
      GO TO 50
      END
$STORAGE:2
C
C     SUBROUTINE MOVE moves the cursor 1 unit in any of the 8 defined
C     directions while the program is in the dumb mode. MOVE is called
C     from SUBROUTINES SPACE and BKSPCE.
C
C     ORI   Paul Broderick   October, 1984
      SUBROUTINE MOVE(KHAR,IX,IY)
      IMPLICIT INTEGER*2(A-Z)
      COMMON /CD/ MAXX,MAXY
      COMMON /CUR/ ICUR
C
      IF (KHAR.EQ.22) THEN
         IY = IY - 1
      ELSE IF (KHAR.EQ.23) THEN
         IX = IX + 1
         IY = IY - 1
      ELSE IF (KHAR.EQ.24) THEN
         IX = IX + 1
      ELSE IF (KHAR.EQ.25) THEN
         IX = IX + 1
         IY = IY + 1
      ELSE IF (KHAR.EQ.28) THEN
         IY = IY + 1
      ELSE IF (KHAR.EQ.29) THEN
         IX = IX - 1
         IY = IY + 1
      ELSE IF (KHAR.EQ.30) THEN
         IX = IX - 1
      ELSE IF (KHAR.EQ.31) THEN
         IX = IX - 1
         IY = IY - 1
      ENDIF
      IF (IX.GT.MAXX) THEN
         IX = MAXX
      ELSE IF (IX.LT.1) THEN
         IX = 1
      ENDIF
      IF (IY.GT.MAXY) THEN
         IY = MAXY
      ELSE IF (IY.LT.1) THEN
         IY = 1
      ENDIF
```

```
C
      ICUR = 1
      CALL CURSOR(IX,IY)
      RETURN
      END
C
        SUBROUTINE CURSOR(IX,IY)
        IMPLICIT INTEGER*2 (A-Z)
        COMMON /SIZZE/ MULTX,MULTY
        COMMON /CUR/ ICUR
        COMMON /HEAD/ MW(12),ISTATE,PAGE
        COMMON /DARK/ OCUR
        DATA XCUR /-1/
C
C       CONVERT COORDINATES TO RASTER
        IF (PAGE.LE.1) CALL SETSCR(2)
        INTX = (IX*MULTX)
        INTY = (IY*MULTY)
        CALL MOVTCA(INTX,INTY)
        IF (OCUR.EQ.1) THEN
           IF (ICUR.NE.XCUR) CALL INITHC(3,3,ICUR)
           HINTX = INTX - 1
           HINTY = INTY + 1
           IF (ICUR.NE.0) CALL MOVHCA(HINTX,HINTY)
        ENDIF
        XCUR = ICUR
        IF (PAGE.EQ.1) CALL SETSCR(1)
        RETURN
        END
C
        SUBROUTINE INPUTX(KAR,IX,IY)
        IMPLICIT INTEGER*2 (A-Z)
        CHARACTER*82 BLNK90
        COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /SIZZE/ MULTX,MULTY
        COMMON /OLD/ IOX,IOY
        COMMON /HEAD/ MW(12),ISTATE,PAGE
        COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
        COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
        COMMON /CUR/ ICUR
        COMMON /ISTATE/ ISTAT
        COMMON /PROB/ IPROB,JPROB
        COMMON /BLANK/BLNK90
        COMMON /CD/ MAXX,MAXY
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /WARN/ ERR
        IOX=IX
C       SAVE OLD COORDINATES FOR VALENCE CALL PRIOR TO DOTDIS
        IOY=IY
1       CONTINUE
        CALL GETCR(KAR,IX,IY)
        IF (((KAR.EQ.74).AND.(ISTATE.NE.8)).OR.(KAR.GE.128)) THEN
           IF (KAR.EQ.131) THEN
              IF (((LEVEL.EQ.1).AND.(ISTATE.GE.3).AND.(ISTATE.LE.7))
     *           .OR.(ISTATE.EQ.11).OR.(ISTATE.EQ.12)) THEN
                 GO TO 2
              ELSE
                 KAR = 13
                 GO TO 2
              ENDIF
           ENDIF
           CALL ERRMSG(KAR)
           GO TO 1
        ENDIF
2       CONTINUE
        IF (PAGE.EQ.0) THEN
           IF (IY.LE.2) THEN
              ICUR = 0
              CALL CURSOR(IX,IY)
              ICUR = 1
           ENDIF
           CALL FTSIZE(2,18)
           CALL FTLOCA(4,1)
           CALL FTEXT(BLNK90)
           PAGE = 2
           CALL FTSIZE(1,10)
```

```
          IF (LOY.LE.2) THEN
             DO 10 I = LOX,HIX+6,6
                KX = MINO(I,MAXX)
                CALL REPLCE(KX,1,1,1,0,0,2)
10           CONTINUE
             CALL RELONG
             CALL CURSOR(IX,IY)
          ENDIF
       ELSE IF (PAGE.LE.1) THEN
          CALL SETCOL(0)
          CALL CLR
          CALL SETCOL(1)
          IF (ERR.NE.100) THEN
             PAGE = 2
             CALL SETSCR(2)
             CALL DISPLA(2)
             CALL FTSIZE(1,10)
          ENDIF
       ENDIF
       RETURN
       END
$STORAGE:2
       SUBROUTINE CONTEX(KAR,IX,IY,INCX,INCY,IERR)
       IMPLICIT INTEGER*2 (A-Z)
       INTEGER*4 MM,IDTPIX
       LOGICAL*2 BAR,CNTX
       COMMON /CD/ MAXX,MAXY
       COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
       COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
       COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
       COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
       COMMON /SIZZE/ MULTX,MULTY
       COMMON /LABELS/ NR,NJLAST,NJNEXT
       COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
       COMMON /PROB/ IPROB,JPROB
       COMMON /WARN/ ERR
CXT    CHER indicates to which HALO page error messages are to be written.
       COMMON /QTVLNC/ OERR,CHER
       COMMON /CUR/ ICUR
       COMMON /HEAD/ MW(12),ISTATE,PAGE
CXT    BAR, in conjunction with NOCHG controls bond typ settings in
CXT    in relation to bond type defaults.
       COMMON /BTPDIR/ BAR
CXT    CNTX acts to inform SUBROUTINE MARKER that is being called by
CXT    SUBROUTINE CONTEX and to set parameters accordingly.
       COMMON /CNTX/ CNTX
C
C        This routine determines the corrected location for the next
C position.  Subroutine DRAW has already TENTATIVELY selected an IX,IY
C to the right of a character or Luhn dot, or one grid space beyond the
C end of a bond (in the bond's direction).  For this 'a priori' context
C analysis are the current and previous character (KAR,MCHAR), current
C and previous character type(ICHAR,JCHAR).
C
       ICUR = 1
C Insert dot if first input is a bond:
       IF (ICHAR.EQ.1) THEN
CXT       Edge of screen problems are precluded.
          IF (IX.GE.MAXX) THEN
             IX = MAXX
             X1 = 0
             NX1 = 1
          ELSE IF (IX.LE.1) THEN
             IX = 1
             NX1 = 0
             X1 = 1
          ELSE
             X1 = 1
             NX1 = 1
          ENDIF
```

```
         IF (IY.GE.MAXY) THEN
            IY = MAXY
            Y1 = 0
            NY1 = 1
         ELSE IF (IY.LE.1) THEN
            IY = 1
            NY1 = 0
            Y1 = 1
         ELSE
            Y1 = 1
            NY1 = 1
         ENDIF
         IF ((MM(IX-NX1,IY)+MM(IX,IY)+
     2      MM(IX+X1,IY)+MM(IX-NX1,IY-NY1)+MM(IX,IY-NY1)+
     3      MM(IX+NX1,IY-NY1)+MM(IX-NX1,IY+Y1)+MM(IX,IY+Y1)+
     4      MM(IX+X1,IY+Y1).EQ.0)) THEN
            CNTX = .TRUE.
            CALL MARK(KAR,IX,IY,IERR)
            CNTX = .FALSE.
         ENDIF
      ENDIF
C
C Replace Luhn dot with uppercase if typed immed after it
      IF ((KAR.EQ.46).OR.(ICHAR.EQ.1)) GOTO 1
      IX = IX - 1
      IF ((MM(IX,IY).NE.46).OR.(IX.EQ.0)) THEN
         IX = IX + 1
         GO TO 1
      ENDIF
      MM(IX,IY) = 0
      CALL REPLCE(IX,IY,0,0,0,0,1)
C
C The following code, through label 41, determines, if the Luhn dot is
C being replaced by an uppercase, whether you are in fact replacing a
C lower case marker with an uppercase element symbol.  If so, the marker
C is removed from the list of markers in LABL and replaced in LABL
C with negative numbers, indicating availability for reuse.
C
    DO 40 I=1,260
C End of markers in use
      IF (LABL(I,1)+LABL(I,2).EQ.0) GOTO 41
C No match
      IF ((LABL(I,1).NE.IX) .OR. (LABL(I,2).NE.IY)) GOTO 40
C Neg value indicates discarded marker available for reuse (see MARK).
              LABL(I,1)=-999
              LABL(I,2)=-999
C Jump out of loop
              GOTO 41
40            CONTINUE
41    CONTINUE
C Reset cursor to exact corner, else char is offset to insert new character
      ICUR = 1
      CALL CURSOR(IX,IY)
      RETURN
C
C
C Character after character: tentative position OK:
1     IF((JCHAR.LT.11) .AND. (ICHAR.LT.11).AND. (JCHAR.GT.1) .AND.
    2    (ICHAR.GT.1))     RETURN
C Character after a bond--tentative position is OK:
      IF ((ICHAR.EQ.1) .OR. (JCHAR.NE.1)) GOTO 2
      RETURN
C
C Bond after character--move left to nearest uppercase(or .or?) &
C proceed one unit in bond direction.
2        IF ((JCHAR.LE.1) .OR. (ICHAR.NE.1)) GOTO 4
      DO 3 I=0,5
C Look left
      MX=IX-I
      IF (MX.LE.0) GO TO 3
      LL = LMM(MX,IY)
C (Non-uppercase or . or ?)
      IF ((LL.NE.46).AND.(LL.NE.63).AND.((LL.LT.65).OR.(LL.GT.90)))
    2      GOTO 3
C Skip over H which is not He, Hq, etc.
```

```
      IF((LL.EQ.72).AND.((MM(MX+1,IY).LE.97).OR.(MM(MX+1,IY).GE.122
     2    ))) GOTO 3
      IX = IX-I
      LL=0
      GOTO 7
3     CONTINUE
C Position bond correctly wrt character
7     IX=IX + INCX
      IY=IY + INCY
      RETURN
C
C 2 similar bonds in a row:
4     IF ((ICHAR.NE.1) .OR. (JCHAR.NE.1)) GOTO 5
C Same bond direction--tentative location is OK
      IF (IBDIR.NE.JBDIR) GO TO 9
C Bonds in same dir, diff type get dot
      IF (IBTYPE.NE.JBTYPE) GO TO 6
C Keep bond type unchanged
      NOCHG=1
      ICUR = 0
      RETURN
C Opposite direction
9     CONTINUE
      IF (IABS(IBDIR-JBDIR).NE.4) THEN
         IF ((ISTATE.EQ.3).OR.(ISTATE.EQ.5).OR.(ISTATE.EQ.12)) THEN
            IF (.NOT.BAR) NOCHG = 0
            BAR = .FALSE.
         ENDIF
         GO TO 6
      ENDIF
C Return to  end of bond
10    IX=IX+INCX
      IY=IY+INCY
C     Follow back bond to node
      IF ((LMM(IX,IY).GT.256).OR.((IBTYPE.EQ.0).AND.(MM(IX,IY).EQ.0))
     1 .OR. ((MM(IX,IY).GE.50).AND.
     2 (MM(IX,IY).LE.57)) .OR. ((MM(IX,IY).GE.97).AND.
     3 (MM(IX,IY).LE.122)).OR.((MM(IX,IY).EQ.72).AND.((MM(IX+1,IY)
     4 .LT.97).OR.(MM(IX+1,IY).GT.122)))) GOTO 10
      IX=IX+1
      ICUR = 1
      CALL CURSOR (IX,IY)
C Flag to line 4900 of draw
      MCHAR=-999
      KAR=MCHAR
      JCHAR=ICHAR
      ICHAR=2
C Keep bond type unchanged
      NOCHG=1
      RETURN
C Automatically drawn dot, then. . .
6     CNTX = .TRUE.
      CALL MARK(KAR,IX,IY,IERR)
      CNTX = .FALSE.
C     Keep NOCHG what it was:  zero unless set to one in number state
C     to introduce new bond type.
C . . .continue as above--bond after character.
      IF (IERR.NE.48) GOTO 2
         RETURN
C Initial letter
5     IF (MCHAR.EQ.0) RETURN
      IERR=13
C Contex error
      CHER = 2
      CALL MYERR(IERR,MCHAR,MCHAR)
      CHER = 0
      JPROB = 1
      RETURN
      END
C
      SUBROUTINE MARK(KAR,IX,IY,IERR)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM,IDTPIX
```

```
      LOGICAL*2 NOMSG,CNTX
      CHARACTER*1 HALO(3)
      CHARACTER*1 KAN
      COMMON /CD/ MAXX,MAXY
      COMMON /RANGE/ LOX,HIX,LOY,HIY
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
      COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
      COMMON /LABELS/ NR,NJLAST,NJNEXT
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
C     What is displayed; State of line 2
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /CUR/ ICUR
      COMMON /OLD/ IOX,IOY
      COMMON /LEAPER/ NOMSG
      COMMON /CNTX/ CNTX
C
C This routine puts the next available marker on the screen.  It
C stores the last line number used as NJNEXT.  NJNEXT is incremented to
C the next line, where LABL(NJNEXT,*)=0.  Previously used but deleted
C labels (where LABL(J,*)=-999are not reused to avoid confusion on
C where a jump will take p.)  The program puts
C IX & IY into LABL on the new line, prints the appropriate label on the
C screen, inserts IDOT=46 (Luhn dot) into MM(IX,IY), moves the cursor to
C IX+1,IY, and sets KAR to IDOT=46 and ICHAR to 2, as if a Luhn dot
C were typed in directly.
C
      ICUR = 1
      IF ((IX.LT.1).OR.(IX.GT.MAXX).OR.(IY.LT.1).OR.(IY.GT.MAXY))
   *     THEN
         IX = IOX
         IY = IOY
         ICUR = 1
         CALL CURSOR(IX,IY)
         CALL MYERR(36,KAR,KAR)
         RETURN
      ENDIF
      HALO(1) = KAN
      HALO(3) = KAN
C
C Line # for next marker--Don't reuse old ones because
C too much confusion in where you're jumping.
      IF (MM(IX,IY).EQ.0) GO TO 10
         IERR = 48
         GO TO 11
C Check adjacent nodal values.
10       DO 1122 I = -1,1
            MX = IX + I
            IF ((MX.LE.0).OR.(MX.GT.MAXX)) GO TO 1122
            DO 12 J = -1,1
               MY = IY + J
               IF ((MY.LE.0).OR.(MY.GT.MAXY)) GO TO 12
               L = LMM(MX,MY)
               IF ((L.EQ.0).OR.(L.GE.256)) GO TO 12
               IF ((MM(MX,MY).GT.2**13).OR.
   *              ((L.GE.50).AND.(L.LE.57).AND.((MM(MX-1,MY).GT.
   *              2**13).OR.((IABS(I+J).NE.1)
   *              .AND.(MM(MX-1,MY).EQ.72))).AND.(MX-1.GT.0))
   *              .OR. (L .EQ. 34))GO TO 12
               IF (NOMSG) GO TO 13
               IERR = 48
               IF (CNTX) GO TO 13
               GO TO 11
12          CONTINUE
1122     CONTINUE
C
      NJNEXT=NJNEXT+1
      IF (NJNEXT.LE.260) GO TO 99
      IERR=16
C Issue message - decrement counter and return
      NJNEXT=NJNEXT-1
```

```
C We've used up all labels
11      CALL MYERR(IERR,KAR,KAR)
13      RETURN
C
99      LINE=NJNEXT
C Letter to be typed
        NR = NJNEXT
        LET=MOD(LINE,26)
C Label 'z'
        IF (LET.EQ.0) LET=26
C ASCII equivalent
        LET=LET+96
C
C Insert coordinates into table of labels.
        LABL(LINE,1)=IX
        LABL(LINE,2)=IY
C Luhn dot into data table
        MM(IX,IY)=IDOT
        HALO(2) = CHAR(LET)
        IF (IX.LT.LOX) THEN
           LOX = IX
        ELSE IF (IX.GT.HIX) THEN
           HIX = IX
        ENDIF
        IF (IY.LT.LOY) THEN
           LOY = IY
        ELSE IF (IY.GT.HIY) THEN
           HIY = IY
        ENDIF
        CALL CURSOR(IX,IY)
        CALL TEXT(HALO)
C Cursor to next location
        IX=IX+1
C As if dot or uppercase were just typed in

        JCHAR=2
        IF (.NOT.CNTX). THEN
           ICHAR=2
           IF ((ISTATE.NE.9).AND.(IBTYPE.NE.0).AND.(IBTYPE.NE.4).AND.
     2        (IBTYPE.NE.8)) IBTYPE=1
        ENDIF
        CALL HEADER
        KAR=IDOT
        MCHAR=IDOT
        ICUR = 1
        CALL CURSOR(IX,IY)
        RETURN
        END
C
        SUBROUTINE DOT(IX,IY,IERR)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
        COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
        COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /SIZZE/ MULTX,MULTY
        COMMON /CD/ MAXX,MAXY
        COMMON /RANGE/ LOX,HIX,LOY,HIY
C
C This subroutine generates 'automatic' Luhn dots & updates position
C and parameters as if generated by keyboard entry.
        IF (IX.GT.MAXX) THEN
           IX = MAXX
        ELSE IF (IX.LT.1) THEN
           IX = 1
        ENDIF
        IF (IY.GT.MAXY) THEN
           IY = MAXY
        ELSE IF (IY.LT.1) THEN
           IY = 1
        ENDIF
        IERR = 0
```

```
      IF (MM(IX,IY).NE.0) GO TO 1144
C Check adjacent nodal values.
      DO 12 I = -1,1
         MX = IX + I
         IF ((MX.LE.0).OR.(MX.GT.MAXX)) GO TO 12
         DO 1122 J = -1,1
            MY = IY + J
            IF ((MY.LE.0).OR.(MY.GT.MAXY)) GO TO 1122
            L = LMM(MX,MY)
            IF ((L.EQ.0).OR.(L.GE.256)) GO TO 1122
            IF ((MM(MX,MY).GT.2**13).OR.
     *         ((L.GE.50).AND.(L.LE.57).AND.((MM(MX-1,MY).GT.2**13)
     *         .OR.((IABS(I+J).NE.1)
     *         .AND.(MM(MX-1,MY).EQ.72))).AND.(MX-1.GT.0)) .OR.
     *         (L.EQ.34)) GO TO 1122
            GO TO 1144
1122     CONTINUE
12    CONTINUE
C Draw a Luhn dot.
      JX = IX * MULTX - 6
      JY = IY * MULTY - 4
      J3X = JX + 3
      J3Y = JY - 3
      CALL BAR(JX,JY,J3X,J3Y)
      MM(IX,IY)=IDOT
C Expand picture boundaries.
      IF (IX.LT.LOX) THEN
         LOX = IX
      ELSE IF (IX.GT.HIX) THEN
         HIX = IX
      ENDIF
      IF (IY.LT.LOY) THEN
         LOY = IY
      ELSE IF (IY.GT.HIY) THEN
         HIY = IY
      ENDIF
      MCHAR=IDOT
      JCHAR=2
      IX=IX+1
      RETURN
1144  CONTINUE
      IERR = 48
      RETURN
      END
C
      SUBROUTINE LEAP (KAR,IX,IY)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM,IDTPIX
      LOGICAL*2 NOMSG
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
      COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
      COMMON /LABELS/ NR,NJLAST,NJNEXT
      COMMON /MKSKP/ ISKIP
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
      COMMON /CUR/ ICUR
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /LEAPER/ NOMSG
C
C  This routine moves the cursor to the location of a given lower case
C  label.  A counter NR is placed at the line of the last label jumped
C  to, and is used as a starting point for the next jump.  When all al-
C  phabets have been used, NR returns to the top.  When a previously-
C  deleted label is addressed (LABL < 0), the next alphabet down is
C  addressed.
C
C This subroutine is called by the operator by typing a lower case
C letter without the '$' precedance code.
```

```
C
       ICUR = 1
C Flag for how many times you have gone to top this jump
10     ITEST=0
C Sequence number within the lowercase alphabet
       NJ=KAR-96
C Same label twice: next alphabet.
       IF (NJ.EQ.NJLAST) GOTO 1
C The alphabet # where currently located.
30     NALPH=(NR+25)/26
C Tentative line in LABL of desired coords.
       NQ=NJ+(NALPH-1)*26
C End of array--go to top.
       IF (NQ.GT.260) GOTO 2
C Tentative X coord of label
       JX=LABL(NQ,1)
       JY=LABL(NQ,2)
       IF (JX+JY) 1,2,3
C Discarded marker: try next alphabet
1      NR=NR+26
       GOTO 30
C Beyond end of useful data: try top
2      NR=1
C Started at top again in this CALL MARK.
       ITEST=ITEST+1
C No such label
       IF (ITEST.GT.1) THEN
          CALL ERRMSG(KAR)
C No such label
          RETURN
       ENDIF
       GOTO 30
C Relocate cursor as if dot were typed here.
3      IF ((ISKIP.NE.1).AND.(JCHAR.EQ.1)) THEN
          NOMSG = .TRUE.
          CALL MARK(ZAR,IX,IY,IERR)
          NOMSG = .FALSE.
       ENDIF
       IX=JX+1
       IY=JY
       CALL CURSOR (IX,IY)
       KAR=IDOT
       JCHAR=2
       ICHAR=2
       MCHAR=IDOT
       NJLAST=NJ
       RETURN
       END
C
       SUBROUTINE CHARGE(KAR,IX,IY,NCHRG)
       IMPLICIT INTEGER*2 (A-Z)
       INTEGER*4 MM,M
       LOGICAL*2 NONLOC
       CHARACTER*1 HALO(3)
       CHARACTER*1 KAN
       COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
       COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
       COMMON /CD/ MAXX,MAXY
       COMMON /RANGE/ LOX,HIX,LOY,HIY
       COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
       COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
       COMMON /HEAD/ MW(12),ISTATE,PAGE
       COMMON /HP/IHP
       COMMON /IPLUS/ IHIGH(14,2)
       COMMON /CUR/ ICUR
       DATA NONLOC /.FALSE./
C
C This subroutine, called when an initial + or - sign is entered, searche
C for a diagonal location for the charge, and types it in.  When subseque
C + or - signs are entered, respectively, the previous charge value is
C increments by 1.
       IF ((JCHAR.EQ.6).AND.(NCHRG.GT.1)) THEN
          IF (NONLOC) THEN
             GO TO 5402
```

```
            ELSE
               GO TO 4501
            ENDIF
         ENDIF
         HALO(1) = KAN
         HALO(3) = KAN
         ICUR = 0
         IC=0
C Search back for the node, if any:
         JJJ=0
         DO 428 I=0,-3,-1
         IF (IX+I.LE.0) GO TO 428
         IF (((MM(IX+I,IY).GE.65).AND.(MM(IX+I,IY).LE.90).AND.(MM(IX+I,
     2      IY).NE.72)) .OR. ((MM(IX+I,IY).EQ.72).AND.(MM(IX+I+1,IY).GE.
     3      97).AND.(MM(IX+I+1,IY).LE.122)).OR.(MM(IX+I,IY).EQ.46)) THEN
            JJJ=IX+I
            GO TO 117
         ENDIF
428      CONTINUE
C Delocalized charge
117      IF (JJJ.LE.0) GOTO 430
C
C Look for space for charge up & to the right:
         IF ((JJJ+2.GT.MAXX).OR.(IY+2*IHP.LE.0).OR.(IY+2*IHP.GT.MAXY))
     * GO TO 431
         IF (MM(JJJ+1,IY+IHP)+MM(JJJ+2,IY+IHP)+MM(JJJ+2,IY+2*IHP)+
     *      MM(JJJ+1,IY+2*IHP).NE.0) GOTO 431
         IF (JJJ+3.LE.MAXX) THEN
            IF (MM(JJJ+3,IY+IHP).NE.0) GO TO 431
         ENDIF
         JX=JJJ+1
         JY = IY + 1 *IHP
         IC=4
         GOTO 450
C
C Look down & right:
431      IF ((JJJ+2.GT.MAXX).OR.(IY-2*IHP.GT.MAXY)
     * .OR. (IY-2*IHP.LE.0)) GO TO 118
         IF (MM(JJJ+1,IY-IHP)+MM(JJJ+2,IY-IHP)+MM(JJJ+2,IY-2*IHP)+
     *      MM(JJJ+1,IY-2*IHP).NE.0) GOTO 118
         IF (JJJ+3.LE.MAXX) THEN
            IF (MM(JJJ+3,IY-IHP).NE.0) GO TO 118
         ENDIF
         JX=JJJ+1
         JY = IY -1*IHP
         IC=13
         GOTO 450
C
C Look up & left:
118      IF ((JJJ-2.LE.0).OR.(IY+2*IHP.LE.0)
     * .OR. (IY+2*IHP.GT.MAXY)) GO TO 433
         IF (MM(JJJ-2,IY+IHP)+MM(JJJ-1,IY+IHP)+MM(JJJ-2,IY+2*IHP)+
     * MM(JJJ-1,IY+2*IHP).NE.0) GOTO 433
         IF (JJJ-3.GT.0) THEN
            IF (MM(JJJ-3,IY+IHP)+MM(JJJ-3,IY+2*IHP).NE.0) GO TO 433
         ENDIF
         JX = JJJ - 1
         JY = IY + 1*IHP
         IC=2
         GOTO 450
C
C Look down and left:
433      IF ((JJJ-2.LE.0).OR.(IY-2*IHP.GT.MAXY)
     * .OR. (IY-2*IHP.LE.0)) GO TO 434
         IF (MM(JJJ-2,IY-IHP)+MM(JJJ-1,IY-IHP)+MM(JJJ-1,IY-2*IHP)
     *      +MM(JJJ-2,IY-2*IHP).NE.0) GOTO 434
         IF (JJJ-3.GT.0) THEN
            IF (MM(JJJ-3,IY-IHP)+MM(JJJ-3,IY-2*IHP).NE.0) GO TO 434
         ENDIF
         JX = JJJ - 1
         JY = IY - 1*IHP
CXT      IC=10
CXT      IF (NCHRG.LE.1) THEN
```

```
CXT     JX=JX+1
        IC=11
CXT     ENDIF
        GOTO 450
C
434     CONTINUE
C No room exists for the charge on the diagonals.
           PAGE = 0
           CALL FTSIZE(2,18)
           CALL FTLOCA(4,1)
           CALL FTEXT('^NO ROOM FOR CHARGES. TRY DUMB MODE. ^')
           NCHRG=0
           KAR = 13
           ICHAR = JCHAR
           CALL FTSIZE(1,10)
           ICUR = 1
           CALL CURSOR(IX,IY)
        RETURN
C
C Draw charges in:
450     CONTINUE
CXT The existance of a previous charge on the node is checked.
        ICNT = 0
        DO 400 I = -2,2
           IF ((JJJ+I.GT.MAXX).OR.(JJJ+I.LE.0)) GO TO 400
           DO 300 J = -1,1
              IF ((IY+J.GT.MAXY).OR.(IY+J.LE.0)) GO TO 300
              IF ((LMM(JJJ+I,IY+J).NE.43).AND.(LMM(JJJ+I,IY+J).NE.45))
     *           GO TO 300
              ILC = IHMM(JJJ+I,IY+J)
              IF (ILC.EQ.0) GO TO 300
              IF ((I.NE.IHIGH(ILC,1)).OR.(J.NE.(-IHP)*IHIGH(ILC,2)))
     *  GO TO 300
              ICNT = ICNT + 1
300        CONTINUE
400     CONTINUE
        IF (ICNT.EQ.0) GO TO 4500
        IERR = 38
        CALL MYERR(IERR,IERR,IERR)
        ICHAR = JCHAR
        KAR = 13
        NCHRG = 0
        RETURN
4500    CONTINUE
CXT The charges sign is drawn with the first entry of a + or -.
        NONLOC = .FALSE.
        HALO(2) = CHAR(KAR)
        CALL CURSOR (JX,JY)
        CALL TEXT(HALO)
        SHFKAR = KAR
        IF (JX.LT.LOX) LOX = JX
        IF (JX+1.GT.HIX) HIX = JX + 1
        IF (JY.LT.LOY) THEN
           LOY = JY
        ELSE IF (JY.GT.HIY) THEN
           HIY = JY
        ENDIF
4501    CONTINUE
        IF (NCHRG.EQ.2) THEN
           IF ((IC.EQ.2).OR.(IC.EQ.11)) THEN
              IF (IC.EQ.2) THEN
                 IC = 1
              ELSE IF (IC.EQ.11) THEN
                 IC = 10
              ENDIF
              CALL FTLOCA(JY,JX)
              CALL FTEXT('^ ^')
              MM(JX,JY) = 0
              HALO(2) = CHAR(SHFKAR)
              JX = JX - 1
              CALL CURSOR(JX,JY)
              CALL TEXT(HALO)
```

```
            ENDIF
            FX = JX + 1
         ELSE IF (NCHRG.GT.2) THEN
            CALL FTLOCA(JY,FX)
            CALL FTEXT('^ ^')
         ENDIF
C Store location of charge in high order part of MM.
         MM(JX,JY)=KAR +IC * 2**13
         IF (NCHRG.LE.1) GOTO 60
         CALL CURSOR(JX+1,JY)
         KHAR=NCHRG+48
C Type integer digit
         HALO(2) = CHAR(KHAR)
         CALL TEXT(HALO)
         MM(JX+1,JY)=KHAR
60       IX=JJJ+1
CXT      NCHRG=1
         ICUR = 1
         CALL CURSOR(IX,IY)
CXT      IF (MM(IX-1,IY) .EQ. 46) KAR=46
         RETURN
C
C Delocalized charge--find clear area:
430      JJJ=IX
         NONLOC = .TRUE.
493      M=0
         DO 223 I=JJJ-1,JJJ+2
         DO 223 J=IY-1,IY+1
            M = M + MM(I,J)
223      CONTINUE
         IF (M.LE.0) GOTO 4320
         IF (JJJ+2.GT.MAXX) GO TO 434
         JJJ=JJJ+1
         GO TO 493
CXT When the clear area is found, the existance of any other non-local
CXT is checked - only 1 non-local charge per structure.
4320     DO 4345 I = LOX,HIX
            DO 4345 J = LOY,HIY
               IF ((MM(I,J).NE.45).AND.(MM(I,J).NE.43)) GO TO 4345
               IF (MM(I-1,J).NE.42) GO TO 4300
4345     CONTINUE
         GO TO 432
4300     CONTINUE
            IERR = 4
            CALL MYERR(IERR,IERR,IERR)
            ICHAR = JCHAR
            KAR = 13
            NCHRG = 0
            RETURN
432      CONTINUE
C The charge sign is entered.
         HALO(2) = CHAR(KAR)
         CALL CURSOR(JJJ,IY)
         CALL TEXT(HALO)
CXT Picture boundaries are expanded.
         IF (JJJ.LT.LOX) LOX = JJJ
         IF (JJJ+1.GT.HIX) HIX = JJJ + 1
         IF (IY.LT.LOY) THEN
            LOY = IY
         ELSE IF (IY.GT.HIY) THEN
            HIY = IY
         ENDIF
CXT The successive charge increment is entered and drawn.
5402     MM(JJJ,IY)=KAR
         IF (NCHRG.LE.1) GOTO 60
         KHAR=NCHRG+48
         IF (NCHRG.EQ.2) THEN
            FX = JJJ + 1
         ELSE
            CALL FTLOCA(IY,FX)
            CALL FTEXT('^ ^')
         ENDIF
         CALL CURSOR (FX,IY)
```

```
      HALO(2) = CHAR(KHAR)
      CALL TEXT(HALO)
      MM(JJJ+1,IY)=KHAR
      GOTO 60
      END
C
C     SUBROUTINE IND1 is called to enter undetermined bond site
C     markers in smart mode.  The marker is drawn in the first
C     available corner cell.  The default corners are first upper
C     left, then lower left, then upper right, and lower right last.
      SUBROUTINE IND1(KAR,IX,IY,IDRAW,IERR)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM
      CHARACTER*1 HALO(3)
      CHARACTER*1 KAN
      COMMON /CD/ MAXX,MAXY
      COMMON /RANGE/ LOX,HIX,LOY,HIY
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /CUR/ ICUR
      COMMON /HP/IHP
      COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
C
      HALO(1) = KAN
      HALO(3) = KAN
      ICUR = 0
C Search back for the node, if any:
      JJJ=0
      DO 428 I=0,-3,-1
      IF (IX+I.LE.0) GO TO 428
      IF(((MM(IX+I,IY).GE.65).AND.(MM(IX+I,IY).LE.90).AND.(MM(IX+I,
     2   IY).NE.72)) .OR. ((MM(IX+I,IY).EQ.72).AND.(MM(IX+I+1,IY).GE.
     3   97).AND.(MM(IX+I+1,IY).LE.122)).OR.(MM(IX+I,IY).EQ.46)) THEN
         JJJ=IX+I
         GO TO 117
      ENDIF
428   CONTINUE
C If no node found, jump to error message.
117   IF (JJJ.LE.0) GOTO 434
C     Check for duplicate "s.
      IF (NBD1.EQ.0) GO TO 4511
         DO 527 I = 1,NBD1
            IF ((JJJ.EQ.DSCNC(3,I)).AND.(IY.EQ.DSCNC(4,I))) GO TO 892
527      CONTINUE
         GO TO 4511
892      IERR = 47
         IF (IDRAW.EQ.1) RETURN
         CALL MYERR(IERR,IERR,IERR)
         RETURN
4511  CONTINUE
C
C Look for space for " up & to the right:
      IF ((JJJ+1.GT.MAXX).OR.(IY+IHP.LE.0).OR.(IY+IHP.GT.MAXY))
     * GO TO 431
      IF (MM(JJJ+1,IY+IHP).NE.0) GOTO 431
      JX=JJJ+1
      JY = IY +IHP
      NBD1 = NBD1 + 1
      DSCNC(2,NBD1) = 2
      DSCNC(3,NBD1) = JJJ
      DSCNC(4,NBD1) = IY
      DSCNC(5,NBD1) = JX
      DSCNC(6,NBD1) = JY
      GOTO 450
C
C Look down & right:
431   IF ((JJJ+1.GT.MAXX).OR.(IY-IHP.GT.MAXY).OR. (IY-IHP.LE.0))
     * GO TO 118
      IF (MM(JJJ+1,IY-IHP).NE.0) GO TO 118
      JX=JJJ+1
      JY = IY -IHP
      NBD1 = NBD1 + 1
```

```
      DSCNC(2,NBD1) = 4
      DSCNC(3,NBD1) = JJJ
      DSCNC(4,NBD1) = IY
      DSCNC(5,NBD1) = JX
      DSCNC(6,NBD1) = JY
      GOTO 450
C
C Look up & left:
118   IF ((JJJ-1.LE.0).OR.(IY+IHP.LE.0).OR. (IY+IHP .GT. MAXY))
     * GO TO 433
      IF (MM(JJJ-1,IY+IHP).NE.0) GOTO 433
      JX=JJJ-1
      JY = IY + IHP
      NBD1 = NBD1 + 1
      DSCNC(2,NBD1) = 8
      DSCNC(3,NBD1) = JJJ
      DSCNC(4,NBD1) = IY
      DSCNC(5,NBD1) =.JX
      DSCNC(6,NBD1) = JY
      GOTO 450
C
C Look down and left:
433   IF ((JJJ-1.LE.0).OR.(IY-IHP.GT.MAXY).OR. (IY-IHP .LE.0))
     * GO TO 119
      IF (MM(JJJ-1,IY-IHP).NE.0) GOTO 119
      JX=JJJ-1
      JY = IY -IHP
      NBD1 = NBD1 + 1
      DSCNC(2,NBD1) = 6
      DSCNC(3,NBD1) = JJJ
      DSCNC(4,NBD1) = IY
      DSCNC(5,NBD1) = JX
      DSCNC(6,NBD1) = JY
      GOTO 450
C
C No node was found.
119   CONTINUE
         IERR = 57
         IF (IDRAW.EQ.1) RETURN
         PAGE = 0
         CALL FTSIZE(2,18)
         CALL FTLOCA(4,1)
         CALL FTEXT('^NO ROOM FOR UNDETERMINED BOND SITE MARKER. TRY D
     *UMB MODE. ^')
         CALL FTSIZE(1,10)
         ICUR = 1
         CALL CURSOR(IX,IY)
         RETURN
434   CONTINUE
      IERR = 34
      IF (IDRAW.EQ.1) RETURN
      CALL MYERR(IERR,IERR,IERR)
      RETURN
C
C Draw bond site marker in:
450   CONTINUE
      IF (JX.LT.LOX) LOX = JX
      IF (JX+1.GT.HIX) HIX = JX + 1
      IF (JY.LT.LOY) THEN
         LOY = JY
      ELSE IF (JY.GT.HIY) THEN
         HIY = JY
      ENDIF
      MM(JX,JY)=KAR
      IF (IDRAW.EQ.1) RETURN
      HALO(2) = CHAR(KAR)
      CALL CURSOR (JX,JY)
      CALL TEXT(HALO)
60    IX=JJJ+1
      ICUR = 1
      CALL CURSOR(IX,IY)
      IF (MM(IX-1,IY) .EQ. 46) KAR=46
      RETURN
      END
```

```
$STORAGE:2
C
        SUBROUTINE VALNCE(II,IX,IY,INCX,INCY)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,IDTPIX
        CHARACTER*1 HALO(3)
        CHARACTER*1 KAN
        COMMON /ELECHR/ IELEM(126,5)
        COMMON /CD/ MAXX,MAXY
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
C       MM(I,J) CONTAINS BOND OR ATOM TYPE, & BOND DIRECTION
C       FOR EACH OF MAXX * MAXY LOCATIONS.
        COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
        COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
        COMMON /PROB/ IPROB,JPROB
        COMMON /IPLUS/ IHIGH(14,2)
        COMMON /LABELS/ NR,LJLAST,NJNEXT
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /CUR/ ICUR
        COMMON /HP/IHP
CXT     If CHER = 2, error messages are output on HALO screen page 1,
CXT     otherwise they are output to page 2.  If CHER = 1, SUBROUTINE
CXT     NOD is calling VALNCE.
        COMMON /QTVLNC/ OERR,CHER
CXT     MLARGE is used to mark distance to node whose valence is being
CXT     computed.
        COMMON /VLNPRV/ MLARGE
CXT     ELENOD carries the current element position code to  SUBROUTINE NOD.
        COMMON /ELENOD/ IELT
        HALO(1) = KAN
        HALO(3) = KAN
        MAR=0
C Filler atoms not triggered by bond.
        IF (II.GT.2) THEN
            JX = IX
            JY = IY
            IF (CHER.EQ.1) THEN
                IF (MM(JX,JY).EQ.46) THEN
                    IELT = 126
                    GO TO 800
                ENDIF
                GO TO 87
            ENDIF
C If element is in DOTDIS compute no valence.
            DO 444 JJ = 0,MAXX
                IF ((MM(JX-JJ,JY).EQ.0).OR.(LMM(JX-JJ,JY).GE.256).OR.
     *              (JX-JJ.LE.0)) THEN
                    GO TO 445
                ELSE IF (MM(JX-JJ,JY).EQ.42) THEN
                    RETURN
                ENDIF
444         CONTINUE
445         CONTINUE
            GO TO 1000
        ELSE IF (II.EQ.1) THEN
C Look at grid space BEFORE bond.
            JX=IX-(MLARGE+1)*INCX
C (NLARGE+1) removes incrementing done in DRAW.
            JY=IY-(MLARGE+1)*INCY
CXT
        ELSE IF (II.EQ.2) THEN
C If overdrawing an existing bond, II=2.
            JX=IX-INCX
            JY=IY-INCY
        ENDIF
C If to right of element, skip back over lower case second letter:
23      IF ((MM(JX,JY).GT.96) .AND. (MM(JX,JY).LT.123)) JX=JX-1
C If bond didn't originate at a (non-dot) node (i.e. cap letter), return
        IF(MM(JX,JY).EQ.46) GO TO 63
        IF ((MM(JX,JY).LT.65) .OR. (MM(JX,JY).GT.90)) THEN
```

```
            MLARGE = NLARGE
            RETURN
         ENDIF
         IF (((MM(JX,JY).EQ.68).OR.(MM(JX,JY).EQ.77)).AND.
     *      (MM(JX+1,JY).GE.112).AND.(MM(JX+1,JY).LE.120)) THEN
            MLARGE = NLARGE
            RETURN
         ENDIF
 C If element is in DOTDIS compute no valence.
         DO 1444 JJ = 0,MAXX
            IF ((MM(JX-JJ,JY).EQ.0).OR.(LMM(JX-JJ,JY).GE.256).OR.(JX-JJ
     *         .LE.0)) THEN
               GO TO 1445
            ELSE IF (MM(JX-JJ,JY).EQ.42) THEN
               MLARGE = NLARGE
               RETURN
            ENDIF
 1444    CONTINUE
 1445    CONTINUE
         GO TO 87
 C IS THIS A MARKER OR FAT DOT
 63      DO 64 I=1,NJNEXT
         IF (JX.EQ.LABL(I,1).AND.JY.EQ.LABL(I,2)) THEN
            MLARGE = NLARGE
            RETURN
         ENDIF
 64      CONTINUE
        MAR=1
C IF FAT DOT SET PARAMS FOR CARBON
        LET1=67
        LET2=0
        IELT=1
        GO TO 800
C First letter of symbol
87      LET1=LMM(JX,JY)
        LET2=0
C Second letter, if 2-letter symbol
        IF ((MM(JX+1,JY).GE.97) .AND. (MM(JX+1,JY).LE.122))
     2          LET2=MM(JX+1,JY)
C Dont check H2,ETC
CXT     IF ((LET1.EQ.72) .AND. (LET2.EQ.0)) THEN
CXT        MLARGE = NLARGE
CXT        RETURN
CXT     ENDIF
C count of OCCUPIED valence positions
        IVALNC=0
C Element number of node at JX,JY
        IELT=0
C
C search for element in element table
                DO 1 I=1,125
                IF ((LET1.NE.IELEM(I,1)) .OR. (LET2.NE.IELEM(I,2)))
     2                  GOTO 1
C Records row number of correct element
                IELT=I
C No valence in table
                IF (IELEM(IELT,3).EQ.0) THEN
                   MLARGE = NLARGE
                   RETURN
                ENDIF
                GOTO 2
1               CONTINUE
C
2       IF (IELT.NE.0) GO TO 800
C ELEMENT NOT FOUND - ISSUE MESSAGE AND CONTINUE
        IERR=11
        CALL MYERR(IERR,LET1,LET2)
C BEWARE I DON'T KNOW ALL THE IMPLICATIONS OF THIS RETURN
        MLARGE = NLARGE
        RETURN
C
C Now search around node for bonds, charges, for 'valence users'.
C
C Indicates presence(=1) or absence(=0) of bond on left
800     CONTINUE
```

```
C              where to put filler H's if there is room on both sides.
C       BEWARE - VAA MODIFIED LOOP 3 - THE MODIFICATION IS TO DETECT
C       CHARGES ON THE RIGHT DIAGONALS OF THE SECOND LETTER OF A 2
C       LETTER ELEMENT NAME
C Count of bonds 'used'.
        IVALNC=0
C search around node - LOOP CHANGED TO 2 BY VAA
        DO 3 IDIRX=-1,2
        DO 3 IDIRY=-1,1
        IF ((IDIRX.EQ.0) .AND. (IDIRY.EQ.0)) GOTO 3
        IF((IDIRX .EQ. 2) .AND. (IDIRY .EQ.0)) GO TO 3
C WE DON'T NEED TO CHECK THIS ONE
C WE WILL CATCH A CHARGE AT THIS LOCATION
C WHEN X=1 AND Y=0
C Nearby array location to look for bonds
        NEWX=JX + IDIRX
        NEWY=JY + IDIRY
C Off the edge
7       IF ((NEWX.LT.1) .OR. (NEWX.GT.MAXX)) GOTO 3
        IF ((NEWY.LT.1) .OR. (NEWY.GT.MAXY))  GOTO 3
C Blank space
        IF (MM(NEWX,NEWY).EQ.0) GOTO 3
C Bonds are >256
        IF (LMM(NEWX,NEWY).LT.256)  GOTO 4
C WE ARE ONLY LOOKING
        IF (IDIRX .EQ. 2) GO TO 3
C FOR CHARGES AT THIS PLACE - NOT BONDS
C Bond extracted for type
        JBOND=LMM(NEWX,NEWY)/2**8
C  Following 5 lines skip bonds not pointed to node being analyzed:
C Direction of bond
        JDIR=LMM(NEWX,NEWY)-JBOND*2**8
        IF ((IDIRX*IDIRY.EQ.-1).AND.(MOD(JDIR,4).NE.2)) GOTO 3
        IF ((IDIRX*IDIRY.EQ.1).AND.(MOD(JDIR,4).NE.0)) GOTO 3
        IF ((IDIRX.EQ.0) .AND. (MOD(JDIR,4).NE.1)) GOTO 3
        IF ((IDIRY.EQ.0) .AND. (MOD(JDIR,4).NE.3)) GOTO 3
C Useful for bondtypes 1-3 others revised below
        IVAL = JBOND
C Stereo bonds are single.
        IF (JBOND.GT.3) IVAL=1
        IVALNC = IVALNC + IVAL
C Used below at label 41 to determine where to put H's. Set here
C only if a valence-using bond is on this side.
        GOTO 3
C Charges
4       IF ((LMM(NEWX,NEWY).NE.43) .AND. (LMM(NEWX,NEWY).NE.45))GOTO 5
4444    LOC=IHMM(NEWX,NEWY)
        IFX=NEWX-IHIGH(LOC,1)
        IFY=NEWY+IHP*IHIGH(LOC,2)
C IS CHARGE ASSOCIATED
        IF(JX.NE.IFX .OR.JY.NE.IFY) GO TO 5
C WITH THIS NODE
C Set the sign from ASCII char
        ISIGN = 44 - LMM(NEWX,NEWY)
        IF ((MM(NEWX+1,NEWY).LT.50).OR.(MM(NEWX+1,NEWY).GT.57)) GOTO 6
C       Number of charges>1
        ISIGN = ISIGN * (LMM(NEWX+1,NEWY) - 48)
C       Correct # of valencies used for chg
6       IVALNC=IVALNC + IABS(ISIGN)
        ISIGN=0
C Used below at label 41 to deter-
CXT         IF ((IDIRX.EQ.1).AND.(IDIRY.EQ.0)) JRIGHT=1
C mine where to put H's. Set here
CXT         IF ((IDIRX.EQ.-1).AND.(IDIRY.EQ.0)) JLEFT=1
C                only if a valence-using bond is on this side.
        GOTO 3
C
C  H, lowercase, numerals, etc, keep looking
5       NEWX = NEWX + IDIRX
C H, lc, OR NUMERAL CAN'T
        IF (IDIRX .EQ. 0) GO TO 3
C CONTRIBUTE TO VALENCE IN THIS LOC
C BEWARE CHANGED BY VAA - TO FIX
C ENDLESS LOOP FOUND BY GREG
        GOTO 7
```

```
C Close loop of looking around each node.
3       CONTINUE
C
C Following code (through label 200) adds to IVALNC those bonds 'used'
C  by long bonds:
C Beginning & ending nodes of long bond
        DO 200 I=0,2,2
C Up to 100 long bonds stored
        DO 201 J=1,100
C Done with this column of node
        IF (LNGBND(J,I+1).EQ.0) GOTO 200
C  Check if current nodeJX,JY is listed as a node of a long bond:
        IF ((LNGBND(J,I+1).NE.JX) .OR. (LNGBND(J,I+2).NE.JY)) GOTO 201
C   Use of valence from this long bond
        IVAL = 1
        IF (LNGBND(J,5).EQ.2) IVAL=2
        IF (LNGBND(J,5).EQ.3) IVAL=3
        IVALNC = IVALNC + IVAL
201     CONTINUE
200     CONTINUE
C
C Number of H's required at this node. neg no for test
        IHYD=-7
C elect smallest valence from IELEM which would
                DO 10 M=3,5
C                              satisfy all existing bonds.
                IF(IELEM(IELT,M).LT.IVALNC) GOTO 10
                IHYD = IELEM(IELT,M) - IVALNC
                GOTO 11
10              CONTINUE
C Now draw hydrogens
11      CONTINUE
        IF (IHYD.GE.0 .AND. MAR .EQ. 0)  GO TO 1000
        IF (IHYD.GE.0 .AND. MAR.EQ.1) THEN
           MLARGE = NLARGE
           RETURN

        ENDIF
C TOO MANY BONDS FOR VALENCY
        IERR=12
        OERR = IERR
        CALL MYERR(IERR,IVALNC,KAR)
1000    CONTINUE
        IF (MM(JX,JY).EQ.46) THEN
           MLARGE = NLARGE
           RETURN
        ENDIF
C
C Now look left & right to determine where filler atoms can fit:
C
C Done if no filler atoms needed.
        IF (IHYD) 111,111,30
C =1 means there IS room for H('s) on left
30      ILEFT=1
C similarly
        IRIGHT=1
C
C       two-letter symbol
        IF (LET2.GT.0) THEN
           MX=JX+2
           NX = JX + 1
        ELSE
C       MX is first position to right of node.
           MX=JX+1
           NX = JX
        ENDIF
C Look right to see if there is room for H('s):
C number of chars needed for H('s):=1 or 2
        KHYD=1
        IF (IHYD.GT.1) KHYD = 2
C
C       Edge of screen problems are checked.
        IF (NX+2.GT.MAXX) THEN
           DO 31 I = 1,KHYD+1
              DG = LMM(JX-I,JY)
```

```
              IF (((DG.LT.256).AND.(DG.GT.0)).OR.((DG.GE.256).AND.
     *           (MOD(IDIR(DG),4).NE.3))) GO TO 9394
 31        CONTINUE
           GO TO 42
        ELSE IF (JX-2.LT.1) THEN
           DO 32 I = 1,KHYD+1
              DG = LMM(NX+I,JY)
              IF (((DG.LT.256).AND.(DG.GT.0)).OR.((DG.GE.256).AND.
     *           (MOD(IDIR(DG),4).NE.3))) GO TO 9394
 32        CONTINUE
           GO TO 43
        ENDIF
 C
 C      If CHER = 1, SUBROUTINE NOD is converting chain markers to "C"s
        IF (CHER.EQ.1) THEN
           IF (KHYD.EQ.2) THEN
              SHF = 1
           ELSE
              SHF = 0
           ENDIF
           DG1 = LMM(NX+KHYD+1,JY)
           DG2 = LMM(NX+KHYD-SHF,JY)

           DG3 = LMM(NX+KHYD,JY)
           U1 = LMM(NX+KHYD+1,JY-1)
           U2 = LMM(NX+KHYD-SHF,JY-1)
           U3 = LMM(NX+KHYD,JY-1)
           L1 = LMM(NX+KHYD+1,JY+1)
           L2 = LMM(NX+KHYD-SHF,JY+1)
           L3 = LMM(NX+KHYD,JY+1)
           IF (((DG1.GT.0).AND.(DG1.LT.256)).OR.((DG2.GT.0).AND.
     *        (DG2.LT.256)).OR.((DG3.GT.0).AND.(DG3.LT.256))) GO TO 402
           IF (((DG1.GE.256).AND.(MOD(IDIR(DG1),4).NE.3)).OR.
     *        ((DG2.GE.256).AND.(MOD(IDIR(DG2),4).NE.3)).OR.
     *        ((DG3.GE.256).AND.(MOD(IDIR(DG3),4).NE.3))) GO TO 402
           IF ((U1.EQ.46).OR.((U1.GE.65).AND.(U1.LE.122)).OR.
     *        ((U1.GE.50).AND.(U1.LE.57).AND.(U3.NE.43).AND.
     *        (U3.NE.45))) GO TO 402
           IF ((L1.EQ.46).OR.((L1.GE.65).AND.(L1.LE.122)).OR.
     *        ((L1.GE.50).AND.(L1.LE.57).AND.(L3.NE.43).AND.
     *        (L3.NE.45))) GO TO 402
           IF ((U3.EQ.46).OR.((U3.GE.65).AND.(U3.LE.122)).OR.
     *        ((U3.GE.50).AND.(U3.LE.57).AND.(LMM(NX+KHYD-1,JY-1)
     *        .NE.43).AND.(LMM(NX+KHYD-1,JY-1).NE.45))) GO TO 402
           IF ((L3.EQ.46).OR.((L3.GE.65).AND.(L3.LE.122)).OR.
     *        ((L3.GE.50).AND.(L3.LE.57).AND.(LMM(NX+KHYD-1,JY+1)
     *        .NE.43).AND.(LMM(NX+KHYD-1,JY+1).NE.45))) GO TO 402
           IF (SHF.EQ.1) THEN
              IF ((U2.EQ.46).OR.((U2.GE.65).AND.(U2.LE.122)).OR.
     *           ((U2.GE.50).AND.(U2.LE.57).AND.(LMM(NX+KHYD-2,JY-1)
     *           .NE.43).AND.(LMM(NX+KHYD-2,JY-1).NE.45))) GO TO 402
              IF ((L2.EQ.46).OR.((L2.GE.65).AND.(L2.LE.122)).OR.
     *           ((L2.GE.50).AND.(L2.LE.57).AND.(LMM(NX+KHYD-2,JY+1)
     *           .NE.43).AND.(LMM(NX+KHYD-2,JY+1).NE.45))) GO TO 402
           ENDIF
           GO TO 43
 402       CONTINUE
           DG1 = LMM(JX-KHYD-1,JY)
           DG2 = LMM(JX-KHYD+SHF,JY)
           DG3 = LMM(JX-KHYD,JY)
           U1 = LMM(NX-KHYD-1,JY-1)
           U2 = LMM(NX-KHYD+SHF,JY-1)
           U3 = LMM(NX-KHYD,JY-1)
           L1 = LMM(NX-KHYD-1,JY+1)
           L2 = LMM(NX-KHYD+SHF,JY+1)
           L3 = LMM(NX-KHYD,JY+1)
           IF (((DG1.GT.0).AND.(DG1.LT.256)).OR.((DG2.GT.0).AND.
     *        (DG2.LT.256)).OR.((DG3.GT.0).AND.(DG3.LT.256)).OR.
     *        ((DG1.GE.256).AND.(MOD(IDIR(DG1),4).NE.3)).OR.
     *        ((DG2.GE.256).AND.(MOD(IDIR(DG2),4).NE.3)).OR.
     *        ((DG3.GE.256).AND.(MOD(IDIR(DG3),4).NE.3))) GO TO 9394
           IF ((U3.EQ.46).OR.((U3.GE.65).AND.(U3.LE.122)).OR.
     *        ((U3.GE.50).AND.(U3.LE.57).AND.(U1.NE.43).AND.
     *        (U1.NE.45))) GO TO 9394
           IF ((L3.EQ.46).OR.((L3.GE.65).AND.(L3.LE.122)).OR.
```

```
     *        ((L3.GE.50).AND.(L3.LE.57).AND.(L1.NE.43).AND.
     *        (L1.NE.45))) GO TO 9394
            IF (SHF.EQ.1) THEN
              IF ((U2.EQ.46).OR.((U2.GE.65).AND.(U2.LE.122)).OR.
     *          ((U2.GE.50).AND.(U2.LE.57).AND.(U3.NE.43)
     *          .AND.(U3.NE.45))) GO TO 9394
              IF ((L2.EQ.46).OR.((L2.GE.65).AND.(L2.LE.122)).OR.
     *          ((L2.GE.50).AND.(L2.LE.57).AND.(L3.NE.43)
     *          .AND.(L3.NE.45))) GO TO 9394
            ENDIF
            IF ((U1.EQ.46).OR.((U1.GE.65).AND.(U1.LE.122)).OR.
     *        ((U1.GE.50).AND.(U1.LE.57).AND.(LMM(NX-KHYD-2,JY-1)
     *        .NE.43).AND.(LMM(NX-KHYD-2,JY-1).NE.45))) GO TO 9394
            IF ((L1.EQ.46).OR.((L1.GE.65).AND.(L1.LE.122)).OR.
     *        ((L1.GE.50).AND.(L1.LE.57).AND.(LMM(NX-KHYD-2,JY+1)
     *        .NE.43).AND.(LMM(NX-KHYD-2,JY+1).NE.45))) GO TO 9394
            GO TO 42
          ENDIF
C
C         Check for bad bonds coming in on the left diagonals.
          L1 = LMM(MX-1,JY-1)
          L2 = LMM(MX-1,JY+1)
          IF (((L1.EQ.0).OR.((L1.GT.256).AND.(MOD(IDIR(L1),4).NE.0)))
     *      .AND.((L2.EQ.0).OR.((L2.GT.256).AND.(MOD(IDIR(L2),4).NE.
     *      2)))) GO TO 522
            IRIGHT = 0
            GO TO 34
C
C The actual search-right algorithm loop.
522          DO 33 I=0,KHYD
               IF (MM(MX+I,JY).EQ.0) THEN
                 GO TO 330
               ELSE IF (LMM(MX+I,JY) .LT. 256) THEN
                 GO TO 400
               ENDIF
               ITEST=LMM(MX+I,JY)/256
               ITEST=LMM(MX+I,JY)-ITEST*256
C              CHECK FOR BOND IN LEFT OR RIGHT DIR
               IF (ITEST.EQ.3 .OR. ITEST.EQ.7) GO TO 330
C If non-blank or non-bond on right within
400            IRIGHT=0
C KHYD+1 to right of node, can't put H('s)there
               GOTO 34
330          CONTINUE
             L1 = LMM(MX+I,JY-1)
             L2 = LMM(MX+I,JY+1)
             L3 = LMM(MX+I-1,JY-1)
             L4 = LMM(MX+I-1,JY+1)
             IF ((L1.EQ.0).AND.(L2.EQ.0)) GO TO 33
             IF (I.LE.2) THEN
               IF (((L1.EQ.46).OR.((L1.GE.65).AND.(L1.LE.122))).OR.
     *           ((L1.GE.50).AND.(L1.LE.57).AND.(L3.NE.43).AND.
     *           (L3.NE.45))) GO TO 400
               IF (((L2.EQ.46).OR.((L2.GE.65).AND.(L2.LE.122))).OR.
     *           ((L2.GE.50).AND.(L2.LE.57).AND.(L4.NE.43).AND.
     *           (L4.NE.45))) GO TO 400
             ENDIF
             IF ((I.EQ.KHYD).AND.(((L1.GT.256).AND.
     *         (MOD(IDIR(L1),4).EQ.2)).OR.((L2.GT.256)
     *         .AND.(MOD(IDIR(L2),4).EQ.0)))) GO TO 400
             IF ((KHYD.EQ.1).AND.(I.EQ.0).AND.((
     *         (L1.GE.256).AND.(MOD(IDIR(L1),4).EQ.1)).OR.(
     *         (L2.GT.256).AND.(MOD(IDIR(L2),4).EQ.1)))) GO TO 400
             IF ((KHYD.EQ.2).AND.(I.EQ.0).AND.((
     *         (L1.GE.256).AND.((MOD(IDIR(L1),4).EQ.1).OR.
     *         (MOD(IDIR(L1),4).EQ.0))).OR.(
     *         (L2.GT.256).AND.((MOD(IDIR(L2),4).EQ.1).OR.
     *         (MOD(IDIR(L2),4).EQ.2))))) GO TO 400
             IF ((KHYD.EQ.2).AND.(I.EQ.1).AND.((
     *         (L1.GE.256).AND.((MOD(IDIR(L1),4).EQ.1).OR.
     *         (MOD(IDIR(L1),4).EQ.2))).OR.(
     *         (L2.GT.256).AND.((MOD(IDIR(L2),4).EQ.1).OR.
     *         (MOD(IDIR(L2),4).EQ.0))))) GO TO 400
33             CONTINUE
```

```
            IF (IRIGHT.EQ.1) GO TO 36
C Now look left to see if filler atoms can be put there:
C Look left for non-blank,non-bonds.
34          L1 = LMM(JX,JY-1)
            L2 = LMM(JX,JY+1)
            IF (((L1.EQ.0).OR.((L1.GT.256).AND.(MOD(IDIR(L1),4).NE.2)))
     *         .AND.((L2.EQ.0).OR.((L2.GT.256).AND.(MOD(IDIR(L2),4)
     *         .NE.0)))) GO TO 3441
            ILEFT = 0
            GO TO 36
3441        DO 35 I=1,KHYD+1
               IF (MM(JX-I,JY).EQ.0) GOTO 3555
               IF(LMM(JX-I,JY) .LT. 256) GO TO 401
               ITEST=LMM(JX-I,JY)/256
               ITEST=LMM(JX-I,JY)-ITEST*256
               IF (ITEST.EQ.3 .OR. ITEST.EQ.7) GO TO 3555
401            ILEFT=0
               GOTO 36
3555        L1 = LMM(JX-I,JY-1)
            L2 = LMM(JX-I,JY+1)
            L3 = LMM(JX-I-1,JY-1)
            L4 = LMM(JX-I-1,JY+1)
            IF ((L1.EQ.0).AND.(L2.EQ.0)) GO TO 35
            IF (((L1.EQ.46).OR.((L1.GE.65).AND.(L1.LE.122))).OR.
     *         ((L1.GE.50).AND.(L1.LE.57).AND.(L3.NE.43).AND.
     *         (L3.NE.45))) GO TO 401
            IF (((L2.EQ.46).OR.((L2.GE.65).AND.(L2.LE.122))).OR.
     *         ((L2.GE.50).AND.(L2.LE.57).AND.(L4.NE.43).AND.
     *         (L4.NE.45))) GO TO 401
            IF ((I.EQ.KHYD+1).AND.(((L1.GT.256).AND.
     *         (MOD(IDIR(L1),4).EQ.0)).OR.((L2.GT.256)
     *         .AND.(MOD(IDIR(L2),4).EQ.2)))) GO TO 401
            IF ((KHYD.EQ.1).AND.(I.EQ.1).AND.(((L1.GE.256)
     *         .AND.(MOD(IDIR(L1),4).EQ.1)).OR.((L2.GT.256)
     *         .AND.(MOD(IDIR(L2),4).EQ.1)))) GO TO 401
            IF ((KHYD.EQ.2).AND.(I.EQ.2).AND.(((L1.GE.256)
     *         .AND.((MOD(IDIR(L1),4).EQ.1).OR.
     *         (MOD(IDIR(L1),4).EQ.0))).OR.((L2.GT.256)
     *         .AND.((MOD(IDIR(L2),4).EQ.1).OR.
     *         (MOD(IDIR(L2),4).EQ.2))))) GO TO 401
            IF ((KHYD.EQ.2).AND.(I.EQ.1).AND.(((L1.GE.256)
     *         .AND.((MOD(IDIR(L1),4).EQ.1).OR.
     *         (MOD(IDIR(L1),4).EQ.2))).OR.((L2.GT.256)
     *         .AND.((MOD(IDIR(L2),4).EQ.1).OR.
     *         (MOD(IDIR(L2),4).EQ.0))))) GO TO 401
35          CONTINUE
C
C See if ILEFT, IRIGHT, or both equal 1. If one is, insert H('s) there.
C If both equal 1, use criteria to decide which side to put H('s) on.
C If neither equals 1, call error message that there is no room for H.
C
36      CONTINUE
        IF (ILEFT+IRIGHT.NE.0) THEN
           IF (IRIGHT.EQ.0) THEN

              GO TO 42
           ELSE
              GO TO 43
           ENDIF
        ENDIF
CXT     IF (ILEFT+IRIGHT.GT.0) GO TO 38
9394    CONTINUE
CXT
CXT     Vertical positioning of attached hydrogens to nodes is attempted.
        MBOND = 0
        DO 9395 IN = IHP,-IHP,-IHP*2
           FY = JY + IN
           IF (((MM(JX,FY).EQ.0).OR.(LMM(JX,FY).GE.256)).AND.(FY.GT.0)
     *        .AND.(FY.LE.MAXY)) THEN
CXT           Check adjacent cells.
              DO 939 KK = -1,2
                 IF ((KK.EQ.2).AND.(KHYD.LE.1)) GO TO 939
                 DO 938 JJ = 0,1
                    IL = JX + KK
                    JL = FY + (JJ * IN)
```

```
              IF ((MM(IL,JL).GT.0).AND.(LMM(IL,JL).LT.256).AND.
     *           (MM(IL,JL).NE.34).AND.(LMM(IL,JL).NE.43).AND.
     *           (LMM(IL,JL).NE.45)) GO TO 9395
  938       CONTINUE
  939     CONTINUE
  CXT
          IF (KHYD.GT.1) THEN
            FX = JX + 1
            IF (MM(FX,FY).EQ.0) THEN
              IF (LMM(JX,FY).GT.256) THEN
                MBOND = MM(JX,FY)
                MM(JX,FY) = 0
                CALL REPLCE(JX,FY,0,1,0,0,1)
                IF (IN.EQ.1) CALL REPLCE(JX,JY,0,1,0,0,1)
              ENDIF
              MM(JX,FY) = 72
              MM(FX,FY) = IHYD + 48
              HALO(2) = 'H'
              ICUR = 0
              CALL CURSOR(JX,FY)
              CALL TEXT(HALO)
              HALO(2) = CHAR(MM(FX,FY))
              CALL CURSOR(FX,FY)
              CALL MOVTCR(0,2)
              CALL TEXT(HALO)
              CALL MOVTCR(0,-2)
              IF (((ICHAR.EQ.1).AND.(INCY.EQ.IN)).OR.(CHER.EQ.1))
     *          THEN
                IF (CHER.NE.1) THEN
                  INC = (IN * NLARGE) + IN
                  IX = JX + (NLARGE * INCX) + INCX
                  IF ((NLARGE.EQ.1).AND.(INCX.EQ.0)) INC=INC+IN
                  IY = JY + INC
                ENDIF
                IF (MBOND.GT.256) THEN
                  FY = FY + IN
                  CALL DRAW2(JX,FY,MBOND)
                  ICHAR = 1
                ENDIF

              IF (FX.GT.HIX) HIX = FX
              GO TO 9396
            ELSE
              GO TO 9395
            ENDIF
          ELSE
            IF (LMM(JX,FY).GT.256) THEN
              MBOND = MM(JX,FY)
              MM(JX,FY) = 0
              CALL REPLCE(JX,FY,0,1,0,0,1)
              IF (IN.EQ.1) CALL REPLCE(JX,JY,0,1,0,0,1)
            ENDIF
            MM(JX,FY) = 72
            HALO(2) = 'H'
            ICUR = 0
            CALL CURSOR(JX,FY)
            CALL TEXT(HALO)
            IF (((ICHAR.EQ.1).AND.(INCY.EQ.IN)).OR.(CHER.EQ.1))
     *        THEN
              IF (CHER.NE.1) THEN
                INC = (IN * NLARGE) + IN
                IX = JX + (NLARGE * INCX) + INCX
                IF ((NLARGE.EQ.1).AND.(INCX.EQ.0)) INC=INC+IN
                IY = JY + INC
              ENDIF
              IF (MBOND.GE.256) THEN
                FY = FY + IN
                CALL DRAW2(JX,FY,MBOND)
                ICHAR = 1
              ENDIF
            ENDIF
            GO TO 9396
          ENDIF
        ENDIF
 9395   CONTINUE
```

```
          GO TO 9397
 9396     CONTINUE
             IF (IY.LT.LOY) THEN
                LOY = IY
             ELSE IF (IY.GT.HIY) THEN
                HIY = IY
             ENDIF
             ICUR = 1
             CALL CURSOR(IX,IY)
             MLARGE = NLARGE
             RETURN
 9397     IERR=14
          JPROB=1
C ERROR IN DECIDING WHERE TO PUT H'S
          CHER = 2
          CALL MYERR(IERR,KAR,KAR)
          CHER = 0
          MLARGE = NLARGE
          RETURN
C         41 IF BOTH 1; 42 OK LEFT; 43 OK RIGHT ONLY
C
C Selection of left vs right for filler H's if there is room on either
C side.  JLEFT & JRIGHT, calculated during the valence count in the DO 3
C loop above, represent the presenc(1) or absence(0) of bonds on the
C left & right sides of the node.  Select the right if there are
C bonds on the left, or bonds on neither left or right, or bonds on
C both sides.  Otherwise, select the left(i.e. bonds on right,none left)
C
C         Draw H on left:
C Saved for possible extension of bond
 42       MBOND=LMM(JX-1,JY)
          IF (MBOND.GE.256) THEN
             FX = JX - KHYD
             CALL FTLOCA(JY,FX)
             CALL FTEXT('^ ^')
          ENDIF
C Move to H location
          CALL CURSOR(JX-KHYD,JY)
C ASCII H into array
          MM(JX-KHYD,JY)=72
C Insert H here
          HALO(2) = 'H'
          IF ((JX-2).LT.LOX) LOX = MIN0(JX-2,1)
          CALL TEXT(HALO)
C Skip subscript if not necessary.
          IF (KHYD.LE.1) GOTO 45
          IF (MBOND.GE.256) THEN
             FX = JX - 1
             CALL FTLOCA(JY,FX)
             CALL FTEXT('^ ^')
          ENDIF
C Move to cursor position: one left of node.
          ICUR = 0
          CALL CURSOR(JX-1,JY)
C ASCII for typing
          IJ=IHYD+48
C backspace
          IBACK=8
C Drop down, type subscript,raise up
          HALO(2) = CHAR(IJ)
          CALL MOVTCR(0,2)
          CALL TEXT(HALO)
          CALL MOVTCR(0,-2)
C ASCII of numeral into array
          MM(JX-1,JY)=IJ
C
C If blank now to the left of H, extend whatever bond was covered over
C by the H and/or subscript,if any.(If MBOND=0,there was no bond there):
 45       IF (MM(JX-KHYD-1,JY).NE.0) GOTO 111
          CALL DRAW2(JX-KHYD-1,JY,MBOND)
C Move cursor
          IF ((IBDIR.EQ.7) .AND. (ILEFT.EQ.1)) IX=JX-KHYD-2
          IF (MBOND.GT.256) ICHAR=1
C beyond the end of the extended bond.
```

```
C Done with valence after left insertion.
        ICUR = 1
        CALL CURSOR (IX,IY)
111     CONTINUE
        MLARGE = NLARGE
        RETURN
C
C  Insert (H's) on right:
C Position for H on right of node
43      MX = JX + 1
        IF (LET2.GT.0) MX=JX+2
C Save for possible bond extension.
        MBOND = LMM(MX,JY)
        IF (MBOND.GE.256) THEN
           CALL FTLOCA(JY,MX)
           CALL FTEXT('^ ^')
        ENDIF
        CALL CURSOR(MX,JY)
C Insert H.
        HALO(2) = 'H'
        IF ((JX+2).GT.HIX) HIX = MAX0(JX+2,MAXX)
        CALL TEXT(HALO)
C ASCII H into array
        MM(MX,JY)=72
C No subscript needed
        IF (KHYD.LE.1) GOTO 44
        IF (MBOND.GE.256) THEN
           FX = MX + 1
           CALL FTLOCA(JY,FX)
           CALL FTEXT('^ ^')
        ENDIF
C Position of subscript
        ICUR = 0
        CALL CURSOR(MX+1,JY)
C ASCII for subscript
        IJ=IHYD+48
        IBACK=8
C Type blank, drop down, type sub, raise
        HALO(2) = CHAR(IJ)
        CALL MOVTCR(0,2)
        CALL TEXT(HALO)
        CALL MOVTCR(0,-2)
C ASCII of numeral into array
        MM(MX+1,JY)=IJ
C If H and subscript covered over all of bond (if any), replace with one
C length of bond, using DRAW2:
44      IF (MM(MX+KHYD,JY).EQ.0) CALL DRAW2(MX+KHYD,JY,MBOND)
        IF ((IBDIR.EQ.3).AND.(IRIGHT.EQ.1)) THEN
           IF (IBTYPE.EQ.0) THEN
              IX = MX + KHYD + MLARGE
           ELSE IF (NLARGE.EQ.1) THEN
              IX = MX + KHYD + 1
           ELSE
              IX = MX + MLARGE
           ENDIF
        ENDIF
        ICUR = 1
        CALL CURSOR(IX,IY)
        MLARGE = NLARGE
C Completed with insertion of H on right
        RETURN
        END
C
        SUBROUTINE CLRHYD(KX,KY)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,ITEMP1
        COMMON /CD/ MAXX,MAXY
        COMMON /SIZZE/ MULTX,MULTY
        COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /CUR/ ICUR
        COMMON /HP/IHP
C This subroutine clears valence hydrogens from the vicinity of nodes
C and extends bonds as needed, before re-calculation of valences.
C       In earlier versions, this code was contained in DRAW. 3/16/83 GMK
```

```
C
C       DO NOTHING IF AT A MARKER OR DOT
1        IF ((MM(KX-1,KY).EQ.46).OR.(MM(KX,KY).EQ.46)) RETURN
         ICUR = 0
C        Look right for H's & subscripts & eliminate them:
C        Increment for looking across for H & subscripts
         INC=1
         MBOND=0
C        2 let element
         IF( (MM(KX+1,KY).GE.97) .AND. (MM(KX+1,KY).LE.122)) INC=2
         IF (MM(KX+INC,KY).NE.72) GOTO 40
C        Bond on rt of H
         MBOND=MAX0 (LMM(KX+INC+1,KY),LMM(KX+INC+2,KY))
         LBLOB=MOD(MBOND,256)
         IF (LBLOB .NE. 3 .AND. LBLOB .NE. 7) MBOND=0
         CALL CURSOR(KX+INC,KY)
C        Undraw H
         FX = KX + INC
         CALL FTLOCA(KY,FX)
         CALL FTEXT('^ ^')
         MM(KX+INC,KY)=0
C        Reinstall bond
         CALL DRAW2(KX+INC,KY,MBOND)
         IF ((MM(KX+INC+1,KY).LT.50).OR.(MM(KX+INC+1,KY).GT.57)) GOTO43
C        Erase subscript on right
         CALL CURSOR (KX+INC+1,KY)
C        Erase bond
         FX = KX + INC + 1
         CALL FTLOCA(KY,FX)
         CALL FTEXT('^ ^')
         CALL CURSOR(KX+INC+1,KY)
         ITEMP1 = MM(KX+INC+1,KY)
         FX = KX + INC + 1
         CALL FTLOCA(KY,FX)
         CALL FTEXT('^ ^')
         IF (IHP .NE. 1) THEN
         IF (MOD((KY*10),40).EQ.0) THEN
            IF ((KY.EQ.8).OR.(KY.EQ.28).OR.(KY.EQ.16)) THEN
               FY = ((KY * 10) / 11) + 1
               CALL FTSIZE(1,11)
            ELSE
               FY = ((KY * 10) / 9) + 1
               CALL FTSIZE(1,9)
            ENDIF
         ELSE
            FY = ((KY * 10) / 8) + 1
            CALL FTSIZE(1,8)
         ENDIF
         CALL FTLOCA(FY,FX)
         CALL FTEXT('^ ^')
         ENDIF
         CALL FTSIZE(1,10)
         MM(KX+INC+1,KY)=0
         IF (MM(KX+INC+1,KY+1).NE.0) CALL REPLCE(KX+INC+1,KY+1,0,0,0,0,0)
         CALL DRAW2(KX+INC+1,KY,MBOND)
C Here completh undrawing H's & subscripts on right

         GOTO 43
C
C  Now look on left for H & subscripts:
40       MBOND=0
C Look left for H, subscript, MBOND to copy
         DO 42 INC=-3,-1
         IF ((MM(KX-1,KY).LT.50) .OR. (MM(KX-1,KY).GT.72)) GOTO 43
         IF (LMM(KX+INC,KY).GT.256) MBOND=MM(KX+INC,KY)
C
         IF (LMM(KX+INC,KY).NE.72) GOTO 42
         CALL CURSOR (KX+INC,KY)
C Untype H
         FX = KX + INC
         CALL FTLOCA(KY,FX)
         CALL FTEXT('^ ^')
         MM(KX+INC,KY)=0
         LBLOB=MOD(MBOND,256)
         IF (LBLOB .NE. 3 .AND. LBLOB .NE. 7) MBOND=0
```

```
C Replace H with bond
        CALL DRAW2(KX+INC,KY,MBOND)
C  Look for number to right of H, on left of node
        IF ((MM(KX+INC+1,KY).LT.50) .OR. (MM(KX+INC+1,KY).GT.57))
     2     GOTO 43
C If no number,skip out of loop: done here
        CALL CURSOR(KX+INC+1,KY)
C Erase bond
        FX = KX + INC + 1
        CALL FTLOCA(KY,FX)
        CALL FTEXT('^ ^')
        CALL CURSOR(KX+INC+1,KY)
C Untype subscript
        ITEMP1 = MM(KX+INC+1,KY)
        FX = KX + INC + 1
        CALL FTLOCA(KY,FX)
        CALL FTEXT('^ ^')
        IF (IHP .NE. 1) THEN
        IF (MOD((KY*10),40).EQ.0) THEN
           IF ((KY.EQ.8).OR.(KY.EQ.28).OR.(KY.EQ.16)) THEN
              FY = ((KY * 10) / 11) + 1
              CALL FTSIZE(1,11)
           ELSE
              FY = ((KY * 10) / 9) + 1
              CALL FTSIZE(1,9)
           ENDIF
        ELSE
           FY = ((KY * 10) / 8) + 1
           CALL FTSIZE(1,8)
        ENDIF
        CALL FTLOCA(FY,FX)
        CALL FTEXT('^ ^')
        CALL FTSIZE(1,10)
        ENDIF
        MM(KX+INC+1,KY)=0
        IF (MM(KX+INC+1,KY+1).NE.0) CALL REPLCE(KX+INC+1,KY+1,0,0,0,0,0)
        CALL DRAW2(KX+INC+1,KY,MBOND)
C At this point, filler H's are removed
42      CONTINUE
43      CONTINUE
C
C       Look above and below to remove H's.

        DO 50 I = -1,1,2
           FY = KY + I
           IF (MM(KX,FY).EQ.72) THEN
              MM(KX,FY) = 0
              CALL FTLOCA(FY,KX)
              CALL FTEXT('^ ^')
              FX = KX + 1
              IF ((MM(FX,FY).GE.50).AND.(MM(FX,FY).LE.57)) THEN
                 MM(FX,FY) = 0
                 CALL REPLCE(FX,FY,0,0,0,0,1)
              ENDIF
              MBOND = LMM(KX,FY+I)
              IF ((MBOND.GE.256).AND.(MOD(IDIR(MBOND),4).EQ.1))
     *           CALL DRAW2(KX,FY,MBOND)
           ENDIF
50      CONTINUE
        ICUR = 1
C
        RETURN
        END
$STORAGE:2
C
        SUBROUTINE SPACE(IX,IY)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,IDTPIX
        LOGICAL*2 FOUND
        CHARACTER*1 HALO(3),HLO(3)
        CHARACTER*3 HALOE
        EQUIVALENCE (HALOE,HALO(1))
        CHARACTER*1 KAN
        CHARACTER*1 ISTAT
        COMMON /CD/ MAXX,MAXY
```

```
      COMMON /HP/IHP
      COMMON /RANGE/ LOX,HIX,LOY,HIY
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
      COMMON /ISTATE/ ISTAT
      COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /IPLUS/ IHIGH(14,2)
      COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
      COMMON /CUR/ ICUR
C
      HALO(1) = KAN
      HALO(3) = KAN
C
C  This routine moves right until the cursor is in a 'clear' area, i.e.
C  one with nothing around current cursor location.
C
      LEFT2 = 0
      ICUR = 1
      ISTAT='S'
      ISP=1
      IF (ICHAR.EQ.25) IX = IX + 1
      CALL CURSOR(IX,IY)
C
C Following code is for terminal going 'dumb' after a space.  Exactly
C the same as in subroutine BKSPCE.
475   ISMART=0
      KHAR=0
      ISTATE=8
      CALL HEADER
100   CALL INPUTX(KHAR,IX,IY)
      IF ((LEFT2.NE.0).AND.((KHAR.LT.50).OR.(KHAR.GT.57))) THEN
CXT      If a charge has been entered to the left of a node and no
CXT      digit attaches it to the node, its validity as a standalone
CXT      charge is determined, and the operator warned.
         DO 20 I = LOX,HIX
            DO 20 J = LOY,HIY
               IF ((MM(I,J).EQ.43).OR.(MM(I,J).EQ.45)) THEN
                  IERR = 4
                  CALL MYERR(IERR,IERR,IERR)
                  MM(OX,OY) = 0
                  CALL FTLOCA(OY,OX)
                  CALL FTEXT('^ ^')
                  GO TO 30
               ENDIF
20       CONTINUE
         IERR = 28
         CALL MYERR(IERR,IERR,IERR)
         MM(OX,OY) = LEFT2
         LEFT2 = 0
         IX = IX - 1
         CALL CURSOR(IX,IY)
         GO TO 100
      ENDIF
30    CONTINUE
      LEFT2 = 0
      IF (IHP .EQ. 1 .AND. ((KHAR .GE. 22) .AND. (KHAR .LE. 31)))
     1 GO TO 200       !Exit if this is a bond and we are using an HP
CXT   If F1 is entered return to calling state.
      IF (KHAR.EQ.21) GO TO 200
      IF ((KHAR.LE.31).AND.(KHAR.GE.22).AND.(KHAR.NE.26).AND.
     *   (KHAR.NE.27)) THEN
C        The cursor moves freely.
         CALL MOVE(KHAR,IX,IY)
         MCHAR = 0
         GO TO 100
      ENDIF
      IF ((KHAR.GT.32).AND.(KHAR.NE.127)) THEN
C
C        The character is put to the screen.
         IF (KHAR.EQ.94) THEN
            HLO(1) = '/'
            HLO(2) = CHAR(KHAR)
```

```
            HLO(3) = '/'
            CALL TEXT(HLO)
         ELSE
            HALO(2) = CHAR(KHAR)
            CALL TEXT(HALO)
         ENDIF
C        New picture boundaries are expanded.
         IF (IX.LT.LOX) THEN
            LOX = IX
         ELSE IF (IX.GT.HIX) THEN
            HIX = IX
         ENDIF
         IF (IY.LT.LOY) THEN
            LOY = IY

         ELSE IF (IY.GT.HIY) THEN
            HIY = IY
         ENDIF
      ENDIF
      IF (KHAR .NE. 43.AND.KHAR .NE. 45) GO TO 199
C
C     WE FOUND A + OR -    ...  NOW FIND ITS NODE
C
C     The logical variable FOUND is set to TRUE when a node adjacent
C     to the charge is found.  The loop that searches for adjacent
C     nodes is continued until all positions adjacent to the charge
C     are checked to ensure the charge placement is not ambiguous.
C     If a second adjacent node is found, the charge is erased, an
C     error message prompting the user to use another position is
C     issued, and the loop is exited.
      FOUND = .FALSE.
C LOOK AROUND FOR NODE
      DO 50 I=-2,2
      DO 50 J=-1,1
C DON'T CHECK THIS BOX
      IF(I.EQ.0 .AND. J .EQ. 0) GO TO 50
      IIX=IX+I
      IIY=IY - J
      IF (((MM(IIX,IIY).GE.65).AND.(MM(IIX,IIY).LE.90)).OR.
     *   (MM(IIX,IIY).EQ.46)) GO TO 47
C CHECK FOR UC LETTER - IF WE FIND ONE - THEN CHECK
C FOR OTHER REQUIREMENTS
C ITS NOT A UC - CAN'T BE A NODE
      GO TO 50
C IF X = -2 THEN WE NEED UC FOLLOWED BY lc
47    IF ((I.EQ.-2).AND.(MM(IIX+1,IIY).GE. 97
     1  .AND. MM(IIX+1,IIY) .LE.122)) THEN
         IF (FOUND) THEN
            IERR = 42
            CALL MYERR(IERR,IERR,IERR)
            CALL FTLOCA(IY,IX)
            CALL FTEXT('^ ^')
            GO TO 999
         ENDIF
         II = -I
         JJ = J
         NIX = IIX
         NIY = IIY
         FOUND = .TRUE.
         GO TO 50
      ENDIF
C IF X=2 WE NEED DIGIT TO RIGHT OF CHARGE
      IF (I.EQ.-2) GO TO 50
49    IF (MM(IIX,IIY).NE.72) THEN
         IF (FOUND) THEN
            IERR = 42
            CALL MYERR(IERR,IERR,IERR)
            CALL FTLOCA(IY,IX)
            CALL FTEXT('^ ^')
            GO TO 999
         ENDIF
         II = -I
         JJ = J
         NIX = IIX
         NIY = IIY
```

```
            FOUND = .TRUE.
            GO TO 50
         ENDIF
         IF (MM(IIX+1,IIY).GE.97.AND.MM(IIX+1,IIY).LE.122) THEN
            IF (FOUND) THEN
               IERR = 42
               CALL MYERR(IERR,IERR,IERR)
               CALL FTLOCA(IY,IX)
               CALL FTEXT('^ ^')
               GO TO 999
            ENDIF
            II = -I
            JJ = J
            NIX = IIX
            NIY = IIY
            FOUND = .TRUE.
            GO TO 50
         ENDIF
C IF UC = H IT MUST BE FOLLOWED BY 1c
50       CONTINUE
         IF (FOUND) GO TO 55
C CAN'T FIND NODE - CALL IT DELOCALIZED CHARGE
C        Check that there is only 1 delocalized charge.
         DO 4345 I = LOX,HIX
            DO 4345 J = LOY,HIY
               IF ((MM(I,J).NE.45).AND.(MM(I,J).NE.43)) GO TO 4345
               IF (MM(I-1,J).NE.42) GO TO 4300
4345     CONTINUE
         GO TO 51
4300       IERR = 4
           CALL MYERR(IERR,IERR,IERR)
           CALL FTLOCA(IY,IX)
           CALL FTEXT('^ ^')
           IX = IX - 1
           GO TO 999
C CAN'T FIND NODE - CALL IT DELOCALIZED CHARGE
51       IERR=28
         CALL MYERR(IERR,KHAR,MAR)
         LEFT2 = 0
         GO TO 99
55       CONTINUE
         ICNT = 0
         DO 300 I = -2,2
            DO 300 J = -1,1
               IF ((LMM(NIX+I,NIY+J).NE.43).AND.(LMM(NIX+I,NIY+J).NE.45))
     *            GO TO 300
               ILC = IHMM(NIX+I,NIY+J)
               IF (ILC.EQ.0) GO TO 300
               IF ((I.NE.IHIGH(ILC,1)).OR.(J.NE.(-IHP)*IHIGH(ILC,2)))
     *   GO TO 300
               ICNT = ICNT + 1
               PREX = NIX + I
               PREY = NIY + J
300      CONTINUE
         IF (ICNT.EQ.0) GO TO 4500
         IERR = 38
         CALL MYERR(IERR,IERR,IERR)
         CALL FTLOCA(IY,IX)
         IF ((IX.NE.PREX).OR.(IY.NE.PREY)) THEN
            CALL FTEXT('^ ^')
            MM(IX,IY) = 0
         ELSE IF (LMM(IX,IY).EQ.43) THEN
            CALL FTEXT('^+^')
         ELSE
            CALL FTEXT('^-^')
         ENDIF
         IX = IX - 1
         GO TO 999
4500     CONTINUE
         DO 56 I=1,14
            KK = I
            IF (IHIGH(I,1).EQ.II.AND.(-IHP)*IHIGH(I,2).EQ.JJ) THEN
               IF (II.EQ.-2) THEN
```

```
              LEFT2 = KHAR
              OX = IX
              OY = IY
            ENDIF
            GO TO 57
          ENDIF
C LOOK UP NODE ASSOCIATOR IN IHIGH
56      CONTINUE
C COULDN'T FIND ONE - CALL IT DELOCALIZED
        GO TO 51
C STORE SIGN WITH NODE ASSOCIATOR
57      CONTINUE
        IF ((MM(IX,IY).EQ.43).OR.(MM(IX,IY).EQ.45)) THEN
          CALL FTLOCA(IY,IX)
          HALO(2) = CHAR(KHAR)
          CALL FTEXT(HALOE)
          CALL FTSIZE(2,18)
          CALL FTLOCA(4,1)
          PAGE = 0
          CALL FTEXT('^CHARGE IS NOW LOCAL^')
          CALL FTSIZE(1,10)
        ENDIF
        MM(IX,IY) = KHAR + KK*2**13
        GO TO 999
C
199     CONTINUE
C
C       UNDETERMINED BOND SITE MARKERS ARE ENTERED.
C
        IF (KHAR.NE.34) GO TO 99
C       The logical variable FOUND is set to TRUE when a node adjacent
C       to the marker is found.  The loop that searches for adjacent
C       nodes is continued until all positions adjacent to the marker
C       are checked to ensure the marker placement is not ambiguous.
C       If a second adjacent node is found, the marker is erased, an
C       error message prompting the user to use another position is
C       issued, and the loop is exited.
        FOUND = .FALSE.
        DO 150 I=-2,1
        DO 150 J=-1,1
C DON'T CHECK THIS BOX
        IF (I.EQ.0 .AND. J .EQ. 0) GO TO 150
        IIX = IX+I
        IIY = IY - J
        IF (((MM(IIX,IIY).GE.65).AND.(MM(IIX,IIY).LE.90)).OR.
     *     (MM(IIX,IIY).EQ.46)) GO TO 147
C CHECK FOR UC LETTER - IF WE FIND ONE - THEN CHECK
C FOR OTHER REQUIREMENTS
C ITS NOT A UC - CAN'T BE A NODE
C       IF X = -2 THEN WE NEED UC FOLLOWED BY 1c
        GO TO 150
147     IF ((I.EQ.-2).AND.(MM(IIX+1,IIY).GE. 97
     1     .AND. MM(IIX+1,IIY) .LE.122)) THEN
          IF (FOUND) THEN
            IERR = 42
            CALL MYERR(IERR,IERR,IERR)
            CALL FTLOCA(IY,IX)
            CALL FTEXT('^ ^')
            GO TO 999
          ENDIF
          II = -I
          JJ = J
          NIX = IIX
          NIY = IIY
          FOUND = .TRUE.
          GO TO 150
        ENDIF
        IF (I.EQ.-2) GO TO 150
149     IF (MM(IIX,IIY).NE.72) THEN
          IF (FOUND) THEN
            IERR = 42
            CALL MYERR(IERR,IERR,IERR)
            CALL FTLOCA(IY,IX)
            CALL FTEXT('^ ^')
            GO TO 999
```

```
          ENDIF
          II = -I
          JJ = J
          NIX = IIX
          NIY = IIY
          FOUND = .TRUE.
          GO TO 150
       ENDIF
       IF (MM(IIX+1,IIY).GE.97.AND.MM(IIX+1,IIY).LE.122) THEN
          IF (FOUND) THEN
             IERR = 42
             CALL MYERR(IERR,IERR,IERR)
             CALL FTLOCA(IY,IX)
             CALL FTEXT('^ ^')
             GO TO 999
          ENDIF
          II = -I
          JJ = J
          NIX = IIX
          NIY = IIY
          FOUND = .TRUE.
          GO TO 150
       ENDIF
C IF UC = H IT MUST BE FOLLOWED BY lc
150    CONTINUE
       IF (FOUND) GO TO 155
C      CAN'T FIND NODE
151    IERR = 34
       CALL MYERR(IERR,IERR,IERR)
       CALL FTLOCA(IY,IX)
       CALL FTEXT('^ ^')
       IX = IX - 1
       GO TO 999
155    CONTINUE
       IF (NBD1.EQ.0) GO TO 157
C      Check for " already on this node.
         DO 527 I = 1,NBD1
            KK = I
            IF ((NIX.EQ.DSCNC(3,I)).AND.(NIY.EQ.DSCNC(4,I))) GO TO 892
527      CONTINUE
         GO TO 157
892      IERR = 47
         CALL MYERR(IERR,IERR,IERR)
         IF ((IX.NE.DSCNC(5,KK)).OR.(IY.NE.DSCNC(6,KK))) THEN
            CALL FTLOCA(IY,IX)
            CALL FTEXT('^ ^')
         ENDIF
         GO TO 999
C STORE SIGN WITH NODE ASSOCIATOR
157    MM(IX,IY) = KHAR
       NBD1 = NBD1 + 1
       DSCNC(3,NBD1) = NIX
       DSCNC(4,NBD1) = NIY
       DSCNC(5,NBD1) = IX
       DSCNC(6,NBD1) = IY
       IF (II.GE.1) THEN
          IF (JJ.EQ.IHP) THEN
             DSCNC(2,NBD1) = 2
          ELSE IF (JJ.EQ.0) THEN
             DSCNC(2,NBD1) = 3
          ELSE
             DSCNC(2,NBD1) = 4
          ENDIF
       ELSE IF (II.EQ.0) THEN
          IF (JJ.EQ.-IHP) THEN
             DSCNC(2,NBD1) = 5
          ELSE
             DSCNC(2,NBD1) = 1
          ENDIF
       ELSE
          IF (JJ.EQ.-IHP) THEN
             DSCNC(2,NBD1) = 6
          ELSE IF (JJ.EQ.0) THEN
```

```
              DSCNC(2,NBD1) = 7
           ELSE
              DSCNC(2,NBD1) = 8
           ENDIF
        ENDIF
        GO TO 999
C Put KHAR into data array.
C TRANSLATE FOR D1'S AND M1'S.
99      IF ((KHAR.GE.49).AND.(KHAR.LE.57).AND.
     *     ((MM(IX-1,IY).EQ.68).OR.(MM(IX-1,IY).EQ.77)))
     *     KHAR = KHAR + 63
        IF ((KHAR.GT.32).AND.(KHAR.NE.127)) THEN
           IF (MM(IX,IY).EQ.46) THEN
              DO 505 I = 1,260
                 IF ((IX.EQ.LABL(I,1)).AND.(IY.EQ.LABL(I,2))) THEN
                    LABL(I,1) = -999
                    LABL(I,2) = -999
                    GO TO 506
                 ENDIF
505           CONTINUE
           ENDIF
506        CONTINUE
           MM(IX,IY) = KHAR
        ENDIF
C Non-printing characters
C ERASE CHAR - WE HAD A DEL
C DEL WAS ENTERED
        IF (((KHAR.EQ.127).OR.(KHAR.EQ.32).OR.(KHAR.EQ.8)).AND.
     *     (MM(IX,IY).NE.0)) THEN
           ICUR = 0
           CALL CURSOR(IX,IY)
           IF ((LMM(IX,IY).GE.256).AND.(MOD(IDIR(IX,IY),2).EQ.0)) THEN
              FX = IX - 1
        IF (IHP .EQ. 1) THEN
        CALL BERASE(IX,IY)
        ELSE
              CALL FTLOCA(IY,FX)
              CALL FTEXT('^   ^')
        ENDIF
              IF (MM(FX,IY).NE.0) CALL REPLCE(FX,IY,0,0,0,0,0)
              FX = IX + 1
              IF (MM(FX,IY).NE.0) CALL REPLCE(FX,IY,0,0,0,0,0)
              INKX = 1
              INKY = 1
           ELSE
              CALL FTLOCA(IY,IX)
              CALL FTEXT('^ ^')
              INKX = 0
              INKY = 0
           ENDIF
           IF ((MM(IX,IY).EQ.46).OR.(LMM(IX,IY).GE.256).OR.(MM(IX,IY)
     *        .EQ.44).OR.((MM(IX,IY).GE.50).AND.(MM(IX,IY).LE.57).AND.
     *        (LMM(IX-1,IY).NE.43).AND.(LMM(IX-1,IY).NE.45)).OR.
     *        (MM(IX,IY).EQ.103).OR.(MM(IX,IY).EQ.106).OR.(MM(IX,IY).EQ
     *        .112).OR.(MM(IX,IY).EQ.113).OR.(MM(IX,IY).EQ.121).OR.
     *        (MM(IX,IY).EQ.95).OR.(MM(IX,IY).EQ.59)) THEN
              IF (MOD((IY*10),40).EQ.0) THEN
                 IF ((IY.EQ.8).OR.(IY.EQ.28).OR.(IY.EQ.16)) THEN
                    FY = ((IY * 10) / 11) + 1
                    CALL FTSIZE(1,11)
                 ELSE
                    FY = ((IY * 10) / 9) + 1
                    CALL FTSIZE(1,9)
                 ENDIF
              ELSE
                 FY = ((IY * 10) / 8) + 1
                 CALL FTSIZE(1,8)
              ENDIF
              IF ((LMM(IX,IY).GE.256).AND.(MOD(IDIR(IX,IY),2).EQ.0))THEN
                 FX = IX - 1
        IF (IHP .EQ. 1) THEN
        CALL BERASE(IX,IY)
        ELSE
```

```
                    CALL FTLOCA(FY,FX)
                    CALL FTEXT('^   ^')
                    CALL FTSIZE(1,10)
          ENDIF
                    FY = IY + 1
                    IF (MM(FX,FY).NE.0) CALL REPLCE(FX,FY,0,0,0,0,0)
                    IF (MM(IX,FY).NE.0) CALL REPLCE(IX,FY,0,0,0,0,0)
                    FX = IX + 1
                    IF (MM(FX,FY).NE.0) CALL REPLCE(FX,FY,0,0,0,0,0)
                ELSE
          IF (IHP .EQ.1) THEN
          CALL BERASE(IX,IY)
          ELSE
                    CALL FTLOCA(FY,IX)
                    CALL FTEXT('^ ^')
                    CALL FTSIZE(1,10)
          ENDIF
                    FY = IY + 1
                    IF (MM(IX,FY).NE.0) CALL REPLCE(IX,FY,0,0,0,0,0)
                ENDIF
            ENDIF
            IF (LMM(IX,IY).GE.256) THEN
               MM(IX,IY) = 0
               FY = IY - 1
               CALL REPLCE(IX,FY,INKX,INKY,0,0,1)
            ELSE
              IF (MM(IX,IY).EQ.46) THEN
                 DO 515 I = 1,260
                    IF ((IX.EQ.LABL(I,1)).AND.(IY.EQ.LABL(I,2))) THEN
                       LABL(I,1) = -999
                       LABL(I,2) = -999
                       GO TO 516
                    ENDIF
515              CONTINUE
              ENDIF
516           CONTINUE
              IF (MM(IX,IY).EQ.34) THEN
                 DO 519 I = 1,NBD1
                    IF ((DSCNC(5,I).EQ.IX).AND.(DSCNC(6,I).EQ.IY)) THEN
                       DO 518 K = I,NBD1
                          DO 517 J = 1,6
                             IF (K.LT.50) THEN
                                DSCNC(J,K) = DSCNC(J,K+1)
                             ELSE
                                DSCNC(J,K) = 0
                             ENDIF
517                       CONTINUE
                          IF (DSCNC(K,2).EQ.0) THEN
                             NBD1 = NBD1 - 1
                             GO TO 520
                          ENDIF
518                    CONTINUE
                    ENDIF
519              CONTINUE
520              CONTINUE
              ENDIF
              MM(IX,IY) = 0
            ENDIF
        ENDIF
999     IX=IX+1
        IF (KHAR.EQ.8) IX=IX-2
C BACKUP ONE SPACE IF A DEL
        IF (KHAR.EQ.127) IX=IX-1
        IF (IX.LT.1) IX = 1
        ICUR = 1
        CALL CURSOR(IX,IY)
C Next character
        GOTO 100
200     ISMART=1
        ISTATE=0
C End graphics text mode
        CALL HEADER
        RETURN
        END
```

```
C
      SUBROUTINE BKSPCE(IX,IY)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM,IDTPIX
      LOGICAL*2 FOUND
      CHARACTER*1 HALO(3),HLO(3)
      CHARACTER*3 HALOE
      EQUIVALENCE (HALOE,HALO(1))
      CHARACTER*1 KAN
      CHARACTER*1 ISTAT
      COMMON /CD/ MAXX,MAXY
      COMMON /RANGE/ LOX,HIX,LOY,HIY
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
      COMMON /HP/IHP
      COMMON /ISTATE/ ISTAT
      COMMON /IPLUS/ IHIGH(14,2)
      COMMON /SIZZE/ MULTX,MULTY
      COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
      COMMON /CUR/ ICUR
C
C  This routine, called when a backspace (Ctl-H, or ASCII 8) is typed
C  in.  Free text is entered onto he graphics screen and into the data
C  array MM. Any bond key ll return you to regular input. Input of a *
C  will be interpreted in the analysis program as preceeding a dot-
C  disconnected substructure.
C
C Input character ASCII equiv; distinct from KAR.
      LEFT2 = 0
      ICUR = 1
      KHAR=0
      ISTAT='B'
      ISTATE=8
      CALL HEADER
      IX=IX-1
      IF (IX.LT.1) IX = 1
      CALL CURSOR(IX,IY)
      HALO(1) = KAN
      HALO(3) = KAN
10    CALL INPUTX(KHAR,IX,IY)
      IF ((LEFT2.NE.0).AND.((KHAR.LT.50).OR.(KHAR.GT.57))) THEN
         DO 2 I = LOX,HIX
            DO 2 J = LOY,HIY
               IF ((MM(I,J).EQ.43).OR.(MM(I,J).EQ.45)) THEN
                  IERR = 4
                  CALL MYERR(IERR,IERR,IERR)
                  MM(OX,OY) = 0
                  CALL FTLOCA(OY,OX)
                  CALL FTEXT('^ ^')
                  GO TO 3
               ENDIF
2        CONTINUE
         IERR = 28
         CALL MYERR(IERR,IERR,IERR)
         MM(OX,OY) = LEFT2
         LEFT2 = 0
         IX = IX - 1
         CALL CURSOR(IX,IY)
         GO TO 10
      ENDIF
3     CONTINUE
      LEFT2 = 0
      IF (IHP .EQ. 1 .AND. ((KHAR .GE. 22) .AND. (KHAR .LE. 31)))
     1 GO TO 20
      IF (KHAR.EQ.21) GO TO 20
      IF ((KHAR.LE.31).AND.(KHAR.GE.22).AND.(KHAR.NE.26).AND.(KHAR.NE.
     *   27)) THEN
         CALL MOVE(KHAR,IX,IY)
         MCHAR = 0
         GO TO 10
```

```
      ENDIF
      IF ((KHAR.GT.32).AND.(KHAR.NE.127)) THEN
         IF (MM(IX,IY).NE.0) THEN
            ICUR = 0
            CALL CURSOR(IX,IY)
            HALO(2) = ' '
            IF ((LMM(IX,IY).GE.256).AND.(MOD(IDIR(IX,IY),2).EQ.0))
     *         THEN
               FX = FX - 1
      IF (IHP .EQ. 1) THEN
      CALL ERASE(IX,IY)
      ELSE
               CALL FTLOCA(IY,FX)
               CALL FTEXT('^   ^')
      ENDIF
               IF (MM(FX,IY).NE.0) CALL REPLCE(FX,IY,0,0,0,0,0)
               FX = IX + 1
               IF (MM(FX,IY).NE.0) CALL REPLCE(FX,IY,0,0,0,0,0)
               INKX = 1
               INKY = 1
            ELSE
               CALL FTLOCA(IY,IX)
               CALL FTEXT(HALOE)
               INKX = 0
               INKY = 0
            ENDIF
            IF ((MM(IX,IY).EQ.46).OR.(LMM(IX,IY).GE.256).OR.
     *         ((MM(IX,IY).GE.50).AND.(MM(IX,IY).LE.57)).AND.
     *         ((LMM(IX-1,IY).NE.43).AND.(LMM(IX-1,IY).NE.45)).OR.
     *         (MM(IX,IY).EQ.103).OR.(MM(IX,IY).EQ.106).OR.(MM(IX,IY)
     *         .EQ.112).OR.(MM(IX,IY).EQ.113).OR.(MM(IX,IY).EQ.121)
     *         .OR.(MM(IX,IY).EQ.95).OR.(MM(IX,IY).EQ.44).OR.
     *         (MM(IX,IY).EQ.59)) THEN
               IF (MOD((IY*10),40).EQ.0) THEN
                  IF ((IY.EQ.8).OR.(IY.EQ.28).OR.(IY.EQ.16)) THEN
                     FY = ((IY * 10) / 11) + 1
                     CALL FTSIZE(1,11)
                  ELSE
                     FY = ((IY * 10) / 9) + 1
                     CALL FTSIZE(1,9)
                  ENDIF
               ELSE
                  FY = ((IY * 10) / 8) + 1
                  CALL FTSIZE(1,8)
               ENDIF
            ENDIF
            IF ((LMM(IX,IY).GE.256).AND.(MOD(IDIR(IX,IY),2).EQ.0))
     *         THEN
               FX = IX - 1
      IF (IHP .EQ. 1) THEN
      CALL ERASE(IX,IY)
      ELSE
               CALL FTLOCA(FY,FX)
               CALL FTEXT('^   ^')
               CALL FTSIZE(1,10)
      ENDIF
               FY = IY + 1
               IF (MM(FX,FY).NE.0) CALL REPLCE(FX,FY,0,0,0,0,0)
               IF (MM(IX,FY).NE.0) CALL REPLCE(IX,FY,0,0,0,0,0)
               FX = IX + 1
               IF (MM(FX,FY).NE.0) CALL REPLCE(FX,FY,0,0,0,0,0)
            ELSE
      IF (IHP .EQ. 1) THEN
      CALL ERASE(IX,IY)
      ELSE
               CALL FTLOCA(FY,IX)
               CALL FTEXT('^ ^')
               CALL FTSIZE(1,10)
      ENDIF
               FY = IY + 1
               IF (MM(IX,FY).NE.0) CALL REPLCE(IX,FY,0,0,0,0,0)
            ENDIF
```

```
            ENDIF
            IF (LMM(IX,IY).GE.256) THEN
               MM(IX,IY) = 0
               FY = IY - 1
               CALL REPLCE(IX,FY,INKX,INKY,0,0,1)
            ENDIF
            ICUR = 1
            CALL CURSOR(IX,IY)
            IF (KHAR.GT.32) THEN
               IF (IX.LT.LOX) THEN
                  LOX = IX
               ELSE IF (IX.GT.HIX) THEN
                  HIX = IX
               ENDIF
               IF (IY.LT.LOY) THEN
                  LOY = IY
               ELSE IF (IY.GT.HIY) THEN
                  HIY = IY
               ENDIF
            ENDIF
            IF (KHAR.EQ.94) THEN
               HLO(1) = '/'
               HLO(2) = CHAR(KHAR)
               HLO(3) = '/'
               CALL TEXT(HLO)
            ELSE
               HALO(2) = CHAR(KHAR)
               CALL TEXT(HALO)
            ENDIF
         ENDIF
C
         IF (KHAR .NE. 43.AND.KHAR .NE. 45) GO TO 199
C
C        WE FOUND A + OR -    ...  NOW FIND ITS NODE
C
C        The logical variable FOUND is set to TRUE when a node adjacent
C        to the charge is found.  The loop that searches for adjacent
C        nodes is continued until all positions adjacent to the charge
C        are checked to ensure the charge placement is not ambiguous.
C        If a second adjacent node is found, the charge is erased, an
C        error message prompting the user to use another position is
C        issued, and the loop is exited.
         FOUND = .FALSE.
C LOOK AROUND FOR NODE
         DO 50 I=-2,2
         DO 50 J=-1,1
C DON'T CHECK THIS BOX
         IF(I.EQ.0 .AND. J .EQ. 0) GO TO 50
         IIX=IX+I
         IIY=IY - J
         IF (((MM(IIX,IIY).GE.65).AND.(MM(IIX,IIY).LE.90)).OR.
     *     (MM(IIX,IIY).EQ.46)) GO TO 47
C CHECK FOR UC LETTER - IF WE FIND ONE - THEN CHECK
C FOR OTHER REQUIREMENTS
C ITS NOT A UC - CAN'T BE A NODE
         GO TO 50
C IF X = -2 THEN WE NEED UC FOLLOWED BY lc
47       IF ((I.EQ.-2).AND.(MM(IIX+1,IIY).GE. 97
     1     .AND. MM(IIX+1,IIY) .LE.122)) THEN
            IF (FOUND) THEN
               IERR = 42
               CALL MYERR(IERR,IERR,IERR)
               CALL FTLOCA(IY,IX)
               CALL FTEXT('^ ^')
               GO TO 999
            ENDIF
            II = -I
            JJ = J
            NIX = IIX
            NIY = IIY
            FOUND = .TRUE.
            GO TO 50
```

```
      ENDIF
C IF X=2 WE NEED DIGIT TO RIGHT OF CHARGE
      IF (I.EQ.-2) GO TO 50
49    IF (MM(IIX,IIY).NE.72) THEN
         IF (FOUND) THEN
            IERR = 42
            CALL MYERR(IERR,IERR,IERR)
            CALL FTLOCA(IY,IX)
            CALL FTEXT('^ ^')
            GO TO 999
         ENDIF
         II = -I
         JJ = J
         NIX = IIX
         NIY = IIY
         FOUND = .TRUE.
         GO TO 50
      ENDIF
      IF (MM(IIX+1,IIY).GE.97.AND.MM(IIX+1,IIY).LE.122) THEN
         IF (FOUND) THEN
            IERR = 42
            CALL MYERR(IERR,IERR,IERR)
            CALL FTLOCA(IY,IX)
            CALL FTEXT('^ ^')
            GO TO 999
         ENDIF
         II = -I
         JJ = J
         NIX = IIX
         NIY = IIY
         FOUND = .TRUE.
         GO TO 50
      ENDIF
C IF UC = H IT MUST BE FOLLOWED BY lc
50    CONTINUE
      IF (FOUND) GO TO 55
C CAN'T FIND NODE - CALL IT DELOCALIZED CHARGE
C     Check that there is only 1 delocalized charge.
      DO 4345 I = LOX,HIX
         DO 4345 J = LOY,HIY
            IF ((MM(I,J).NE.45).AND.(MM(I,J).NE.43)) GO TO 4345
            IF (MM(I-1,J).NE.42) GO TO 4300
4345  CONTINUE
      GO TO 51
4300    IERR = 4
        CALL MYERR(IERR,IERR,IERR)
        CALL FTLOCA(IY,IX)
        CALL FTEXT('^ ^')
        IX = IX - 1
        GO TO 999
C CAN'T FIND NODE - CALL IT DELOCALIZED CHARGE
51    IERR=28
      CALL MYERR(IERR,KHAR,MAR)
      LEFT2 = 0
      GO TO 99
55    CONTINUE
      ICNT = 0
      DO 300 I = -2,2
         DO 300 J = -1,1
            IF ((LMM(NIX+I,NIY+J).NE.43).AND.(LMM(NIX+I,NIY+J).NE.45))
     *         GO TO 300
            ILC = IHMM(NIX+I,NIY+J)
            IF (ILC.EQ.0) GO TO 300
            IF ((I.NE.IHIGH(ILC,1)).OR.(J.NE.(-IHP)*IHIGH(ILC,2)))
     * GO TO 300
            ICNT = ICNT + 1
            PREX = NIX + I
            PREY = NIY + J
300   CONTINUE
      IF (ICNT.EQ.0) GO TO 4500
      IERR = 38
      CALL MYERR(IERR,IERR,IERR)
      CALL FTLOCA(IY,IX)
```

```
        IF ((IX.NE.PREX).OR.(IY.NE.PREY)) THEN
           CALL FTEXT('^ ^')
           MM(IX,IY) = 0
        ELSE IF (LMM(IX,IY).EQ.43) THEN
           CALL FTEXT('^+^')
        ELSE
           CALL FTEXT('^-^')
        ENDIF
        IX = IX - 1
        GO TO 999
4500    CONTINUE
        DO 56 I=1,14
           KK = I
           IF (IHIGH(I,1).EQ.II.AND.(-IHP)*IHIGH(I,2).EQ.JJ) THEN
              IF (II.EQ.-2) THEN
                 LEFT2 = KHAR
                 OX = IX
                 OY = IY
              ENDIF
              GO TO 57
           ENDIF
C LOOK UP NODE ASSOCIATOR IN IHIGH
56      CONTINUE
C COULDN'T FIND ONE - CALL IT DELOCALIZED
        GO TO 51
C STORE SIGN WITH NODE ASSOCIATOR
57      CONTINUE
        IF ((MM(IX,IY).EQ.43).OR.(MM(IX,IY).EQ.45)) THEN
           CALL FTLOCA(IY,IX)
           HALO(2) = CHAR(KHAR)
           CALL FTEXT(HALOE)
           CALL FTSIZE(2,18)
           CALL FTLOCA(1,1)
           PAGE = 0
           CALL FTEXT('^CHARGE IS NOW LOCAL^')
           CALL FTSIZE(1,10)
        ENDIF
        MM(IX,IY) = KHAR + KK*2**13
        GO TO 999
C
199     CONTINUE
C
C       UNDETERMINED BOND SITE MARKER ENTRY.
C
        IF (KHAR.NE.34) GO TO 99
C       The logical variable FOUND is set to TRUE when a node adjacent
C       to the marker is found.  The loop that searches for adjacent
C       nodes is continued until all positions adjacent to the marker
C       are checked to ensure the charge placement is not ambiguous.
C       If a second adjacent node is found, the marker is erased, an
C       error message prompting the user to use another position is
C       issued, and the loop is exited.
        FOUND = .FALSE.
        DO 150 I=-2,1
        DO 150 J=-1,1
C DON'T CHECK THIS BOX
        IF (I.EQ.0 .AND. J .EQ. 0) GO TO 150
        IIX=IX+I
        IIY=IY - J
        IF (((MM(IIX,IIY).GE.65).AND.(MM(IIX,IIY).LE.90)).OR.
     *     (MM(IIX,IIY).EQ.46)) GO TO 147
C CHECK FOR UC LETTER - IF WE FIND ONE - THEN CHECK
C FOR OTHER REQUIREMENTS
C ITS NOT A UC - CAN'T BE A NODE
C ITS NOT A UC - CAN'T BE A NODE
C       IF X = -2 THEN WE NEED UC FOLLOWED BY 1c
        GO TO 150
147     IF ((I.EQ.-2).AND.(MM(IIX+1,IIY).GE. 97
     1     .AND. MM(IIX+1,IIY) .LE.122)) THEN
           IF (FOUND) THEN
              IERR = 42
              CALL MYERR(IERR,IERR,IERR)
              CALL FTLOCA(IY,IX)
```

```
            CALL FTEXT('^ ^')
            GO TO 999
         ENDIF
         II = -I
         JJ = J
         NIX = IIX
         NIY = IIY
         FOUND = .TRUE.
         GO TO 150
      ENDIF
      IF (I.EQ.-2) GO TO 150
149   IF (MM(IIX,IIY).NE.72) THEN
         IF (FOUND) THEN
            IERR = 42
            CALL MYERR(IERR,IERR,IERR)
            CALL FTLOCA(IY,IX)
            CALL FTEXT('^ ^')
            GO TO 999
         ENDIF
         II = -I
         JJ = J
         NIX = IIX
         NIY = IIY
         FOUND = .TRUE.
         GO TO 150
      ENDIF
      IF (MM(IIX+1,IIY).GE.97.AND.MM(IIX+1,IIY).LE.122) THEN
         IF (FOUND) THEN
            IERR = 42
            CALL MYERR(IERR,IERR,IERR)
            CALL FTLOCA(IY,IX)
            CALL FTEXT('^ ^')
            GO TO 999
         ENDIF
         II = -I
         JJ = J
         NIX = IIX
         NIY = IIY
         FOUND = .TRUE.
         GO TO 150
      ENDIF
C IF UC = H IT MUST BE FOLLOWED BY lc
150   CONTINUE
      IF (FOUND) GO TO 155
C CAN'T FIND NODE
151   IERR = 34
      CALL MYERR(IERR,IERR,IERR)
      CALL FTLOCA(IY,IX)
      CALL FTEXT('^ ^')
      IX = IX - 1
      GO TO 999
155   CONTINUE
C STORE SIGN WITH NODE ASSOCIATOR
      IF (NBD1.EQ.0) GO TO 157
C     Check for " already on this node.
         DO 527 I = 1,NBD1
            KK = I
            IF ((NIX.EQ.DSCNC(3,I)).AND.(NIY.EQ.DSCNC(4,I))) GO TO 892
527      CONTINUE
         GO TO 157
892      IERR = 47
         CALL MYERR(IERR,IERR,IERR)
         IF ((IX.NE.DSCNC(5,KK)).OR.(IY.NE.DSCNC(6,KK))) THEN
            CALL FTLOCA(IY,IX)
            CALL FTEXT('^ ^')
         ENDIF
         CALL FTLOCA(IY,IX)
         CALL FTEXT('^ ^')
         GO TO 999
157   MM(IX,IY) = KHAR
      NBD1 = NBD1 + 1
      DSCNC(3,NBD1) = NIX
      DSCNC(4,NBD1) = NIY
```

```
      DSCNC(5,NBD1) = IX
      DSCNC(6,NBD1) = IY
      IF (II.GE.1) THEN
         IF (JJ.EQ.IHP) THEN
            DSCNC(2,NBD1) = 2
         ELSE IF (JJ.EQ.0) THEN
            DSCNC(2,NBD1) = 3
         ELSE
            DSCNC(2,NBD1) = 4
         ENDIF
      ELSE IF (II.EQ.0) THEN
         IF (JJ.EQ.-IHP) THEN
            DSCNC(2,NBD1) = 5
         ELSE
            DSCNC(2,NBD1) = 1
         ENDIF
      ELSE
         IF (JJ.EQ.-IHP) THEN
            DSCNC(2,NBD1) = 6
         ELSE IF (JJ.EQ.0) THEN
            DSCNC(2,NBD1) = 7
         ELSE
            DSCNC(2,NBD1) = 8
         ENDIF
      ENDIF
      GO TO 999
C Put KHAR into data array.
C TRANSLATE D1'S AND M1'S.
99    IF ((KHAR.EQ.47).AND.(KHAR.LE.57).AND.((MM(IX-1,IY)
     *    .EQ.68).OR.(MM(IX-1,IY).EQ.77))) KHAR = KHAR + 63
      IF ((KHAR.GT.32).AND.(KHAR.NE.127)) THEN
         IF (MM(IX,IY).EQ.46) THEN
            DO 505 I = 1,260
               IF ((IX.EQ.LABL(I,1)).AND.(IY.EQ.LABL(I,2))) THEN
                  LABL(I,1) = -999
                  LABL(I,2) = -999
                  GO TO 506
               ENDIF
505         CONTINUE
         ENDIF
506      CONTINUE
         MM(IX,IY) = KHAR
      ENDIF

C Non printing chars
C ERASE CHAR - WE HAD A DEL
      IF (((KHAR.EQ.127).OR.(KHAR.EQ.32).OR.(KHAR.EQ.8)).AND.
     *    (MM(IX,IY).NE.0)) THEN
         ICUR = 0
         CALL CURSOR(IX,IY)
         HALO(2) = ' '
         IF ((LMM(IX,IY).GE.256).AND.(MOD(IDIR(IX,IY),2).EQ.0)) THEN
            FX = IX - 1
        IF (IHP .EQ.1) THEN
        CALL ERASE(IX,IY)
        ELSE
            CALL FTLOCA(IY,FX)
            CALL FTEXT('^   ^')
        ENDIF
            IF (MM(FX,IY).NE.0) CALL REPLCE(FX,IY,0,0,0,0,0)
            FX = IX + 1
            IF (MM(FX,IY).NE.0) CALL REPLCE(FX,IY,0,0,0,0,0)
            INKX = 1
            INKY = 1
         ELSE
            CALL FTLOCA(IY,IX)
           CALL FTEXT(HALOE)
            INKX = 0
            INKY = 0
         ENDIF
         IF ((MM(IX,IY).EQ.46).OR.(LMM(IX,IY).GE.256).OR.
     *       ((MM(IX,IY).GE.50).AND.(MM(IX,IY).LE.57)).AND.
     *       ((LMM(IX-1,IY).NE.43).AND.(LMM(IX-1,IY).NE.45)).OR.
     *       (MM(IX,IY).EQ.103).OR.(MM(IX,IY).EQ.106).OR.(MM(IX,IY)
     *       .EQ.112).OR.(MM(IX,IY).EQ.113).OR.(MM(IX,IY).EQ.121).OR.
```

```
*        (MM(IX,IY).EQ.95).OR.(MM(IX,IY).EQ.44).OR.(MM(IX,IY).EQ.
*        59)) THEN
         IF (MOD((IY*10),40).EQ.0) THEN
            IF ((IY.EQ.8).OR.(IY.EQ.28).OR.(IY.EQ.16)) THEN
               FY = ((IY * 10) / 11) + 1
               CALL FTSIZE(1,11)
            ELSE
               FY = ((IY * 10) / 9) + 1
               CALL FTSIZE(1,9)
            ENDIF
         ELSE
            FY = ((IY * 10) / 8) + 1
            CALL FTSIZE(1,8)
         ENDIF
      ENDIF
      IF ((LMM(IX,IY).GE.256).AND.(MOD(IDIR(IX,IY),2).EQ.0))
*        THEN
         FX = IX - 1
    IF (IHP .EQ. 1) THEN
    CALL ERASE(IX,IY)
    ELSE
         CALL FTLOCA(FY,FX)
         CALL FTEXT('^   ^')
         CALL FTSIZE(1,10)
    ENDIF
         FY = IY + 1
         IF (MM(FX,FY).NE.0) CALL REPLCE(FX,FY,0,0,0,0,0)
         IF (MM(IX,FY).NE.0) CALL REPLCE(IX,FY,0,0,0,0,0)
         FX = IX + 1
         IF (MM(FX,FY).NE.0) CALL REPLCE(FX,FY,0,0,0,0,0)
      ELSE
    IF (IHP .EQ. 1) THEN
    CALL ERASE(IX,IY)
    ELSE
         CALL FTLOCA(FY,IX)
         CALL FTEXT(HALOE)
         CALL FTSIZE(1,10)
    ENDIF
         FY = IY + 1
         IF (MM(IX,FY).NE.0) CALL REPLCE(IX,FY,0,0,0,0,0)
      ENDIF
      IF (LMM(IX,IY).GE.256) THEN
         MM(IX,IY) = 0
         FY = IY - 1
         CALL REPLCE(IX,FY,INKX,INKY,0,0,1)
      ELSE
         IF (MM(IX,IY).EQ.46) THEN
            DO 515 I = 1,260
               IF ((IX.EQ.LABL(I,1)).AND.(IY.EQ.LABL(I,2))) THEN
                  LABL(I,1) = -999
                  LABL(I,2) = -999
                  GO TO 516
               ENDIF
515         CONTINUE
         ENDIF
516      CONTINUE
         IF (MM(IX,IY).EQ.34) THEN
            DO 519 I = 1,NBD1
               IF ((DSCNC(5,I).EQ.IX).AND.(DSCNC(6,I).EQ.IY)) THEN
                  DO 518 K = I,NBD1
                     DO 517 J = 1,6
                        IF (K.LT.50) THEN
                           DSCNC(J,K) = DSCNC(J,K+1)
                        ELSE
                           DSCNC(J,K) = 0
                        ENDIF
517                  CONTINUE
                     IF (DSCNC(K,2).EQ.0) THEN
                        NBD1 = NBD1 - 1
                        GO TO 520
                     ENDIF
518               CONTINUE
               ENDIF
```

```
519             CONTINUE
520             CONTINUE
             ENDIF
             MM(IX,IY) = 0
          ENDIF
       ENDIF
C DEL WAS ENTERED
999     IX=IX+1
        IF (KHAR.EQ.8 ) IX=IX-2
C BACKUP ONE IF DEL
        IF (KHAR .EQ. 127) IX=IX-1
        IF (IX.LT.1) IX = 1
        ICUR = 1
        CALL CURSOR(IX,IY)
C Next char
        GOTO 10
20      ISMART=1
        ISTATE=0
        CALL HEADER
        RETURN
        END
$STORAGE:2
C
        SUBROUTINE REDRAW(IX,IY,INCX,INCY,NBTYPE)
        IMPLICIT INTEGER*2 (A-Z)
        REAL A
        INTEGER*4 MM,IDTPIX
        LOGICAL*2 RDBACK,SKIP,RETR
        CHARACTER*1 HALO(3)
        COMMON /CD/ MAXX,MAXY
        COMMON /IOFFST/IOFF
        COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /SIZZE/ MULTX,MULTY
        COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /BONDS/ A(5,3,4,4),B(2,3,4)
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /CUR/ ICUR
        COMMON /HP/IHP
CXT     RDBACK = TRUE indicates bond is being patched by SUBROUTINE DRAW.
        COMMON /PTCH/ RDBACK
CXT     SKIP = TRUE indicates a bond of type 0 is to skim over existing
CXT     bond.
        COMMON /BOSKIP/ SKIP
CXT     RETR is set in SUBROUTINE RETRIEVE to ensure proper screen
CXT     replacement activity with respect to arrays MM and IDTPIX.
        COMMON /RETDRW/ RETR
C
C This subroutine replaces existing bonds with bonds of a new type code.
C The parameter NBTYPE is the type of the old bond, the IBTYPE is that
C of the new one.  This routine is only called by DRAW when attempting
C to retrace an existing bond with one of a new bondtye.
C
C Existing bond direction.
        IF (RETR) THEN
           SKIP = .FALSE.
           RDBACK = .FALSE.
        ENDIF
        LX=IX
        LY=IY
        ICUR = 0
        CALL CURSOR(LX,LY)
C
C       Undraw existing bond:
100     CONTINUE
        IF ((.NOT.RDBACK).AND.(.NOT.SKIP)) THEN
           IF (IABS(INCX*INCY).EQ.1) THEN
        IF (IHP .EQ. 1) THEN
        CALL BERASE(LX,LY)
        ELSE
              FX = LX - 1
              CALL FTLOCA(LY,FX)
              CALL FTEXT('^   ^')
```

```
      ENDIF
         ELSE
            FX = LX
            CALL FTLOCA(LY,FX)
            CALL FTEXT('^ ^')
         ENDIF
      ENDIF
      CALL FTSIZE(1,10)
C
C     Close NLINES loop
C     If NBTYPE = 0 REDRAW just skims existing bond to next node
C     (IBTYPE = 0 and starting node is not a marker).
      IF (.NOT.SKIP) THEN
         IF (MM(LX,LY).GT.256) MM(LX,LY) = MM(LX,LY) * (-1)
         IF (MM(LX+INCX,LY+INCY).GT.256) MM(LX+INCX,LY+INCY) =
     *      MM(LX+INCX,LY+INCY) * (-1)
         CALL REPLCE(LX,LY,INCX,INCY,0,0,1)
      ENDIF
      LX = LX + INCX
      LY = LY + INCY
      IF (IABS(LMM(LX,LY)).GT.256) GO TO 100
      IF (SKIP) GO TO 645
      IF (INCY.NE.0) THEN
         FX = IX - INCX
         FY = IY - INCY
         CALL REPLCE(FX,FY,INCX,INCY,0,0,1)
         CALL REPLCE(LX,LY,INCX,INCY,0,0,1)
      ENDIF
      LX = IX
      LY = IY
200   CONTINUE
      IF (IBTYPE.EQ.0) GOTO 635
C
C     number of line segments req'd to draw bond--max 3
      NLINES=3
C     double bond needs 2 line segments
      IF (IBTYPE.EQ.2)   NLINES=2
      IF (IBTYPE.EQ.4) NLINES = 1
C     single or stereo
      IF ((MOD(IBTYPE,4).EQ.1)) NLINES=1
C     define & select dashed line--stereo
      IF (IBTYPE.EQ.5) CALL SETLNS(2)
C
C     Conversion of bond type to first A array coordinate value IBOND:
      IBOND=1
      IF (IBTYPE.LE.3)  IBOND=IBTYPE
      IF (IBTYPE.EQ.4) IBOND = 1
      IF (IBTYPE.EQ.6)   IBOND=4
      IF (IBTYPE .EQ. 8) IBOND=3
      IF (IBTYPE.EQ.7)   IBOND=5
C
      JKL=IBDIR
      JKM = IBDIR
      IF (JKL.GT.4) JKL=JKL-4
      IF ((IBOND.GE.4).AND.(IBDIR.GT.4)) IBOND=9-IBOND
C
C
C     Start drawing the bond:
      NX=LX*MULTX - 8*IOFF
C     Screen coordinates of lower left corner of 7x10 area
      NY=LY*MULTY - 11*IOFF
C     Draw each segment separately
      DO 1153 J=1,NLINES
         IF (IBTYPE.EQ.8) THEN
            IF (J.EQ.1) THEN
               CALL SETLNS(2)
            ELSE IF (J.EQ.2) THEN
               CALL SETLNS(1)
            ELSE IF (J.EQ.3) THEN
               CALL SETLNS(3)
            ENDIF
          ENDIF
```

```
C          Calc plotting coords
           IF (MOD(JKM,2).EQ.1) THEN
              JKJ = JKL
              IF ((IBOND.EQ.5).AND.(JKM.EQ.1)) THEN
                 BND = 4
              ELSE IF ((IBOND.EQ.4).AND.(JKM.EQ.1)) THEN
                 BND = 5
              ELSE
                 BND = IBOND
              ENDIF
           ELSE
              BND = IBOND
              IF (JKL.EQ.2) THEN
                 JKJ = 4
              ELSE IF (JKL.EQ.4) THEN
                 JKJ = 2
              ENDIF
           ENDIF
           IF ((JKM.EQ.5).AND.((IBOND.EQ.4).OR.(IBOND.EQ.5))) THEN
              IF (IBOND.EQ.4) THEN
                 BND = 2
              ELSE
                 BND = 1
              ENDIF
              I1X = NX + B(BND,J,1)
              I2X = NX + B(BND,J,2)
              I1Y = NY + B(BND,J,3)
              I2Y = NY + B(BND,J,4)
           ELSE
              I1X = NX + A(BND,J,JKJ,1)
C             I1X,I1Y = start
              I2X = NX + A(BND,J,JKJ,3)
C             I2X,I2Y = end
              I1Y = NY + A(BND,J,JKJ,2)
              I2Y = NY + A(BND,J,JKJ,4)
           ENDIF
C          Do the actual drawing here:
           CALL MOVABS(I1X,I1Y)
           CALL LNABS(I2X,I2Y)
C        Close NLINES loop
1153     CONTINUE
C       Replace old data in array.
CXT     Directional defaults for wedge bonds are set.
        IF ((IBTYPE.EQ.6).AND.((INCX.LT.0).OR.(INCX+INCY.LT.0)).AND.
     *     (.NOT.RDBACK)) THEN
           ZBTYPE = 7
           ZBDIR = IBDIR + 4
           IF (ZBDIR.GT.8) ZBDIR = ZBDIR - 8
        ELSE IF ((IBTYPE.EQ.7).AND.((INCX.LT.0).OR.(INCX+INCY.LT.0))
     *     .AND.(.NOT.RDBACK)) THEN
           ZBTYPE = 6
           ZBDIR = IBDIR + 4
           IF (ZBDIR.GT.8) ZBDIR = ZBDIR - 8
        ELSE
           ZBTYPE = IBTYPE
           ZBDIR = IBDIR
        ENDIF
        MM(LX,LY)=2**8*ZBTYPE + ZBDIR
        CALL SETLNS(1)
C       Return to solid linetype
635     CONTINUE
        IF (IBTYPE.EQ.0) MM(LX,LY) = 0
        LX=LX+INCX
        LY=LY+INCY
        IF (MM(LX,LY).LE.-256) GO TO 200
C       Do next piece of bond.
645     IF (RETR) THEN
           CALL VLNCE(1,IX,IY,0,0,IERR)
        ELSE
           CALL VALNCE(1,IX,IY,0,0)
        ENDIF
        IX = LX
        IY = LY
```

```
      IF (LBLEN.GT.0) CALL RELONG
      ICUR = 0
      CALL CURSOR(IX,IY)
      SKIP = .FALSE.
      RETURN
      END
C
      SUBROUTINE DRAW2(LX,LY,MBOND)
      IMPLICIT INTEGER*2 (A-Z)
      REAL A
      INTEGER*4 MM
      COMMON /CD/ MAXX,MAXY
C     LX represents MX, MX+1, NX, etc. as location of former H or subscript.
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /RANGE/ LOX,HIX,LOY,HIY
      COMMON /SIZZE/ MULTX,MULTY
      COMMON /IOFFST/IOFF
C     Line segments to draw bonds--see DRAW.
      COMMON /BONDS/ A(5,3,4,4),B(2,3,4)
C
C  This routine draws in individual bond segments at location LX,LY,
C  and of the form of bond MBOND.
C  It is patterned after the drawing routines in subroutine DRAW, but is
C  simplified, and is used primarily to fill in gaps in bonds of length
C  3 or more made when an H or numerical subsript is erased when
C  drawing a bond from a node in subroutine DRAW.
C
C  The type and direction of bond to be used as filler is supplied as
C  MBOND by the calling program.
C
C     END DRAWing if it isn't a bond.
      IF (MBOND.LT.256) RETURN
      IF (LX.LT.LOX) THEN
         LOX = LX
      ELSE IF (LX.GT.HIX) THEN
         HIX = LX
      ENDIF
      IF (LY.LT.LOY) THEN
         LOY = LY
      ELSE IF (LY.GT.HIY) THEN
         HIY = LY
      ENDIF
C     Extract bond type
      KBTYPE = MBOND/2**8
C     Extract bond direction
      KBDIR = MBOND - KBTYPE*2**8
C     Put data in permanent array
      MM(LX,LY) = MBOND
C
C  Conversion of bond type to the first coordinate of 'A' (drawing coordin-
C  ate array:
      IBOND=1
C     IBOND is 1st coord of A; max 5
      IF (KBTYPE.LE.3) IBOND=KBTYPE
C     Wedges:
      IF ((KBTYPE.EQ.6) .OR. (KBTYPE.EQ.7)) IBOND=KBTYPE-2
C
C     Number of line segments req'd to draw the bond-Max 3
      NLINES=3
C     single=1; double=2 line segments
      IF (IBOND.LE.2) NLINES=IBOND
C
C     Set line type if necessary to change:
C     Go to solid line type first
      CALL SETLNS(1)
C     Set dashed line for stereo down
      IF (KBTYPE.EQ.5) CALL SETLNS(2)
C
C     Correct direction error for wedge bond inherent in A array in DRAW:
      JKL=KBDIR
      JKM = KBDIR
      IF (JKL.GT.4) JKL=JKL-4
      IF ((IBOND.GE.4) .AND. (KBDIR.GT.4)) IBOND= 9 - IBOND
C
C     Start drawing the bond:
      NX=LX*MULTX - 8*IOFF
```

```
C       Screen coordinates of lower left corner of 7x10 area
        NY=LY*MULTY - 11*IOFF
        IF (KBTYPE.EQ.8) GO TO 40
C       Draw each segment separately
        DO 153 J=1,NLINES
           IF (MOD(JKM,2).EQ.1) THEN
              JKJ = JKL
              IF ((IBOND.EQ.5).AND.(JKM.EQ.1)) THEN
                 BND = 4
              ELSE IF ((IBOND.EQ.4).AND.(JKM.EQ.1)) THEN
                 BND = 5
              ELSE
                 BND = IBOND
              ENDIF
           ELSE
              BND = IBOND
              IF (JKL.EQ.2) THEN
                 JKJ = 4
              ELSE IF (JKL.EQ.4) THEN
                 JKJ = 2
              ENDIF
           ENDIF
           IF ((JKM.EQ.5).AND.((IBOND.EQ.4).OR.(IBOND.EQ.5))) THEN
              IF (IBOND.EQ.4) THEN
                 BND = 2
              ELSE
                 BND = 1
              ENDIF
              I1X = NX + B(BND,J,1)
              I2X = NX + B(BND,J,2)
              I1Y = NY + B(BND,J,3)
              I2Y = NY + B(BND,J,4)
           ELSE
C             Calc plotting coords
              I1X = NX + A(BND,J,JKJ,1)
C             I1X,I1Y = start
              I2X = NX + A(BND,J,JKJ,3)
C             I2X,I2Y = end
              I1Y = NY + A(BND,J,JKJ,2)
              I2Y = NY + A(BND,J,JKJ,4)
           ENDIF
C          Do the actual drawing here:
           CALL MOVABS(I1X,I1Y)
           CALL LNABS(I2X,I2Y)
C       Close NLINES loop
153     CONTINUE
        GO TO 70
C       DRAWING OF TYPE 8 BOND - WIGGLY LINE
C       draw each segment separately
40      DO 66 J=1,3
           IF (J.EQ.1) CALL SETLNS(2)
           IF (J.EQ.2) CALL SETLNS(1)
           IF (J.EQ.3) CALL SETLNS(3)
C          Calculate plotting
           IF (MOD(JKM,2).EQ.1) THEN
              JKJ = JKL
           ELSE
              IF (JKL.EQ.2) THEN
                 JKJ = 4
              ELSE IF (JKL.EQ.4) THEN
                 JKJ = 2
              ENDIF
           ENDIF
           I1X = NX + A(3,J,JKJ,1)
C          Coodinates;1=start
           I2X = NX + A(3,J,JKJ,3)
C          2=end
           I1Y = NY + A(3,J,JKJ,2)
           I2Y = NY + A(3,J,JKJ,4)
           CALL MOVABS(I1X,I1Y)
           CALL LNABS(I2X,I2Y)
66      CONTINUE
```

```
70          CONTINUE
C           Return to solid linetype
            CALL SETLNS(1)
         RETURN
         END
C
         SUBROUTINE DRAW(KAR,IX,IY,INCX,INCY)
         IMPLICIT INTEGER*2 (A-Z)
         REAL A
         INTEGER*4 MM,IDTPIX,LLUP,LLDN
         LOGICAL*2 NEWO,PCROS,XCROS,RDBACK,BONDEL,SKIP,BARR,RETR,NEWDIR
         CHARACTER*1 HALO(3)
         CHARACTER*1 KAN
         CHARACTER*3 HALOE
         COMMON /CD/ MAXX,MAXY
         COMMON /IOFFST/IOFF
         COMMON /RANGE/ LOX,HIX,LOY,HIY
         COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
         COMMON /SIZZE/ MULTX,MULTY
         COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
         COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
         COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
C        Relative coords for dwg bonds in 7x10 areas
         COMMON /BONDS/ A(5,3,4,4),B(2,3,4)
C        0,0 in lower left corner.
C        1st coord is bondtype (1=single,2=double,3=triple,4=wedge in,5=Out)
C        2nd coord is line segment # for dwg each bond (eg triple has 3segments)
C        3rd coord is bond direction, modulo 4 (up=1)
C        4th coord is Xstart,Ystart,Xend,Yend drawing coordinates.
         COMMON /LABELS/ NR,NJLAST,NJNEXT
         COMMON /HEAD/ MW(12),ISTATE,PAGE
         COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
         COMMON /WARN/ ERR
         COMMON /ITERM/ ITER
         COMMON /CUR/ ICUR
         COMMON /OLD/ IOX,IOY
CXT      OCUR is set by SUBROUTINES RING and CHAIN to darken cursor and
CXT      facilitate ring and chain bond drawing.
         COMMON /DARK/ OCUR
         COMMON /ELECHR/ IELEM(126,5)
CXT      RDBACK = TRUE indicates to SUBROUTINE REDRAW that a bond is
CXT      being patched.
         COMMON /PTCH/ RDBACK
CXT
CXT      NEWBND is set by SUBROUTINE REPEAT to indicate the drawing of a
CXT      new bond.
         COMMON /REPBND/ NEWBND
CXT
CXT      MLARGE is passed to SUBROUTINE VALNCE to note the distance between
CXT      the cursor and the node whose valence hydrogens are computed.
         COMMON /VLNPRV/ MLARGE
CXT
CXT      BONDEL = TRUE if a bond has been drawn between 2 nodes so a
CXT      subsequent deletion will delete the bond, not a node.
         COMMON /DELBND/ BONDEL
CXT
CXT      SKIP informs SUBROUTINE REDRAW that a retracing, not a replacing
CXT      of a bond with a bond of type 0 occurs.
         COMMON /BOSKIP/ SKIP
CXT
CXT      BARR in used in conjunction with NOCHG to set bond types in
CXT      relation to their defaults.
         COMMON /BTPDIR/ BARR
CXT
CXT      RETR is set by SUBROUTINE RETRIEVE to replace screen values
CXT      with SUBROUTINE REPLCE involving both array MM and array IDTPIX.
         COMMON /RETDRW/ RETR
C
         EQUIVALENCE (HALOE,HALO(1))
         HALO(1) = KAN
         HALO(3) = KAN
         IERR = 0
```

```
C Skip following code if not a bond.
        IF (ICHAR.NE.1) GO TO 10
        BEGX = IX
        BEGY = IY
        RETR = .FALSE.
        SKIP = .FALSE.
        RDBACK = .FALSE.
        NEWDIR = .FALSE.
        IF (MM(IX,IY).EQ.42) THEN
           IERR = 25
           CALL MYERR(IERR,IERR,IERR)
           ICHAR = JCHAR
           KAR = MCHAR
           IBDIR = JBDIR
           RETURN
        ENDIF
C X & Y increment depend on bond direction.
        INCY = -1*ITER
        IF ((IBDIR.GE.4).AND.(IBDIR.LE.6)) INCY = 1*ITER
        IF (MOD(IBDIR,4).EQ.3)  INCY=0
        INCX=1
        IF ((IBDIR.GE.6) .AND. (IBDIR.LE.8)) INCX=-1
        IF (MOD(IBDIR,4).EQ.1) INCX=0
C
        CALL CONTEX(KAR,IX,IY,INCX,INCY,IERR)
        IF (IERR.NE.48) GO TO 11448
        CALL MYERR(IERR,IERR,IERR)
        DBDIR = JBDIR
        CALL DELTA(DBDIR,INCX,INCY)
        IX = IOX
        IY = IOY
        IF (LMM(IX-INCX,IY-INCY).GE.256) THEN
           JCHAR = 1
           CALL DEL(KAR,IX,IY,INCX,INCY,0)
           JCHAR = 2
        ENDIF
        CALL CURSOR(IX,IY)
        ICHAR = JCHAR
        KAR = MCHAR
        IBDIR = JBDIR
        RETURN
C
11448   IF ((ICHAR.EQ.2).AND.(MCHAR.LT.0)) RETURN
        JIX = IX - INCX
        JIY = IY - INCY
        IF (MM(JIX,JIY).NE.0) GO TO 11446
        CALL MARK(KAR,JIX,JIY,IERR)
        IF (IERR.NE.48) GO TO 11446
           CALL MYERR(IERR,IERR,IERR)
           ICUR = 1
        IX=IOX
        IY=IOY
           CALL CURSOR(IX,IY)
           ICHAR = JCHAR
           KAR = MCHAR
           IBDIR = JBDIR
           RETURN
11446   CONTINUE
        NEWX = IX + INCX
        NEWY = IY + INCY
        IF ((NEWX.LE.0).OR.(NEWX.GT.MAXX).OR.(NEWY.LE.0).OR.
     *     (NEWY.GT.MAXY)) THEN
           IERR = 36
           CALL MYERR(IERR,KAR,KAR)
           IX = IOX
           IY = IOY
          CALL CURSOR(IX,IY)
          ICHAR = JCHAR
          KAR = MCHAR
          IBDIR = JBDIR
          RETURN
        ELSE IF ((MM(IX,IY).EQ.46).OR.((MM(IX,IY).GE.65).AND.
     *     (MM(IX,IY).LE.90).AND.((MM(IX,IY).NE.72).OR.
     *     ((MM(IX+1,IY).GE.97).AND.(MM(IX+1,IY).LE.122))))
```

```
*       THEN
          IERR = 40
          CALL MYERR(IERR,KAR,KAR)
          IX = IOX
          IY = IOY
          ICUR = 1
          CALL CURSOR(IX,IY)
          ICHAR = JCHAR
          KAR = MCHAR
          IBDIR = JBDIR
          RETURN
        ELSE IF (IBTYPE.EQ.0) THEN
          KX = IX
          KY = IY
987       IF (MM(KX,KY).EQ.0) THEN
            NEWO = .TRUE.
            GO TO 804
          ELSE IF (LMM(KX,KY).GT.256) THEN
            DIR = MM(KX,KY)
            IF (MOD(IDIR(DIR),4).EQ.MOD(IBDIR,4)) THEN
              NEWO = .FALSE.
            ELSE
              NEWO = .TRUE.
            ENDIF
          ELSE
            KX = KX + INCX
            KY = KY + INCY
            GO TO 987
          ENDIF
        ELSE
          NEWO = .FALSE.
        ENDIF
C       Ret bondtype to 1
        IF ((NOCHG.EQ.0).AND.(IBTYPE.NE.0).AND.(IBTYPE.NE.4).AND.
     2     (IBTYPE.NE.8)) IBTYPE=1
C                or newly-entered number
C
        IBOND = 1
        NLINES = 1
C number of line segments req'd to draw bond--max 3
        IF (IBTYPE.EQ.3) THEN
          NLINES=3
          IBOND = 3
C double bond needs 2 line segments
        ELSE IF (IBTYPE.EQ.2) THEN
          NLINES=2
          IBOND = 2
        ELSE IF (IBTYPE.EQ.6) THEN
          IBOND=4
          NLINES = 3
        ELSE IF (IBTYPE.EQ.7) THEN
          IBOND=5
          NLINES = 3
C single or stereo
        ELSE IF (IBTYPE.EQ.4) THEN
          GOTO 805
        ENDIF
C Following code (thru label 804) handles bond type 4:
C
C Conversion of bond type to first A array coordinate value IBOND:
C
        JKL=IBDIR
        JKM = IBDIR
        IF (JKL.GT.4) JKL=JKL-4
        IF ((IBOND.GE.4).AND.(IBDIR.GT.4)) IBOND=9-IBOND
        GOTO 804
805     KX=IX-INCX
        KY=IY-INCY
C Search around node
        DO 3 IDIRX=-1,1
        DO 3 IDIRY=-1,1
        IF ((IDIRX.EQ.0) .AND. (IDIRY.EQ.0)) GOTO 3
C Nearby array location to look for bonds
        NEWX=KX + IDIRX
        NEWY=KY + IDIRY
```

```
C Off the edge
802     IF ((NEWY.LT.1) .OR. (NEWY.GT.MAXY))  GOTO 3
        IF ((NEWX.LT.1) .OR. (NEWX.GT.MAXX)) GOTO 3
C Blank space
        IF (MM(NEWX,NEWY).EQ.0) GOTO 3
C Bonds are >256
        IF (LMM(NEWX,NEWY).GT.256)  GOTO 806
C Look beyond characters
        NEWY=NEWY+IDIRY
        NEWX=NEWX+IDIRX
        GOTO 802
C Bond extracted for type
806     JBOND=LMM(NEWX,NEWY)/2**8
C Not a double bond
        IF ((JBOND.NE.2).AND.(JBOND.NE.3)) GOTO 3
C Following 5 lines skip bonds not pointed to node being analyzed:
C Direction of bond
        JDIR=LMM(NEWX,NEWY)-JBOND*2**8
        IF ((IDIRX*IDIRY.EQ.-1).AND.(MOD(JDIR,4).NE.2)) GO TO 3
        IF ((IDIRX*IDIRY.EQ.1).AND.(MOD(JDIR,4).NE.0)) GO TO 3
        IF ((IDIRX.EQ.0) .AND. (MOD(JDIR,4).NE.1)) GOTO 3
        IF ((IDIRY.EQ.0) .AND. (MOD(JDIR,4).NE.3)) GOTO 3
        NLINES=1
        IBOND=1
        JKL = IBDIR
        JKM = IBDIR
        IF (JKL.GT.4) JKL = JKL - 4
        GOTO 803
3       CONTINUE
C
C See if there exists a double or triple longbond at this node
C
        DO 40 I=0,2,2
        DO 4141 J=1,100
        IF (LNGBND(J,I+1) .EQ. 0) GO TO 40
        IF ((LNGBND(J,I+1) .NE. KX) .OR.
     1  (LNGBND(J,I+2) .NE. KY)) GO TO 4141
        IF (LNGBND(J,5) .NE. 2 .AND. LNGBND(J,5) .NE. 3) GO TO 4343
        IBOND=1
        NLINES=1
        GO TO 44
4141    CONTINUE
40      CONTINUE
C
4343    IBOND=2
        NLINES=2
44      JKL=IBDIR
        JKM = IBDIR
        IF (JKL.GT.4) JKL=JKL-4
803     IF (LMM(IX-INCX,IY-INCY).LE.256) GOTO 804
C Bond type of immediate preceeding.
        IBT4=LMM(IX-INCX,IY-INCY)/2**8
C       bond, if no dot or marker interposed.
        IBOND=IBT4
        NLINES=IBT4
C Check for DOTDIS structure.
804     CONTINUE
        DO 444 JJ = 1,MAXX
           IF ((MM(BEGX-JJ,BEGY).EQ.0).OR.(LMM(BEGX-JJ,BEGY).GE.256).OR.
     *        (BEGX-JJ.LE.0)) THEN
              GO TO 445
           ELSE IF (MM(BEGX-JJ,BEGY).EQ.42) THEN
              IERR = 25
              CALL MYERR(IERR,IERR,IERR)
              IX = IOX
              IY = IOY
              KAR = MCHAR
              ICHAR = JCHAR
              IBDIR = JBDIR
              CALL SETLNS(1)
              ICUR = 1
              CALL CURSOR(IX,IY)
              RETURN
           ENDIF
```

```
444     CONTINUE
445     CONTINUE
C
C
C Start drawing bonds:
C Enlargement factor NLARGE
        DO 5 I = 1,NLARGE
           II = I
           ICUR = 0
           CALL CURSOR(IX,IY)
C Don't do any redrawing if retracing your path.
C Null bond type
        IF ((IBTYPE.EQ.0).AND.(.NOT.NEWO)) THEN
           IF (I.EQ.1) THEN
              KX = IX - INCX
              KY = IY - INCY
              CALL CLRHYD(KX,KY)
           ENDIF
           GO TO 7777
        ENDIF
C Only eliminate H's once.
        IF (I.GT.1) GO TO 1236
C Erease all H's & subscripts.
        KX=IX-INCX
        KY=IY-INCY
C Only @ nodes
        IF ((MM(KX,KY).LT.65) .OR. (MM(KX,KY).GT.90)) GOTO 43
C
        CALL CLRHYD(KX,KY)
C
C At this point filler H's are removed; IX and IY are
C poised at first position for new (or retraced) bond. If MM(IX,IY)=0,
C skip to 41 & just draw the bond.  If not, glide along it to next
C node or empty space, reset ICHAR accordingly, and leave this subroutine:
C Move one right if 2-letter element & bond dir=3
43      IF ((IBDIR.EQ.3).AND.(MM(IX,IY).GE.97).AND.(MM(IX,IY).LE.122))
     2     IX=IX+1
        IXX=IX
        IYY=IY
        IF (MM(IX,IY).EQ.0) GOTO 1232
C Save first position of bond being traced over
C Existing bond type
        DIR = LMM(IX,IY)
CXT
CXT
        IF ((DIR.LT.256).OR.(MOD(IBDIR,4).NE.MOD(IDIR(DIR),4))) GO TO 52
CXT
        NBTYPE=DIR/2**8
C Following line takes care of wedge in-from looks like wedge out-to.
        IF ((NBTYPE*IBTYPE.EQ.36).OR.(NBTYPE*IBTYPE.EQ.49)) GOTO 75
C Don't redraw if same bondtype
        IF ((NBTYPE.EQ.IBTYPE).OR.((OCUR.EQ.0).AND.(.NOT.BARR))) THEN
           IF (OCUR.EQ.0) NEWDIR = .TRUE.
           GOTO 52
        ENDIF
        IF (IBTYPE.EQ.4 .AND.(NBTYPE.EQ.2.OR.NBTYPE.EQ.1))GOTO 52
C Don't redraw if bondtype = alternating and existing bond is single or
C double.
C These 4 lines of code allow change of bond
75      DO 123 K=1,260
C Type only if starting @ marker.
        IF (LABL(K,1).EQ.0) GOTO 52
        IF ((KX.EQ.LABL(K,1)).AND.(KY.EQ.LABL(K,2))) GOTO 74
123     CONTINUE
C Redraw new bond 'over' old
74      CONTINUE
        IF (LMM(KX+INCX,KY+INCY).GE.256) THEN
           CALL REDRAW(IX,IY,INCX,INCY,NBTYPE)
           IF (OCUR.EQ.1) NOCHG = 0
C Don't increment past first bond segment first time.
           GOTO 52
        ELSE
           IX = KX
           IY = KY
        ENDIF
```

```
C Track along bond till its end
51      CONTINUE
        IX=IX+INCX
        IY=IY+INCY
C Shorthand for seeing what is on bond's track
52      CONTINUE
        LL=LMM(IX,IY)
        L2=LMM(IX+1,IY)
     IF ((LL.EQ.43).OR.(LL.EQ.45).OR.(LL.EQ.34).OR.
  *     ((LL.GE.49).AND.(LL.LE.57).AND.((MOD(IBDIR,4).NE.3).OR.
  *     (MM(IX-1,IY).NE.72)))) THEN
        IERR = 45
        CALL MYERR(IERR,IERR,IERR)
        IF (LMM(IX-INCX,IY-INCY).GE.256) THEN
           JCHAR = 1
           CALL DEL(KAR,IX,IY,INCX,INCY,0)
           JCHAR = 2
        ELSE
           IX = IOX
           IY = IOY
        ENDIF
        ICUR = 1
        CALL CURSOR(IX,IY)
        KAR = MCHAR
        ICHAR = JCHAR
        IBDIR = JBDIR
        CALL SETLNS(1)
        RETURN
     ENDIF
825  CONTINUE
C See if bond intersection is on bond path.
     IF ((LL.GT.256).AND.(MOD(IBDIR,4).NE.MOD(IDIR(LL),4))) THEN
        IERR = 23
        CALL MYERR(IERR,IERR,IERR)
        IF ((LMM(IX-INCX,IY-INCY).GE.256).AND.
  *        ((LMM(IX,IY).GE.256).OR.(MM(IX,IY).EQ.0))) THEN
           JCHAR = 1
           CALL DEL(KAR,IX,IY,INCX,INCY,0)
           JCHAR = 2
        ELSE
            IX = IOX
            IY = IOY
        ENDIF
        KAR = MCHAR
        ICHAR = JCHAR
        IBDIR = JBDIR
        CALL SETLNS(1)
        ICUR = 1
        CALL CURSOR(IX,IY)
        RETURN
     ENDIF
C Following line bypasses bond segments, numerals, lowercase, and H's
C not followed by lowercases, inorder to find the 'other' end of bond:
     IF (((LL.NE.0).AND.(LL.NE.46).AND.(LL.NE.63).AND.(LL.LT.65))
  *     .OR.(LL.GT.90).OR.((LL.EQ.72).AND.((L2.LT.97).OR.
  *     (L2.GT.122)))) GO TO 51
     CALL VALNCE(2,IXX,IYY,INCX,INCY)
     ICUR = 1
     CALL CURSOR(IX,IY)
C Bond tracked to empty slot.
     IF (MM(IX,IY).EQ.0) THEN
        CALL SETLNS(1)
        RETURN
     ENDIF
C New location is already a node
     ICHAR=2
     IF (IBTYPE.NE.0) BONDEL = .TRUE.
C This part of code simulates IDENT.
     KAR=LMM(IX,IY)
C Tentative location, as if after typing uppercase.
     IX=IX+1
     CALL CURSOR(IX,IY)
     CALL SETLNS(1)
     RETURN
C Back to jam mode
```

```
1232    CONTINUE
        DISTX = NLARGE * INCX + IX
        DISTY = NLARGE * INCY + IY
        IF ((DISTX.GE.2).AND.(DISTX.LT.MAXX).AND.(DISTY.GE.2).AND.
     *     (DISTY.LT.MAXY)) GO TO 1235
        IF (((IX.LE.1).AND.(IBDIR.GE.6)).OR.((IY.GE.MAXY).AND.
     *     (IBDIR.GE.4).AND.(IBDIR.LE.6)).OR.((IY.LE.1).AND.
     *     ((IBDIR.LE.2).OR.(IBDIR.EQ.8))).OR.((IX.GE.MAXX).AND.
     *     (IBDIR.GE.2).AND.(IBDIR.LE.4)).OR.
     *     (DISTX.GT.MAXX).OR.(DISTX.LT.1).OR.(DISTY.GT.MAXY).OR.
     *     (DISTY.LT.1)) THEN
           IF (((MM(IOX,IOY).LT.256).AND.(NLARGE.EQ.1).AND.
     *        (DISTX.LT.1).AND.(IOX.EQ.2).AND.(IBDIR.GE.6)).OR.
     *        ((DISTY.LT.1).AND.(IY.LE.2).AND.((IBDIR.LE.2).OR.
     *        (IBDIR.EQ.8)))) THEN
              GO TO 1233
           ELSE IF ((NLARGE.EQ.1).AND.(JCHAR.EQ.1).AND.
     *     (IBDIR.EQ.JBDIR).AND.(IBTYPE.EQ.JBTYPE)) THEN
               IF ((IBDIR.GE.4).AND.(IBDIR.LE.6).AND.
     *            (DISTY.LE.MAXY)) GO TO 1234
               IF ((DISTX.LT.1).OR.(DISTX.GE.MAXX).OR.(DISTY.LT.1)
     *            .OR.(DISTY.GT.MAXY)) GO TO 1233
           ENDIF
           IF ((IY.LE.1).AND.((DISTX.LE.1).OR.(DISTX.GE.MAXX)))
     *        THEN
              GO TO 1233
           ELSE IF ((IY.GE.MAXY).AND.((DISTX.LE.1).OR.
     *        (DISTX.GE.MAXX))) THEN
              GO TO 1233
           ELSE IF ((IX.LE.1).AND.((DISTY.LE.1).OR.(DISTY.GE.MAXY)))
     *        THEN
              GO TO 1233
           ELSE IF ((IX.GE.MAXX).AND.((DISTY.LE.1).OR.
     *        (DISTY.GE.MAXY))) THEN
              GO TO 1233
           ENDIF
           IF (((IX.GE.MAXX).OR.(IX.LE.1)).AND.(INCX.EQ.0))
     *        GO TO 1234
           IF (((IY.GE.MAXY).OR.(IY.LE.1)).AND.(INCY.EQ.0))
     *        GO TO 1234
1233       CALL MYERR(36,KAR,KAR)
           IX = IOX
           IY = IOY
           ICUR = 1
           CALL CURSOR(IX,IY)
           ICHAR = JCHAR
           KAR = MCHAR
           IBDIR = JBDIR
           CALL SETLNS(1)
           RETURN
1234     CONTINUE
        ENDIF
1235  CONTINUE
C
C The drawing of overlapping bonds is prevented.
      GIX = IX
      GIY = IY
      XCROS = .FALSE.
      PCROS = .FALSE.
1237  CONTINUE
      GOX = GIX + 1
      NOX = GIX - 1
      GOY = GIY + 1
      NOY = GIY - 1
C
C This segment prevents the overlapping of diagonal bonds when one
C node lies adjacent to a non attaching bond. OCUR is checked to
C disable the segment during chain and ring drawing.
      DIR1 = LMM(GOX,GIY)
      DIR2 = LMM(GIX,GOY)
      DIR3 = LMM(NOX,GIY)
      DIR4 = LMM(GIX,NOY)
      IF ((OCUR.EQ.1).AND.((MM(GIX,GIY).EQ.0).OR.(LMM(GIX,GIY).GT.256))
     *   .AND.(MOD(IBDIR,2).EQ.0).AND.
     *   (((DIR1.GE.256).AND.
     *   (MOD(IDIR(DIR1),2).EQ.0).AND.
```

```
     *   (MOD(IBDIR,4).NE.MOD(IDIR(DIR1),4))).OR.
     *   ((DIR2.GE.256).AND.
     *   (MOD(IDIR(DIR2),2).EQ.0).AND.
     *   (MOD(IBDIR,4).NE.MOD(IDIR(DIR2),4))).OR.
     *   ((DIR3.GE.256).AND.
     *   (MOD(IDIR(DIR3),2).EQ.0).AND.
     *   (MOD(IBDIR,4).NE.MOD(IDIR(DIR3),4))).OR.
     *   ((DIR4.GE.256).AND.
     *   (MOD(IDIR(DIR4),2).EQ.0).AND.
     *   (MOD(IBDIR,4).NE.MOD(IDIR(DIR4),4)))))
     *   XCROS = .TRUE.
C
C Diagonal overlaps are prevented.
      IF (PCROS) XCROS = .TRUE.
      DIR1 = LMM(GIX,GIY+INCX)
      DIR2 = LMM(GIX+INCX,GIY)
      IF ((MOD(IBDIR,2).EQ.0).AND.
     *   (((DIR1.GE.256).AND.
     *   (MOD(IDIR(DIR1),2).EQ.0).AND.
     *   (MOD(IBDIR,4).NE.MOD(IDIR(DIR1),4))).OR.
     *   ((DIR2.GE.256).AND.
     *   (MOD(IDIR(DIR2),2).EQ.0).AND.
     *   (MOD(IBDIR,4).NE.MOD(IDIR(DIR2),4)))))
     *   PCROS = .TRUE.
      IF (IBDIR.EQ.7) THEN
         GX = GIX - 1
      ELSE
         GX = GIX
      ENDIF
C
C Attempted overlap meets error message.
      IF (((MM(GX,GIY).NE.0).OR.(XCROS)).AND.((ISTATE.NE.9).OR.
     *   ((ISTATE.EQ.9).AND.(NEWBND.EQ.1)))) THEN
         DIR1 = LMM(GX,GIY)
         DIR2 = LMM(GX-2*INCX,GIY-2*INCY)
         IF (((DIR1.GE.256).AND.(MOD(IBDIR,4).NE.MOD(IDIR(DIR1),4)))
     *      .OR.XCROS) THEN
            IERR = 23
            CALL MYERR(IERR,IERR,IERR)
            IF (OCUR.EQ.0) GO TO 1239
            IF ((LMM(IX-INCX,IY-INCY).GE.256).AND.
     *         ((LMM(IX,IY).GE.256).OR.(MM(IX,IY).EQ.0))) THEN
               JCHAR = 1
               CALL DEL(KAR,IX,IY,INCX,INCY,0)
               JCHAR = 2
            ELSE
               IX = IOX
               IY = IOY
            ENDIF
            KAR = MCHAR
            ICHAR = JCHAR
            IBDIR = JBDIR
            CALL SETLNS(1)
            ICUR = 1
            CALL CURSOR(IX,IY)
            RETURN
C Check for need of bond patching.
         ELSE IF ((DIR1.GE.256).AND.(DIR2.GE.256).AND.
     *      (MOD(IDIR(DIR1),4).EQ.MOD(IDIR(DIR2),4)).AND.
     *      ((DIR1/256.EQ.DIR2/256).OR.((DIR1/256+DIR2/256.EQ.13).AND.
     *      ((DIR1/256.EQ.6).OR.(DIR2/256.EQ.6))))) THEN
            IBTYPE = DIR2 / 256
            NBTYPE = DIR1 / 256
            MM(GX-INCX,GIY-INCY) = DIR2
            DBDIR = IDIR(DIR2)
            CALL DELTA(DBDIR,INCX,INCY)
            IBDIR = DBDIR
            DO 3400 LL = 1,MAXX
               LX = GX - LL*INCX
               LY = GIY - LL*INCY
               IF ((MM(LX,LY).EQ.0).OR.(MM(LX,LY).EQ.46).OR.
     *            (MM(LX,LY).EQ.63).OR.((MM(LX,LY).GE.65).AND.
     *            (MM(LX,LY).LE.90))) THEN
                  IX = LX + INCX
```

```
               IY = LY + INCY
               GO TO 3410
             ENDIF
3400       CONTINUE
3410       CONTINUE
           RDBACK = .TRUE.
           CALL REDRAW(IX,IY,INCX,INCY,NBTYPE)
           CALL VALNCE(2,LX,LY,INCX,INCY)
           CALL SETLNS(1)
           ICUR = 1
           CALL CURSOR(IX,IY)
           RETURN
         ENDIF
1239   CONTINUE
       ENDIF
       GIX = GIX + INCX
       GIY = GIY + INCY
       IF ((GIX.EQ.DISTX+INCX).AND.(GIY.EQ.DISTY+INCY)) GO TO 1238
       IF ((MM(GIX,GIY).GT.0).AND.(MM(GIX,GIY).LT.256)) GO TO 1238
       GO TO 1237
1238   CONTINUE
       IF (DISTX.LT.LOX) THEN
          LOX = DISTX
       ELSE IF (DISTX.GT.HIX) THEN
          HIX = DISTX
       ENDIF
       IF (DISTY.LT.LOY) THEN
          LOY = DISTY
       ELSE IF (DISTY.GT.HIY) THEN
          HIY = DISTY
       ENDIF
1236   CONTINUE
       IF (NEWO) THEN
          IF (I.EQ.1) THEN
             GIX = DISTX
             GIY = DISTY
          ENDIF
          GO TO 778
       ENDIF
C Draw in jam mode, solid line.
         CALL SETMOD(4)  !Set JAM mode
         CALL SETLNS(1)
C Define & select dashed line--stereo
       IF (IBTYPE.EQ.5) CALL SETLNS(2)
C Scale to graphic coordinates
         NX = IX * MULTX -  8*IOFF
         NY = IY * MULTY - 11*IOFF
         IF (IBTYPE .EQ. 8) GO TO 77
C        Draw each segment separately
C
         DO 6 J=1,NLINES
            IF (MOD(JKM,2).EQ.1) THEN
               IF ((IBTYPE.EQ.6).AND.(JKM.EQ.1)) THEN
                  BND = 5
               ELSE IF ((IBTYPE.EQ.7).AND.(JKM.EQ.1)) THEN
                  BND = 4
               ELSE
                  BND = IBOND
               ENDIF
               IF ((JKM.EQ.5).AND.((IBTYPE.EQ.6).OR.(IBTYPE.EQ.7))) THEN
                  IF (IBOND.EQ.4) THEN
                     BND = 2
                  ELSE
                     BND = 1
                  ENDIF
                  I1X = NX + B(BND,J,1)
                  I2X = NX + B(BND,J,2)
                  I1Y = NY + B(BND,J,3)
                  I2Y = NY + B(BND,J,4)
               ELSE
C                 Calculate plotting
                  I1X=NX + A(BND,J,JKL,1)
C                 Coodinates;1=start
                  I2X=NX + A(BND,J,JKL,3)
C                 2=end
```

```
            I1Y=NY + A(BND,J,JKL,2)
            I2Y=NY + A(BND,J,JKL,4)
         ENDIF
         CALL MOVABS(I1X,I1Y)
         CALL LNABS(I2X,I2Y)
      ELSE
         IF (JKL.EQ.2) THEN
            JKJ = 4
         ELSE IF (JKL.EQ.4) THEN
            JKJ = 2
         ENDIF
         I1X = NX + A(IBOND,J,JKJ,1)
         I2X = NX + A(IBOND,J,JKJ,3)
         I1Y = NY + A(IBOND,J,JKJ,2)
         I2Y = NY + A(IBOND,J,JKJ,4)
         CALL MOVABS(I1X,I1Y)
         CALL LNABS(I2X,I2Y)
      ENDIF
C Draw bond line segment
6     CONTINUE
      GO TO 777
C
C DRAWING OF TYPE 8 BOND - WIGGLY LINE
C Draw each segment separately
77    DO 66 J=1,3
         IF (J.EQ.1) CALL SETLNS(2)
         IF (J.EQ.2) CALL SETLNS(1)
         IF (J.EQ.3) CALL SETLNS(3)
         IF (MOD(JKM,2).EQ.1) THEN
C           Calculate plotting
            I1X=NX + A(3,J,JKL,1)
C           coodinates;1=start
            I2X=NX + A(3,J,JKL,3)
C           2=end
            I1Y=NY + A(3,J,JKL,2)
            I2Y = NY + A(3,J,JKL,4)
            CALL MOVABS(I1X,I1Y)
            CALL LNABS(I2X,I2Y)
         ELSE
            IF (JKL.EQ.2) THEN
               JKJ = 4
            ELSE IF (JKL.EQ.4) THEN
               JKJ = 2
            ELSE
               JKJ = JKL
            ENDIF
            I1X = NX + A(3,J,JKJ,1)
            I2X = NX + A(3,J,JKJ,3)
            I1Y = NY + A(3,J,JKJ,2)
            I2Y = NY + A(3,J,JKJ,4)
            CALL MOVABS(I1X,I1Y)
            CALL LNABS(I2X,I2Y)
         ENDIF
66    CONTINUE
C
C Calculate 256(bond type1-8) + (bond direction) for storage in MM array.
C This is NOT the format required by the analysis program.
777   CONTINUE
         IF (IBTYPE.NE.4) THEN
CXT         Directional defaults for wedge bonds are set.
            IF ((IBTYPE.EQ.6).AND.((INCX.LT.0).OR.
     *         (INCX+INCY.LT.0))) THEN
               ZBTYPE = 7
               ZBDIR = IBDIR + 4
               IF (ZBDIR.GT.8) ZBDIR = ZBDIR - 8
            ELSE IF ((IBTYPE.EQ.7).AND.((INCX.LT.0).OR.
     *         (INCX+INCY.LT.0))) THEN
               ZBTYPE = 6
               ZBDIR = IBDIR + 4
               IF (ZBDIR.GT.8) ZBDIR = ZBDIR - 8
            ELSE
               ZBTYPE = IBTYPE
               ZBDIR = IBDIR
            ENDIF
            MM(IX,IY) = 2**8*ZBTYPE + ZBDIR
         ELSE
```

```
              MM(IX,IY)=2**8*IBOND + IBDIR
           ENDIF
C Analysis pgm has direc UP=DOWN=0 & max 3 [here UP=1, max 8 incr clkwise]
C Analysis pgm recognizes only 3 incoming bond types:single,double;trple
C Analysis pgm recognizes and converts some to tautomer(8), ring(1-3) etc.  Here,
C chain(5,6,7) and converts some to tautomer(8), ring(1-3) etc.  Here,
C bond types include stereo wedge bonds (6,7), dotted stereo(5),etc.
C
7       CONTINUE
C Move location counters
778     IX = IX + INCX
        IY = IY + INCY
C
        IF (((IX.EQ.GIX).AND.(IY.EQ.GIY)).OR.(MM(IX,IY).GT.0)) THEN
           MLARGE = I
           IF (MM(IX,IY).GT.0) NOCHG = 0
           GO TO 5555
        ENDIF
C Close NLARGE loop
5       CONTINUE
C
C
5555    CONTINUE
C Restore H('s)
        CALL VALNCE(1,IX,IY,INCX,INCY)
7777    CONTINUE
C
CXT Bond type 0 overskipping an existing bond (from a non-marker) occurs.
        IF ((IBTYPE.NE.0).OR.(NEWO)) GOTO 7778
           ICUR = 0
           CALL CURSOR(IX,IY)
C Only erase bond if starting at marker
           DO 779 K=1,260
C
              IF ((IX-INCX.EQ.LABL(K,1)).AND.(IY-INCY.EQ.LABL(K,2)))
     *           THEN
                 GO TO 780
              ELSE IF ((LABL(K,1).EQ.0).OR.(K.EQ.260)) THEN
                 SKIP = .TRUE.
                 GO TO 780
              ENDIF
779        CONTINUE
C This code skipped above
780        NBTYPE=LMM(IX,IY)/2**8
C
           IXX = KX + INCX
           IYY = KY + INCY
C When IBTYPE=0
           CALL REDRAW(IX,IY,INCX,INCY,NBTYPE)
           IF (OCUR.EQ.1) NOCHG = 0
           IF ((NBTYPE.GT.0).AND.(IBTYPE.EQ.0))
     *        CALL VALNCE(2,IXX,IYY,INCX,INCY)
C
7778    CONTINUE
        DO 1444 JJ = 0,MAXX
           IF ((MM(IX-JJ,IY).EQ.0).OR.(LMM(IX-JJ,IY).GE.256).OR.
     *        (IX-JJ.EQ.0)) THEN
              GO TO 1445
           ELSE IF (MM(IX-JJ,IY).EQ.42) THEN
              IERR = 25
              CALL MYERR(IERR,IERR,IERR)
              JCHAR = 1
              CALL DEL(KAR,IX,IY,INCX,INCY,0)
              JCHAR = 2
              KAR = MCHAR
              ICHAR = JCHAR
              IBDIR = JBDIR
              CALL SETLNS(1)
              ICUR = 1
              CALL CURSOR(IX,IY)
              RETURN
           ENDIF
1444    CONTINUE
1445    CONTINUE
```

```
C Following lines (through label 55) look for existing node @ end
C of newly drawn bond:
      IF (MM(IX,IY).EQ.0) GOTO 55
      MIX=IX
C SAVE OLD IX AND IY IN CASE WE CAN'T FIND NODE
      MIY=IY
56    LL=LMM(IX,IY)
      L2=LMM(IX+1,IY)
      L3 = LMM(IX+INCX,IY)
      IF ((LL.GT.0).AND.((LL.LE.48).AND.(LL.NE.46))) GO TO 5557
      IF ((LL.GE.97).AND.(LL.LE.122).AND.((MM(IX-1,IY).LT.65).OR.
     *   (MM(IX-1,IY).GT.90).OR.(IBDIR.NE.7)))
     *   GO TO 5557
C     Various ways to approach and identify node vs. non-node.
      IF (((LL.GE.65).AND.(LL.LE.90).AND.(LL.NE.72)) .OR. (LL.EQ.46)
     2    .OR. (LL.EQ.63) .OR. ((LL.EQ.72).AND.(L2.GE.97).AND.(L2.LE.
     3    122)).OR.(LL.GE.256)) GOTO 57
      IF ((LL.GE.49).AND.(LL.LE.57).AND.((IBDIR.NE.7).OR.
     *   (MM(IX-1,IY).NE.72))) GO TO 5557
      IF ((MOD(IBDIR,4).NE.3).AND.(MOD(IBDIR,4).NE.1)) GO TO 5557
      IF (((LL.GE.58).AND.(LL.LE.62)).OR.(LL.EQ.64).OR.
     *   ((LL.GE.91).AND.(LL.LE.96)).OR.(LL.GE.123)) GO TO 5557
      IF ((LL.EQ.72).OR.((LL.GE.49).AND.(LL.EQ.57))) THEN
         IF (IBDIR.EQ.7) THEN
            IF ((LL.GE.49).AND.(LL.LE.57)) THEN
               II = 2
            ELSE
               II = 1
            ENDIF
            IF ((MM(IX-II,IY).GE.65).AND.(MM(IX-II,IY).LE.122))
     *         THEN
               GO TO 57
            ELSE
               IX = IX + 1
               GO TO 5557
            ENDIF
         ELSE IF (IBDIR.EQ.3) THEN
            DO 915 II = 1,2
               IF ((MM(IX+II,IY).GE.65).AND.(MM(IX+II,IY).LE.90))
     *            GO TO 57
               IF (MM(IX+II,IY).EQ.0) GO TO 5557
915         CONTINUE
            GO TO 5557
         ELSE IF (IBDIR.EQ.1) THEN
            IF ((MM(IX,IY-1).GE.65).AND.(MM(IX,IY-1).LE.90))
     *         THEN
               IY = IY - 1
               GO TO 57
            ELSE
               IF ((MM(IX,IY+1).GE.65).AND.(MM(IX,IY+1).LE.90)) THEN
                  GO TO 55
               ELSE
                  GO TO 5557
               ENDIF
            ENDIF
         ELSE IF (IBDIR.EQ.5) THEN
            IF ((MM(IX,IY+1).GE.65).AND.(MM(IX,IY+1).LE.90))
     *         THEN
               IY = IY + 1
               GO TO 57
            ELSE
               IF ((MM(IX,IY+1).GE.65).AND.(MM(IX,IY+1).LE.90)) THEN
                  GO TO 55
               ELSE
                  GO TO 5557
               ENDIF
            ENDIF
         ELSE
            GO TO 5557
         ENDIF
      ENDIF
      IX=IX+INCX
      IY=IY+INCY
```

```
      IF (IX.GE.1.AND.IX.LE.MAXX.AND.IY.GE.1.AND.IY.LE.MAXY)
     1 GO TO 56
5557  CONTINUE
      IERR = 45
C Found space conflict - ERROR MESSAGE
      CALL MYERR(IERR,KAR,KAR)
      IF (LMM(IX-INCX,IY-INCY).GE.256) THEN
         JCHAR = 1
         CALL DEL(KAR,IX,IY,INCX,INCY,0)
         JCHAR = 2
      ELSE
         IX = MIX
         IY = MIY
      ENDIF
      GO TO 55
C Simulating IDENT as if this node were typed in
57    CONTINUE
      ICHAR=2
      IF (IBTYPE.NE.0) BONDEL = .TRUE.
      KAR=LL
C Tentative location after 'typing' node
      IX=IX+1
C Move cursor to new position
55    CONTINUE
      ICUR = 1
      CALL CURSOR(IX,IY)
      CALL HEADER
C Return to solid linetype (if nec)
      CALL SETLNS(1)
C End of normal bond drawing.
      RETURN
C
C Typed alphameric characters
10    CONTINUE
      ICUR = 1
      NOCHG = 0
      IF ((IX.GT.MAXX).OR.(IX.LT.1).OR.(IY.GT.MAXY).OR.(IY.LT.1))
     *   THEN
         IF ((IX.GT.MAXX).AND.(IY.GE.1).AND.(IY.LE.MAXY).AND.
     *      (KAR.GE.65).AND.(KAR.LE.90).AND.(MM(MAXX,IY).EQ.46))
     *      GO TO 11111
         CALL MYERR(36,KAR,KAR)
         IX = IOX
         IY = IOY
         CALL CURSOR(IX,IY)
         RETURN
      ENDIF
C Charges done in separate subroutine
      IF (IX.LT.LOX) THEN
         LOX = IX
      ELSE IF (IX.GT.HIX) THEN
         HIX = IX
      ENDIF
      IF (IY.LT.LOY) THEN
         LOY = IY
      ELSE IF (IY.GT.HIY) THEN
         HIY = IY
      ENDIF
11111 CONTINUE
      IF (ICHAR.NE.4) CALL CONTEX(KAR,IX,IY,INCX,INCY,IERR)
      IF (IX.GT.MAXX) THEN
         IX = MAXX
      ELSE IF (IX.LT:1) THEN
         IX = 1
      ENDIF
C Return bond type to 1 after any typed char(incl dot), unless it was 4,8,0:
      IF ((IBTYPE.NE.0).AND.(IBTYPE.NE.4).AND.(IBTYPE.NE.8)) IBTYPE=1
C Draw in jam mode
C 46 is Luhn dot--draw as 'fat dot'.
      IF (KAR.NE.IDOT) GOTO 14
      IF (MM(IX,IY).NE.0) GO TO 1144
      DO 12 I = -1,1
         MX = IX + I
         IF ((MX.LE.0).OR.(MX.GT.MAXX)) GO TO 12
```

```
          DO 1122 J = -1,1
             MY = IY + J
             IF ((MY.LE.0).OR.(MY.GT.MAXY)) GO TO 1122
             L = LMM(MX,MY)
             IF ((L.EQ.0).OR.(L.GE.256)) GO TO 1122
             IF ((L.EQ.34).OR.(MM(MX,MY).GT.8192).OR.
     *          ((L.GE.49).AND.(L.LE.57).AND.((LMM(MX-1,MY).EQ.
     *          43).OR.(LMM(MX-1,MY).EQ.45).OR.((IABS(I+J).NE.1)
     *          .AND.(MM(MX-1,MY).EQ.72)).AND.(MX-1.GE.0))))
     *          GO TO 1122
             GO TO 1144
1122      CONTINUE
12      CONTINUE
C Draw 3x3 fat dot
        I1X = IX * MULTX - 6
        I1Y = IY * MULTY - 4
        I3X = I1X + 3
        I3Y = I1Y - 3
        CALL BAR(I1X,I1Y,I3X,I3Y)
        MM(IX,IY)=IDOT
        IX=IX+1
        CALL CURSOR(IX,IY)
        RETURN
14      CONTINUE
        LL = LMM(IX,IY)
        IF ((KAR.LT.49).OR.((KAR.GT.57).AND.(KAR.LT.97)).OR.
     *     (KAR.GT.122)) THEN
           IF (LL.EQ.0) THEN
              GO TO 2222
           ELSE
              GO TO 1144
           ENDIF
        ENDIF
C Space is found for 2nd letter of 2 letter atomic symbol.
        LLUP = MM(IX+1,IY-1)
        LLDN = MM(IX+1,IY+1)
        IF ((LLUP.GE.256).AND.(MOD(IDIR(LLUP),4).EQ.2)) GO TO 1898
        IF ((LLUP.GT.0).AND.(LLUP.NE.34).AND.(LLUP.NE.43).AND.
     *     (LLUP.NE.45).AND.(LLUP.LT.256)) GO TO 1898
        IF ((LLDN.GE.256).AND.(MOD(IDIR(LLDN),4).EQ.0)) GO TO 1898
        IF ((LLDN.GT.0).AND.(LLDN.NE.34).AND.(LLDN.NE.43).AND.
     *     (LLDN.NE.45).AND.(LLDN.LT.256)) GO TO 1898
        IF (((LL.EQ.0).OR.((LL.GE.256).AND.((IDIR(LL).EQ.3).OR.
     *     (IDIR(LL).EQ.7)))).AND.((LMM(IX+1,IY).GE.256).OR.
     *     (MM(IX+1,IY).EQ.0))) GO TO 2003
1898       FX = IX - 1
           CALL FTLOCA(IY,FX)
           CALL FTEXT('^ ^')
           MM(FX,IY) = 0
           IOX = IOX - 1
           GO TO 1144
2003    CONTINUE
        IELT = 0
        IF (IX-1.LE.0) GO TO 2008
C Element is identified.
        LET1 = LMM(IX-1,IY)
        IF ((KAR.GE.49).AND.(KAR.LE.57).AND.(((MM(IX-1,IY)
     *     .EQ.68).OR.(MM(IX-1,IY).EQ.77)).AND.(IX-1.GT.0))) THEN
           LET2 = KAR + 63
        ELSE
           LET2 = KAR
        ENDIF
        DO 2007 I = 1,126
           IF ((LET1.EQ.IELEM(I,1)).AND.(LET2.EQ.IELEM(I,2))) GO TO 2323
2007    CONTINUE
2008    IERR = 11
        CALL MYERR(IERR,LET1,LET2)
        ICHAR = 30
        GO TO 1146
C
2323    CONTINUE
C Available space for 2nd letter of 2 letter element symbol is cleared.
        IF (ICHAR.EQ.4) THEN
           IF (MM(IX,IY).NE.0) THEN
              CALL FTLOCA(IY,IX)
```

```
            CALL FTEXT('^ ^')
          ENDIF
          GO TO 2333
        ENDIF
2222    CONTINUE
C
C Clear space for new node is verified.
        DO 2001 I = -1,1
          MX = IX + I
          IF ((MX.LE.0).OR.(MX.GT.MAXX)) GO TO 2001
          DO 2000 J = -1,1
            MY = IY + J
            IF ((MY.LE.0).OR.(MY.GT.MAXY)) GO TO 2000
            IF ((I.EQ.0).AND.(J.EQ.0)) GO TO 2000
            LL = LMM(MX,MY)
            IF (MX-1.LE.0) THEN
              LL2 = 0
            ELSE
              LL2 = LMM(MX-1,MY)
            ENDIF
            IF (LL.EQ.0) GO TO 2000
            IF ((MM(MX,MY).GT.8192).OR.(LL.EQ.34)) GO TO 2000
            IF ((LL.GE.49).AND.(LL.LE.57).AND.((MM(MX-1,MY).GT.
     *        8192).OR.((IABS(I+J).NE.1).AND.(LL2.EQ.72))))
     *        GO TO 2000
            IF (LL.GE.256) GO TO 2000
            GO TO 1144
2000      CONTINUE
2001    CONTINUE
2333    CALL CURSOR(IX,IY)
C
C Nodal or remaining character of atomic symbol is entered on screen.
        HALO(2) = CHAR(KAR)
        CALL TEXT(HALOE)
C
C Set H=J for storage so we won't have valence problems with H's
        IF (KAR .EQ. 72) KAR=74
C Translate D1-D9 and M1-M9 to Dp-Dx and Mp-Mx for internal storage.
        IF ((KAR.GE.49).AND.(KAR.LE.57).AND.(((MM(IX-1,IY)
     *    .EQ.68).OR.(MM(IX-1,IY).EQ.77)).AND.(IX-1.GT.0)))
     *    KAR = KAR + 63
        MM(IX,IY)=KAR
        IX=IX+1
        CALL CURSOR(IX,IY)
        RETURN
1144    CONTINUE
        IERR = 48
        CALL MYERR(IERR,IERR,IERR)
        ICHAR = JCHAR
        KAR = MCHAR
        IBDIR = JBDIR
1146    CONTINUE
        IX = IOX
        IY = IOY
        ICUR = 1
        CALL CURSOR(IX,IY)
        RETURN
        END
$STORAGE:2
        SUBROUTINE STRDRW(ISWIT)
        IMPLICIT INTEGER*2 (A-Z)
        REAL A,THETA,SLOPE,DELX,DELY,DTHETA,THETA2,DX,DY
        INTEGER*4 MM,IDTPIX,IPACK,LN
        CHARACTER*1 HALO(3)
        COMMON /CD/ MAXX,MAXY
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /IOFFST/IOFF
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /SIZZE/ MULTX,MULTY
        COMMON /HP/IHP
C       Relative coords for dwg bonds in 7x10 areas
        COMMON /BONDS/ A(5,3,4,4),B(2,3,4)
C       0,0 in lower left corner.
C       1st coord is bondtype (1=single,2=double,3=triple,4=wedge in,5=Out)
```

```
C       2nd coord is line segment # for dwg each bond (eg triple has 3segments)
C       3rd coord is bond direction, modulo 4 (up=1)
C       4th coord is Xstart,Ystart,Xend,Yend drawing coordinates.
        COMMON /CUR/ ICUR
C
        HALO(1) = '^'
        HALO(3) = '^'
C Counter for array LABL
        ICUR = 0
        CALL CURSOR(1,1)
        MRKLEN=0
        IGTEXT=1
C       If ISWIT = 0 markers are displayed
C       as Luhn dots - If ISWIT .NE. 0
C       markers are displayed as lower case letters
        IF (ISWIT .EQ. 0) GO TO 41
        DO 40 I=1,260
        IF (LABL(I,1).EQ.0) GO TO 40
        MRKLEN=MRKLEN+1
40      CONTINUE
C
41      DO 1000 IY= LOY,HIY
        DO 1000 IX= LOX,HIX
        IF (MM(IX,IY).EQ.0) GO TO 1000
        ISUBSC=1
C
C       UNPACK ARRAY
        IC=0
        IBDIR=0
        IBTYPE=0
        IPACK = MM(IX,IY)
        IF (IPACK.LT.256) GO TO 700
        IF ((LMM(IX,IY).EQ.43).OR.(LMM(IX,IY).EQ.45)) GO TO 800
C
C IDENTIFY BONDS
        IBDIR=MOD(IPACK,256)
        IBTYPE=(IPACK-IBDIR)/256
C Conversion of bond type to the first coordinate of 'A' (drawing coordin-
C ate array:
        IBOND=1
C IBOND is 1st coord of A; max 5
        IF (IBTYPE.LE.3) IBOND=IBTYPE
C We need 3 lines for type 8 bond
        IF (IBTYPE.EQ.8) IBOND=3
C Wedges:
        IF ((IBTYPE.EQ.6) .OR. (IBTYPE.EQ.7)) IBOND=IBTYPE-2
C
C Number of line segments req'd to draw the bond-Max 3
        NLINES=3
C single=1; double=2 line segments
        IF (IBOND.LE.2) NLINES=IBOND
C
Correct direction error for wedge bond inherent in A array in DRAW:
        JKL=IBDIR
        JKM = IBDIR
        IF (JKL.GT.4) JKL=JKL-4
        IF ((IBOND.GE.4) .AND. (IBDIR.GT.4)) IBOND= 9 - IBOND
C
C Start drawing the bond:
        NX=IX*MULTX - 8*IOFF
C Screen coordinates of lower left corner of 7x10 area
        NY=IY*MULTY - 11*IOFF
C
        IPAT=1
        IF (IBTYPE.EQ.5) IPAT=5
C
C       Draw each segment separately
        DO 600 J=1,NLINES
           IF (MOD(JKM,2).EQ.1) THEN
              JKJ = JKL
              IF ((IBOND.EQ.5).AND.(JKM.EQ.1)) THEN
                 BND = 4
              ELSE IF ((IBOND.EQ.4).AND.(JKM.EQ.1)) THEN
                 BND = 5
              ELSE
```

```
                 BND = IBOND
              ENDIF
           ELSE
              BND = IBOND
              IF (JKL.EQ.2) THEN
                 JKJ = 4
              ELSE IF (JKL.EQ.4) THEN
                 JKJ = 2
              ENDIF
           ENDIF
           IF ((JKM.EQ.5).AND.((IBOND.EQ.4).OR.(IBOND.EQ.5))) THEN
              IF (IBOND.EQ.4) THEN
                 BND = 2
              ELSE
                 BND = 1
              ENDIF
              I1X = NX + B(BND,J,1)
              I2X = NX + B(BND,J,2)
              I1Y = NY + B(BND,J,3)
              I2Y = NY + B(BND,J,4)
           ELSE
C          Calc plotting coords
              I1X = NX + A(BND,J,JKJ,1)
C             I1X,I1Y = start
              I2X = NX + A(BND,J,JKJ,3)
C             I2X,I2Y = end
              I1Y = NY + A(BND,J,JKJ,2)
              I2Y = NY + A(BND,J,JKJ,4)
           ENDIF
           IF (IBTYPE.EQ.8) IPAT=IPAT+1
           CALL LINE(IGTEXT,IPAT,I1X,I1Y,I2X,I2Y)
600     CONTINUE
        GO TO 1000
C
C IDENTIFY CHARACTERS
700     CONTINUE
        NX=IX*MULTX - 8*IOFF
        NY=IY*MULTY - 2*IOFF
        IF (IPACK.EQ.46) GO TO 770
        IF (IPACK.LT.48.OR.IPACK.GT.57) GO TO 900
        IF (IX.LE.ISUBSC) GO TO 900
        LN = LMM(IX-ISUBSC,IY)
C       (LEFT NEIGHBOR)
        IF (LN.EQ.42) GO TO 900
        IF ((LN.EQ.43).OR.(LN.EQ.45)) GO TO 650
        IF((LN.GE.65.AND.LN.LE.90).OR.(LN.GE.97.AND.LN.LE.122))
     *  NY=NY-IHP*2
        IF (LN.GE.48.AND.LN.LE.57) GO TO 730
        GO TO 900
730     CONTINUE
        ISUBSC=ISUBSC+1
        GO TO 700
C
C       DIGIT ASSOCIATED WITH CHARGE
C       SEE IF CHARGE IS PART OF DOTDIS - IF SO RAISE DIGIT FOR DISPLAY
C
650     DO 652 I=IX-1,1,-1
           IF ((MM(I,IY).EQ.0).OR.(IY.EQ.1)) GO TO 900
           IF (MM(I,IY).EQ.42) GO TO 950
652     CONTINUE
        GO TO 900
C
C REENTER MARKERS
770     CONTINUE
C LUHN DOT - NOT MARKER
        IF (MRKLEN .EQ. 0) GO TO 750
        DO 780 K=1,MRKLEN
        IF (LABL(K,1).EQ.IX.AND.LABL(K,2).EQ.IY) GO TO 790
780     CONTINUE
C LUHN DOT - NOT MARKER
        GO TO 750
790     CONTINUE
        IPACK=MOD(K-1,26)+97
        GO TO 900
C
```

```
C       DRAW FAT DOT
750     CONTINUE
        IGTEXT = 0
        JX = (IX * MULTX) - 6
        JY = (IY * MULTY) - 4
        J3X = JX + 3
        J3Y = JY - 3
        CALL BAR(JX,JY,J3X,J3Y)
        GO TO 1000
C
C IDENTIFY CHARGES
800     CONTINUE
        NX=IX*MULTX - 8*IOFF
        NY=IY*MULTY - 2*IOFF
        IPACK=MOD(IPACK,2**13)
        IC=(MM(IX,IY)-IPACK)/2**13
C SEE IF CHARGE IS PART OF DOTDIS. IF SO RAISE
C CURSOR FOR DISPLAY
        DO 500 I=IX-1,1,-1
          IF (MM(I,IY).EQ.0) GO TO 900
          IF (MM(I,IY).EQ.42) GO TO 950
500     CONTINUE
        GO TO 900
C WE FOUND DOTDIS CHARGE
950     NY = NY +IHP*10
C
900     CONTINUE
        IGTEXT=1
C Display J's (which are stereo hydrogens) as H's
        IF (IPACK .EQ. 74) IPACK=72
        IF ((IPACK.GE.112).AND.(IPACK.LE.120).AND.
     *     ((MM(IX-1,IY).EQ.68).OR.(MM(IX-1,IY).EQ.77)))
     *     IPACK = IPACK - 63
        CALL MOVTCA(NX,NY)
        HALO(2) = CHAR(IPACK)
        CALL TEXT(HALO)
        IBOND=0
        IBTYPE=0
        IBDIR=0
        IC=0
1000    CONTINUE
C
C IDENTIFY LONG BONDS
        DO 2000 K=1,LBLEN
        IF (LNGBND(K,1).EQ.0) GO TO 2000
        IX1=LNGBND(K,1)
        IY1=LNGBND(K,2)
        IX2=LNGBND(K,3)
        IY2=LNGBND(K,4)
        IBTYPE=LNGBND(K,5)
C Now calculate bond endpoints, based on circle of rad 6 surrounding node
168     DX=MULTX*(IX2-IX1)
        DY=MULTY*(IY2-IY1)
        SLOPE = 0.0
        IF (IHP .NE. 1) THEN
        IF (DX.EQ.0.0) THEN
           IF (IY1.GT.IY2) THEN
              DELV1 = -4
              DELV2 = 8
           ELSE
              DELV1 = 8
              DELV2 = -4
           ENDIF
           DELX = 0.0
           DELY = 0.0
        ELSE
           DELV1 = 0
           DELV2 = 0
           SLOPE=DY/DX
           THETA=ATAN(SLOPE)
           IF ((THETA.LE.0.).AND.(DX.LT.0.0)) THETA = THETA - 3.14159265
C          Principal value problem
           IF ((THETA.GT.0.).AND.((DX.LT.0.0).OR.(DY.LT.0.0)))
     2         THETA = THETA + 3.14159265
```

```
C          Bond connects to circle of rad pixels from center of node
           DELX=6*COS(THETA)
           DELY=6*SIN(THETA)
        ENDIF
        JX1=IX1*MULTX - 4+DELX
        JY1=IY1*MULTY - 9 + DELY + DELV1
        JX2=IX2*MULTX - 4-DELX
        JY2=IY2*MULTY - 9 - DELY + DELV2
        IF ((SLOPE.LT.1.0).AND.(SLOPE.NE.0.0).AND.(SLOPE.GT.-1.0)) THEN
              JY2 = JY2 + 3
              JY1 = JY1 + 3
        ELSE IF (ABS(SLOPE).GT.1.0) THEN
           IF (JY1.GT.JY2) THEN
              JY1 = JY1 + 6
              JY2 = JY2 + 3
           ELSE
              JY1 = JY1 + 3
              JY2 = JY2 + 6
           ENDIF
        ELSE IF (ABS(SLOPE).EQ.1.0) THEN
           IF (JY1.GT.JY2) THEN
              JY1 = JY1 - 2
              JY2 = JY2 + 3
           ELSE
              JY1 = JY1 + 3
              JY2 = JY2 - 2
           ENDIF
       ELSE IF (DY.EQ.0.0) THEN
          JY1 = JY1 + 3
          JY2 = JY2 + 3
          IF (JX1.GT.JX2) JY2 = JY2 + 1
       ENDIF
        ELSE
        IF (DX .EQ. 0) THEN
        IF (IY2 .GT. IY1) THEN
        DELV1=6
        DELV2=-6
        THETA=1.571
        ELSE
        DELV1=-6
        DELV2=6
        THETA=-1.571
        ENDIF
        DELX=0
        DELY=0
        ELSE
        DELV1=0
        DELV2=0
           SLOPE = DY/DX
           THETA=ATAN(SLOPE)
           IF ((THETA.LE.0.) .AND. (DX.LT.0)) THETA = THETA - 3.14159265
C          Principal value problem
           IF ((THETA.GT.0.) .AND. ((DX.LT.0) .OR. (DY.LT.0)))
     2        THETA = THETA + 3.14159265
C          Bond connects to circle of rad 6 pixels from center of node
           DELX=6*COS(THETA)
           DELY=6*SIN(THETA)
        ENDIF
        JX1=IX1*MULTX+4+DELX
        JY1=IY1*MULTY+5+DELY+DELV1
        JX2=IX2*MULTX+4-DELX
        JY2=IY2*MULTY+5-DELY+DELV2
        ENDIF
C Now determine bond type to draw.
        IPAT=1
        IF (IBTYPE.EQ.5) IPAT=5
        IF (IBTYPE.EQ.8) IPAT=3
        IBOND=1
        IF (IBTYPE.LE.3) IBOND=IBTYPE
        IF (IBOND.EQ.1.OR.IBOND.EQ.3)
     2     CALL LINE(IGTEXT,IPAT,JX1,JY1,JX2,JY2)
        IF (IBTYPE .EQ. 8) GO TO 1700
C No more lines to draw
        IF (IBOND.EQ.1) GOTO 2000
C
```

```
C  Calculate side lines for double or triple bonds:
C  Use angle of +-.6 radians from center for side lines for triple;
C .3 for double
1700    CONTINUE
        IF (IBOND.EQ.2) THEN
           DTHETA = .2
        ELSE IF ((IBOND.EQ.3).OR.(IBTYPE.EQ.8)) THEN
           DTHETA = .6
        ENDIF
C
C Change sign
        DO 1550 I=1,-1,-2
        IF (IHP .NE. 1) THEN
        IF (DX.EQ.0.0) THEN
           DELX = I * 2.0
           DELY = 0.0
           IF (IY1.GT.IY2) THEN
              DELV1 = -4
              DELV2 = 8
           ELSE
              DELV1 = 8
              DELV2 = -4
           ENDIF
        ELSE
           DELV1 = 0
           DELV2 = 0
           THETA2 = THETA + DTHETA*I
           DELX = (6*COS(THETA2))
           DELY=(6*SIN(THETA2))
        ENDIF
        JX1 = IX1 * MULTX - 4 + DELX
        JY1 = IY1 * MULTY - 9 + DELY + DELV1
        IF (DX.NE.0.0) THEN
           THETA2 = 3.14159265 + THETA - I*DTHETA
           DELX=(6*COS(THETA2))
           DELY=(6*SIN(THETA2))
        ENDIF
        JX2 = IX2 * MULTX - 4 + DELX
        JY2 = IY2 * MULTY - 9 + DELY + DELV2
        IF (IBTYPE.EQ.8) IPAT=3+I
        IF ((SLOPE.LT.1.0).AND.(SLOPE.NE.0.0).AND.(SLOPE.GT.-1.0)) THEN
           JY2 = JY2 + 3
           JY1 = JY1 + 3
        ELSE IF (ABS(SLOPE).GT.1.0) THEN
           IF (JY1.GT.JY2) THEN
              JY1 = JY1 + 6
              JY2 = JY2 + 3
           ELSE
              JY1 = JY1 + 3
              JY2 = JY2 + 6
           ENDIF
        ELSE IF (ABS(SLOPE).EQ.1.0) THEN
           IF (JY1.GT.JY2) THEN
              JY1 = JY1 - 2
              JY2 = JY2 + 3
           ELSE
              JY1 = JY1 + 3
              JY2 = JY2 - 2
           ENDIF
        ELSE IF (DY.EQ.0.0) THEN
           IF ((IBOND.EQ.3).OR.(IBTYPE.EQ.8)) THEN
              IF (DX.GT.0.0) THEN
                 IF (I.EQ.-1) THEN
                    JY1 = JY1 + 5
                    JY2 = JY2 + 5
                 ELSE
                    JY1 = JY1 + 2
                    JY2 = JY2 + 2
                 ENDIF
              ELSE
                 IF (I.EQ.-1) THEN
                    JY1 = JY1 + 2
                    JY2 = JY2 + 2
                 ELSE
                    JY1 = JY1 + 5
                    JY2 = JY2 + 5
```

```
            ENDIF
         ENDIF
      ELSE IF (IBOND.EQ.2) THEN
         JY1 = JY1 + 4
         JY2 = JY2 + 4
      ENDIF
      ENDIF
      IF ((SLOPE.NE.0.0).AND.((IBOND.EQ.3).OR.(IBTYPE.EQ.8))) THEN
         IF (SLOPE.GT.0.0) THEN
            IF (JY1.GT.JY2) THEN
               JY1 = JY1 + I
               JY2 = JY2 + I
            ELSE
               JY1 = JY1 - I
               JY2 = JY2 - I
            ENDIF
         ELSE
             IF (JY1.GT.JY2) THEN
               JY1 = JY1 - I
               JY2 = JY2 - I
            ELSE
               JY1 = JY1 + I
               JY2 = JY2 + I
            ENDIF
         ENDIF
      ENDIF
       ELSE
       THETA2 = THETA + DTHETA*I
       DELX= (6*COS(THETA2))
       DELY=(6*SIN(THETA2))
       JX1 = IX1 * MULTX + 4 + DELX
       JY1 = IY1 * MULTY + 5 + DELY
       THETA2 = 3.14159265 + THETA - I*DTHETA
       DELX=(6*COS(THETA2))
       DELY=(6*SIN(THETA2))
       JX2 = IX2 * MULTX + 4 + DELX
       JY2 = IY2 * MULTY + 5 + DELY
       ENDIF
      CALL LINE(IGTEXT,IPAT,JX1,JY1,JX2,JY2)
1550  CONTINUE
2000  CONTINUE
8500  CONTINUE
      ICUR = 1
      RETURN
      END
C
       SUBROUTINE LONG(KAR,IX,IY)
       IMPLICIT INTEGER*2 (A-Z)
       REAL THETA,DTHETA,THETA2,DELX,DELY,SLOPE,DX,DY
       INTEGER*4 MM,IDTPIX
       LOGICAL*2 RPLC
       CHARACTER*1 ISTAT
       COMMON /CD/ MAXX,MAXY
       COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
       COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
       COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
       COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
       COMMON /HEAD/ MW(12),ISTATE,PAGE
       COMMON /LABELS/ NR,NJLAST,NJNEXT
       COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
       COMMON /SIZZE/ MULTX,MULTY
       COMMON /ISTATE/ ISTAT
       COMMON /CUR/ ICUR
       COMMON /HP/ IHP
C
C This routine allows drawing of 'long bonds' between current location
C (if it is a marker) and any active marker.  The routine is called by
C entering a '%'.  Any number of calls to 'LEAP' can be made while in
C the routine.  When a second '%' is
C entered, a long bond is drawn between the initial node and the last
C marker jumped to.
C
C Long Bond state
       ICUR = 1
       ISTATE=7
```

```
        ISTAT='%'
        CALL HEADER
        IX2 = -99
        IY2 = -99
        IX1 = -99
        IY1 = -99
        RPLC = .FALSE.
C
        K = 0
        IF (IX.GT.2) K = LMM(IX-1,IY)
        IF (K.EQ.46) GO TO 123
C Return to previous state
        ISTATE=0
        KAR=0
        IF (MOD(IBTYPE,4).NE.0) IBTYPE=1
        LASTN=0
        CALL HEADER
        CALL CURSOR(IX,IY)
        CALL ERRMSG(0)
        RETURN
C
123     IX1 = IX - 1
        IY1 = IY
        CALL CURSOR(IX1,IY1)
2       IKAR=KAR
77      CALL INPUTX(KAR,IX,IY)
C Second entry of '%'
        IF (KAR.EQ.LBOND) GOTO 3
        IF ((KAR.EQ.13).OR.(KAR.EQ.81)) GO TO 95
C       These lines are commented out to lock out entry of elements in
C       LONG.
C Lowercase for jump
        IF ((KAR.GE.97).AND.(KAR.LE.122)) GOTO 4
C digit = set bond type
        IF ((KAR .GE. 48) .AND. (KAR .LE. 57)) GO TO 21
C '#' set marker
        IF (KAR.EQ.ITAG) GOTO 25
        CALL ERRMSG(KAR)
        GO TO 2
51      IERR=9
        GO TO 96
95      IERR=2
96      CALL MYERR(IERR,KAR,KAR)
5       LASTN=0
        ISTATE=0
        IF (MOD(IBTYPE,2).NE.0) IBTYPE=1
        CALL HEADER
        CALL CURSOR(IX,IY)
C Erroneous input
        RETURN
C
C set marker after '#'
25      CALL MARK(KAR,IX,IY)
        IX2=IX-1
        IY2=IY
        GOTO 2
C
700     ICHAR=4
CLC AFTER $
        CALL DRAW(KAR,IX,IY,INCX,INCY)
        MCHAR=KAR
        JCHAR=ICHAR
        IX2=IX-2
        IY2=IY
        GO TO 2
C
900     ICHAR=2
C       UC
        CALL DRAW(KAR,IX,IY,INCX,INCY)
        MCHAR=KAR
        JCHAR=ICHAR
        IX2=IX-1
        IY2=IY
        GO TO 2
C
C use digit to set bond type
```

```
21      IBTYPE=KAR-48
        CALL HEADER
C for more input
        GOTO 2
4       CALL LEAP(KAR,IX,IY)
        IX2=IX-1
        IY2=IY
        GOTO 2
C
C Zero-length bond
3       IF ((IX1.EQ.IX2) .AND. (IY1.EQ.IY2)) GOTO 51
C No endpoint specified
        IF (IX2.LE.0 .OR.IY2.LE.0) GOTO 51
C No starting point specified
        IF (IX1.LE. 0 .OR.IY1.LE.0) GO TO 51
        IF ((IBTYPE.EQ.4).OR.(IBTYPE.EQ.6).OR.(IBTYPE.EQ.7)) THEN
           IERR = 53
           CALL MYERR(IERR,KAR,MAR)
           IBTYPE = 1
        ENDIF
C
C  Actual drawing of long bond; hence ICHAR<10
        ICHAR=8
        JCHAR=8
C Put info into longbond array:
10      DO 9 I=1,100
        II = I
        IF ((LNGBND(I,1).EQ.IX1) .AND. (LNGBND(I,2).EQ.IY1) .AND.
     2     (LNGBND(I,3).EQ.IX2) .AND. (LNGBND(I,4).EQ.IY2)) THEN
           KX1 = IX1
           KY1 = IY1
           GOTO 166
C       If repeating an existing
C       long bond, don't re-enter into long bond table.
        ELSE IF ((LNGBND(I,1).EQ.IX2).AND.(LNGBND(I,2).EQ.IY2).AND.
    2     (LNGBND(I,3).EQ.IX1).AND.(LNGBND(I,4).EQ.IY1)) THEN
          KX1 = IX2
          KY1 = IY2
          GO TO 166
       ENDIF
       IF (LNGBND(I,1)+LNGBND(I,2)+LNGBND(I,3)+LNGBND(I,4).GT.0) GOTO 9
       IF (IBTYPE .EQ. 0) GO TO 5
       LNGBND(I,1)=IX1
       LNGBND(I,2)=IY1
       LNGBND(I,3)=IX2
       LNGBND(I,4)=IY2
       LNGBND(I,5)=IBTYPE
       ICUR = 0
       CALL CURSOR(IX,IY)
       GOTO 168
9      CONTINUE
C
166    IF (((LNGBND(II,5).EQ.IBTYPE).AND.(IBTYPE.NE.0)).OR.
    *    (MM(IX1,IY1).NE.46)) GO TO 5
C Don't redraw if bond type is the same or if initial
C point is not a marker
       IWHICH = II
       KXX = KX1
       KYY = KY1
       RPLC = .TRUE.
       CALL DEL(KAR,KXX,KYY,INCX,INCY,IWHICH)
C Set new bond type
       IF (IBTYPE .EQ. 0) GO TO 16
       LNGBND(II,5)=IBTYPE
       LNGBND(II,1) = KX1
C
C Now calculate bond endpoints, based on circle of rad 6 surrounding node
168    CONTINUE
       DX=MULTX*(IX2-IX1)
       DY=MULTY*(IY2-IY1)
       SLOPE = 0.0
       IF (IHP .NE. 1) THEN
       IF (DX.EQ.0.0) THEN
          IF (IY1.GT.IY2) THEN
             DELV1 = -4
```

```
            DELV2 = 8
         ELSE
            DELV1 = 8
            DELV2 = -4
         ENDIF
         DELX = 0.0
         DELY = 0.0
      ELSE
         DELV1 = 0
         DELV2 = 0
         SLOPE = DY/DX
         THETA=ATAN(SLOPE)
         IF ((THETA.LE.0.) .AND. (DX.LT.0)) THETA = THETA - 3.14159265
C        Principal value problem
         IF ((THETA.GT.0.) .AND. ((DX.LT.0) .OR. (DY.LT.0)))
     2      THETA = THETA + 3.14159265
C        Bond connects to circle of rad 6 pixels from center of node
         DELX=6*COS(THETA)
         DELY=6*SIN(THETA)
      ENDIF
      JX1=IX1*MULTX - 4+DELX
      JY1=IY1*MULTY - 9 + DELY + DELV1
      JX2=IX2*MULTX - 4-DELX
      JY2=IY2*MULTY - 9 - DELY + DELV2
      IF ((SLOPE.LT.1.0).AND.(SLOPE.NE.0.0).AND.(SLOPE.GT.-1.0)) THEN
         JY2 = JY2 + 3
         JY1 = JY1 + 3
      ELSE IF (ABS(SLOPE).GT.1.0) THEN
         IF (JY1.GT.JY2) THEN
            JY1 = JY1 + 6
            JY2 = JY2 + 3
         ELSE
            JY1 = JY1 + 3
            JY2 = JY2 + 6
         ENDIF
      ELSE IF (ABS(SLOPE).EQ.1.0) THEN
         IF (JY1.GT.JY2) THEN
            JY1 = JY1 - 2
            JY2 = JY2 + 3
         ELSE
            JY1 = JY1 + 3
            JY2 = JY2 - 2
         ENDIF
      ELSE IF (DY.EQ.0.0) THEN
         JY1 = JY1 + 3
         JY2 = JY2 + 3
         IF (JX1.GT.JX2) JY2 = JY2 + 1
      ENDIF
      ELSE
      IF (DX .EQ. 0) THEN
      IF (IY2 .GT. IY1) THEN
      DELV1=6
      DELV2=-6
      THETA=1.571
      ELSE
      DELV1=-6
      DELV2=6
      THETA=-1.571
      ENDIF
      DELX=0
      DELY=0
      ELSE
      DELV1=0
      DELV2=0
         SLOPE = DY/DX
         THETA=ATAN(SLOPE)
         IF ((THETA.LE.0.) .AND. (DX.LT.0)) THETA = THETA - 3.14159265
C        Principal value problem
         IF ((THETA.GT.0.) .AND. ((DX.LT.0) .OR. (DY.LT.0)))
     2      THETA = THETA + 3.14159265
C        Bond connects to circle of rad 6 pixels from center of node
         DELX=6*COS(THETA)
         DELY=6*SIN(THETA)
      ENDIF
      JX1=IX1*MULTX+4+DELX
      JY1=IY1*MULTY+5+DELY+DELV1
```

```
        JX2=IX2*MULTX+4-DELX
        JY2=IY2*MULTY+5-DELY+DELV2
        ENDIF
C Now determine bond type to draw.
        IBOND=1
        IF (IBTYPE.LE.3) IBOND=IBTYPE
C Set mode, solid line
        CALL SETLNS(1)
CWIGGLY LINE - BOND TYPE 8
        IF (IBTYPE.EQ.5) CALL SETLNS(2)
C Single or triple: draw central line:
        IF ((IBOND.EQ.1).OR.(IBOND.EQ.3)) THEN
           CALL MOVABS(JX1,JY1)
           CALL LNABS(JX2,JY2)
        ENDIF
        IF (IBTYPE .EQ. 8) GO TO 70
C No more lines to draw
        IF (IBOND.EQ.1) GOTO 56
C
C  Calculate side lines for double or triple bonds:
C  Use angle of +-.6 radians from center for side lines for triple;
C .3 for double
70      CONTINUE
        IF (IBOND.EQ.2) THEN
           DTHETA = .2
        ELSE IF ((IBTYPE.EQ.8).OR.(IBOND.EQ.3)) THEN
           DTHETA = .6
        ENDIF
C Change sign
        DO 55 I=1,-1,-2
           IF ((IBTYPE.EQ.8).AND.(I.EQ.1)) CALL SETLNS(2)
           IF ((IBTYPE.EQ.8).AND.(I.EQ.-1)) CALL SETLNS(3)
        IF (IHP .NE. 1) THEN
        IF (DX.EQ.0.0) THEN
           DELX = I * 2.0
           IF (IY1.GT.IY2) THEN
              DELY = 0.0
              DELV1 = -4
              DELV2 = 8
           ELSE
              DELY = 0.0
              DELV1 = 8
           DELV2 = -4
         ENDIF
      ELSE
         DELV1 = 0
         DELV2 = 0
         THETA2 = THETA + DTHETA*I
         DELX= (6*COS(THETA2))
         DELY=(6*SIN(THETA2))
      ENDIF
      JX1 = IX1 * MULTX - 4 + DELX
      JY1 = IY1 * MULTY - 9 + DELY + DELV1
      IF (DX.NE.0.0) THEN
         THETA2 = 3.14159265 + THETA - I*DTHETA
         DELX=(6*COS(THETA2))
         DELY=(6*SIN(THETA2))
      ENDIF
      JX2 = IX2 * MULTX - 4 + DELX
      JY2 = IY2 * MULTY - 9 + DELY + DELV2
      IF ((SLOPE.LT.1.0).AND.(SLOPE.NE.0.0).AND.(SLOPE.GT.-1.0)) THEN
         JY2 = JY2 + 3
         JY1 = JY1 + 3
      ELSE IF (ABS(SLOPE).GT.1.0) THEN
         IF (JY1.GT.JY2) THEN
            JY1 = JY1 + 6
            JY2 = JY2 + 3
         ELSE
            JY1 = JY1 + 3
            JY2 = JY2 + 6
         ENDIF
      ELSE IF (ABS(SLOPE).EQ.1.0) THEN
          IF (JY1.GT.JY2) THEN
             JY1 = JY1 - 2
             JY2 = JY2 + 3
```

```
      ELSE
         JY1 = JY1 + 3
         JY2 = JY2 - 2
      ENDIF
   ELSE IF (DY.EQ.0.0) THEN
      IF ((IBOND.EQ.3).OR.(IBTYPE.EQ.8)) THEN
         IF (DX.GT.0.0) THEN
            IF (I.EQ.-1) THEN
               JY1 = JY1 + 5
               JY2 = JY2 + 5
            ELSE
               JY1 = JY1 + 2
               JY2 = JY2 + 2
            ENDIF
         ELSE
            IF (I.EQ.-1) THEN
               JY1 = JY1 + 2
               JY2 = JY2 + 2
            ELSE
               JY1 = JY1 + 5
               JY2 = JY2 + 5
            ENDIF
         ENDIF
      ELSE IF (IBOND.EQ.2) THEN
         JY1 = JY1 + 4
         JY2 = JY2 + 4
      ENDIF

         ENDIF
         IF ((SLOPE.NE.0.0).AND.((IBOND.EQ.3).OR.(IBTYPE.EQ.8))) THEN
            IF (SLOPE.GT.0.0) THEN
               IF (JY1.GT.JY2) THEN
                  JY1 = JY1 + I
                  JY2 = JY2 + I
               ELSE
                  JY1 = JY1 - I
                  JY2 = JY2.- I
               ENDIF
            ELSE
               IF (JY1.GT.JY2) THEN
                  JY1 = JY1 - I
                  JY2 = JY2 - I
               ELSE
                  JY1 = JY1 + I
                  JY2 = JY2 + I
               ENDIF
            ENDIF
         ENDIF
         ELSE
         THETA2 = THETA + DTHETA*I
         DELX= (6*COS(THETA2))
         DELY=(6*SIN(THETA2))
         JX1 = IX1 * MULTX + 4 + DELX
         JY1 = IY1 * MULTY + 5 + DELY
         THETA2 = 3.14159265 + THETA - I*DTHETA
         DELX=(6*COS(THETA2))
         DELY=(6*SIN(THETA2))
         JX2 = IX2 * MULTX + 4 + DELX
         JY2 = IY2 * MULTY + 5 + DELY
         ENDIF
         CALL MOVABS(JX1,JY1)
         CALL LNABS(JX2,JY2)
55       CONTINUE
56       CONTINUE
         IF (.NOT.RPLC) LBLEN = LBLEN + 1
16       CALL SETLNS(1)
C Solid line
C Following code is copied from DRAW & also appears in DEL:
C  ERASE ALL H's & SUBSCRIPTS:  **********
         KX=IX1
         KY=IY1
COnly@nodes
         IF ((LMM(KX,KY).LE.65) .OR. (LMM(KX,KY).GT.90)) GOTO 43
C
C Clear old valence hydrogens
         CALL CLRHYD(KX,KY)
```

```
        CALL VALNCE(2,IX1,IY1,0,0)
43      CONTINUE
        ICUR = 1
        CALL CURSOR(IX2+1,IY2)
972     IF(IBTYPE.NE.4 .AND. IBTYPE.NE.8 .AND. IBTYPE.NE.0) IBTYPE=1
        ISTATE=0
        CALL HEADER
        RETURN
        END
C     SUBROUTINE RELONG redraws all remaining long bonds after a bond
C     deletion to ensure that no long bond is only part visible.
C
      SUBROUTINE RELONG
      IMPLICIT INTEGER*2 (A-Z)
      REAL THETA,DTHETA,THETA2,DELX,DELY,SLOPE,DX,DY
      INTEGER*4 MM,IDTPIX
      COMMON /SIZZE/ MULTX,MULTY
      COMMON /CD/ MAXX,MAXY
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
C
      DO 1000 LB = 1,LBLEN
         IF (LNGBND(LB,1).NE.0) THEN
            IX1 = LNGBND(LB,1)
            IY1 = LNGBND(LB,2)
            IX2 = LNGBND(LB,3)
            IY2 = LNGBND(LB,4)
            KBTYPE = LNGBND(LB,5)
C           Now calculate bond endpoints, based on circle of rad 6
C           surrounding node.
            DX=MULTX*(IX2-IX1)
            DY=MULTY*(IY2-IY1)
            SLOPE = 0.0
        IF (DX .EQ. 0) THEN
        IF (IY2 .GT. IY1) THEN
        DELV1=6
        DELV2=-6
        THETA=1.571
        ELSE
        DELV1=-6
        DELV2=6
        THETA=-1.571
        ENDIF
        DELX=0
        DELY=0
        ELSE
        DELV1=0
        DELV2=0
           SLOPE = DY/DX
           THETA=ATAN(SLOPE)
           IF ((THETA.LE.0.) .AND. (DX.LT.0)) THETA = THETA - 3.14159265
C          Principal value problem
           IF ((THETA.GT.0.) .AND. ((DX.LT.0) .OR. (DY.LT.0)))
     2        THETA = THETA + 3.14159265
C          Bond connects to circle of rad 6 pixels from center of node
           DELX=6*COS(THETA)
           DELY=6*SIN(THETA)
        ENDIF
        JX1=IX1*MULTX+4+DELX
        JY1=IY1*MULTY+5+DELY+DELV1
        JX2=IX2*MULTX+4-DELX
        JY2=IY2*MULTY+5-DELY+DELV2
C
C           Now determine bond type to draw.
            IBOND=1
            IF (KBTYPE.LE.3) IBOND=KBTYPE
C           Set mode, solid line
            CALL SETLNS(1)
C           WIGGLY LINE - BOND TYPE 8
            IF (KBTYPE.EQ.5) CALL SETLNS(2)
C           Single or triple: draw central line:
            IF ((IBOND.EQ.1).OR.(IBOND.EQ.3)) THEN
```

```
            CALL MOVABS(JX1,JY1)
            CALL LNABS(JX2,JY2)
         ENDIF
         IF (KBTYPE .EQ. 8) GO TO 70
C        No more lines to draw
         IF (IBOND.EQ.1) GOTO 100
C
C        Calculate side lines for double or triple bonds:
C        Use angle of +-.6 radians from center for side lines for triple;
C        .3 for double
70       CONTINUE
         IF (IBOND.EQ.2) THEN
            DTHETA = .2
         ELSE IF ((KBTYPE.EQ.8).OR.(IBOND.EQ.3)) THEN
            DTHETA = .6
         ENDIF
C        Change sign
         DO 55 I=1,-1,-2
            IF ((KBTYPE.EQ.8).AND.(I.EQ.1)) CALL SETLNS(2)
            IF ((KBTYPE.EQ.8).AND.(I.EQ.-1)) CALL SETLNS(3)
      THETA2 = THETA + DTHETA*I
      DELX= (6*COS(THETA2))
      DELY=(6*SIN(THETA2))
      JX1 = IX1 * MULTX + 4 + DELX
      JY1 = IY1 * MULTY + 5 + DELY
      THETA2 = 3.14159265 + THETA - I*DTHETA
      DELX=(6*COS(THETA2))
      DELY=(6*SIN(THETA2))
      JX2 = IX2 * MULTX + 4 + DELX
      JY2 = IY2 * MULTY + 5 + DELY
         CALL MOVABS(JX1,JY1)
         CALL LNABS(JX2,JY2)
55       CONTINUE
100      CONTINUE
         CALL SETLNS(1)
C        Solid line
       ENDIF
1000  CONTINUE
      RETURN
      END
C
      SUBROUTINE LINE(IGTEXT,IPAT,I1X,I1Y,I2X,I2Y)
      IMPLICIT INTEGER*2 (A-Z)
C
      IGTEXT=0
C Will print solid line.
      IF (IPAT.LE.0.OR.IPAT.GE.10) IPAT=1
C
      GO TO (100,200,300,400,500,100,100,100,100),IPAT
      GO TO 1000
C
100   CONTINUE
C Set mode, solid line
      CALL SETLNS(1)
      GO TO 1000
C
C     (ENTRIES 200-400 BELOW RESULT IN WIGGLY LINE)
200   CONTINUE
      CALL SETLNS(2)
      GO TO 1000
C
300   CONTINUE
CWIGGLY LINE - BOND TYPE 8
      CALL SETLNS(1)
      GO TO 1000
C
400   CONTINUE
      CALL SETLNS(3)
      GO TO 1000
C
500   CONTINUE
C Will print dashed line--stereo
      CALL SETLNS(2)
      GO TO 1000
C
```

```
1000    CONTINUE
        CALL MOVABS(I1X,I1Y)
        CALL LNABS(I2X,I2Y)
C Solid line
        CALL SETLNS(1)
        RETURN
        END
$STORAGE:2
C
        SUBROUTINE REPLCE(KX,KY,INKX,INKY,DLX,DLY,EDGE)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,IDTPIX
        CHARACTER*1 HALO(3)
        LOGICAL*2 RETR
        COMMON /CD/ MAXX,MAXY
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
        COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
        COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /LABELS/ NR,NJLAST,NJNEXT
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /SIZZE/ MULTX,MULTY
        COMMON /CUR/ ICUR
        COMMON /HP/IHP
CXT     RETR is set in SUBROUTINE RETRIEVE to ensure proper screen
CXT     screen replacement between arrays MM and IDTPIX.
        COMMON /RETDRW/ RETR
        COMMON /TEMP/ LLBOND(100,5),LLABL(260,2),MCHN(260)
C
C ERASE CELL(S) TO CLEAR BOND FRAGMENTS, AND RESTORE ANY CELL VALUES.
        ICUR = 0
        CALL CURSOR(KX,KY)
        IX = KX
        IY = KY
        INCX = INKX
        INCY = INKY
        IF (EDGE.EQ.0) THEN
           PASY2 = 0
        ELSE
        PASY2 = 1
        IF (EDGE.EQ.1) THEN
           IF (IABS(INCX*INCY).EQ.1 .AND. IHP .EQ.1) THEN
              FX = IX - 2
              CALL FTLOCA(IY,FX)
              CALL FTEXT('^     ^')
          ELSE
             CALL FTLOCA(IY,IX)
             CALL FTEXT('^ ^')
          ENDIF
       IF (IHP .NE. 1) THEN
            IF (MOD((IY*10),40).EQ.0) THEN
               IF ((IY.EQ.8).OR.(IY.EQ.28).OR.(IY.EQ.16)) THEN
                  FY = ((IY * 10) / 11) + 1
                  CALL FTSIZE(1,11)
               ELSE
                  FY = ((IY * 10) / 9) + 1
                  CALL FTSIZE(1,9)
               ENDIF
            ELSE
               FY = ((IY * 10) / 8) + 1
               CALL FTSIZE(1,8)
            ENDIF
            IF (IABS(INCX*INCY).EQ.1) THEN
               CALL FTLOCA(FY,FX)
               CALL FTEXT('^     ^')
               CALL FTSIZE(1,10)
            ELSE
               CALL FTLOCA(FY,IX)
               CALL FTEXT('^ ^')
               CALL FTSIZE(1,10)
            ENDIF
        ENDIF
        ENDIF
       ENDIF
          IF (IABS(INCX*INCY).EQ.1) THEN
             DO 4000 YY = IY,IY+PASY2
```

```
      IF (YY.LE.MAXY) THEN
      DO 3000 KKK = IX-2,IX+3
         IF (((MM(KKK,YY).GT.0).OR.RETR).AND.(KKK.GE.1).AND.
     *      (KKK.LE.MAXX)) THEN
            IF (RETR) THEN
               IF ((IDTPIX(KKK,YY).NE.0).AND.(MM(KKK,YY).EQ.0))
     *            THEN
                  MM(KKK,YY) = IDTPIX(KKK,YY)
               ELSE
                  GO TO 3000
               ENDIF
            ENDIF
            YYY = YY
            KKKK = KKK
            IF (MM(KKKK,YY).EQ.46) THEN
               IF (RETR) THEN
                  DO 2019 LBL = 1,260
                     IF ((LLABL(LBL,1).EQ.KKKK).AND.
     *                  (LLABL(LBL,2).EQ.YY)) THEN
                        CALL CURSOR(KKKK,YYY)
                        IF (MOD(LBL,26).EQ.0) THEN
                           HALO(2) = 'z'
                        ELSE
                           HALO(2) = CHAR(MOD(LBL,26)+96)
                        ENDIF
                        CALL TEXT(HALO)
                        GO TO 2029
                     ELSE IF (((LLABL(LBL,1).EQ.0).AND.
     *                  (LLABL(LBL,2).EQ.0)).OR.(LBL.EQ.260))
     *                  THEN
                        JX = KKK * MULTX - 6
                        JY = YYY * MULTY - 4
                        J3X = JX + 3
                        J3Y = JY - 3
                        CALL BAR(JX,JY,J3X,J3Y)
                        GO TO 2029
                     ENDIF
 2019             CONTINUE
 2029             CONTINUE
               ELSE
                  DO 2020 LBL = 1,260
                     IF ((LABL(LBL,1).EQ.KKKK).AND.(LABL(LBL,2)
     *                  .EQ.YY)) THEN
                        CALL CURSOR(KKKK,YYY)
                        IF (MOD(LBL,26).EQ.0) THEN
                           HALO(2) = 'z'
                        ELSE
                           HALO(2) = CHAR(MOD(LBL,26)+96)
                        ENDIF
                        CALL TEXT(HALO)
                        GO TO 2030
                     ELSE IF (((LABL(LBL,1).EQ.0).AND.
     *                  (LABL(LBL,2).EQ.0)).OR.(LBL.EQ.260))
     *                  THEN
                        JX = KKK * MULTX - 6
                        JY = YYY * MULTY - 4
                        J3X = JX + 3
                        J3Y = JY - 3
                        CALL BAR(JX,JY,J3X,J3Y)
                        GO TO 2030
                     ENDIF
 2020             CONTINUE
 2030             CONTINUE
               ENDIF
            ELSE IF (LMM(KKKK,YYY).LT.256) THEN
               IF ((MM(KKK,YY).GE.112).AND.(MM(KKK,YY).LE.
     *            120).AND.((MM(KKK-1,YY).EQ.68).OR.
     *            (MM(KKK-1,YY).EQ.77))) THEN
                  HALO(2) = CHAR(MM(KKK,YY) - 63)
               ELSE
                  HALO(2) = CHAR(LMM(KKKK,YYY))
                  IF (HALO(2).EQ.'J') HALO(2) = 'H'
               ENDIF
               CALL CURSOR(KKKK,YYY)
               IF ((MM(KKK,YY).GE.50).AND.(MM(KKK,YY).LE.57)
```

```
     *                   .AND.(((MM(KKK-1,YY).GE.65).AND.(MM(KKK-1,YY)
     *                   .LE.90)).OR.((MM(KKK-1,YY).GE.97).AND.
     *                   (MM(KKK-1,YY).LE.122)))) THEN
                         CALL MOVTCR(0,2)
                         CALL TEXT(HALO)
                         CALL MOVTCR(0,-2)
                      ELSE IF (((LMM(KKKK,YYY).EQ.43).OR.(LMM(KKKK,YYY)
     *                   .EQ.45)).OR.((MM(KKK,YYY).GE.49).AND.(MM(KKK,
     *                   YYY).LE.57).AND.((LMM(KKK-1,YYY).EQ.43).OR.
     *                   (LMM(KKK-1,YYY).EQ.45)))) THEN
                         DO 2060 LX = KKK,1,-1
                            IF (MM(LX,YYY).EQ.42) THEN
                               CALL MOVTCR(0,-10)
                               CALL TEXT(HALO)
                               CALL MOVTCR(0,10)
                               GO TO 2070
                            ELSE IF ((MM(LX,YYY).EQ.0).OR.(LX.EQ.1))
     *                         THEN
                               CALL TEXT(HALO)
                               GO TO 2070
                            ENDIF
 2060                    CONTINUE
 2070                    CONTINUE
                      ELSE
                         CALL TEXT(HALO)
                      ENDIF
                   ELSE IF ((KKK.NE.DLX).OR.(YY.NE.DLY)) THEN
                      MBOND = LMM(KKKK,YYY)
                      CALL DRAW2(KKKK,YYY,MBOND)
                   ENDIF
                   IF (RETR) MM(KKK,YY) = 0
                ENDIF
 3000        CONTINUE
             ENDIF
 4000        CONTINUE
          ELSE
             DO 5000 YY = IY,IY+PASY2
                IF (((MM(IX,YY).GT.0).OR.RETR).AND.(YY.LE.MAXY)) THEN
                   YYY = YY
                   IF (RETR) THEN
                      IF ((IDTPIX(IX,YY).NE.0).AND.(MM(IX,YY).EQ.0))
     *                   THEN
                         MM(IX,YY) = IDTPIX(IX,YY)
                      ELSE
                         GO TO 5000
                      ENDIF
                   ENDIF
                   IF (MM(IX,YY).EQ.46) THEN
                      IF (RETR) THEN
                         DO 4019 LBL = 1,260
                            IF ((LLABL(LBL,1).EQ.IX).AND.
     *                         (LLABL(LBL,2).EQ.YY)) THEN
                               CALL CURSOR(IX,YYY)
                               IF (MOD(LBL,26).EQ.0) THEN
                                  HALO(2) = 'z'
                               ELSE
                                  HALO(2) = CHAR(MOD(LBL,26)+96)
                               ENDIF
                               CALL TEXT(HALO)
                               GO TO 4029
                            ELSE IF (((LLABL(LBL,1).EQ.0).AND.
     *                         (LLABL(LBL,2).EQ.0)).OR.(LBL.EQ.260))
     *                         THEN
                               JX = IX * MULTX - 6
                               JY = YY * MULTY - 4
                               J3X = JX + 3
                               J3Y = JY - 3
                               CALL BAR(JX,JY,J3X,J3Y)
                               GO TO 4029
                            ENDIF
 4019                    CONTINUE
 4029                    CONTINUE
                      ELSE
                         DO 4020 LBL = 1,260
```

```
                  IF ((LABL(LBL,1).EQ.IX).AND.(LABL(LBL,2)
     *            .EQ.YY)) THEN
                     CALL CURSOR(IX,YYY)
                     IF (MOD(LBL,26).EQ.0) THEN
                        HALO(2) = 'z'
                     ELSE
                        HALO(2) = CHAR(MOD(LBL,26)+96)
                     ENDIF
                     CALL TEXT(HALO)
                     GO TO 4030
                  ELSE IF (((LABL(LBL,1).EQ.0).AND.
     *            (LABL(LBL,2).EQ.0)).OR.(LBL.EQ.260)) THEN
                     JX = IX * MULTX - 6
                     JY = YYY * MULTY - 4
                     J3X = JX + 3
                     J3Y = JY - 3
                     CALL BAR(JX,JY,J3X,J3Y)
                     GO TO 4030
                  ENDIF
4020           CONTINUE
4030        CONTINUE
         ENDIF
      ELSE IF (LMM(IX,YYY).LT.256) THEN
         CALL CURSOR(IX,YYY)
         IF ((MM(IX,YY).GE.112).AND.(MM(IX,YY).LE.
     *      120).AND.((MM(IX-1,YY).EQ.68).OR.
     *      (MM(IX-1,YY).EQ.77))) THEN
            HALO(2) = CHAR(MM(IX,YY) - 63)
         ELSE
            HALO(2) = CHAR(LMM(IX,YYY))
            IF (HALO(2).EQ.'J') HALO(2) = 'H'
         ENDIF
         IF ((MM(IX,YY).GE.50).AND.(MM(IX,YY).LE.57).AND.
     *      (((MM(IX-1,YY).GE.65).AND.(MM(IX-1,YY).LE.90))
     *      .OR.((MM(IX-1,YY).GE.97).AND.(MM(IX-1,YY).LE.
     *      122)))) THEN
            CALL MOVTCR(0,2)
            CALL TEXT(HALO)
            CALL MOVTCR(0,-2)
         ELSE IF (((LMM(IX,YYY).EQ.43).OR.(LMM(IX,YYY).EQ.
     *      45)).OR.((MM(IX,YY).GE.49).AND.(MM(IX,YY)
     *      .LE.57).AND.((LMM(IX-1,YYY).EQ.43).OR.(LMM(IX-1,
     *      YYY).EQ.45)))) THEN
            DO 4060 LX = IX,1,-1
               IF (MM(LX,YYY).EQ.42) THEN
                  CALL MOVTCR(0,-10)
                  CALL TEXT(HALO)
                  CALL MOVTCR(0,10)
                  GO TO 4070
               ELSE IF ((MM(LX,YYY).EQ.0).OR.(LX.EQ.1)) THEN
                  CALL TEXT(HALO)
                  GO TO 4070
               ENDIF
4060        CONTINUE
4070        CONTINUE
         ELSE
            CALL TEXT(HALO)
         ENDIF
      ELSE IF ((IX.NE.DLX).OR.(YY.NE.DLY)) THEN
         MBOND = LMM(IX,YYY)
         CALL DRAW2(IX,YYY,MBOND)
      ENDIF
      IF (RETR) MM(IX,YYY) = 0
   ENDIF
5000  CONTINUE
   ENDIF
   RETURN
   END
C
      SUBROUTINE DEL(KAR,IX,IY,INCX,INCY,IWHICH)
      IMPLICIT INTEGER*2 (A-Z)
      REAL SLOPE,DX,DY,THETA,ROUNDX,ROUNDY(2),DIAG
      INTEGER*4 MM,IDTPIX
      INTEGER*2 RTNX(10),RTNY(10)
      CHARACTER*1 HALO(3)
```

```
        LOGICAL*2 BONDEL
        COMMON /CD/ MAXX,MAXY
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
        COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
        COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /LABELS/ NR,NJLAST,NJNEXT
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /SIZZE/ MULTX,MULTY
        COMMON /IPLUS/ IHIGH(14,2)
        COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
        COMMON /CUR/ ICUR
        COMMON /HP/IHP
        COMMON /HEAD/ MW(12),ISTATE,PAGE
CXT     BONDEL = TRUE if a bond was last drawn between 2 nodes by
CXT     SUBROUTINE DRAW.
        COMMON /DELBND/ BONDEL
C
C  This subroutine handles, on input of a delete (ASCII 127), removal
C  of the most recently entered character, bond, or long bond.
C
        ICUR = 0
        CALL CURSOR(IX,IY)
        IF ((JCHAR.EQ.2).AND.BONDEL) THEN
           IX = IX - 1
           GO TO 11111
        ENDIF
C Erase bonds here, chars below.
        IF (JCHAR.NE.1) GOTO 1
11111   DLX = IX - INCX
        DLY = IY - INCY
        IF ((MM(DLX,DLY).EQ.46).OR.((MM(DLX,DLY).GE.65).AND.
     *     (MM(DLX,DLY).LE.122)).OR.((MM(DLX,DLY).GE.48).AND.
     *     (MM(DLX,DLY).LE.57))) THEN
           IX = IX - INCX
           IY = IY - INCY
           GO TO 11111
C If there is nothing to delete, the cursor is left stationary.
        ELSE IF (MM(DLX,DLY).EQ.0) THEN
           ICUR = 1
           CALL CURSOR(IX,IY)
           RETURN
        ENDIF
        BEGX = IX
        BEGY = IY
        IF (LMM(DLX,DLY).GE.256) THEN
           BONDEL = .TRUE.
           IF ((INCY.NE.0).AND.(LMM(IX,IY).LT.256))
     *        CALL REPLCE(IX,IY,INCX,INCY,DLX,DLY,1)
        ELSE
           BONDEL = .FALSE.
        ENDIF
        VHSCR = 0
C
C Back up one notch
2       CONTINUE
        IX = IX - INCX
        IY = IY - INCY
C
C Erase bonds and filler atoms until the next node:
        IF ((LMM(IX,IY).GT.256).OR.((MM(IX,IY).GE.50).AND.
     2     (MM(IX,IY).LE.57)) .OR. ((MM(IX,IY).EQ.72) .AND.
     3     ((MM(IX+1,IY).LT.97).OR.(MM(IX+1,IY).GT.122)))) THEN
           IF ((INCX.EQ.0).AND.(MM(IX,IY).EQ.72)) THEN
              IF ((MM(IX+1,IY).GE.50).AND.(MM(IX+1,IY).LE.57)) VHSCR = 1
           ENDIF
22         CONTINUE
           IF ((BONDEL).AND.(IABS(INCX*INCY).EQ.1)) THEN
                IF (IHP .EQ. 1) THEN
                CALL BERASE(IX,IY)
                ELSE
                FX = IX -1
              CALL FTLOCA(IY,FX)
              CALL FTEXT('^    ^')
                ENDIF
```

```
            ELSE
               CALL FTLOCA(IY,IX)
         IF (IHP .EQ. 1) THEN
         CALL ERASE(IX,IY)
         ELSE
               CALL FTEXT('^ ^')
         ENDIF
            ENDIF
            IF (((MM(IX,IY).GE.50).AND.(MM(IX,IY).LE.57).AND.
     *         (LMM(IX-1,IY).NE.43).AND.(LMM(IX-1,IY).NE.45)).OR.
     *         (BONDEL)) THEN
               IF (MOD((IY*10),40).EQ.0) THEN
                  IF ((IY.EQ.8).OR.(IY.EQ.28).OR.(IY.EQ.16)) THEN
                     FY = ((IY * 10) / 11) + 1
                     CALL FTSIZE(1,11)
                  ELSE
                     FY = ((IY * 10) / 9) + 1
                     CALL FTSIZE(1,9)
                  ENDIF
               ELSE
                  FY = ((IY * 10) / 8) + 1
                  CALL FTSIZE(1,8)
               ENDIF
               IF((BONDEL).AND.(IABS(INCX*INCY).EQ.1))THEN
                 IF (IHP .EQ. 1) THEN
                 CALL BERASE(IX,IY)
                 ELSE
                  CALL FTLOCA(FY,FX)
                  CALL FTEXT('^   ^')
                  CALL FTSIZE(1,10)
                 ENDIF
                  MM(IX,IY) = 0
                  FY = IY - IHP
                  CALL REPLCE(IX,IY,INCX,INCY,IX,IY,0)
                  IF (INCY.LT.0) THEN
                     FX = IX - INCX
                     CALL REPLCE(IX,FY,INCX,INCY,FX,FY,0)
                  ELSE
                     CALL REPLCE(IX,FY,INCX,INCY,0,0,0)
                  ENDIF
               ELSE
                  CALL FTLOCA(FY,IX)
                 IF (IHP .EQ. 1) THEN
                 CALL ERASE(IX,IY)
                 ELSE
                  CALL FTEXT('^ ^')
                 ENDIF
                  CALL FTSIZE(1,10)
                  MM(IX,IY) = 0
                  IF (INCY.EQ.0) THEN
                     FY = IY -IHP
                     CALL REPLCE(IX,FY,INCX,INCY,0,0,0)
                  ENDIF
               ENDIF
            ENDIF
            IF (VHSCR.EQ.1) THEN
               IX = IX + 1
               VHSCR = 2
               GO TO 22
            ELSE IF (VHSCR.EQ.2) THEN
               FY = IY + 1
               CALL REPLCE(IX,FY,INCX,INCY,0,0,0)
               IX = IX - 1
               VHSCR = 0
            ENDIF
C Keep deleting this bond
      GOTO 2
      ENDIF
C
3     CONTINUE
      IF (INCY.NE.0) THEN
         CALL REPLCE(IX,IY,INCX,INCY,0,0,1)
         CALL REPLCE(BEGX,BEGY,INCX,INCY,0,0,1)
      ENDIF
      IF (LBLEN.GT.0) CALL RELONG
```

```
      IF (LEVEL.EQ.0) ICUR = 1
      CALL CURSOR(IX,IY)
      IF (MM(IX,IY).LE.0) GOTO 7
      K=LMM(IX,IY)
      IF (K.EQ.46) GOTO 23
C IF STEREO H IS ERASED, REPLACE WITH STEREO H, NOT INTERNALLY
C STORED J.
       IF (K .EQ. 74) K=72
C TRANSLATE Dp-Dx to D1-D9 and Mp-Mx to M1-M9 for redisplay.
       IF ((K.GE.112).AND.(K.LE.120).AND.((MM(IX-1,IY).EQ.
    *    68).OR.(MM(IX-1,IY).EQ.77))) K = K - 63
       HALO(2) = CHAR(K)
       CALL TEXT(HALO)
C retype letter
C RECONVERT Dp to D1 and Mp to M1.
      IF ((K.GE.49).AND.(K.LE.57).AND.((MM(IX-1,IY).EQ.
    *    68).OR.(MM(IX-1,IY).EQ.77))) K = K + 63
       IF (K.NE.46) GOTO 10
C Loop to retype marker--not nec if dot only
23              DO 21 I=1,260
                IF (LABL(I,1).LT.0) GOTO 21
                IF (LABL(I,1).EQ.0) GO TO 5000
                IF ((LABL(I,1).NE.IX).OR.(LABL(I,2).NE.IY)) GOTO 21
C ASCII marker
                MARK=MOD(I,26)+96
                IF (MARK.EQ.96) MARK=122
                CALL CURSOR (IX,IY)
                HALO(2) = CHAR(MARK)
                CALL TEXT(HALO)
C retype marker
                GOTO 10
21           CONTINUE
5000         CONTINUE
             JX = IX * MULTX - 6
             JY = IY * MULTY - 4
             J3X = JX + 3
             J3Y = JY - 3
             CALL BAR(JX,JY,J3X,J3Y)
C       Identify cap, '.', AND '?'.
10      IF (.NOT.((K.EQ.46) .OR. (K.EQ.63) .OR. ((K.GE.65).AND.(K.LE.90)
    2     )))  GOTO 6
C identify as if this node was just typed.
        KAR=K
        ICHAR=2
        IX=IX+1
        GOTO 7
6       IF ((K.LT.97) .OR. (K.GT.122)) GOTO 7
        KAR=LMM(IX-1,IY)
        ICHAR=2
7       CONTINUE
        IF (IX.GT.MAXX) THEN
           IX = MAXX
        ELSE IF (IX.LT.1) THEN
           IX = 1
        ENDIF
        IF (IY.GT.MAXY) THEN
           IY = MAXY
        ELSE IF (IY.LT.1) THEN
           IY = 1
        ENDIF
        BONDEL = .FALSE.
        ICUR = 1
        CALL CURSOR (IX,IY)
        RETURN
C
1       IF (JCHAR.EQ.8) GOTO 60
        IF (JCHAR.EQ.6) GO TO 40
        IF (JCHAR.EQ.9) GO TO 140
        IX=IX-1
CXT
C If there is nothing to delete, the cursor is left stationary.
        IF (MM(IX,IY).EQ.0) THEN
           IX = IX + 1
           ICUR = 1
           CALL CURSOR(IX,IY)
```

```
            RETURN
         ENDIF
C Delete prevous char


         CALL FTLOCA(IY,IX)
         IF (IHP .EQ. 1) THEN      !Use this undrawing section if using
                                   !an HP terminal
         CALL ERASE(IX,IY)         !Erase pixel
         ELSE
         CALL FTEXT('^ ^')
         IF ((MM(IX,IY).EQ.46).OR.
     *      ((MM(IX,IY).GE.50).AND.(MM(IX,IY).LE.57).AND.
     *      (LMM(IX-1,IY).NE.43).AND.(LMM(IX-1,IY).NE.45)).OR.(MM(IX,
     *      IY).EQ.103).OR.(MM(IX,IY).EQ.106).OR.(MM(IX,IY).EQ.112)
     *      .OR.(MM(IX,IY).EQ.113).OR.(MM(IX,IY).EQ.121)) THEN
            IF (MOD((IY*10),40).EQ.0) THEN
               IF ((IY.EQ.8).OR.(IY.EQ.28).OR.(IY.EQ.16)) THEN
                  FY = ((IY * 10) / 11) + 1
                  CALL FTSIZE(1,11)
               ELSE
                  FY = ((IY * 10) / 9) + 1
                  CALL FTSIZE(1,9)
               ENDIF
            ELSE
               FY = ((IY * 10) / 8) + 1
               CALL FTSIZE(1,8)
            ENDIF
            CALL FTLOCA(FY,IX)
            CALL FTEXT('^ ^')
            CALL FTSIZE(1,10)
            FY = IY + 1
            CALL REPLCE(IX,FY,0,0,0,0,0)
         ENDIF
         ENDIF
         CALL CURSOR(IX,IY)
         IF (MM(IX,IY).NE.46) GOTO 4
C Elim erased symbols from marker list
                DO 5 I=1,260
                IF (LABL(I,1)+LABL(I,2).EQ.0) GOTO 4
                IF ((LABL(I,1).NE.IX).OR.(LABL(I,2).NE.IY)) GOTO 5
                LABL(I,1)=-999
                LABL(I,2)=-999
                MRKCHN(I)=0
                GOTO 4
5               CONTINUE
C
4        MM(IX,IY)=0
         JX=IX-1
         K=LMM(JX,IY)
         IF (.NOT.((K.GE.30).AND.(K.LT.123))) GOTO 1110
         IX=IX-1
         GO TO 10
1110     NODE=0
         DO 50 IDIRX=-1,1
         DO 50 IDIRY=-1,1
         NEWX=IX+IDIRX
         NEWY=IY+IDIRY
         IF ((IDIRX.EQ.0).AND.(IDIRY.EQ.0)) GOTO 50
C Off edge
17       IF ((NEWX.LT.1) .OR. (NEWX.GT.MAXX)) GOTO 50
         IF ((NEWY.LT.1) .OR. (NEWY.GT.MAXY)) GOTO 50
C Blank space
         IF (MM(NEWX,NEWY).EQ.0) GOTO 50
C Bonds are > 256
         IF (LMM(NEWX,NEWY).LT.256) GOTO 14
C Bond extracted for type
         JBOND=LMM(NEWX,NEWY)/2**8
C Following 5 lines skip bonds not pointed to node being analyzed
C Bond direction
         JDIR=LMM(NEWX,NEWY) - JBOND*2**8
         IF ((IDIRX*IDIRY.EQ.-1).AND.(MOD(JDIR,4).NE.2)) GO TO 50
         IF ((IDIRX*IDIRY.EQ.1).AND.(MOD(JDIR,4).NE.0)) GO TO 50
         IF ((IDIRX.EQ.0) .AND. (MOD(JDIR,4).NE.1)) GOTO 50
```

```
        IF ((IDIRY.EQ.0) .AND. (MOD(JDIR,4).NE.3)) GOTO 50
        NODE=1
        GOTO 51
C
C H, lowercase, numerals, signs etc.
14      NEWX=NEWX+IDIRX
C This aboids endless loop.
        IF (IDIRX .EQ. 0) GO TO 50
        GOTO 17
50      CONTINUE
51      CONTINUE
C Picture boundary limits are adjusted.
        IF (IX.GT.MAXX) THEN
           IX = MAXX
        ELSE IF (IX.LT.1) THEN
           IX = 1
        ENDIF
        IF (IY.GT.MAXY) THEN
           IY = MAXY
        ELSE IF (IY.LT.1) THEN
           IY = 1
        ENDIF
        IF (NODE.LE.0) THEN
           ICUR = 1
           CALL CURSOR(IX,IY)
           RETURN
        ENDIF
C
C BOND
        JCHAR=1
        ICHAR=1
        IBDIR=JDIR
        IBTYPE=JBOND
        KAR=LMM(NEWX,NEWY)
        IF (IX.GT.MAXX) THEN
           IX = MAXX
        ELSE IF (IX.LT.1) THEN
           IX = 1
        ENDIF
        IF (IY.GT.MAXY) THEN
           IY = MAXY
        ELSE IF (IY.LT.1) THEN
           IY = 1
        ENDIF
        ICUR = 1
        CALL CURSOR(IX,IY)
        RETURN
C We are deleting a charge
40      IX=IX-1
        IF(LMM(IX,IY).EQ.43 .OR. LMM(IX,IY).EQ.45)GO TO 45
C Charge at a node
        IIX=IX
        IF (MM(IX,IY).EQ.46.OR.MM(IX,IY).EQ.63.OR.
     1  (MM(IX,IY).GE. 65).AND.(MM(IX,IY) .LE.90)) GO TO 41
        IX=IX-1
        IF((MM(IX,IY).GE.65).AND.(MM(IX,IY).LE.90)) GOTO 41
C Can't find good node
        IERR=24
        CALL MYERR(IERR,KAR,KAR)
        IX=IIX+1
        ICUR = 1
        CALL CURSOR(IX,IY)
        RETURN
41      JX=IX+1
        JY = IY - 1
        IF((LMM(JX,JY).EQ.43.OR.LMM(JX,JY).EQ.45) .AND.
     1  (IX .EQ. (JX-IHIGH(IHMM(JX,JY),1))) .AND.
     2  (IY .EQ. (JY+IHP*IHIGH(IHMM(JX,JY),2)))) GO TO 47
        JY = IY + 1
        IF((LMM(JX,JY).EQ.43.OR.LMM(JX,JY).EQ.45).AND.
     1  (IX .EQ. (JX-IHIGH(IHMM(JX,JY),1))) .AND.
     2  (IY .EQ. (JY+IHP*IHIGH(IHMM(JX,JY),2)))) GO TO 47
        JX=IX-1
        IF((LMM(JX,JY).EQ.43.OR.LMM(JX,JY).EQ.45) .AND.
     1  (IX .EQ. (JX-IHIGH(IHMM(JX,JY),1))) .AND.
     2  (IY .EQ. (JY+IHP*IHIGH(IHMM(JX,JY),2)))) GO TO 47
```

```
      JY = IY - 1
      IF((LMM(JX,JY).EQ.43.OR.LMM(JX,JY).EQ.45) .AND.
     1 (IX .EQ. (JX-IHIGH(IHMM(JX,JY),1))) .AND.
     2 (IY .EQ. (JY+IHP*IHIGH(IHMM(JX,JY),2)))) GO TO 47
      JX=JX-1
      IF((LMM(JX,JY).EQ.43.OR.LMM(JX,JY).EQ.45) .AND.
     1 (IX .EQ. (JX-IHIGH(IHMM(JX,JY),1))) .AND.
     2 (IY .EQ. (JY+IHP*IHIGH(IHMM(JX,JY),2)))) GO TO 47
      JY = IY + 1
      IF((LMM(JX,JY).EQ.43.OR.LMM(JX,JY).EQ.45).AND.
     1 (IX .EQ. (JX-IHIGH(IHMM(JX,JY),1))) .AND.
     2 (IY .EQ. (JY+IHP*IHIGH(IHMM(JX,JY),2)))) GO TO 47
      IERR=24
      CALL MYERR(IERR,KAR,KAR)
C Can't find charge
      IX=IIX+1
      CALL CURSOR(IX,IY)
      IF (IX.GT.MAXX) THEN
         IX = MAXX
      ELSE IF (IX.LT.1) THEN
         IX = 1
      ENDIF
      IF (IY.GT.MAXY) THEN
         IY = MAXY
      ELSE IF (IY.LT.1) THEN
         IY = 1
      ENDIF
      ICUR = 1
      RETURN
C Clear cell
47    MM(JX,JY)=0
      CALL FTLOCA(JY,JX)
      CALL FTEXT('^ ^')
C Erase charge
      IF ((MM(JX+1,JY).GE.50).AND.(MM(JX+1,JY).LE.57)) THEN
C Clear cell
         MM(JX+1,JY)=0
         FX = JX + 1
         CALL FTLOCA(JY,FX)
         CALL FTEXT('^ ^')
      ENDIF
C Erase digit
      IX=IIX+1
      CALL CURSOR(IX,IY)
      KAR=LMM(IIX,IY)
      ICHAR=2
      IF((KAR.GE.97).AND.(KAR.LE.122))ICHAR=4
C Make it look like we just entered node
      IF (IX.GT.MAXX) THEN
         IX = MAXX
      ELSE IF (IX.LT.1) THEN
         IX = 1
      ENDIF
      IF (IY.GT.MAXY) THEN
         IY = MAXY
      ELSE IF (IY.LT.1) THEN
         IY = 1
      ENDIF
      ICUR = 1
      CALL CURSOR(IX,IY)
      RETURN
C Clear MM cell - we have a delocalized charge
45    MM(IX,IY)=0
      CALL FTLOCA(IY,IX)
      CALL FTEXT('^ ^')
C Erase charge
      IF((MM(IX+1,IY).LT.48) .OR. MM(IX+1,IY).GT.57) GO TO 46
C Charge is followed by digit - del that also
      IX=IX+1
```

```
C Clear cell
        MM(IX,IY)=0
        CALL FTLOCA(IY,IX)
        CALL FTEXT('^ ^')
C Erase digit
46      CALL CURSOR(IX,IY)
        KAR=13
        ICHAR=26
C Return witg kar = CARR RETURN - I.E. NOP
        MODE=1
        IF (IX.GT.MAXX) THEN
           IX = MAXX
        ELSE IF (IX.LT.1) THEN
           IX = 1
        ENDIF
        IF (IY.GT.MAXY) THEN
           IY = MAXY
        ELSE IF (IY.LT.1) THEN
           IY = 1
        ENDIF
        ICUR = 1
        CALL CURSOR(IX,IY)
        RETURN
C We are deleting a "
140     IX=IX-1
C At a node
        IIX=IX
        IF (MM(IX,IY).EQ.46.OR.MM(IX,IY).EQ.63.OR.
     1  (MM(IX,IY).GE. 65).AND.(MM(IX,IY) .LE.90)) GO TO 141
        IX=IX-1
        IF((MM(IX,IY).GE.65).AND.(MM(IX,IY).LE.90)) GOTO 141
C Can't find good node
        IERR=24
        CALL MYERR(IERR,KAR,KAR)
        IX=IIX+1
        ICUR = 1
        CALL CURSOR(IX,IY)
        RETURN
C
141     CONTINUE
        JX=IX+1
        JY = IY - 1
        IF ((MM(JX,JY).EQ.34).AND.(DSCNC(3,NBD1).EQ.IX).AND.
     *     (DSCNC(4,NBD1).EQ.IY)) GO TO 147
        JY = IY + 1
        IF ((MM(JX,JY).EQ.34).AND.(DSCNC(3,NBD1).EQ.IX).AND.
     *     (DSCNC(4,NBD1).EQ.IY)) GO TO 147
        JX= IX - 1
        IF ((MM(JX,JY).EQ.34).AND.(DSCNC(3,NBD1).EQ.IX).AND.
     *     (DSCNC(4,NBD1).EQ.IY)) GO TO 147
        JY = IY - 1
        IF ((MM(JX,JY).EQ.34).AND.(DSCNC(3,NBD1).EQ.IX).AND.
     *     (DSCNC(4,NBD1).EQ.IY)) GO TO 147
        IERR=24
        CALL MYERR(IERR,KAR,KAR)
C Can't cind "
        IX=IIX+1
        CALL CURSOR(IX,IY)
        IF (IX.GT.MAXX) THEN
           IX = MAXX
        ELSE IF (IX.LT.1) THEN
           IX = 1
        ENDIF
        IF (IY.GT.MAXY) THEN
           IY = MAXY
        ELSE IF (IY.LT.1) THEN
           IY = 1
        ENDIF
        ICUR = 1
        RETURN
C Clear cell
147     MM(JX,JY)=0
        CALL FTLOCA(JY,JX)
        CALL FTEXT('^ ^')
        DO 1444 K = 1,6
```

```
           DSCNC(K,NBD1) = 0
1444     CONTINUE
         NBD1 = NBD1 - 1
148      IX=IIX+1
         CALL CURSOR(IX,IY)
         KAR=LMM(IIX,IY)
         ICHAR=2
         IF((KAR.GE.97).AND.(KAR.LE.122))ICHAR=4
C Make it look like we just entered node.
         IF (IX.GT.MAXX) THEN
            IX = MAXX
         ELSE IF (IX.LT.1) THEN
            IX = 1
         ENDIF
         IF (IY.GT.MAXY) THEN
            IY = MAXY
         ELSE IF (IY.LT.1) THEN
            IY = 1
         ENDIF
         ICUR = 1
         CALL CURSOR(IX,IY)
         RETURN
145      MM(IX,IY)=0
         CALL FTLOCA(IY,IX)
         CALL FTEXT('^ ^')
         RETURN
C Following code (thru END) deletes last long bond entered:
C
C If IWHICH not 0 then delete long bond # IWHICH
60       LINE=IWHICH
         IF(IWHICH .NE. 0) GO TO 62
         LINE=0
C Find last long bond entered in LNGBND.
                 DO 61 I=1,200
                 IF (LNGBND(I,1).EQ.0) GOTO 62
                 LINE=I
61               CONTINUE
C
62       CONTINUE
         IF (IHP .EQ. 1) THEN
         CALL HPLONG(LINE)
         ELSE
       IX1=LNGBND(LINE,1)
         IY1=LNGBND(LINE,2)
         IX2=LNGBND(LINE,3)
         IY2=LNGBND(LINE,4)
         IBOND=LNGBND(LINE,5)
         DY = IY2 - IY1
         IF (DY.GT.0) THEN
            DY = (-1) * DY
            BGX = IX2
            BGY = IY2
            FNX = IX1
            FNY = IY1
         ELSE
            BGX = IX1
            BGY = IY1
            FNX = IX2
            FNY = IY2
         ENDIF
         DX = FNX - BGX
         KX = BGX
         KY = BGY
         SLOPE = 0.0
         IF (DX.NE.0.0) THEN
            SLOPE = DY / DX
            THETA = ATAN(SLOPE)
            IF ((THETA.LE.0.).AND.(DX.LT.0.)) THETA = THETA - 3.14159265
C           Principal value problem
            IF ((THETA.GT.0.) .AND. ((DX.LT.0.) .OR. (DY.LT.0.)))
     2           THETA = THETA + 3.14159265
         ENDIF
         IF (DX.GT.0.0) THEN
            INKX = 1
            ROUNDX = 0.0
```

```
      ELSE IF (DX.EQ.0.0) THEN
         INKX = 0
         ROUNDX = 0.0
      ELSE
         INKX = -1
         ROUNDX = 0.0
      ENDIF
      IF (DY.LT.0.0) THEN
         INKY = -1
         ROUNDY(1) = 1.0
         ROUNDY(2) = -1.0
      ELSE
         INKY = 0
      ENDIF
      DIAG = ABS(SLOPE)
      IF ((0.86666.LT.DIAG).AND.(DIAG.LT.1.15385)) THEN
         THRI = 0
         XL = 3
         XR = 4
         RY = BGY
      ELSE IF ((DX*DY.NE.0.0).AND.(ABS(DX).GT.ABS(DY))) THEN
         THRI = 0
         XL = 3
         XR = 4
      ELSE
         THRI = -1
         XL = 3
         XR = 5
      ENDIF
      NDDCHG = 0
2311  CONTINUE
      ICUR = 0
      IF (DX.EQ.0.0) THEN
         KY = KY + INKY
      ELSE IF (DY.EQ.0.0) THEN
         KX = KX + INKX
      ELSE IF ((0.86666.LT.DIAG).AND.(DIAG.LT.1.15385)) THEN
         IF (THRI.GT.0) THEN
            KY = RY + ROUNDY(THRI)
         ELSE
            KX = KX + INKX
            RY = RY + INKY
            KY = RY
         ENDIF
      ELSE IF (ABS(DX).GE.ABS(DY)) THEN
         IF (THRI.GT.0) THEN
            KY = RY + ROUNDY(THRI)
         ELSE
            KX = FLOAT(KX) + FLOAT(INKX)
            RY = (FLOAT(IABS(KX-BGX)) * SIN(THETA)) + FLOAT(BGY)
            KY = RY
         ENDIF
      ELSE IF (ABS(DX).LT.ABS(DY)) THEN
         KY = KY + INKY
         KX = (FLOAT(IABS(KY-BGY)) * COS(THETA)) + FLOAT(BGX)
      ENDIF
      IF (IABS(INKX*INKY).EQ.1) THEN
         IF (THRI.EQ.-1) THEN
            FX = KX - 3
            CALL FTLOCA(KY,FX)
            CALL FTEXT('^        ^')
         ELSE
            FX = KX - 3
            CALL FTLOCA(KY,FX)
            CALL FTEXT('^        ^')
         ENDIF
      ELSE
         FX = KX
         CALL FTLOCA(KY,FX)
         CALL FTEXT('^ ^')
      ENDIF
      IF (MOD((KY*10),40).EQ.0) THEN
         IF ((KY.EQ.8).OR.(KY.EQ.28).OR.(KY.EQ.16)) THEN
            FY = ((KY * 10) / 11) + 1
            CALL FTSIZE(1,11)
```

```
            ELSE
               FY = ((KY * 10) / 9) + 1
               CALL FTSIZE(1,9)
            ENDIF
         ELSE
            FY = ((KY * 10) / 8) + 1
            CALL FTSIZE(1,8)
         ENDIF
         IF (IABS(INKX*INKY).EQ.1) THEN
            CALL FTLOCA(FY,FX)
            CALL FTEXT('^         ^')
            CALL FTSIZE(1,10)
         ELSE
            CALL FTLOCA(FY,FX)
            CALL FTEXT('^ ^')
            CALL FTSIZE(1,10)
         ENDIF
C
         IF (IABS(INKX*INKY).EQ.1) THEN
            DO 4000 YY = KY,KY+1
               DO 3000 KKK = KX-XL,KX+XR
                  IF (MM(KKK,YY).GT.0) THEN
                     YYY = YY
                     KKKK = KKK
                     IF (MM(KKKK,YY).EQ.46) THEN
                        DO 2020 LBL = 1,260
                           IF ((LABL(LBL,1).EQ.KKKK).AND.(LABL(LBL,2)
     *                        .EQ.YY)) THEN
                              CALL CURSOR(KKKK,YYY)
                              IF (MOD(LBL,26).EQ.0) THEN
                                 HALO(2) = 'z'
                              ELSE
                                 HALO(2) = CHAR(MOD(LBL,26)+96)
                              ENDIF
                              CALL TEXT(HALO)
                              GO TO 2030
                           ELSE IF (((LABL(LBL,1).EQ.0).AND.
     *                        (LABL(LBL,2).EQ.0)).OR.(LBL.EQ.260)) THEN
                              JX = KKK * MULTX - 6
                              JY = YYY * MULTY - 4
                              J3X = JX + 3
                              J3Y = JY - 3
                              CALL BAR(JX,JY,J3X,J3Y)
                              GO TO 2030
                           ENDIF
 2020                   CONTINUE
 2030                   CONTINUE
                     ELSE IF (LMM(KKKK,YYY).LT.256) THEN
                        IF ((MM(KKK,YY).GE.112).AND.(MM(KKK,YY).LE.
     *                     120).AND.((MM(KKK-1,YY).EQ.68).OR.
     *                     (MM(KKK-1,YY).EQ.77))) THEN
                           HALO(2) = CHAR(MM(KKK,YY) - 63)
                        ELSE
                           HALO(2) = CHAR(LMM(KKKK,YYY))
                           IF (HALO(2).EQ.'J') HALO(2) = 'H'
                        ENDIF
                        CALL CURSOR(KKKK,YYY)
                        IF ((MM(KKK,YY).GE.50).AND.(MM(KKK,YY).LE.57)
     *                     .AND.(((MM(KKK-1,YY).GE.65).AND.(MM(KKK-1,YY)
     *                     .LE.90)).OR.((MM(KKK-1,YY).GE.97).AND.
     *                     (MM(KKK-1,YY).LE.122)))) THEN
                           CALL MOVTCR(0,2)
                           CALL TEXT(HALO)
                           CALL MOVTCR(0,-2)
                        ELSE IF (((LMM(KKK,YYY).EQ.43).OR.(LMM(KKK,YYY)
     *                     .EQ.45)).OR.((MM(KKK,YY).GE.49).AND.(MM(KKK
     *                     ,YY).LE.57).AND.((LMM(KKK-1,YYY).EQ.43).OR.
     *                     (LMM(KKK-1,YYY).EQ.45)))) THEN
                           DO 2060 LX = KKK,1,-1
                              IF (MM(LX,YY).EQ.42) THEN
                                 DO 2050 LLXX = 1,NDDCHG
                                    IF ((RTNX(LLXX).EQ.KKK).AND.
     *                                 (RTNY(LLXX).EQ.YY)) GO TO 2070
 2050                            CONTINUE
                                 NDDCHG = NDDCHG + 1
```

```
                          RTNX(NDDCHG) = KKK
                          RTNY(NDDCHG) = YY
                          GO TO 2070
                       ELSE IF ((MM(LX,YY).EQ.0).OR.(LX.EQ.1))
     *                    THEN
                          CALL TEXT(HALO)
                          GO TO 2070
                       ENDIF
 2060               CONTINUE
 2070               CONTINUE
                 ELSE
                    CALL TEXT(HALO)
                 ENDIF
              ELSE
                 MBOND = LMM(KKKK,YYY)
                 CALL DRAW2(KKKK,YYY,MBOND)
              ENDIF
           ENDIF
 3000   CONTINUE
 4000   CONTINUE
     ELSE
        DO 6000 YY = KY,KY+1
           IF (MM(KX,YY).GT.0) THEN
              YYY = YY
              IF (MM(KX,YY).EQ.46) THEN
              DO 4020 LBL = 1,260
                 IF ((LABL(LBL,1).EQ.KX).AND.(LABL(LBL,2).EQ.YY))
     *              THEN
                    CALL CURSOR(KX,YYY)
                    IF (MOD(LBL,26).EQ.0) THEN
                       HALO(2) = 'z'
                    ELSE
                       HALO(2) = CHAR(MOD(LBL,26)+96)
                    ENDIF
                    CALL TEXT(HALO)
                    GO TO 4030
                 ELSE IF (((LABL(LBL,1).EQ.0).AND.(LABL(LBL,2)
     *              .EQ.0)).OR.(LBL.EQ.260)) THEN
                    JX = KX * MULTX - 6
                    JY = YYY * MULTY - 4
                    J3X = JX + 3
                    J3Y = JY - 3
                    CALL BAR(JX,JY,J3X,J3Y)
                    GO TO 4030
                 ENDIF
 4020         CONTINUE
 4030         CONTINUE
           ELSE IF (LMM(KX,YYY).LT.256) THEN
              CALL CURSOR(KX,YYY)
              IF ((MM(KX,YY).GE.112).AND.(MM(KX,YY).LE.
     *           120).AND.((MM(KX-1,YY).EQ.68).OR.
     *           (MM(KX-1,YY).EQ.77))) THEN
                 HALO(2) = CHAR(MM(KX,YY) - 63)
              ELSE
                 HALO(2) = CHAR(LMM(KX,YYY))
                 IF (HALO(2).EQ.'J') HALO(2) = 'H'
              ENDIF
              IF ((MM(KX,YY).GE.50).AND.(MM(KX,YY).LE.57).AND.
     *           (((MM(KX-1,YY).GE.65).AND.(MM(KX-1,YY).LE.90))
     *           .OR.((MM(KX-1,YY).GE.97).AND.(MM(KX-1,YY).LE.
     *           122)))) THEN
                 CALL MOVTCR(0,2)
                 CALL TEXT(HALO)
                 CALL MOVTCR(0,-2)
              ELSE IF (((LMM(KX,YYY).EQ.43).OR.(LMM(KX,YYY).EQ.
     *           45)).OR.((MM(KX,YY).GE.49).AND.(MM(KX,YY).LE.
     *           57).AND.((LMM(KX-1,YYY).EQ.43).OR.(LMM(KX-1,
     *           YYY).EQ.45)))) THEN
                 DO 4060 LX = KX,1,-1
                    IF (MM(LX,YYY).EQ.42) THEN
                       DO 4050 LLXX = 1,NDDCHG
                          IF ((RTNX(LLXX).EQ.KX).AND.
     *                       (RTNY(LLXX).EQ.YYY)) GO TO 4070
 4050                  CONTINUE
                       NDDCHG = NDDCHG + 1
                       RTNX(NDDCHG) = KX
```

```
                        RTNY(NDDCHG) = YYY
                        GO TO 4070
                     ELSE IF ((MM(LX,YYY).EQ.0).OR.(LX.EQ.1)) THEN
                        CALL TEXT(HALO)
                        GO TO 4070
                     ENDIF
4060              CONTINUE
4070              CONTINUE
               ELSE
                  CALL TEXT(HALO)
               ENDIF
            ELSE
               MBOND = LMM(KX,YYY)
               CALL DRAW2(KX,YYY,MBOND)
            ENDIF
         ENDIF
6000     CONTINUE
      ENDIF
         IF ((((KX.GE.FNX-4).AND.(KX.LE.FNX+4).AND.(INKY.NE.0))
     *      .OR.((KX.GE.FNX-1).AND.(KX.LE.FNX+1))).AND.((KY.EQ.FNY)
     *      .OR.(KY.EQ.FNY-INKY))) GO TO 3368
         IF ((KX.LT.0).OR.(KX.GT.MAXX).OR.(KY.LT.0).OR.(KY.GT.MAXY))
     *      THEN
            CALL MYERR(24,KAR,KAR)
            GO TO 43
         ENDIF
         IF (THRI.EQ.2) THEN
            THRI = 0
         ELSE IF (THRI.GE.0) THEN
            THRI = THRI + 1
         ENDIF
         GO TO 2311
3368  CONTINUE
      CALL REPLCE(IX1,IY1,INKX,INKY,0,0,1)
      CALL REPLCE(IX2,IY2,INKX,INKY,0,0,1)
      IF (NDDCHG.GT.0) THEN
         DO 3369 I = 1,NDDCHG
            HALO(2) = CHAR(MM(RTNX(I),RTNY(I)))
            ICUR = 0
            CALL CURSOR(RTNX(I),RTNY(I))
            CALL MOVTCR(0,-10)
            CALL TEXT(HALO)
            CALL MOVTCR(0,10)
3369     CONTINUE
         ICUR = 1
         CALL CURSOR(IX1,IY1)
      ENDIF
      ENDIF
C
C Now zero out the last line of LNGBND.
C     SKIP THIS "ZERO" CODE IF WE ARE GOING TO REDRAW A LONG BOND
107   CONTINUE
      LNGBND(LINE,1) = 0
      IF ((IWHICH.NE.0).AND.(IBTYPE.NE.0)) GO TO 666
         DO 63 I=2,5
            LNGBND(LINE,I) = 0
63       CONTINUE
         IF (LBLEN.GT.LINE) THEN
            DO 65 I = LINE,LBLEN
               IF (I.LT.100) THEN
                  DO 64 J = 1,5
                     LNGBND(I,J) = LNGBND(I+1,J)
64                CONTINUE
               ENDIF
65          CONTINUE
         ENDIF
         LBLEN = LBLEN - 1
666   CONTINUE
      IF (LBLEN.GT.0) CALL RELONG
C ERASE ALL H's & SUBSCRIPTS:  **********
      KX=IX1
      KY=IY1
C Only@nodes
      IF ((MM(KX,KY).LE.65) .OR. (MM(KX,KY).GT.90)) GOTO 43
C
```

```
      CALL CLRHYD(KX,KY)
      CALL VALNCE(2,IX1,IY1,0,0)
43    CONTINUE
      ICUR = 1
      CALL CURSOR(IX2+1,IY2)
      RETURN
      END
$STORAGE:2
C
      SUBROUTINE ERRMSG(KAR)
      IMPLICIT INTEGER*2 (A-Z)
      CHARACTER*82 BLNK90
      CHARACTER*1 HALO(3)
      CHARACTER*3 HALOE
      EQUIVALENCE (HALOE,HALO(1))
      CHARACTER*1 KAN
      COMMON /CHARS/IES, IDOT,ITAG,IJUMP,LBOND,KAN,ISPACE
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /BLANK/ BLNK90
      COMMON /QTVLNC/ OERR,CHER
C
      CALL FTSIZE(2,18)
      IF (PAGE.EQ.0) THEN
         CALL FTLOCA(1,1)
         CALL FTEXT(BLNK90)
      ENDIF
      PAGE = 0
      IF (CHAR(KAR).NE.KAN) THEN
         HALO(1) = KAN
         HALO(3) = KAN
      ELSE
         HALO(1) = '/'
         HALO(3) = '/'
      ENDIF
      IF (KAR.EQ.0) GOTO 101
      CALL FTLOCA(4,1)
      IF (KAR.GE.128) THEN
        CALL FTEXT('^NON-RELEVANT KEY PRESSED. REENTER.^')
        GO TO 9
      ENDIF
      IF (KAR.EQ.13) GO TO 25
         HALO(2) = CHAR(KAR)
         CALL FTEXT(HALOE)
         CALL FTEXT('^ IS AN ILLEGAL INPUT. REENTER.^')
         GO TO 9
25    CONTINUE
      CALL FTEXT('^CR IS AN ILLEGAL INPUT. REENTER.^')
      GOTO 9
101   CONTINUE
      CALL FTLOCA(4,1)
      CALL FTEXT('^MUST BEGIN LONG BOND AT A MARKER! REENTER.^')
9     CONTINUE
      CALL FTSIZE(1,10)
      RETURN
      END
C
C     ERROR MESSAGE SUBROUTINE
C
      SUBROUTINE MYERR(IERR,KAR,MAR)
      IMPLICIT INTEGER*2 (A-Z)
      CHARACTER*82 BLNK90
      CHARACTER*54 MSBUF(61)
      CHARACTER*1 HALO(3)
      CHARACTER*3 HALOE
      EQUIVALENCE (HALOE,HALO(1))
      CHARACTER*1 KAN
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /BLANK/ BLNK90
      COMMON /WARN/ ERR
      COMMON /QTVLNC/ OERR,CHER
      DATA MSBUF(1)
     1 /'^NO SPACE AVAILABLE FOR CHAIN/GROUP-ENTER CMD OR ESC ^'/
      DATA MSBUF(2)
     1 /'^CMD STRING INTERRUPTED BY CR/Q - COMMAND ABORTED    ^'/
      DATA MSBUF(3)
```

```
1   /'^BAD ENVIRONMENT FOR CHAIN OR GROUP-ENTER CMD OR ESC ^'/
    DATA MSBUF(4)
1   /'^ONLY 1 NONLOCAL CHARGE ALLOWED - CMD ABORTED        ^'/
    DATA MSBUF(5)
1   /'^MUST ENTER BOND TYPE -OR- CR                         ^'/
    DATA MSBUF(6)
1   /'^BAD/NO REPEAT CMD - REENTER CMD - (CR TO GND)        ^'/
    DATA MSBUF(7)
1   /'^BAD BOND/NO BOND FOUND - REPEAT ABORTED              ^'/
    DATA MSBUF(8)
1   /'^" BOND MARKER AND Dx NODE ARE NOT MATCHED            ^'/
    DATA MSBUF(9)
1   /'^BAD LONG BOND - (O LEN/NO ENDPOINT)- CMD ABORTED     ^'/
    DATA MSBUF(10)
1   /'^INVALID CHARACTER                                    ^'/
    DATA MSBUF(11)
1   /'^ ELEMENT DOES NOT EXIST IN ELEMENT TABLE             ^'/
    DATA MSBUF(12)
1   /'^WARNING: TOO MANY BONDS FOR VALENCY                  ^'/
    DATA MSBUF(13)
1   /'^CONTEXT ERROR - UNFORESEEN PROBLEM                   ^'/
    DATA MSBUF(14)
1   /'^NO ROOM FOR FILLER HYDROGENS                         ^'/
    DATA MSBUF(15)
1   /'^ERROR IN DECIDING WHERE TO PUT H''S                  ^'/
    DATA MSBUF(16)
1   /'^ALL MARKERS USED- OR -NOT ENOUGH MARKERS FOR CHAIN   ^'/
    DATA MSBUF(17)
1   /'^BAD ANGLE DATA FOR GROUP - CMD ABORTED               ^'/
    DATA MSBUF(18)
1   /'^NULL CONNECTION TABLE                                ^'/
    DATA MSBUF(19)
1   /'^RETURNING TO NEW STRUCTURE MENU-DATA WILL BE LOST    ^'/
    DATA MSBUF(20)
1   /'^DOT DISCONNECTED UNIT NOT STANDARD TO PROGRAM        ^'/
    DATA MSBUF(21)
1   /'^PROBLEM HANDLING DOT DISCONNECTED STRUCTURE          ^'/
    DATA MSBUF(22)
1   /'^SUM OF *M LENGTHS EXCEEDS MAXIMUM                    ^'/
    DATA MSBUF(23)
1   /'^BAD BOND - USE LONGBOND TO CROSS BOND                ^'/
    DATA MSBUF(24)
1   /'^CAN''T FIND NODE/CHARGE IN DEL - CMD ABORTED         ^'/
    DATA MSBUF(25)
1   /'^SPACE CONFLICT IN DOTDIS - CMD ABORTED               ^'/
    DATA MSBUF(26)
1   /'^TOO MANY CONNECTIONS/NODE                            ^'/
    DATA MSBUF(27)
1   /'^NO SUBSTRUCTURE FILES ON DISK - RETRIEVE ABORTED     ^'/
    DATA MSBUF(28)
1   /'^CAN''T FIND NODE FOR(+-)WILL CALL IT DELOCALIZED     ^'/
    DATA MSBUF(29)
1   /'^BAD VALUE FOR RING SIZE - ENTER CMD OR ESC           ^'/
    DATA MSBUF(30)
1   /'^BAD ENVIRONMENT FOR RING - ENTER CMD OR ESC          ^'/
    DATA MSBUF(31)
1   /'^NO SPACE FOR RING - ENTER CMD OR ESC                 ^'/
    DATA MSBUF(32)
1   /'^NO GOOD ORIENTATION FOUND - ENTER NEW COMMAND        ^'/
    DATA MSBUF(33)
1   /'^BOND WITH REDUNDANT LONG BOND BETWEEN SAME 2 NODES   ^'/
    DATA MSBUF(34)
1   /'^NO NODE ADJACENT TO " - CMD ABORTED                  ^'/
    DATA MSBUF(35)
1   /'^CONNECTION TABLE LIMITED TO 255 NODES                ^'/
    DATA MSBUF(36)
1   /'^ATTEMPT TO DRAW OFF SCREEN - CMD ABORTED             ^'/
    DATA MSBUF(37)
1   /'^2 ATTEMPTS AT TRANSMISSION FAILED                    ^'/
    DATA MSBUF(38)
1   /'^NODE ALLOWED ONLY 1 CHARGE - CMD ABORTED             ^'/
    DATA MSBUF(39)
1   /'^ALREADY IN REQUESTED STATE                           ^'/
```

```
      DATA MSBUF(40)
     1 /'^ADJACENT NODES FOUND                                    ^'/
      DATA MSBUF(41)
     1 /'^DANGLING BOND FOUND                                     ^'/
      DATA MSBUF(42)
     1 /'^AMBIGUOUSLY ASSIGNED ENTRY - REPOSITION                 ^'/
      DATA MSBUF(43)
     1 /'^ATTACHING BOND IN WRONG DIR - COMMAND ABORTED           ^'/
      DATA MSBUF(44)
     1 /'^NOT AT BOND OR MARKER - CAN''T ATTACH                   ^'/
      DATA MSBUF(45)
     1 /'^BAD BOND - END IS NOT A NODE                            ^'/
      DATA MSBUF(46)
     1 /'^*M NODE AND DEFINITIONS ARE NOT MATCHED                 ^'/
      DATA MSBUF(47)
     1 /'^NODE ALLOWED ONLY 1 " - CMD ABORTED                     ^'/
      DATA MSBUF(48)
     1 /'^SPACE CONFLICT - CMD ABORTED                            ^'/
      DATA MSBUF(49)
     1 /'^ONLY NEW BOND MAY BE DELETED IN REPEAT                  ^'/
      DATA MSBUF(50)
     1 /'^NOT AT A MARKER - CMD IGNORED                           ^'/
      DATA MSBUF(51)
     1 /'^TOO MANY CHARGES - LIBRARY CMD ABORTED                  ^'/
      DATA MSBUF(52)
     1 /'^INVALID (STRUCTURE+DOTDIS) DETECTED - CMD ABORTED       ^'/
      DATA MSBUF(53)
     1 /'^NO BOND TYPES 4, 6, OR 7 IN LONG - IBTYPE = 1           ^'/
      DATA MSBUF(54)
     1 /'^SUBSTRUCTURE TOO LONG FOR INPUT                         ^'/
      DATA MSBUF(55)
     1 /'^BAD BONDTYPE OR CHARGE VALUE - CMD ABORTED              ^'/
      DATA MSBUF(56)
     1 /'^BAD ENLARGE VALUE                                       ^'/
      DATA MSBUF(57)
     1 /'^SUBSTRUCTURE MUST EMANATE FROM MARKER OR LUHN DOT       ^'/
      DATA MSBUF(58)
     1 /'^NO SUBSTRUCTURE YET INPUT                               ^'/
      DATA MSBUF(59)
     1 /'^BAD INPUT CHAR - ENTER RETURN TWICE                     ^'/
      DATA MSBUF(60)
     1 /'^AMBIGUOUSLY PLACED NONLOCAL CHARGE - REPOSITION         ^'/
      DATA MSBUF(61)
     1 /'^+ - " NOT ALLOWED ON 2 LETTER ELEMENT IN LIBRARY        ^'/
C
      CALL FTSIZE(2,18)
      IF (CHER.EQ.2) THEN
         CALL SETSCR(1)
         PAGE = 1
         CALL DISPLA(1)
         IF (IERR.NE.18) THEN
            CALL SETCOL(0)
            CALL CLR
            CALL SETCOL(1)
            CALL FTLOCA(1,1)
         ELSE
            CALL FTLOCA(2,1)
         ENDIF
      ELSE
         IF (PAGE.EQ.0) THEN
            CALL FTLOCA(4,1)
            CALL FTEXT(BLNK90)
         ENDIF
         PAGE = 0
         CALL FTLOCA(4,1)
      ENDIF
      IF (IERR.EQ.11) GO TO 77
         CALL FTEXT(MSBUF(IERR))
         GO TO 9
77    CONTINUE
         HALO(1) = KAN
         HALO(3) = KAN
         IF (KAR.NE.32) THEN
            EL1 = KAR
            EL2 = MAR
         ENDIF
```

```
         HALO(2) =CHAR(EL1)
         CALL FTEXT(HALOE)
         HALO(2) = CHAR(EL2)
         CALL FTEXT(HALOE)
         CALL FTEXT(MSBUF(IERR))
9     CONTINUE
      IF (CHER.NE.2) CALL SETSCR(2)
      CALL FTSIZE(1,10)
      ERR = IERR
      RETURN
      END
C
      INTEGER*2 FUNCTION ILRRAY(IX,IY)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 IARRAY
      COMMON /STRPIX/LPIX,IARRAY(90,38),LBLEN,LNGBND(100,5)
C     EXTRACT LOW ORDER PORTION OF WORD
      ILRRAY=MOD(IARRAY(IX,IY),2**13)
C     THIS ELIMINATES THE CHARGE LOC INFORMATION
      RETURN
      END
C
      INTEGER*2 FUNCTION IDIR(KAR)
      IMPLICIT INTEGER*2 (A-Z)
C     Set IDIR = -1
      IDIR=-1
C     Not a bond - return IDIR = -1
      IF (KAR .LT. 256) RETURN
      IDIR=KAR/256
      IDIR=KAR-IDIR*256
      RETURN
      END
C
      INTEGER*2 FUNCTION IHMM(IX,IY)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
C     EXTRACT HIGH ORDER PORTION OF WORD
      IHMM=MM(IX,IY)/2**13
C     THIS SHOULD YIELD A NUMBER FROM 0-14
C     THIS ASSOCIATES THE CHARGE WITH THE NODE
C     NOTE - 0 = DELOCALIZED CHARGE
      RETURN
      END
C
      INTEGER*2 FUNCTION LMM(IX,IY)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
C     EXTRACT LOW ORDER PORTION OF WORD
      LMM=MOD(MM(IX,IY),2**13)
C     THIS ELIMINATES THE CHARGE LOC INFORMATION
      RETURN
      END
C
      SUBROUTINE DOTDIS(KAR,IX,IY,IRESET,LFLAG)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM
      LOGICAL*2 TERMN
      CHARACTER*1 HALO(3)
      CHARACTER*1 KAN
      CHARACTER*1 ISTAT
      COMMON /CD/ MAXX,MAXY
      COMMON /RANGE/ LOX,HIX,LOY,HIY
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /ISTATE/ ISTAT
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /BAD/ IBADX(9),IBADY(9)
      COMMON /CUR/ ICUR
      DIMENSION LIST(50)
C
      HALO(1) = KAN
      HALO(3) = KAN
      ISTATE=10
      KKAR=32
```

```
        ISTAT='*'
        MODE=1
        TERMN = .FALSE.
        CALL HEADER
        CALL CURSOR(IX,IY)
        CALL CELL(IX,IY,IGOOD)
        IF (IGOOD .NE.0) GO TO 55
        I=0
        DO 11 J = 1,50
        LIST(J)=0
11      CONTINUE
C TYPE KAR
14      CONTINUE
        HALO(2) = CHAR(KAR)
        CALL TEXT(HALO)
C STORE KAR
35      MM(IX,IY)=KAR
        IF (IX.LT.LOX) THEN
           LOX = IX
        ELSE IF (IX.GT.HIX) THEN
           HIX = IX
        ENDIF
        IF (IY.LT.LOY) THEN
           LOY = IY
        ELSE IF (IY.GT.HIY) THEN
           HIY = IY
        ENDIF
        IF (KAR .NE. 43 .AND. KAR .NE. 45) GO TO 666
C CHARGE IN LOCATION 9 - 2 LETTER NODE
        IF(MM(IX-1,IY).GE.97 .AND. MM(IX-1,IY).LE.122)
     1  MM(IX,IY)=KAR + 9*2**13
C CHARGE IN LOCATION 8 - 1 LETTER NODE
        IF(MM(IX-1,IY).GE.65 .AND. MM(IX-1,IY) .LE. 90)
     1  MM(IX,IY)=KAR + 8*2**13
        IF (MM(IX,IY) .GT. 2**13) GO TO 666
        CALL FTSIZE(2,18)
C Charge not associated with node - cmd rejected
        CALL FTLOCA(1,1)
        CALL FTEXT('^ENTER DIGIT TO ASSIGN VALUE TO CHARGE^')
        CALL FTSIZE(1,10)
        PAGE = 0
C Delete charge
        MM(IX,IY)=0
        IF (IY.GT.1) THEN
           FY = IY - 1
        ELSE
           FY = IY
        ENDIF
        CALL FTLOCA(FY,IX)
        CALL FTEXT('^ ^')
        CALL CURSOR(IX,IY)
        GO TO 65
666     I=I+1
        IX=IX+1
        CALL CURSOR(IX,IY)
        LIST(I)=KAR
        IF (I.EQ.50) GO TO 55
65      CALL INPUTX(KAR,IX,IY)
        IF (KAR.EQ.42) THEN
           IERR = 39
           CALL MYERR(IERR,IERR,IERR)
           GO TO 65
        ENDIF
C KAR = DEL?
        IF (KAR .EQ. 127) GO TO 90
        JX=IX+1
        CALL CELL(JX,IY,IGOOD)
        IF (IGOOD .NE. 0) GO TO 55
        IF (KAR .NE. 32 .AND. KAR .NE. 81) GO TO 44
        IX=IX+3
        CALL CURSOR(IX,IY)
C EXIT IF SPACE
        GO TO 50
C FOUND UC - NOW WHAT
C FOUND A ':' - GO PRINT IT
```

```
44      IF (KAR.EQ.58) GO TO 14
        IF ((KAR.GE.65).AND.(KAR.LE.90)) GO TO 14
20      IF(KAR .EQ. 47 .AND. (LIST(I).GE.48 .AND.
     1  LIST(I) .LE. 57)) GO TO 14
C DO WE HAVE DIGIT
        IF(KAR .LT. 48 .OR. KAR .GT. 57) GO TO 15
C OK IF PRECEEDED BY * OR /
        IF(LIST(I).EQ.47.OR.LIST(I).EQ.42)GO TO 14
C       PRECEEDED BY UC - THUS IS A SUBSCRIPT
C FOUND DIGIT PRECEEDED BY D OR M
        IF ((LIST(I).EQ.68).OR.(LIST(I).EQ.77)) GO TO 57
        IF(LIST(I) .GE.65 .AND. LIST(I).LE.90)GO TO 18
C       PRECEEDED BY A + OR - THUS IS A CHARGE
        IF(LIST(I) .EQ. 43 .OR. LIST(I) .EQ. 45) GO TO 222
C       PRECEEDED BY LC - THUS IS A SUBSCRIPT
        IF(LIST(I) .GE. 97 .AND. LIST(I) .LE. 122) GO TO 18
C IF BAD INPUT SEQUENCE, ISSUE MESSAGE.
        IF ((LIST(I).LT.48).OR.(LIST(I).GT.57)) GO TO 500
C IT'S A SUBSCRIPT.
        IF (((LIST(I-1).GE.65).AND.(LIST(I-1).LE.90)).OR.
     *     ((LIST(I-1).GE.97).AND.(LIST(I-1).LE.122)))GOTO 18
C IT'S A REGULAR INPUT
        GO TO 14
C WE HAVE A CHARGE
15      IF (KAR .EQ. 43 .OR. KAR .EQ. 45) GO TO 222
        IF(KAR .EQ. 36) GO TO 65
C       WE HAVE VALID LC
        IF( (KAR .GE. 97 .AND. KAR .LE. 122).AND.
     1  (LIST(I).GE.65.AND.LIST(I).LE.90))GO TO 14
C BAD CHAR - ISSUE MESSAGE AND GET NEW INPUT
500     CALL ERRMSG(KAR)
        GO TO 65
C DROP FOR A SUBSCRIPT
18      CONTINUE
        ICUR = 0
        CALL CURSOR(IX,IY)
        CALL MOVTCR(0,2)
        HALO(2) = CHAR(KAR)
        CALL TEXT(HALO)
        CALL MOVTCR(0,-2)
        ICUR = 1
C RAISE FROM SUBSCRIPT
        GO TO 35
C NOTHING TO DEL
90      IF(I .EQ. 0) GO TO 65
C DEC LIST COUNTER
        I=I-1
C DECREMENT CURSOR LOC
        IX=IX-1
C MOVE CURSOR BACK
        ICUR = 1
        CALL CURSOR(IX,IY)
C ZERO SPOT IN ARRAY
        IF (MM(IX,IY).EQ. 42) TERMN = .TRUE.
        MM(IX,IY)=0
C WHAT ARE WE TRYING TO DELETE
        J=LIST(I+1)
C IT'S A CHARGE
        IF (J .EQ. 43 .OR. J .EQ. 45) GO TO 95
        IF(J .GE.48 .AND. J .LE. 57) GO TO 98
C ERASE SPOT ON SCREEN
91      CONTINUE
        CALL REPLCE(IX,IY,0,0,0,0,1)
        IF (TERMN) GO TO 50
C MOVE CURSOR BACK AGAIN
66      CONTINUE
        ICUR = 1
        CALL CURSOR(IX,IY)
        GO TO 65
C RAISE FOR CHARGE
95      CONTINUE
        IF (IY.GT.1) THEN
           FY = IY + 1
```

```
         ELSE
            FY = IY
         ENDIF
         CALL FTLOCA(FY,IX)
         CALL FTEXT('^ ^')
C ERASE CHARGE
C DROP FROM CHARGE
         GO TO 66
98       K=LIST(I)
C IT'S A CHARGE
         IF (K .EQ. 43 .OR. K .EQ. 45) GO TO 95
C IT'S A SUBSCRIPT
         IF (K .GE. 65 .AND. K .LE. 90) GO TO 97
C IT'S A SUBSCRIPT
         IF(K .GE. 97 .AND. K .LE. 122) GO TO 97
C IT'S JUST A REGULAR CHAR
         GO TO 91
C DROP FOR SUBSCRIPT
97       CONTINUE
         CALL REPLCE(IX,IY,0,0,0,0,1)
C ERASE SUBSCRIPT
C RAISE FROM SUBSCRIPT
         GO TO 66
C
C RAISE FOR CHARGE
222      CONTINUE
         HALO(2) = CHAR(KAR)
         IF (IY.GT.1) THEN
            CALL MOVTCR(0,-10)
            CALL TEXT(HALO)
            CALL MOVTCR(0,10)
         ELSE
            CALL TEXT(HALO)
         ENDIF
         GO TO 35
C TYPE KAR
C DROP FROM CHARGE
57       CONTINUE
         HALO(2) = CHAR(KAR)
         CALL TEXT(HALO)
         KAR = KAR + 63
         GO TO 35
55       IERR=25
         CALL MYERR(IERR,KAR,KAR)
50       ISTATE=0
         LFLAG=0
C RETURN AND PROCESS Q
         IF (KAR .EQ. 81) LFLAG=1
         CALL HEADER
10       CONTINUE
         RETURN
         END
C
         SUBROUTINE REPEAT(KAR,IX,IY,INCX,INCY,IRESET,LFLAG)
         IMPLICIT INTEGER*2 (A-Z)
         INTEGER*4 MM
         CHARACTER*1 CMD(3),HCMD,CHR,REPATM
         CHARACTER*1 ISTAT
         INTRINSIC ICHAR
         COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
         COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
         COMMON /MODES/ JBTYPE,ICHR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
         COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
         COMMON /HEAD/ MW(12),ISTATE,PAGE
         COMMON /ISTATE/ ISTAT
         COMMON /CUR/ ICUR
         COMMON /FROM/ LCHAR
         COMMON /REP/ HCMD(2)
         COMMON /REPBND/ NEWBND
         COMMON /MSKIP/ ISKIP
         COMMON /WARN/ ERR
         COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
         COMMON /PROB/ IPROB,JPROB
         COMMON /DFAULT/ REPATM(2)
C
```

```
C       SET STATE VARIABLES SO THAT HEADER WILL DISPLAY
C       THE HEADER FOR REPEAT STATE
C       CLEN = LENGTH OF COMMAND STRING
        OSTATE = ISTATE
        ISTATE=9
        ISTAT='@'
        HOLD=NLARGE
        IF ((IBTYPE.EQ.0).OR.(IBTYPE.EQ.4).OR.(IBTYPE.EQ.8)) THEN
           BHOLD = IBTYPE
        ELSE
           BHOLD = 1
        ENDIF
C
C       SAVE NLARGE AND SET TEMPORARILY TO 1
        NLARGE=1
        NOCHG = 1
        ISKIP = 1
        MODE=1
        KAR = 0
        CMD(1) = REPATM(1)
        HCMD(1) = CMD(1)
        IF (REPATM(2).NE.CHAR(0)) THEN
           CMD(2) = '$'
           CMD(3) = REPATM(2)
           CLEN = 3
        ELSE
           CMD(2) = '0'
           CMD(3) = '0'
           CLEN = 1
        ENDIF
        HCMD(2) = CMD(3)
        BTYPE = 50
        IBTYPE = BTYPE - 48
        NEWBND = 0
100     CONTINUE
        CALL HEADER
        ICUR = 1
        CALL CURSOR(IX,IY)
        OKAR = KAR
        CALL INPUTX(KAR,IX,IY)
1010    IF ((KAR.EQ.13).OR.(KAR.EQ.81)) GO TO 27
        IF ((KAR.LT.48).OR.(KAR.GT.56)) GO TO 10
        BTYPE = KAR
        IBTYPE = BTYPE - 48
        GO TO 100
C
10      IF ((KAR.LT.65).OR.(KAR.GT.90)) GO TO 20
        CLEN = 1
        CMD(1) = CHAR(KAR)
        HCMD(1) = CMD(1)
        CMD(2) = '0'
        CMD(3) = '0'
        HCMD(2) = CMD(3)
        GO TO 100
C
20      IF (KAR.NE.36) GO TO 30
        CMD(2) = CHAR(KAR)
        GO TO 100
30      IF ((KAR.LT. 97).OR.(KAR.GT.122)) GO TO 50
CXT
        IF (OKAR.NE.36) THEN
           IF (NEWBND.EQ.1) THEN
              GO TO 1012
           ELSE
              GO TO 40
           ENDIF
        ENDIF
        CMD(3) = CHAR(KAR)
        HCMD(2) = CMD(3)
        CLEN = 3
        GO TO 100
C
40      CALL IDENT(KAR,IX,IY,INCX,INCY,IRESET)
        IF (JPROB.EQ.1) GO TO 27
        GO TO 100
50      IF (KAR.NE.39) GO TO 60
```

```
      IF (MM(IX-1,IY).NE.46) GO TO 70
      DO 55 I = 1,CLEN
         CHR = CMD(I)
         ZAR = ICHAR(CHR)
         ERR = 0
         CALL IDENT(ZAR,IX,IY,INCX,INCY,IRESET)
         IF (JPROB.EQ.1) GO TO 27
         IF (ERR.EQ.48) THEN
            CALL MARK(KAR,IX,IY,IERR)
            GO TO 56
         ENDIF
55    CONTINUE
56    CONTINUE
      IF (IBTYPE.EQ.BTYPE-48) GO TO 100
      IBTYPE = BTYPE - 48
      CALL HEADER
      GO TO 100
C
70    IERR = 50
      CALL MYERR(IERR,KAR,MAR)
      GO TO 100
60    IF ((KAR.LT.22).OR.(KAR.GT.31)) GO TO 85
      ZAR = KAR
      CALL DELTA(ZAR,INCX,INCY)
      ZAR = LMM(IX+INCX-1,IY+INCY)
      IF (ZAR.LT.256) NEWBND = 1
      ZAR = BTYPE
      CALL IDENT(ZAR,IX,IY,INCX,INCY,IRESET)
      CALL IDENT(KAR,IX,IY,INCX,INCY,IRESET)
      IF (JPROB.EQ.1) GO TO 27
      IF ((MM(IX,IY).EQ.0).AND.(LMM(IX-INCX,IY-INCY).GE.256)) NEWBND=1
      OKAR = KAR
      CALL INPUTX(KAR,IX,IY)
      IF (KAR.NE.127) GO TO 1011
351      IF (NEWBND.EQ.1) CALL IDENT(KAR,IX,IY,INCX,INCY,IRESET)
      IF (JPROB.EQ.1) GO TO 27
      IF (NEWBND.EQ.0) THEN
         IERR = 49
         CALL MYERR(IERR,IERR,IERR)
      ENDIF
      NEWBND = 0
      GO TO 100
1011  IF (NEWBND.NE.1) GO TO 1010
      IF ((KAR.LT.97).OR.(KAR.GT.122)) GO TO 1010
1012  CONTINUE
      IF (MM(IX,IY).EQ.0) THEN
      IF (CLEN .EQ. 3) THEN
      ICK=LMM(IX+1,IY)
      JCK=LMM(IX+2,IY)
      KCK=LMM(IX+3,IY)
      IF((ICK .GE. 256) .AND. (ICK .NE. KCK)) THEN
      IF ((MM(IX-1,IY) .NE. 0 ).OR. (MM(IX-2,IY) .NE.0)) THEN
      IERR=48
      CALL MYERR(IERR,IERR,IERR)
      KAR=127
      GO TO 351
      ELSE IF (ICK .NE. JCK) THEN
      MM(IX,IY)=ICK
      IX=IX-1
      ENDIF
      ENDIF
      ENDIF
         DO 655 I = 1,CLEN
            CHR = CMD(I)
            ZAR = ICHAR(CHR)
            CALL IDENT(ZAR,IX,IY,INCX,INCY,IRESET)
            IF (JPROB.EQ.1) GO TO 27
655      CONTINUE
      ENDIF
      NEWBND = 0
      IF (IBTYPE.EQ.(BTYPE-48)) GO TO 40
      IBTYPE = BTYPE - 48
      CALL HEADER
      GO TO 40
```

```
85      IF (KAR.NE.64) GO TO 80
           IERR = 39
           CALL MYERR(IERR,IERR,IERR)
           GO TO 100
80      CALL ERRMSG(KAR)
        GO TO 100
C
27      ISTATE = 0
        LEVEL = 0
        NLARGE = HOLD
        IBTYPE = BHOLD
        NOCHG = 0
        LFLAG = 1
        DO 4576 I = 1,12
4576       MW(I) = 999
        ISTATE = OSTATE
        ISKIP = 0
        CALL HEADER
        RETURN
        END
C
C
C This subroutine sets the parameter NLARGE (i.e. the enlargement
C factor).  If an attempt is made to set the enlargment factor to
C 0 or a number > 99, and error message is issued, NLARGE is set to
C 1, and the subroutine is exited.
C
      SUBROUTINE SETLRG
      IMPLICIT INTEGER*2 (A-Z)
        CHARACTER*1 ISTAT
      COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
      COMMON /ISTATE/ ISTAT
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /ICUR/ CUR
CXT
CXT   MLARGE is used by SUBROUTINE VALNCE to determine the distance
CXT   between the end of the bond and the valence to be computed.
      COMMON /VLNPRV/ MLARGE
C
      ISTAT = '&'
      ICHAR = 15
      ISTATE = 13
      NLARGE = 0
      CALL HEADER
50    CALL INPUTX(KAR,10,10)
      IF (KAR.EQ.38) GO TO 100
      IF ((KAR.LT.48).OR.(KAR.GT.57)) GO TO 90
C
C We have a digit - process it.
      NLARGE = 10 * NLARGE + (KAR - 48)
      IF ((NLARGE.GT.99).OR.(NLARGE.EQ.0)) GO TO 70
      CALL HEADER
      GO TO 50
C Bad input
90    CALL ERRMSG(KAR)
      ICUR = 1
      GO TO 50
C Bad enlargement factor
70    IERR = 56
      CALL MYERR(IERR,IERR,IERR)
      NLARGE = 1
      MLARGE = NLARGE
      LASTN = 0
      ISTATE = 0
      CALL HEADER
      RETURN
C
C Good enlargment factor
100   CONTINUE
      MLARGE = NLARGE
      IF (NLARGE.EQ.0) NLARGE = 1
      ISTATE = 0
      CALL HEADER
      RETURN
      END
```

```
$STORAGE:2
C       SUBROUTINE CELL sees if a 3*3 area is empty.
        SUBROUTINE CELL(IX,IY,IGOOD)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM
        COMMON /BAD/ IBADX(9),IBADY(9)
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        IGOOD=0
        DO 55 I=1,9
        IBADX(I)=0
        IBADY(I)=0
55      CONTINUE
        DO 10 I=-1,1
        DO 10 J=-1,1
        IVALX=IX+I
        IVALY = IY - J
        IF (MM(IVALX,IVALY) .EQ. 0) GO TO 10
        IGOOD=IGOOD+1
        IBADX(IGOOD)=IVALX
        IBADY(IGOOD)=IVALY
10      CONTINUE
        RETURN
        END
C
C       SUBROUTINE CELL2 sees if a 3*3 area is empty.
        SUBROUTINE CELL2(IX,IY,IGOOD)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 IDTPIX
        COMMON /BAD/ IBADX(9),IBADY(9)
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        IGOOD=0
        DO 55 I=1,9
        IBADX(I)=0
        IBADY(I)=0
55      CONTINUE
        DO 10 I=-1,1
        DO 10 J=-1,1
        IVALX=IX+I
        IVALY = IY - J
        IF (IDTPIX(IVALX,IVALY).EQ.0) GO TO 10
        IGOOD=IGOOD+1
        IBADX(IGOOD)=IVALX
        IBADY(IGOOD)=IVALY
10      CONTINUE
        RETURN
        END
C
C       SUBROUTINE SWITCH alters the bond direction back and forth for
C       chains of length 4 of greater.
        SUBROUTINE SWITCH(COMLEN)
        IMPLICIT INTEGER*2 (A-Z)
        COMMON /CHN/ CLARGE,CHBITS(65)
C       INTERCHANGE BONDS
        DO 9005 K=1,COMLEN
        KK=CHBITS(K)
        IF(KK.EQ. 35) GO TO 9005
        KK=KK-21
        IF(KK .GT.4) KK=KK-2
        IF (KK .EQ. 2 .OR. KK .EQ. 6) GO TO 9006
        KK=KK-2
        GO TO 9007
9006    KK=KK+2
9007    KK=KK+21
        IF (KK .GT. 25) KK=KK+2
        CHBITS(K)=KK
9005    CONTINUE
        RETURN
        END
C       SUBROUTINE DOCHN - THIS SUBROUTINE DECIDES WHERE TO DRAW
C                          A CHAIN AND THEN DRAWS IT
C       THIS CODE WAS PULLED OUT OF SUBROUTINE CHAIN WHEN IT WAS
C       DECIDED TO TAKE THE GROUP FUNCTION OUT OF CHAIN AND MAKE GROUP
C       A SEPARATE SUBROUTINE AND ALLOW CHAINS TO BE DRAWN IN GROUP
        SUBROUTINE DOCHN(CLEN,CORF,MRKPNT,COMLEN,CBOND,IX,IY,IERR)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*2 CB(2)
```

```
      INTEGER*4 MM,IDTPIX
      LOGICAL*2 BONDEL,BAR,BONDID
      COMMON /CINFO/ NDIRS(4),BDIRS(8,3)
      COMMON /BAD/ IBADX(9),IBADY(9)
      COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
      COMMON /CUR/ ICUR
      COMMON /DARK/ OCUR
      COMMON /CHN/ CLARGE,CHBITS(65)
      COMMON /CD/ MAXX,MAXY
      COMMON /HP/IHP
      COMMON /XBOND/ GOODB(2,9)
      COMMON /WARN/ ERR
CXT
CXT   BONDEL = TRUE indicates a bond has been drawn between 2 nodes
CXT   and subsequent deletion should delete the bond, not a node.
      COMMON /DELBND/ BONDEL
CXT
CXT   BAR is used in conjunction with NOCHG and BONDID to set bond
CXT   types in relation to default bond types.
      COMMON /BTPDIR/ BAR
C
      OCUR = 0
      CALL INITHC(3,3,OCUR)
      PDIR=0
C USED TO DETERMINE INITIAL BOND IN PUCKERED CHAIN
      CLARGE=NLARGE
CXT
CXT   BONDID is used in conjunction with BAR and NOCHG to set bond
CXT   types in relation to default bond types.
      BONDID = .FALSE.
C SAVE ENLARGE FACTOR FOR WE MAY TEMPORARILY
C CHANGE IT IF WE DRAW A STRAIGHT CHAIN
C
C THEN ESTABLISH CHAIN DIRECTION
C
      CALL NEW(SUM,IX,IY)
C ARE WE STARTING A NEW STRUCTURE
      IF (SUM .NE. 0) GO TO 23
      NODE=0
C YES-SET NODE AND BOND DIR ACCORDINGLY
      NEWS=1
C SET NEWS STRUCTURE CODE TO YES = 1
      IBDIR=3
      GO TO 25
C
C CAN WE FIND A CORRECT POINTER BOND
C
23    IF (MM(IX,IY) .NE.0) GO TO 22
C CAN'T BE A BOND - GO FIND NODE
      CALL FINDB(IBDIR,KBDIR,IX,IY)
      IF (IBDIR .EQ. -1) GO TO 22
C NOT AT A BOND - GO FIND NODE
      NODE = 0
C GOOD RETURN FROM FINDB - WE FOUND A BOND
      PDIR=KBDIR
      GO TO 25
22    DO 333 I=0,5
C WE'RE NOT AT A BOND - FIND THE NODE
      MX=IX-I
C LOOK LEFT
      LL=LMM(MX,IY)
      IF ((LL.NE.46).AND.(LL.NE.63).AND.((LL.LT.65).OR.(LL.GT.90)))
     2 GO TO 333
C NOT UPPERCASE OR DOT OR ?
      IF((LL.EQ.72).AND.((MM(MX+1,IY).LE.97).OR.(MM(MX+1,IY).GE.
     2    122))) GO TO 333
C SKIP OVER H WHICH IS NOT HE,HG, ETC.
      IX=IX-I
      CALL CNTBND(ICNT,IX,IY)
C HOW MANY BONDS AROUND NODE
      IF(ICNT .GT. 1) GO TO 9002
```

```
C MORE THAN ONE BOND AT NODE
C DON'T WORRY ABOUT INITIAL BOND IN PUCKERED CHAIN
        CALL FINDB(DUMMY,PDIR,IX,IY)
C WHAT IS THE DIR OF BOND COMING INTO NODE
9002    NODE=1
        ITRY=1
        NIX=IX
C SAVE INFO FOR SHARP ANGLE CHECK
        NIY=IY
        IBDIR=NDIRS(ITRY)
        IF (MM(IX+1,IY) .EQ. 0) GO TO 25
C NEXT SPACE IS EMPTY
C GO ON AND CHECK CELLS
        IF((MM(IX+1,IY) .GE. 97) .AND. (MM(IX+1,IY) .LE. 122)
     1   .AND. (MM(IX+2,IY) .EQ. 0)) GO TO 266
        IF (MM(IX+1,IY) .NE. 72) GO TO 974
C NEXT CHAR NOT H
C WE CAN'T DRAW A CHAIN IN THIS DIR
        IF(.NOT. (MM(IX+2,IY) .EQ. 0 .OR.
     1  (MM(IX+2,IY) .GE. 49 .AND. MM(IX+2,IY) .LE. 52
     2  .AND. MM(IX+3,IY) .EQ. 0))) GO TO 974
C WE CAN'T DRAW A CHAIN IN THIS DIR
        HYD=1
        CALL CLRHYD(IX,IY)
        GO TO 25
C FOUND THE NODE
333     CONTINUE
        IERR=3
        CALL MYERR(IERR,KAR,KAR)
C FOUND NO BOND OR NODE AND NOT NEW STRUCTURE
            OCUR = 1
            CALL INITHC(3,3,OCUR)
            ICUR = 1
            CALL CURSOR(IX,IY)
        RETURN
C THIS SHOULD NOT HAPPEN - PROBABLY PROGRAM ERROR
266     BIX=IX+1
        GO TO 270
25      CONTINUE
        BIX=IX
270     BIY=IY
475     IF (CLEN .LE. 4) GO TO 81
C CHAIN STRAIGHT OR PUCKERED?
        IF (NODE .EQ. 0) GO TO 742
        CB(1)=BDIRS(IBDIR,1)
C PUCKERED CHAIN - SET BOND DIRS
        CB(2)=BDIRS(IBDIR,2)
        GO TO 82
742     CB(1)=BDIRS(IBDIR,2)
        CB(2)=BDIRS(IBDIR,1)
        GO TO 82
81      CB(1)=BDIRS(IBDIR,3)
C STRAIGHT CHAIN - SET BONDS AND ENLARGE
        CB(2)=CB(1)
82      I=1
        DO 6 J=1,CLEN
C GENERATE COMMANDS FOR PROPOSED CHAIN
        IF(J .NE. 1) GO TO 55
        IF(NODE .EQ. 0) GO TO 60
55      CHBITS(I)=CB(MOD(J+1,2)+1)
        I=I+1
60      CHBITS(I)=ITAG
        I=I+1
6       CONTINUE
        COMLEN=I-1
        IF(NEWS .EQ. 1) GO TO 99
        FIRB=CHBITS(1)
C GET FIRST BOND OF CHAIN
        IF(FIRB.EQ.35) FIRB=CHBITS(2)
        FIRB=FIRB-21
        IF (FIRB .GT. 4) FIRB=FIRB-2
        IF(((FIRB.EQ.2.OR.FIRB.EQ.6) .AND.
     1  (PDIR.EQ.2 .OR. PDIR .EQ.6))) GO TO 9004
C IF BONDS ARE IN THE
```

```
C SAME DIR CHANGE BONDS IN CHAIN
        IF(.NOT.((FIRB.EQ.4 .OR. FIRB .EQ. 8) .AND.
     1  (PDIR .EQ. 4 .OR. PDIR .EQ. 8))) GO TO 9003
9004    CALL SWITCH(COMLEN)
C SWITCH BONDS IN CHAIN
C
C SEE IF THE CHAIN WE PROPOSE TO DRAW CREATES ANY OVERLAPS
C
9003    IF (NODE .EQ. 0) GO TO 89
        BOND=CHBITS(1)
        CALL DELTA(BOND,INCX,INCY)
        CALL SHARP(BOND,NIX,NIY,ISHARP)
C WILL THIS GENERATE A SHARP ANGLE
        IF (ISHARP .EQ. 0) GO TO 27
C NO SHARP ANGLE - GO AHEAD
        IF(CLEN .LE. 4) GO TO 974
C IF STRAIGHT CHAIN - THIS ONE IS NO GOOD
        CALL SWITCH(COMLEN)
C PUCKERED CHAIN - TRY PUCKERING THE OTHER WAY
        BOND=CHBITS(1)
        CALL DELTA(BOND,INCX,INCY)
        CALL SHARP(BOND,NIX,NIY,ISHARP)
C DO WE STILL HAVE A SHARP ANGLE
        IF( ISHARP .EQ. 1) GO TO 974
C IF STILL BAD - GO TO 974
27      BOND=CHBITS(1)
C WHAT BOND?
        CALL DELTA(BOND,INCX,INCY)
C CALCULATE INCX AND INCY
        BIX=BIX+INCX
        BIY=BIY+INCY
        IF (MM(BIX,BIY) .NE. 0) GO TO 974
        LAR=NLARGE
        IF (CLEN .LE. 4 .AND. (IBDIR .EQ. 3 .OR. IBDIR .EQ. 7))
     1  LAR=NLARGE*3
        DO 67 J=2,LAR+1
        BIX=BIX+INCX
        BIY=BIY+INCY
        CALL CHECK(BIX,BIY,ICHECK)
        IF (ICHECK .EQ. 1) GO TO 974
        CALL CELL(BIX,BIY,IGOOD)
        IF(IGOOD .NE. 0) GO TO 974
67      CONTINUE
        IF(COMLEN .LT.3) GO TO 99
        DO 68 J=3,COMLEN,2
        BOND=CHBITS(J)
        CALL DELTA(BOND,INCX,INCY)
        DO 699 I=1,LAR+1
        BIX=BIX+INCX
        BIY=BIY+INCY
        CALL CHECK(BIX,BIY,ICHECK)
        IF (ICHECK .EQ. 1) GO TO 974
        CALL CELL(BIX,BIY,IGOOD)
        IF (IGOOD .NE. 0) GO TO 974
699     CONTINUE
68      CONTINUE
        GO TO 99
974     ITRY=ITRY+1
        IF(ITRY .EQ. 5) GO TO 310
        IBDIR=NDIRS(ITRY)
       IF (HYD .EQ. 1 ) CALL VALNCE(2,IX,IY,0,0)
       IF (HYD .EQ. 1) HYD = 0
       BIX=IX
       BIY=IY
       IF (ITRY.EQ.3) BIY = IY -IHP
       IF (ITRY.EQ.4) BIY = IY +IHP
       IF (MM(BIX,BIY) .NE. 0 .AND. (ITRY .EQ. 3
     1 .OR. ITRY .EQ. 4)) GO TO 974
       IF (ITRY .NE. 2) GO TO 475
       HYD=0
       IF (MM(BIX-1,BIY) .EQ. 0) GO TO 475
       IF (LMM(BIX-1,BIY) .GE. 256) GO TO 974
       IF ((MM(BIX-1,BIY).EQ.72).AND.(MM(BIX-2,BIY).EQ.0)) GO TO 999
       IF (MM(BIX-2,BIY).EQ. 72 .AND. MM(BIX-3,BIY).EQ.0 .AND.
     1 (MM(BIX-1,BIY) .EQ. 51 .OR. MM(BIX-1,BIY) .EQ. 50)) GO TO 999
       GO TO 974
```

```
999     HYD=1
        CALL CLRHYD(IX,IY)
        GO TO 475
89      CALL CHECK(BIX,BIY,ICHECK)
        IF (ICHECK .EQ. 1) GO TO 310
        CALL CELL(BIX,BIY,IGOOD)
C THIS IS THE FIRST
C BOX CHECKED - WE
C SHOULD FIND ONLY ONE
C CELL OCCUPIED - THAT CELL
C CONTAINS THE POINTER BOND
        IF((IGOOD .EQ. 1) .AND. (NODE .EQ.0)) GO TO 301
310     IERR=1
C FOUND TOO MANY CELLS OCCUPIED - NO ROOM
        CALL MYERR(IERR,KAR,KAR)
C FOR CHAIN - ABORT CMD
        OCUR = 1
        CALL INITHC(3,3,OCUR)
        ICUR = 1
        CALL CURSOR(IX,IY)
        RETURN
301     IF(COMLEN .LT.2) GO TO 99
        DO 302 J=2,COMLEN,2
        BOND=CHBITS(J)
C CHECK THE REST OF THE CELLS- THEY SHOULD = 0
        CALL DELTA(BOND,INCX,INCY)
        LAR=NLARGE
        IF (CLEN .LE. 4 .AND. (IBDIR .EQ. 3 .OR. IBDIR .EQ. 7))
     1  LAR=NLARGE*3
        DO 302 I=1,LAR+1
        BIX=BIX+INCX
        BIY=BIY+INCY
        CALL CHECK(BIX,BIY,ICHECK)
        IF(ICHECK .EQ. 1) GO TO 310
        CALL CELL(BIX,BIY,IGOOD)
        IF (IGOOD .NE. 0) GO TO 310
302     CONTINUE
99      NEWS=0
        DO 90 M=1,260
        IF(LABL(M,1) .EQ. 0) GO TO 91
90      CONTINUE
7777    IERR=1
        CALL MYERR(IERR,KAR,KAR)
        OCUR = 1
        CALL INITHC(3,3,OCUR)
        ICUR = 1
        CALL CURSOR(IX,IY)
        RETURN
91      MRKPNT=M
        IF ((MRKPNT+CLEN) .GT. 260) GO TO 7777
        IF (CLEN .LE. 4 .AND. (IBDIR .EQ. 3 .OR. IBDIR .EQ. 7))
     1  NLARGE=NLARGE*3
        ICUR=1
        DO 45 I=1,COMLEN
        KAR=CHBITS(I)
        IF(CHBITS(I) .NE. ITAG) GO TO 93
        MRKCHN(MRKPNT)=1
        MRKPNT=MRKPNT+1
93      IF ((I.EQ.1.OR.I.EQ.2).AND.CHBITS(I).NE.ITAG) IBTYPE = CBOND
        ERR = 0
        IF ((KAR.GE.22).AND.(KAR.LE.31)) BONDID = .TRUE.
        CALL IDENT(KAR,IX,IY,INCX,INCY,IRESET)
        IF (BONDID) THEN
           NOCHG = 0
           BAR = .FALSE.
           BONDID = .FALSE.
           IF ((IBTYPE.NE.0).AND.(IBTYPE.NE.4).AND.(IBTYPE.NE.8))
     *        IBTYPE = 1
        ENDIF
        CBOND = IBTYPE
CXT
        IF (ERR.EQ.48) THEN
           IERR = 48
           STPLEN = I
           ICHAR = 1
```

```
            IX = IX
            IY = IY
            MRKPNT = MRKPNT - 1
            GO TO 46
         ENDIF
45       CONTINUE
46       CONTINUE
         IF (IERR.EQ.48) COMLEN = STPLEN - 1
CXT
         ICUR=0
         ICHAR=13
         CBOND=IBTYPE
         IF (IBTYPE .EQ. 2 .OR. IBTYPE .EQ. 3 .OR. IBTYPE.EQ.5
     1   .OR. IBTYPE .EQ. 6 .OR. IBTYPE .EQ. 7) CBOND=1
         NLARGE=CLARGE
         CORF=1
         OCUR = 1
         CALL INITHC(3,3,OCUR)
         ICUR = 1
         CALL CURSOR(IX,IY)
         RETURN
         END
C
         SUBROUTINE CHAIN(KAR,IX,IY,INCX,INCY,IRESET,LFLAG)
         IMPLICIT INTEGER*2 (A-Z)
         LOGICAL*2 BAR,BONDEL,BONDID
         INTEGER*4 MM,IDTPIX
         CHARACTER*1 ISTAT
         COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
         COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
         COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
         COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
         COMMON /HEAD/ MW(12),ISTATE,PAGE
         COMMON /SIZZE/ MULTX,MULTY
         COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
         COMMON /XBOND/ GOODB(2,9)
         COMMON /PROB/ IPROB,JPROB
         COMMON /CD/ MAXX,MAXY
         COMMON /CHN/ CLARGE,CHBITS(65)
         COMMON /CUR/ ICUR
         COMMON /ISTATE/ ISTAT
         COMMON /FROM/ LCHAR
CXT
CXT      BAR is used in conjunction with NOCHG and BONDID to set bond
CXT      types in relation to default bond types.
         COMMON /BTPDIR/ BAR
CXT
CXT      BONDEL = TRUE indicates a bond has been drawn between 2 nodes
CXT      and subsequent deletion should delete the bond, not a node.
         COMMON /DELBND/ BONDEL
C
C        SET SOME VARIABLES
C
         IF (LCHAR.NE.13) LLCHAR = LCHAR
         BONDID = .FALSE.
10001    CONTINUE
         KKAR=0
         ISTAT='!'
         CBOND=IBTYPE
         IF((IBTYPE.NE.0).AND.(IBTYPE.NE.4).AND.(IBTYPE.NE.8).AND.
     1   (.NOT.BAR)) CBOND=1
         IF (BAR) NOCHG = 1
         HYD=0
         ISTATE=3
         MODE=1
         ICHAR = JCHAR
         CALL HEADER
         LFLAG=0
         NEWS=0
C SET NEW STRUCTURE CODE TO 0 = NOT NEW STRUCTURE
         CLARGE=NLARGE
100      OCHAR=KKAR
         CALL INPUTX(KAR,IX,IY)
         IF (KAR.EQ.27) THEN
            ICUR = 1
```

```
         CALL CURSOR(IX,IY)
         GO TO 100
      ENDIF
      IF (KAR.EQ.33) THEN
         IERR = 39
         CALL MYERR(IERR,IERR,IERR)
         GO TO 100
      ENDIF
      ICUR = 0
C GET INPUT CHARACTER
101   KKAR=KAR
      IF (KAR .EQ. 13 .OR. KAR .EQ. 81) GO TO 900
C IS CHAR A CR OR Q - YES - QUIT OR RETURN TO GND LEVEL
      IF (KAR .NE. 124) GO TO 200

C ********************************************************************
C
C                # ENTRY CODE
C
C ********************************************************************
C
C             CHAR WAS A VERTICAL LINE SO WE WILL BE SETTING
C                 NEW BOND TYPE OR CHARGE VALUE
C
C
     CALL NUMBER(KAR,IX,IY)
     IF (KAR.EQ.81) GO TO 900
     ISTAT = '!'
     ISTATE = 3
     CBOND = IBTYPE
     CALL HEADER
     GO TO 100
C ********************************************************************
C                   END OF # ENTRY CODE
C ********************************************************************
C
200   IF (KAR.LT.49 .OR. KAR.GT.57) GO TO 300
      IF (.NOT.BAR) THEN
         NOCHG = 0
         IF ((IBTYPE.NE.0).AND.(IBTYPE.NE.4).AND.(IBTYPE.NE.8)) THEN
            CBOND = 1
            IBTYPE = 1
         ENDIF
      ENDIF
C KAR NOT DIGIT 1-9
C
C                  CHAIN DRAWING SECTION
C
C               FIRST ESTABLISH CHAIN LENGTH
C
      CLEN=KAR-48
C CLEN = length of chain
      IERR=0
      BIX = IX
      BIY = IY
C Set error code to 0 - We will check it when we return from DOCHN
      CALL DOCHN(CLEN,CORF,MRKPNT,COMLEN,CBOND,IX,IY,IERR)
CXT
      IF (IERR.EQ.48) THEN
         KAR = 127
         ICHAR = 13
         GO TO 750
      ENDIF
CXT
C This is a chain command
C Determine where to draw chain and then draw it
      IF (IERR .EQ. 1) NLARGE=CLARGE
      IF (IERR .NE. 16) GO TO 100
      LFLAG=0
      GO TO 9501
300   IF (KAR.GE.22 .AND. KAR.LE.31) THEN
         BONDID = .TRUE.
         GO TO 400
      ENDIF
C Bond command?
      IF (KAR .GE. 97 .AND. KAR .LE. 122) GO TO 400
```

```
C Lower case?
        IF (KAR .EQ. ITAG) GO TO 400
C Enlarge command?
        IF (KAR.EQ.38) GO TO 4123
C Marker command?
        IF (KAR .EQ. 63) GO TO 400
C Luhn dot?
        IF (KAR.EQ.46) GO TO 400
C Dumb mode
        IF ((KAR.EQ.21).OR.(KAR.EQ.32).OR.(KAR.EQ.8)) THEN
           IF (KAR.EQ.32) THEN
              JX = IX - 1
              CALL CURSOR(JX,IY)
              CALL CLRHYD(JX,IY)
              CALL VALNCE(2,JX,IY,0,0)
              IF (JPROB.EQ.1) GO TO 900
           ENDIF
           CALL SPACE(IX,IY)
           JCHAR = 2
           MCHAR = 0
           GO TO 10001
        ENDIF
        IF (KAR.EQ.34) GO TO 400
        IF ((KAR.EQ.43).OR.(KAR.EQ.45).OR.(KAR.EQ.61)) GO TO 400
C Question mark?
        IF (KAR .EQ. 36) GO TO 400
C Dollar sign?
        IF ((KAR.GE.65 .AND. KAR.LE.90).OR.(KAR.EQ.46)) GO TO 400
C Upper case?
        GO TO 600
CXT
400     CALL IDENT(KAR,IX,IY,INCX,INCY,IRESET)
        IF (BONDID) THEN
           BAR = .FALSE.
           BONDID = .FALSE.
        ENDIF
        CBOND = IBTYPE
        IF (JPROB.EQ.1) GO TO 900
        CALL HEADER
C Let IDENT process command if possible
        GO TO 100
C Set enlargement factor
4123    CALL IDENT(KAR,IX,IY,INCX,INCY,IRESET)
        ISTATE = 3
        IF (JPROB.EQ.1) GO TO 900
        CALL HEADER
        GO TO 100
C
C IF ITS A RING - SPACE - OR USER DEFINED COMMAND
C SET LFLAG = 1 SO WE NEXT GO TO IDENT AND NOT INPUT
600     IF (KAR.NE.94.AND.KAR.NE.60.AND.KAR.NE.32.AND.KAR.NE.95.AND.
     *      KAR.NE.58.AND.KAR.NE.42) GO TO 700
        GO TO 900
700     IF(KAR .NE. 64) GO TO 777
        CALL REPEAT(KAR,IX,IY,INCX,INCY,IRESET,LFLAG)
        LEVEL=1
        ISTATE=3
        ISTAT='C'
        JBDIR=IBDIR
        JBTYPE=IBTYPE
        JCHAR=ICHAR
        IF (JPROB.EQ.1) GO TO 900
        CALL HEADER
        IF (KAR .EQ. 13) GO TO 100
C IF KAR = CR GET NEXT CHAR
        OCHAR=KKAR
        GO TO 101
777     IF(KAR .NE. 37) GO TO 750
        CALL LONG(KAR,IX,IY)
C KAR WAS % - CALL LONG
        ISTAT='C'
        JBDIR=IBDIR
        JBTYPE=IBTYPE
        MCHAR=KAR
        JCHAR=ICHAR
```

```
989     ISTATE=3
        CALL HEADER
        IF(KAR .EQ. 81) GO TO 900
C LONG BOND CMD WAS INTERRUPTED
C BY Q - EXIT AND PASS Q ON
        GO TO 100
750     IF (KAR .NE. 127) GO TO 9981
CXT     IF (KAR .NE. OCHAR) GO TO 978
C 2 DEL'S IN ROW NOT ALLOWED
CXT     IERR=5
C TYPE ERR MSG AND GET NEXT CMD
CXT     CALL MYERR(IERR,KAR,KAR)
CXT     GO TO 100
978     IF (ICHAR .NE. 13) GO TO 781
        I=COMLEN
C DELETE THE LAST CHAIN
        MRKPNT=MRKPNT-1
CXT
        IF (IERR.EQ.48) THEN
           IERR = 0
           GO TO 988
        ENDIF
CXT
977     JCHAR=2
C DELETE MARKER
        IX=LABL(MRKPNT,1)+1
        IY=LABL(MRKPNT,2)
        MRKPNT=MRKPNT-1
        CALL DEL(KAR,IX,IY,INCX,INCY,0)
        JBTYPE=IBTYPE
        JBDIR=IBDIR
        I=I-1
CXT
988     IF (I.EQ.0) GO TO 110
C CHAIN DELETED - GO TO INPUT
        JCHAR=1
C PREPARE TO DELETE BOND
        BOND=CHBITS(I)
        CALL DELTA(BOND,INCX,INCY)
        CALL DEL(KAR,IX,IY,INCX,INCY,0)
        JBDIR=IBDIR
        JBTYPE=IBTYPE
        I=I-1
        IF (I .EQ. 0) GO TO 110
        GO TO 977
110     CONTINUE
        ICUR = 1
        IX = BIX
        IY = BIY
        CALL CURSOR(IX,IY)
        MCHAR=KAR
        JCHAR=ICHAR
        GO TO 100
781     IF (JCHAR .EQ. 1) CALL DELTA(MCHAR,INCX,INCY)
        CALL DEL(KAR,IX,IY,INCX,INCY,0)
C DEL LONG BOND OR LAST INPUT
        JCHAR=ICHAR
        MCHAR=KAR
        GO TO 100
9981    CALL ERRMSG(KAR)
C INVALID INPUT FOR CHAIN
        GO TO 100
C TYPE MESSAGE AND GET NEXT CMD
900     CONTINUE
        IF (KAR.EQ.13) THEN
           LCHAR = LLCHAR
           LFLAG=0
        ELSE
           LCHAR = 13
           LFLAG = 1
        ENDIF
9501    LEVEL=0
        ISTATE=0
        CALL HEADER
        ICUR = 1
800     RETURN
        END
```

```
$STORAGE:2
      SUBROUTINE RING(KAR,IX,IY,INCX,INCY,IRESET,LFLAG)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM,IDTPIX
      INTEGER*2 IPREF(5,10)
      INTEGER*2 PBRING(8,8,2)
      INTEGER*2 TEST(2),FBOND(2),T2BOND(8)
      LOGICAL*2 MATCH,BAR,BONDEL,BONDID
      CHARACTER*1 ISTAT
      COMMON /RINGY/ LBND(8,2),TSBOND(8),RHBIT(10),LAP(40,3),
     *   RINGS(16,2),RINGO(16,2)
      COMMON /BAD/ IBADX(9),IBADY(9)
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
      COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /RCAN/ CAN(10,10)
      COMMON /SIZZE/ MULTX,MULTY
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
      COMMON /CD/ MAXX,MAXY
      COMMON /FUSE/ ITIMES
      COMMON /ISTATE/ ISTAT
      COMMON /FROM/ LCHAR
      COMMON /XRNG/ NORDRW(8,8,2),SOFAR
      COMMON /WARN/ ERR
CXT   BAR is used in conjunction with NOCHG, BONDID, and LASTN
CXT   to control bond type drawing in relation to default bond types.
      COMMON /BTPDIR/ BAR
CXT   BONDEL = TRUE indicates that a bond has been drawn between 2
CXT   nodes so subsequent deletion will delete the bond, not a node.
      COMMON /DELBND/ BONDEL
      COMMON /PROB/ IPROB,JPROB
      DATA IPREF(1,3),IPREF(2,3),IPREF(3,3),IPREF(4,3) /7,3,5,1/
      DATA IPREF(1,4),IPREF(2,4),IPREF(3,4),IPREF(4,4) /1,2,3,4/
      DATA IPREF(1,5),IPREF(2,5),IPREF(3,5),IPREF(4,5)/1,5,3,7/
      DATA IPREF(1,6),IPREF(2,6),IPREF(3,6),IPREF(4,6)/4,6,8,2/
      DATA IPREF(1,7),IPREF(2,7),IPREF(3,7),IPREF(4,7)/2,6,4,8/
      DATA IPREF(1,8),IPREF(2,8) /1,2/
      DATA IPREF(1,9),IPREF(2,9),IPREF(3,9),IPREF(4,9)/1,3,5,7/
      DATA IPREF(1,10),IPREF(2,10),IPREF(3,10),IPREF(4,10)
     *   /2,4,6,8/
      DATA PBRING(3,1,1),PBRING(3,1,2),PBRING(3,2,1),PBRING(3,2,2),
     * PBRING(3,3,1),PBRING(3,3,2),PBRING(3,4,1),PBRING(3,4,2),
     * PBRING(3,5,1),PBRING(3,5,2),PBRING(3,6,1),PBRING(3,6,2),
     * PBRING(3,7,1),PBRING(3,7,2),PBRING(3,8,1),PBRING(3,8,2)
     *   /1,2,2,3,3,4,1,4,2,6,1,7,4,8,2,8/
      DATA PBRING(4,1,1),PBRING(4,1,2),PBRING(4,2,1),PBRING(4,2,2),
     * PBRING(4,3,1),PBRING(4,3,2),PBRING(4,4,1),PBRING(4,4,2),
     * PBRING(4,5,1),PBRING(4,5,2),PBRING(4,6,1),PBRING(4,6,2),
     * PBRING(4,7,1),PBRING(4,7,2),PBRING(4,8,1),PBRING(4,8,2)
     *   /2,2,1,3,2,4,1,5,2,6,1,7,2,8,1,1/
      DATA PBRING(5,1,1),PBRING(5,1,2),PBRING(5,2,1),PBRING(5,2,2),
     * PBRING(5,3,1),PBRING(5,3,2),PBRING(5,4,1),PBRING(5,4,2),
     * PBRING(5,5,1),PBRING(5,5,2),PBRING(5,6,1),PBRING(5,6,2),
     * PBRING(5,7,1),PBRING(5,7,2),PBRING(5,8,1),PBRING(5,8,2)
     *   /1,2,2,3,4,4,1,5,2,6,1,7,3,8,2,1/
      DATA PBRING(6,1,1),PBRING(6,1,2),PBRING(6,2,1),PBRING(6,2,2),
     * PBRING(6,3,1),PBRING(6,3,2),PBRING(6,4,1),PBRING(6,4,2),
     * PBRING(6,5,1),PBRING(6,5,2),PBRING(6,6,1),PBRING(6,6,2),
     * PBRING(6,7,1),PBRING(6,7,2),PBRING(6,8,1),PBRING(6,8,2)
     *   /1,2,1,4,2,4,1,5,1,6,1,8,2,8,1,1/
      DATA PBRING(7,1,1),PBRING(7,1,2),PBRING(7,2,1),PBRING(7,2,2),
     * PBRING(7,3,1),PBRING(7,3,2),PBRING(7,4,1),PBRING(7,4,2),
     * PBRING(7,5,1),PBRING(7,5,2),PBRING(7,6,1),PBRING(7,6,2),
     * PBRING(7,7,1),PBRING(7,7,2),PBRING(7,8,1),PBRING(7,8,2)
     *   /1,2,2,4,4,4,1,5,2,6,1,8,3,8,2,1/
      DATA PBRING(8,1,1),PBRING(8,1,2),PBRING(8,2,1),PBRING(8,2,2),
     * PBRING(8,3,1),PBRING(8,3,2),PBRING(8,4,1),PBRING(8,4,2),
     * PBRING(8,5,1),PBRING(8,5,2),PBRING(8,6,1),PBRING(8,6,2),
     * PBRING(8,7,1),PBRING(8,7,2),PBRING(8,8,1),PBRING(8,8,2)
     *   /1,3,1,4,1,5,2,5,1,6,1,8,1,8,1,1/
C Set a few variables
C
      ERR = 0
```

```
CXT
CXT     BONDID is used in conjnction with BAR, NOCHG and RBOND to control
CXT     bond type drawing in relation to default bond types.
        BONDID = .FALSE.
        IF (LCHAR.NE.12) LLCHAR = LCHAR
        LARGE = NLARGE
10001   CONTINUE
        KKAR=0
        ISTAT='^'
C Save bond type
        RBOND=IBTYPE
C Reset RBOND to 1 if bond
        IF ((IBTYPE .NE. 4).AND.(IBTYPE .NE. 8).AND.(IBTYPE.NE.0)

     *  .AND.(.NOT.BAR)) RBOND = 1
CXT  1  .AND. (LASTN .EQ. 0)) RBOND=1
C       Type is temporary type and it has been used once
C       Set header variable to RING state
888     ISTATE=5
C       Unless changed - upon exit we go to call next input
        LFLAG=0
        KAR1=0
        MODE=1
C       Display RING header
        CALL HEADER
100     OCHAR=KKAR
        ICUR = 1
        CALL CURSOR(IX,IY)
C       Get input char
1060    CALL INPUTX(KAR,IX,IY)
        IF (KAR.EQ.131) GO TO 1060
        IF (KAR.EQ.94) THEN
           IERR = 39
           CALL MYERR(IERR,IERR,IERR)
           GO TO 1060
        ENDIF
        KKAR=KAR
C       Not a valid digit - thus not a ring command
101     IF (KAR .LT. 48 .OR. KAR .GT. 56) GO TO 400
CXT
        IF (.NOT.BAR) THEN
           NOCHG = 0
           IF ((IBTYPE.NE.0).AND.(IBTYPE.NE.4).AND.(IBTYPE.NE.8)) THEN
              RBOND = 1
              IBTYPE = RBOND
           ENDIF
        ENDIF
C       Ring command - find environment
200     ENVIRN=-999
C       Count of bonds pointing to or away from node
        BCNT=0
C       Used to determine if all legal rings have been tried
        ITRY = 1
C       Implies that we are using the standard form of the ring
        IFROM = 0
C       RINGS version of NLARGE - we can't use NLARGE
        LARGE = NLARGE
C       in an automatic way for rings 3,5 and 7 so we do
C       it the hard way
        NLARGE=1
        DO 841 I=1,40
        DO 841 J=1,3
C       Zero overlap table
841     LAP(I,J)=0
C       Zero overlap table counter
        LCNT=0
        CALL CELL (IX,IY,IGOOD)
C       We are at an empty 3X3 area
        IF (IGOOD.NE.0) GO TO 7006
           ENVIRN=-1
           GO TO 207
7006    IF (MM(IX,IY).NE.0) GO TO 7001
           CALL FINDB(SLOB,BLOB,IX,IY)
           IF (SLOB.EQ.-1) GO TO 7001
```

```
            CALL DELTA(BLOB,INCX,INCY)
            IBDIR = BLOB
            ENVIRN = 0
            GO TO 207
 7001     KHAR=LMM(IX-1,IY)
 C        WE ARE AT NODE
          IF(KHAR .EQ. 46 .OR. (KHAR .GE. 65 .AND.
      1   KHAR .LE.90) .OR. (KHAR .GE. 97 .AND.
      2   KHAR .LE. 122)) ENVIRN = 1
          IF(ENVIRN .NE. 1) GO TO 207
 C
 C        Find coordinates of node
 C
          JJJ=0
          IF (KHAR .EQ. 46 .OR. KHAR .EQ. 81) JJJ=IX-1
          DO 428 I=0,-3,-1
          IF (((MM(IX+I,IY).GE.65).AND.(MM(IX+I,IY).LE.90).AND.
      2      (MM(IX+I,IY).NE.72)).OR.((MM(IX+I,IY).EQ.72).AND.
      3      (MM(IX+I+1,IY).GE.97).AND.(MM(IX+I+1,IY).LE.122))) THEN
             JJJ=IX+I
             GO TO 427
          ENDIF
 428      CONTINUE
 427      IF (JJJ .EQ. 0) ENVIRN=-999
 207      IF (ENVIRN .NE. -999) GO TO 201
 C        Could not determine our environment
          IERR= 29
 C        Issue error message and return to GND
          CALL MYERR(IERR,KAR,MAR)
          NLARGE = LARGE
          IF ((MM(IX,IY).EQ.46).OR.((MM(IX,IY).GE.65).AND.(MM(IX,IY).LE.
      *      90))) IX = IX + 1
          GO TO 10001
 C        Set connection value to default
 201      CONN=ENVIRN
 C        If chain (i.e. bond) CONN = 0
 C        If ring (i.e. node) CONN = 1
 C        If digit = 0,1,2 then set CONN to
          DIG=KAR-48
 C        to explicitly requested connection type
 C        -1 = unconnected
 C        0 = SPIRO
 C        1 = At least 1 side fused
 C        2 = 2 sides fused
          COC=1
          IF (DIG .GE. 3) GO TO 202
 C        Set connection type to explicitly requested type
          CONN=DIG
 C        IS THIS A NEW COMMAND OR RETRY AFTER DELETE
 205      IF (KAR1 .EQ. 0) GO TO 2205
          KAR=KAR1
          KAR1=0
          GO TO 2105
 2205     OCHAR=KKAR
 1063     CALL INPUTX(KAR,IX,IY)
          IF (KAR.EQ.131) THEN
             ICUR = 1
             CALL CURSOR(IX,IY)
             NLARGE = LARGE
             GO TO 100
          ELSE IF (KAR.EQ.94) THEN
             IERR = 39
             CALL MYERR(IERR,IERR,IERR)
             GO TO 1063
          ENDIF
          KKAR=KAR
 C        Get ring size
 2105     DIG=KAR-48
 C        Go on if ring size 3 to 8
 202      IF (DIG .GE. 3 .AND. DIG .LE. 8) GO TO 203
          IF (DIG .NE. -35 ) GO TO 2020
          NLARGE=LARGE
          KAR1=0
          GO TO 100
 2020     IERR=30
```

```
C       Bad ring size - display error message
199     CALL MYERR(IERR,DIG,MAR)
C       and await reentry of ring size
        GO TO 205
C       Set ring size
203     RSIZE=DIG
C       Set default # of tries  to 1
        NTEST=1
        IF (CONN .NE. -1) GO TO 300
C
C       We are going to draw an unattached ring
C
        CALL MBIT(RSIZE)
C       Pick up first bond direction
        BONDF = IPREF(1,RSIZE)
C       Now generate full ring command table
        CALL MAKRNG(RSIZE,RCNT,ENVIRN,BONDF,LARGE,COC,1)
        FBOND(1) = BONDF
C
        GO TO 850
300     CONTINUE
        IF (CONN .NE. 0) GO TO 3100
C
C       Ring will have spiro connection
C
        IF (ENVIRN .EQ. 1) GO TO 305
C
C       Spiro connection - ring attached to bond
C
        KHAR=LMM(IX-INCX,IY-INCY)
        FINCX = INCX
        FINCY = INCY
        INBOND=KHAR/256
C       Ring will attach to bond of dir INBOND
        INBOND=KHAR-INBOND*256
C       Put pointer bond in table
        LAP(1,1)=IX-INCX
        LAP(1,2)=IY-INCY
        LCNT=1
        GO TO 308
C
C       Spiro connection - ring attached to node
C
305     KX=JJJ
        KY=IY
C       Clear hydrogens around node
        CALL CLRHYD(KX,KY)
C       so we can more easily find the
C       bonds around the node
C       Locate bonds around the node
        CALL LOCBND(JJJ,KY,BCNT)
C       Set X value
        IX=JJJ
        LAP(1,1)=JJJ
C       Put node in overlap table
        LAP(1,2)=KY
        LCNT=1
9999    IF (BCNT .NE. 0) GO TO 310
C
C       No bonds - draw ring in normal shape and orientation with node
C       incorporated in ring
C
C       Set up ring definition and first bond
        BONDF = IPREF(1,RSIZE)
        CALL MBIT(RSIZE)
        CALL MAKRNG(RSIZE,RCNT,ENVIRN,BONDF,LARGE,COC,1)
        FBOND(1) = BONDF
        GO TO 850
310     IF (BCNT .NE. 1) GO TO 315
C
C       One bond - draw ring with existing node in ring and determine
C       orientation using pointer bond logic
C
C       Pick up bond
        INBOND=LBND(1,1)
C       Reverse pointer bond
317     INBOND=MOD(INBOND+4,8)
```

```
      IF (INBOND .EQ. 0) INBOND=8
      GO TO 308
C
C     2 or more bonds at node - determine pseudo pointer bond
C
315   MAXI=0

      TEST(1)=0
      TEST(2)=0
      MAXGAP=0
C     Find biggest gap
      DO 20 I=1,BCNT
      IF (LBND(I,2) .LE. MAXGAP) GO TO 20
      MAXI=I
      MAXGAP=LBND(I,2)
20    CONTINUE
C
C     Found biggest gap - now calculate pseudo pointer bond
C
      INBOND=MOD((LBND(MAXI,1)+MAXGAP/2),8)
      IF (INBOND .EQ. 0) INBOND = 8
C     If gap = 4
      IF (BCNT .NE.2 .OR. MAXGAP .NE. 4) GO TO 309
C     and there are only 2 bonds on node - there are 2
C     'equal' positions - set TEST(1) and TEST(2) such
C     that rings are positoned in the following order
C     right - left - down - up
      TEST(1)=INBOND
      IF(INBOND .LT. 3 .OR. INBOND .GT. 6) TEST(2)=INBOND
      INBOND=MOD(INBOND+4,8)
      IF(INBOND .EQ. 0) INBOND=8
      IF (INBOND .LT.3 .OR. INBOND .GT. 6) TEST(2)=INBOND
      IF (INBOND .GE.3 .AND. INBOND.LE. 6) TEST(1)=INBOND
      IF (TEST(1) .EQ. 5 .AND. TEST(2) .EQ. 1) THEN
      TEST(1)=1
      TEST(2)=5
      ENDIF           !Fix so ring goes down before up
      INBOND=TEST(1)
      NTEST=2
C     If MAXGAP is not an
309   IF (MOD(MAXGAP,2).EQ.0) GO TO 308
C     even number - we have 2 positions to try
      TEST(1)=INBOND
      INBOND=INBOND+1
      IF(INBOND .GT. 8) INBOND = 1
      TEST(2)=INBOND
      if (mod(inbond,2).eq. 0) then
      ihold=test(1)
      test(1)=test(2)
      test(2)=ihold
      endif
      INBOND=TEST(1)
      NTEST=2
C     First bond in ring will have dir FFBOND
308   FFBOND=PBRING(RSIZE,INBOND,1)
      FFBOND=IPREF(FFBOND,RSIZE)
330   CALL MBIT(RSIZE)
      CALL MAKRNG(RSIZE,RCNT,ENVIRN,FFBOND,LARGE,COC,0)
      BONDF = PBRING(RSIZE,INBOND,2)
C     Convert bond dir to bond command
      CALL MKBND(BONDF)
      FBOND(1) = BONDF
      DO 409 I=1,RCNT
C     See if we have the needed bond
      ISTART = I
      IF (FBOND(1).EQ.RINGO(I,1)) GO TO 410
409   CONTINUE
C     Can't find needed bond - go try next orientation
      GO TO 937
410   CONTINUE
      IF (ISTART .EQ. 1 .AND. ENVIRN .EQ. 0) ISTART=RCNT+1
      IF (ISTART .NE. 1 .AND. ENVIRN .EQ. 0)ISTART=ISTART-1
      DO 411 I=1,RCNT
```

```
C       Copy RING to RINGS so commands are
        RINGS(I,1)=RINGO(ISTART,1)
C       in the right order for DRING
        RINGS(I,2) = RINGO(ISTART,2)
        ISTART=ISTART+1
        IF (ISTART .GT. RCNT) ISTART=1
411     CONTINUE
C
850     KX=IX
        KY=IY
        BIX=IX
C       Start to check if there is room for ring
C       without creating unacceptable collisions
C
852     J=1
        RG1 = RINGS(1,1)
        RG2 = RINGS(2,1)
        BLOB=MIN0(RG1,RG2)
        CALL DELTA(BLOB,INCX,INCY)
C       Pick up ring command
985     BLOB=RINGS(J,1)
C       If it is a marker
        IF (BLOB .EQ. 35) GO TO 854
C       Its a bond - get incs
        CALL DELTA(BLOB,INCX,INCY)
C       Get bond length
        LAR = RINGS(J,2)
        SLOB=BLOB
        DO 990 IK=1,LAR
        KX=KX+INCX
        KY=KY+INCY
C       Check cell
8888    CALL LOOK(KX,KY,ICHECK,LCNT,BLOB)
        RG1 = RINGS(J,2)
        IF (BLOB .EQ. -1) RINGS(J,2) = -IABS(RG1)
C       Not = 0 means invalid conflict
        IF (ICHECK .NE. 0) GO TO 937
        BLOB=SLOB
990     CONTINUE
C       Bond OK - go get next command
        GO TO 971
C
854     IF (J .EQ. 1 .AND. ENVIRN .EQ. 0) GO TO 8854
        KX=KX+INCX
        KY=KY+INCY
C       Check cell
8854    CALL LOOK(KX,KY,ICHECK,LCNT,BLOB)
        RG2 = RINGS(J,2)
        IF (BLOB.EQ.-1) RINGS(J,2) = -IABS(RG2)
C       If bad conflict - go to 937
        IF (ICHECK .NE. 0) GO TO 937
C       OK so far - go check next one
971     J=J+1
C       OK so far - get next command
        IF( J .LE. RCNT) GO TO 985
C
999     BIX=IX
        BIY=IY
C       Now draw ring
        ERR = 0
        CALL DRING(RCNT,IX,IY,TX,TY,RBOND,CONN)
        NLARGE=LARGE
        OCHAR=KKAR
        IF (ERR.EQ.23) THEN
CXT        Crossing diagonal bonds not allowed - delete ring.
           ERR = 0
           KAR = 127
           GO TO 1074
        ELSE IF (ERR.EQ.48) THEN
CXT        Adjacent nodal values not allowed - delete ring.
           KAR = 127
           GO TO 1084
        ENDIF
C       GET INPUT TO CHECK FOR DELETE
```

```
1064    CALL INPUTX(KAR,TX,TY)
        IF (KAR.EQ.131) THEN
           ICUR = 1
           CALL CURSOR(TX,TY)
           GO TO 1064
        ELSE IF (KAR.EQ.94) THEN
           IERR = 39
           CALL MYERR(IERR,IERR,IERR)
           GO TO 1064
        ENDIF
1074    CONTINUE
1084    IDEL=0
        KKAR=KAR
        KAR1=0
C       NOT DEL - GO PROCESS COMMAND
        IF (KAR .NE. 127) THEN
           IF ((MM(TX,TY).EQ.46).OR.((MM(TX,TY).GE.65).AND.(MM(TX,TY)
     *        .LE.90))) THEN
              IX = TX + 1
           ELSE
              IX = TX
           ENDIF
           IY = TY
           GO TO 101
        ENDIF
        CALL CURSOR(IX,IY)
C THIS VARIABLE IS USED TO TRIGGER 'NO GOOD ORIENTATION' MESSAGE
        IDEL=1
        IF ((RINGS(1,1).EQ.35).AND.(ERR.NE.48)) IX=IX-1
C DELETE RINGS
        CALL RNGDEL(RCNT,IX,IY)
        IF (ERR.EQ.48) THEN
           IX = BIX
           IY = BIY
           CALL CURSOR(IX,IY)
           ERR = 0
        ENDIF
C WE DELETED FREE STANDING
        IF (ENVIRN .EQ. -1) GO TO 100
C RING - GO GET NEXT COMMAND
        OCHAR=KKAR
C WE DID A DELETE - DO WE TRY IT AGAIN
1065    CALL INPUTX(KAR,IX,IY)
        IF (KAR.EQ.131) THEN
           ICUR = 1
           CALL CURSOR(IX,IY)
           GO TO 1065
        ELSE IF (KAR.EQ.94) THEN
           IERR = 39
           CALL MYERR(IERR,IERR,IERR)
           GO TO 1065
        ENDIF
        KKAR=KAR
        IF(KAR .LT. 48 .OR. KAR .GT.56) GO TO 400
        OCONN=CONN
        CONN=-999
        ORSIZE=RSIZE
        DIG=KAR-48
        IF (DIG .GE. 3) GO TO 1202
        CONN=DIG
1205    OCHAR=KKAR
1066    CALL INPUTX(KAR1,IX,IY)
        IF (KAR1.EQ.131) THEN
           ICUR = 1
           CALL CURSOR(IX,IY)
           GO TO 1066
        ELSE IF (KAR1.EQ.94) THEN
           IERR = 39
           CALL MYERR(IERR,IERR,IERR)
           GO TO 1066
        ENDIF
        KKAR=KAR1
C GET NEW CONN AND RING SIZE
        DIG=KAR1-48
1202    IF (DIG .GE. 3 .AND. DIG .LE. 8) GO TO 1203
        IERR=30
```

```
      CALL MYERR(IERR,DIG,MAR)
      GO TO 1205
1203  RSIZE=DIG
      IF (CONN .EQ. -999) CONN=ENVIRN
      IF ((IX.NE.BIX).OR.(IY.NE.BIY)) GO TO 7017
      IF (ORSIZE .EQ. RSIZE .AND. CONN .EQ. OCONN) GO TO 937
C IF SAME SIZE AND CONNECTION - TRY NEXT ORIENTATION
C IF NOT - TRY NEW RING
7017  INCX = FINCX
      INCY = FINCY
      NLARGE = LARGE
      GO TO 101
C     We've tried everything - all failed - issue error and get next command
937   IF (ITRY.EQ.NTEST) THEN
         INCX = FINCX
         INCY = FINCY
         GO TO 973
      ENDIF
      ITRY=ITRY+1
      IX=BIX
C Pick up next INBOND and try again
      INBOND=TEST(ITRY)
      GO TO 308
3100  KX=IX
      KY=IY
      IF(ENVIRN .EQ. 1) KX=JJJ
      MX=KX
      MY=KY
      JL=KX+1
      ITIMES=CONN
      IALT=1
C Start loop for alternate ring forms if ring size = 3 or 5.
      IF (RSIZE .EQ. 3 .OR. RSIZE .EQ. 5) IALT=2
C Get all into bonds
      CALL GETABD(JL,KY,TSCNT)
C No bond - too bad
      IF (TSCNT .EQ. 0) GO TO 947
CXT
CXT   Variables used to prevent redrawing of symmetrical rings are
CXT   (re)initiallized.
      IF ((MOD(RSIZE,2).EQ.0).AND.(SOFAR.GT.0)) THEN
         DO 1053 IM = 1,SOFAR
            DO 1052 IN = 1,8
               NORDRW(IM,IN,1) = 0
               NORDRW(IM,IN,2) = 0
1052        CONTINUE
1053     CONTINUE
      ENDIF
      SOFAR = 0
CXT
CXT   Two passes can be made, the first for 2 sided fuses, the second
CXT   for fuses of more than 2 sides, if the operator does not accept
CXT   any 2 sided fuses.  The count of the passes and the count of
CXT   fuses with more then 2 sides are initiallized.
      ATTMPT = 0
      FUSE3 = 0
1061  CONTINUE
      ATTMPT = ATTMPT + 1
CXT
      DO 1001 IKK=1,IALT
      DO 1000 IK=1,TSCNT
      KX=MX
      KY=MY
      LCNT=0
C 0 implies we are at the end of a bond
      IF (ENVIRN .EQ. 0) GO TO 957
      LCNT=LCNT+1
      LAP(LCNT,1)=KX
C Put node in overlap table
      LAP(LCNT,2)=KY
C Get bond dir
957   BDIR=TSBOND(IK)
      CALL DELTA(BDIR,INCX,INCY)
      KX=KX-INCX
      KY=KY-INCY
```

```
C Put bond in overlap table
       BND=LMM(KX,KY)
968    LCNT=LCNT+1
       IF(LCNT .GT. 40) GO TO 947
       LAP(LCNT,1)=KX
       LAP(LCNT,2)=KY
       KX=KX-INCX
       KY=KY-INCY
       GND=LMM(KX,KY)
       IF(GND .EQ. BND) GO TO 968
967    BLEN=LCNT-1
       IF (BLEN .EQ. 0) BLEN=1
       IF(GND .NE. 46) GO TO 947
       LCNT=LCNT+1
       IF(LCNT .GT. 40) GO TO 947
C Put marker in overlap table
       LAP(LCNT,1)=KX
       LAP(LCNT,2)=KY
       LLCNT=LCNT
C Set first bond
4000   FBOND(1)=BDIR
       BONDF1 = FBOND(1)
       FBOND(2)=MOD(FBOND(1)+4,8)
C REVERSE BOND
       IF (FBOND(2) .EQ. 0) FBOND(2)=8
       BONDF2 = FBOND(2)
C Convert bond dir to bond command
       CALL MKBND(BONDF1)
       CALL MKBND(BONDF2)
       FBOND(1) = BONDF1
       FBOND(2) = BONDF2
       DO 991 K=1,4
       DO 8809 IROT=1,2
       COC=1
       RRSIZE=RSIZE
       IF (RSIZE .EQ. 3 .AND. IKK .EQ. 2) RRSIZE=9
       IF (RSIZE .EQ. 5 .AND. IKK .EQ. 2) RRSIZE=10
       FFBOND=IPREF(K,RRSIZE)
C      If no new orientations - try next 'into' bond
       IF (FFBOND .EQ. 0) GO TO 8809
       CALL MBIT(RRSIZE)
       CALL MAKRNG(RSIZE,RCNT,ENVIRN,FFBOND,LARGE,COC,0)
       DO 809 I=1,RCNT
       II = I
       IF(FBOND(IROT).EQ.RINGO(I,1).AND.BLEN.EQ.RINGO(I,2)) GO TO 810
C Can we match bond dir and len
809    CONTINUE
C No - go try next orientation
       GO TO 8809
810    ISTART=II
       IF (IROT .EQ. 2) GO TO 8111
       ISTART=MOD(ISTART+2,RCNT)
       IF (ISTART .EQ. 0) ISTART=RCNT
8111   IF (ISTART .EQ. 1  .AND. ENVIRN .EQ. 0) ISTART=RCNT+1
       IF (ISTART .NE. 1 .AND. ENVIRN .EQ. 0) ISTART=ISTART-1
C Copy RING to RINGS so commands are in
       DO 811  I=1,RCNT
C the right order for DRING
       RINGS(I,1)=RINGO(ISTART,1)
       RINGS(I,2)=RINGO(ISTART,2)
       ISTART=ISTART+1
       IF (ISTART .GT. RCNT) ISTART=1
811    CONTINUE
       J=1
       KX=MX
       KY=MY
       BLOB=MINO(RINGS(1,1),RINGS(2,1))
       CALL DELTA(BLOB,INCX,INCY)
C Pick up ring command
9850   BLOB=RINGS(J,1)
       IF (BLOB .EQ. 35) GO TO 8540
C Its a bond - get incs
994    CALL DELTA(BLOB,INCX,INCY)
C Get bond length
       LAR = RINGS(J,2)
       SLOB=BLOB
```

```
        DO 9990 IM=1,LAR
        KX=KX+INCX
        KY=KY+INCY
C Check cell
        CALL LOOK(KX,KY,ICHECK,LCNT,BLOB)
        IF (BLOB .EQ. -1) RINGS(J,2)=-IABS(RINGS(J,2))
C Not = 0 means invalid conflict
        IF (ICHECK .NE. 0) GO TO 992
        BLOB=SLOB
9990    CONTINUE
C Bond OK - go get next command
        GO TO 9710
C
8540    IF (J.EQ.1 .AND. ENVIRN.EQ.0 ) GO TO 8585
        KX=KX+INCX
        KY=KY+INCY
C Check cell
8585    CALL LOOK(KX,KY,ICHECK,LCNT,BLOB)
        RG2 = RINGS(J,2)
        IF (BLOB .EQ. -1) RINGS(J,2)=-IABS(RG2)
C NEQ NUM IN RINGS(*,2) MEANS FUSED SO DON'T
C REALLY DO THIS COMMAND
C If bad conflict - go to 992
        IF (ICHECK .NE. 0) GO TO 992
C OK so far - go check next one
9710    J=J+1
C OK so far - get next command
        IF( J .LE. RCNT) GO TO 9850
C Reset LCNT for next try
        LCNT=LLCNT
        DO 995  IM=1,LLCNT
        IF (LAP(IM,3) .EQ. 0) GO TO 8809
995     CONTINUE
        IF(ITIMES .EQ. 1) GO TO 9050
        L=0
        LB=0
        DO 714 IM=1,RCNT
        IF (RINGS(IM,2).LT.0) L=L+1
        IF (RINGS(IM,1) .NE. 35 .AND. RINGS(IM,2) .LT.0) LB=LB+1
714     CONTINUE
        ITEST=4
        IF (ENVIRN .EQ.0) ITEST=3
        IF (L .LT. ITEST .OR. LB .LT. 2) GO TO 8809
        IF (L .EQ. RCNT) GO TO 8809
CXT
CXT     If the current number of fuses found by the original algorithm
CXT     is greater than 2 and this is the 1st pass, skip drawing it -or-
CXT     If the current number of fused found by the original algorithm
CXT     equals 2 and this is the second pass, skip the drawing.
        IF ((LB.GT.2).AND.(ATTMPT.EQ.1)) THEN
           FUSE3 = FUSE3 + 1
           GO TO 8809
        ELSE IF ((LB.EQ.2).AND.(ATTMPT.EQ.2)) THEN
           GO TO 8809
        ENDIF
CXT
9050    CONTINUE
CXT
CXT     The next symmetrical ring drawing is compared to previous
CXT     symmetrical drawings to see if it is a duplicate.  X and
CXT     Y coordinates of nodes are computed by tracing bonds and
CXT     compared.
        IF ((MOD(RSIZE,2).EQ.0).AND.(SOFAR.GT.0)) THEN
           DO 9075 IL = 1,SOFAR
              LX = MX
              LY = MY
              MATCH = .FALSE.
              DO 9074 IM = 1,RCNT
                 IF (IABS(RINGS(IM,1)).EQ.35) THEN
                    DO 9072 IN = 1,8
                       IF ((LX.EQ.NORDRW(IL,IN,1)).AND.
   *                      (LY.EQ.NORDRW(IL,IN,2))) THEN
                          MATCH = .TRUE.
                          GO TO 9073
                       ENDIF
```

```
9072                CONTINUE
                    MATCH = .FALSE.
                    GO TO 9075
                 ELSE IF (RINGS(IM,1).NE.0) THEN
                    DRDIR = IABS(RINGS(IM,1))
                    IF (DRDIR.GT.25) DRDIR = DRDIR - 2
                    DRDIR = DRDIR - 21
                    IF ((DRDIR.EQ.1).OR.(DRDIR.EQ.5)) THEN
                       INCKX = 0
                    ELSE IF ((DRDIR.GE.2).AND.(DRDIR.LE.4)) THEN
                       INCKX = 1
                    ELSE IF (DRDIR.GE.6) THEN
                       INCKX = -1
                    ENDIF
                    IF ((DRDIR.EQ.8).OR.(DRDIR.LE.2)) THEN
                       INCKY = -1
                    ELSE IF ((DRDIR.EQ.3).OR.(DRDIR.EQ.7)) THEN
                       INCKY = 0
                    ELSE IF ((DRDIR.GE.4).AND.(DRDIR.LE.6)) THEN
                       INCKY = 1
                    ENDIF
                    LX = LX + (IABS(RINGS(IM,2)) * INCKX) + INCKX
                    LY = LY + (IABS(RINGS(IM,2)) * INCKY) + INCKY
                 ELSE
                    GO TO 9075
                 ENDIF
9073             CONTINUE
9074          CONTINUE
              IF (MATCH) GO TO 8809
9075       CONTINUE
        ENDIF
CXT
        CIX=IX
        CIY=IY
        BX=MX
        BY=MY
        TIMES = ITIMES
        ERR = 0
        CALL DRING(RCNT,BX,BY,TX,TY,RBOND,TIMES)
        NLARGE=LARGE
        OCHAR=KKAR
        IF (ERR.EQ.23) THEN
CXT        Crossing diagonal bonds not allowed - delete ring.
           ERR = 0
           KAR = 127
           GO TO 1077
        ELSE IF (ERR.EQ.48) THEN
CXT        Adjacent nodal values not allowed - delete ring.
           KAR = 127
           IX = BX
           IY = BY
           GO TO 1088
        ENDIF
C GET INPUT TO CHECK FOR DELETE
1067    CALL INPUTX(KAR,TX,TY)
        IF (KAR.EQ.131) THEN
           ICUR = 1
           CALL CURSOR(TX,TY)
           GO TO 1067
        ELSE IF (KAR.EQ.94) THEN
           IERR = 39
           CALL MYERR(IERR,IERR,IERR)
           GO TO 1067
        ENDIF
1077    CONTINUE
1088    IDEL=0
        KKAR=KAR
        KAR1=0
C NOT DEL - GO PROCESS COMMAND
        IF (KAR.NE.127) THEN
           IF ((MM(TX,TY).EQ.46).OR.((MM(TX,TY).GE.65).AND.(MM(TX,TY)
     *        .LE.90))) THEN
              IX = TX + 1
           ELSE
              IX = TX
           ENDIF
```

```
            IY = TY
            GO TO 101
         ENDIF
         CALL CURSOR(IX,IY)
C THIS VARIABLE TRIGGERS THE 'NO GOOD ORIENTATION' MESSAGE
         IDEL=1
CXT      IF (RINGS(RCNT,1).EQ.35) IX = IX - 1
         IF ((RINGS(RCNT,1).EQ.35).AND.(ERR.NE.48)) IX = IX - 1
C DELETE RINGS
         CALL RNGDEL(RCNT,IX,IY)
         ERR = 0
         IX=CIX
         IY=CIY
         IF (IBTYPE.NE.0) THEN
            IF ((MM(IX,IY).GT.0).AND.(MM(IX,IY).LT.256)) IX = IX + 1
            CALL CURSOR(IX,IY)
         ENDIF
         OCHAR=KKAR
C WE DID A DELETE - DO WE TRY IT AGAIN
1068     CALL INPUTX(KAR,IX,IY)
         IF (KAR.EQ.131) THEN
            ICUR = 1
            CALL CURSOR(IX,IY)
            GO TO 1068
         ELSE IF (KAR.EQ.94) THEN
            IERR = 39
            CALL MYERR(IERR,IERR,IERR)
            GO TO 1068
         ENDIF
         KKAR=KAR
         IF(KAR .LT. 48 .OR. KAR .GT.56) GO TO 400
         OCONN=CONN
         CONN=-999
         ORSIZE=RSIZE
         DIG=KAR-48
         IF (DIG .GE. 3) GO TO 3202
         CONN=DIG
3205     OCHAR=KKAR
1069     CALL INPUTX(KAR1,IX,IY)
         IF (KAR1.EQ.131) THEN
            ICUR = 1
            CALL CURSOR(IX,IY)
            GO TO 1069
         ELSE IF (KAR1.EQ.94) THEN
            IERR = 39
            CALL MYERR(IERR,IERR,IERR)
            GO TO 1069
         ENDIF
         KKAR=KAR1
C GET NEW CONN AND RING SIZE
         DIG=KAR1-48
3202     IF (DIG .GE. 3 .AND. DIG .LE. 8) GO TO 3203
         IERR=30
         CALL MYERR(IERR,DIG,MAR)
         GO TO 3205
3203     RSIZE=DIG
         IF (CONN .EQ. -999) CONN=ENVIRN
         IF ((IX.NE.CIX).OR.(IY.NE.CIY)) GO TO 70017
         IF (ORSIZE .EQ. RSIZE .AND. CONN .EQ. OCONN) GO TO 992
C IF SAME SIZE AND CONNECTION - TRY NEXT ORIENTATION
C IF NOT - TRY NEW RING
70017    NLARGE = LARGE
         GO TO 101
992      DO 993 IM=1,40
         LAP(IM,3)=0
993      CONTINUE
         DO 904 IM=1,16
         RG2 = RINGS(IM,2)
904      RINGS(IM,2)=IABS(RG2)
8809     CONTINUE
991      CONTINUE
1000     CONTINUE
1001     CONTINUE
CXT
CXT      If fuses of more than 2 sides have been found possible,
```

```
CXT     attempt pass 2.
        IF ((FUSE3.GT.0).AND.(ATTMPT.EQ.1)) GO TO 1061
CXT
C Can't draw ring - issue error message
973     IF (IDEL .EQ. 1) GO TO 974
        IERR=31
C       Issue error message - reset NLARGE command and get next command
        CALL MYERR(IERR,KAR,MAR)
        NLARGE=LARGE
        KAR1=0
        GO TO 100
974     IDEL=0
        IERR=32
        CALL MYERR(IERR,IERR,IERR)
        KAR1=0
        NLARGE = LARGE
        GO TO 100
C       Bad connections for ring - issue error message - reset NLARGE
C       - get next cmd
947     IERR=29
        CALL MYERR(IERR,IERR,IERR)
        NLARGE=LARGE
        KAR1=0
        IF ((MM(IX,IY).EQ.46).OR.((MM(IX,IY).GE.65).AND.(MM(IX,IY).LE.
     *     90))) IX = IX + 1
        GO TO 10001
CXT
C Check for bond
400     IF (KAR.GE.22 .AND. KAR.LE.31) THEN
           BONDID = .TRUE.
           GO TO 700
        ELSE
           NOCHG = 0
        ENDIF
CXT
        IF (KAR.EQ.13 .OR. KAR .EQ. 81) GO TO 900
C If KAR = CR or Q - Quit or return to GND level
        IF ((KAR.EQ.21).OR.(KAR.EQ.32).OR.(KAR.EQ.8)) THEN
           IF (KAR.EQ.32) THEN
              JX = IX - 1
              CALL CURSOR(JX,IY)
              CALL CLRHYD(JX,IY)
              CALL VALNCE(2,JX,IY,0,0)
              IF (JPROB.EQ.1) GO TO 900
           ENDIF
           CALL SPACE(IX,IY)
           JCHAR = 2
           MCHAR = 0
           NLARGE = LARGE
           GO TO 10001
        ENDIF
        IF (KAR.EQ.33 .OR. KAR.EQ.95 .OR .KAR.EQ.58) GO TO 900
        IF (KAR.EQ.42) GO TO 900
C If KAR is chain, space or backspace (i.e. DUMB) set LFLAG
C so that we exit and go to IDENT not INPUTX
        IF (KAR .EQ. 64 .OR. KAR .EQ. 37) GO TO 800
C We have a REPEAT or LONGBOND command
C Check to UC
        IF ((KAR.GE.65 .AND. KAR.LE.90).OR.(KAR.EQ.46)) GO TO 700
C Check for $
        IF (KAR .EQ. 36) GO TO 700
C Check for &
        IF (KAR.EQ.38) GO TO 71234
C Check for lc
        IF (KAR .GE. 97 .AND. KAR .LE. 122) GO TO 700

CXT
C Check for marker command
        IF (KAR .EQ. 35) GO TO 700
C Check for luhn dot command
        IF (KAR.EQ.46) GO TO 700
C Go to DELETE section
        IF (KAR .EQ. 127) GO TO 700
C Go to NUM ENTRY section
        IF (KAR .EQ. 124) GO TO 600
```

```
       IF ((KAR.EQ.43).OR.(KAR.EQ.45).OR.(KAR.EQ.61)) GO TO 700
       IF (KAR.EQ.34) GO TO 700
       CALL ERRMSG(KAR)
       NLARGE = LARGE
C Invalid RING command - display error message and go try again
       GO TO 100
C
C ********************************************************************
C
C                      # ENTRY CODE
C
C ********************************************************************
C
C           CHAR WAS A VERTICAL LINE SO WE WILL BE SETTING
C                 A NEW BOND TYPE OR CHARGE VALUE
C
600    OCHAR=KKAR
       CALL CURSOR(IX,IY)
       CALL NUMBER(KAR,IX,IY)
       IF (KAR.EQ.81) GO TO 900
       KKAR = KAR
       ISTATE = 5
       ISTAT = '^'
       RBOND = IBTYPE
       CALL HEADER
       GO TO 100
C ********************************************************************
C                     END OF # ENTRY CODE
C ********************************************************************
C      Process command that IDENT can handle
700    CALL IDENT(KAR,IX,IY,INCX,INCY,IRESET)
CXT
       IF (BONDID) THEN
          BONDID = .FALSE.
          BAR = .FALSE.
       ENDIF
       RBOND = IBTYPE
C Get next command
       NLARGE = LARGE
       IF (JPROB.EQ.1) GO TO 900
       CALL HEADER
       GO TO 100
C Set enlargement factor
71234  CALL IDENT(KAR,IX,IY,INCX,INCY,IRESET)
       LARGE = NLARGE
       IF (JPROB.EQ.1) GO TO 900
       ISTATE = 5
       CALL HEADER
       GO TO 100
C Call REPEAT
800    IF (KAR .EQ. 64)
     1 CALL REPEAT(KAR,IX,IY,INCX,INCY,IRESET,LFLAG)
       IF (JPROB.EQ.1) GO TO 900
C Call LONGBOND
       IF (KAR .EQ. 37) CALL LONG(KAR,IX,IY)
C If we returned with
       IF (KAR .EQ. 81) GO TO 900
C a Q - Quit
C Reset variables and get next command
1310   CONTINUE
       LEVEL=1
       ISTATE=5
       ISTAT='^'
       JBDIR=IBDIR
       JBTYPE=IBTYPE
       JCHAR=ICHAR
C Call HEADER to display RING header
       CALL HEADER
       ICUR = 1
       CALL CURSOR(IX,IY)
       NLARGE = LARGE
       GO TO 100
C Set return flag to go to IDENT not INPUTX
900    CONTINUE
```

```
C If CR - then go to INPUTX
        IF (KAR .EQ. 13) THEN
           LCHAR = LLCHAR
           LFLAG=0
        ELSE
           LCHAR = 12
           LFLAG = 1
        ENDIF
        LEVEL=0
        ISTATE=0
C Set LEVEL and ISTATE to GND and call HEADER
        CALL HEADER
        ICUR = 1
        RETURN
        END
$STORAGE:2
C       SUBROUTINE LOCBND(IX,IY,LBND,BCNT)
C
C       THIS SUBROUTINE LOOKS AROUND A NODE AND COUNTS THE
C       BONDS POINTING TO OR FROM THE NODE - INPUT IS IX, IY
C       THE X AND Y COORDINATES OF THE NODE - OUTPUT IS BCNT
C       THE COUNT OF BONDS POINTING TO OR FROM THE NODE AND
C       LBND(1-8), WHICH IS SET TO 1 FOR THOSE LOCATIONS WHICH
C       HAVE EXISTING BONDS - I E - LBND(1) IS SET IF THE CELL
C       WHICH WOULD BE OCCUPIED BY ENTERING A DIR=1 BOND FROM
C       THE NODE CURRENTLY CONTAINS A BOND OF DIRECTION 1 OR 5
C
        SUBROUTINE LOCBND(IX,IY,BCNT)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM
        INTEGER*2 CBOND(8)
        COMMON /RINGY/ LBND(8,2),TSBOND(8),RHBIT(10),LAP(40,3),
     *     RINGS(16,2),RINGO(16,2)
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        DATA CBOND /8,1,2,7,3,6,5,4/
C
C Zero LBND
C
        DO 10 I=1,8
        DO 10 J=1,2
10      LBND(I,J)=0
9999    INDEX=1
C
C See if location contains a bond pointing to or from the node
C
       DO 11 J = -1,1
        DO 11 I=-1,1
C
C Skip node position
C
        IF (I .EQ. 0 .AND. J .EQ. 0) GO TO 11
        KAR = LMM(IX+I,IY+J)
C
C Consider case of 2 letter element code
C
        IF (I .EQ. 1 .AND. J .EQ. 0  .AND.
     1  (MM(IX+I,IY+J) .GE. 97 .AND. MM(IX+I,IY+J).LE.122))
     2  KAR = LMM(IX+I+1, IY+J)
C
C See if KAR is a bond and if so extract dir
C
        DIR = IDIR(KAR)
C Not a bond - go on
        IF(DIR .EQ. -1) GO TO 9
        IF(MOD(DIR,4).EQ. MOD(CBOND(INDEX),4))
     1  LBND(CBOND(INDEX),1)=CBOND(INDEX)
9       INDEX=INDEX+1
11      CONTINUE
C
C COUNT # OF GOOD BONDS FOUND
C
        BCNT=0
        DO 14 I=1,8
        IF(LBND(I,1) .NE. 0) BCNT=BCNT+1
14      CONTINUE
C
C Compress list - so that bond numbers are at the top on the list
```

```
C and 0's are at the bottom
C
      IF (BCNT .EQ. 0) RETURN
      I=1
      DO 15 J=1,8
      IF(LBND(J,1) .EQ. 0) GO TO 15
      LBND(I,1)=LBND(J,1)
      IF (I .NE. J) LBND(J,1)=0
      I=I+1
15    CONTINUE
      IF (BCNT .EQ. 1) RETURN
C
C Now set up LBND so that LBND(I,1) = first bond of gap
C                         LBND(I,2) = width of gap
C
      DO 16 I=2,BCNT
      LBND(I-1,2)=LBND(I,1)-LBND(I-1,1)
16    CONTINUE
      LBND(BCNT,2)=8-LBND(BCNT,1)+LBND(1,1)
C
      RETURN
      END
C
      SUBROUTINE GETABD(IX,IY,TSCNT)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*2 GETB(8,3)
      INTEGER*4 MM
      COMMON /RINGY/ LBND(8,2),TSBOND(8),RHBIT(10),LAP(40,3),
     *   RINGS(16,2),RINGO(16,2)
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      DATA GETB /-1,0,0,0,-1,-2,-2,-2,1,1,0,-1,-1,-1,0,1,
     *   5,6,7,8,1,2,3,4/
      DO 100 I=1,8
100   TSBOND(I)=0
      TSCNT=0
      DO 10 I=1,8
      KX=IX+GETB(I,1)
      KY = IY - GETB(I,2)
      K=LMM(KX,KY)
      KBTYPE=K/256
      KBDIR=K-KBTYPE*256
      IF(KBDIR .NE. GETB(I,3)) GO TO 10
      TSCNT=TSCNT+1
      TSBOND(TSCNT)=KBDIR
10    CONTINUE
      RETURN
      END
C
C     SUBROUTINE MAKRNG(RSIZE,RCNT,ENVIRN,FBOND,LARGE,COC,WCHRNG)
C
C     This subroutine will take the raw data in RHBIT and generate
C     a table of ring commands  - RINGS(I,1) will be the actual
C     ring commands - i.e. markers or bond commands - RINGS(I,2)
C     will give the length of the bonds desired - We do not use
C     NLARGE in an automatic way in RINGS because of multiplicative
C     problems in rings or size 3, 5, and 7. We temporarily set NLARGE
C     to 1 and let RINGS(I,2) represent the actual length on the bonds
C     RSIZE = size of ring - i.e. 3 to 8
C     RCNT = length of RINGS table
C     ENVIRN = type of environment -
C                        -1 = We are at an empty 3X3 area
C                         1 = We are at a node
C                         0 = We are at a bond
C     FBOND = direction of first bond of ring
C     LARGE = pseudo NLARGE
      SUBROUTINE MAKRNG(RSIZE,RCNT,ENVIRN,FBOND,LARGE,COC,WCHRNG)
      IMPLICIT INTEGER*2 (A-Z)
      COMMON /HP/IHP
      COMMON /RINGY/ LBND(8,2),TSBOND(8),RHBIT(10),LAP(40,3),
     *  RINGS(16,2),RINGO(16,2)
      DIMENSION TBOND(8)
      DATA TBOND/5,4,3,2,1,8,7,6/
      RCNT = 1
      DO 101 I=1,16
```

```
C Clear RINGS array
            IF (WCHRNG.EQ.1) THEN
               RINGS(I,1)=0
C Default len is 1
               RINGS(I,2)=1
            ELSE
               RINGO(I,1)=0
               RINGO(I,2)=1
            ENDIF
101      CONTINUE
C
C Generate ring definitions - i.e. markers and bonds
C
         I=1
         DO 6 J=1,RSIZE
C Skip first marker if we are doing SPIRO connection at a node
         IF (ENVIRN .EQ. 1 .AND. J .EQ. 1) GO TO 7
C Marker command
         IF (WCHRNG.EQ.1) THEN
            RINGS(I,1)=35
         ELSE
            RINGO(I,1) = 35
         ENDIF
         I=I+1
C Insert raw bond command
7        CONTINUE
         IF (WCHRNG.EQ.1) THEN
            RINGS(I,1)=RHBIT(J)
         ELSE
            RINGO(I,1) = RHBIT(J)
         ENDIF
         I=I+1
6        CONTINUE
C Length of RINGS table
         RCNT=I-1
         IF(ENVIRN .NE. 1) GO TO 40
         RCNT=RCNT+1
         IF (WCHRNG.EQ.1) THEN
            RINGS(RCNT,1)=35
         ELSE
            RINGO(RCNT,1) = 35
         ENDIF
C
C Now start to convert raw bond command to IDENT acceptable
C commands - i.e. 22-31 - and load RINGS(I,2) with bond length
C
40       PIT = 0
         BIT = FBOND
         DO 111 J=1,RCNT
C No work needed for marker command
         IF (WCHRNG.EQ.1) THEN
            IF(RINGS(J,1) .EQ. 35) GO TO 111
         ELSE
            IF (RINGO(J,1).EQ.35) GO TO 111
         ENDIF
         BIT=BIT+COC*PIT
         IF (BIT .EQ. 0) BIT = 8
         IF (BIT .LT. 0) BIT=BIT+8
         IF (BIT .GT. 8) BIT = BIT - 8
         IT=BIT
         IF (IHP .EQ. 1) IT=TBOND(IT)
         IT=IT+21
         IF (IT .GT. 25) IT=IT+2
         IF (WCHRNG.EQ.1) THEN
            PIT=RINGS(J,1)
         ELSE
            PIT = RINGO(J,1)
         ENDIF
         LEN = (PIT+4)/4
         IF(LEN .GT. 1) PIT=PIT-((LEN-1)*4)
         LEN = LEN*LARGE
         IF (WCHRNG.EQ.1) THEN
            RINGS(J,1)=IT
            RINGS(J,2)=LEN
```

```
      ELSE
         RINGO(J,1) = IT
         RINGO(J,2) = LEN
      ENDIF
111   CONTINUE
      IF (LARGE .EQ. 1) GO TO 12
      IF (RSIZE .NE. 3 .AND. RSIZE .NE. 5) GO TO 70
C
C Alter longest bond if size is 3 or 5 and LARGE > 1
C
      MAXI = 0
      MAXLEN = 0
      DO 15 I=1,RCNT
         IF (WCHRNG.EQ.1) THEN
            IF(RINGS(I,2) .LT.  MAXLEN) GO TO 15
            MAXLEN = RINGS(I,2)
         ELSE
            IF(RINGO(I,2) .LT.  MAXLEN) GO TO 15
            MAXLEN = RINGO(I,2)
         ENDIF
         MAXI=I
15    CONTINUE
          IF (WCHRNG.EQ.1) THEN
             RINGS(MAXI,2)=RINGS(MAXI,2)-(LARGE-1)
          ELSE
             RINGO(MAXI,2)=RINGO(MAXI,2)-(LARGE-1)
          ENDIF
C
70    IF(RSIZE .NE. 7) GO TO 12
C
C Adjust ring of size 7 if LARGE>1
C
       MAXI=0
       MAXLEN=LARGE
       DO 16 I=1,RCNT
          IF (WCHRNG.EQ.1) THEN
             IF(RINGS(I,2) .LT. MAXLEN) GO TO 16
             MAXLEN=RINGS(I,2)
          ELSE
             IF(RINGO(I,2) .LT. MAXLEN) GO TO 16
             MAXLEN=RINGO(I,2)
          ENDIF
          MAXI=I
16     CONTINUE
       INDEX = MAXI + 6
       IF (WCHRNG.EQ.1) THEN
       IF (INDEX.GT.RCNT.AND.RINGS(MAXI-2,2).NE.MAXLEN)INDEX=MAXI-6
       IF(INDEX.GT.RCNT.AND.RINGS(MAXI-2,2).EQ.MAXLEN)INDEX=MAXI-8
       RINGS(INDEX,2)=LARGE*2-1
       ELSE
       IF (INDEX.GT.RCNT.AND.RINGO(MAXI-2,2).NE.MAXLEN)INDEX=MAXI-6
       IF(INDEX.GT.RCNT.AND.RINGO(MAXI-2,2).EQ.MAXLEN)INDEX=MAXI-8
       RINGO(INDEX,2)=LARGE*2-1
       ENDIF
12     CONTINUE
       RETURN
       END
C
       SUBROUTINE DRING(SIZE,IX,IY,RMXCUR,LMYCUR,RBOND,TIMES)
       IMPLICIT INTEGER*2 (A-Z)
       INTEGER*2 REALR(4)
       INTEGER*4 IDTPIX,MM
       LOGICAL*2 DUPSTR,BAR,OPNBAR,BONDEL,BONDID
       COMMON /RINGY/ LBOND(8,2),TSBOND(8),RHBIT(10),LAP(40,3),
     *   RINGS(16,2),RINGO(16,2)
       COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
       COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
       COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
       COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
       COMMON /CUR/ ICUR
       COMMON /DARK/ OCUR
       COMMON /XRNG/ NORDRW(8,8,2),SOFAR
CXT    BAR is used in conjunction with NOCHG, OPNBAR, and BONDID to
CXT    control bond type determination in relation to default bond types.
       COMMON /BTPDIR/ BAR
```

```
CXT     BONDEL = TRUE indicates a bond has been drawn between 2 nodes so
CXT     subsequent deletion can delete the bond, not a node.
        COMMON /DELBND/ BONDEL
        COMMON /WARN/ ERR
C
        RSIZE = SIZE / 2
        OPNBAR = .TRUE.
        OBTYPE = IBTYPE
C
C       Each ring drawing is recorded to bypass later duplication.
        IF ((TIMES.GT.0).AND.(MOD(RSIZE,2).EQ.0)) THEN
           SOFAR = SOFAR + 1
           L = 0
           DUPSTR = .TRUE.
        ELSE
           DUPSTR = .FALSE.
        ENDIF
C
C       The cursor coordinates are initialized to allow cursor end up
C       at lower right corner node of ring.
        RMXCUR = 1
        LMYCUR = 1
        CALL INITHC(3,3,0)
        OCUR = 0
        OLARGE=NLARGE
        DO  11 I = 1,SIZE
        KAR =RINGS(I,1)
        K=KAR
C
C       The x and y coordinates of the ring being drawn are recorded.
        IF ((DUPSTR).AND.(KAR.EQ.35)) THEN
           L = L + 1
           IF ((MM(IX,IY).NE.46).AND.(MM(IX-1,IY).EQ.46)) THEN
              NORDRW(SOFAR,L,1) = IX - 1
           ELSE
              NORDRW(SOFAR,L,1) = IX
           ENDIF
           NORDRW(SOFAR,L,2) = IY
        ENDIF
        IF (KAR.NE.35 .AND.(I.EQ.1.OR.I.EQ.2)) IBTYPE = RBOND
        LEN = RINGS(I,2)
C
C       Test is made for lower rightmost node of ring.
        IF ((KAR.EQ.35).AND.(IX.GE.RMXCUR)) THEN
           IF (IX.GT.RMXCUR) THEN
              LMYCUR = IY
           ELSE IF (IY.GT.LMYCUR) THEN
              LMYCUR = IY
           ENDIF
           RMXCUR = IX
        ENDIF
        IF (LEN.LT.0 .AND. KAR.EQ.35) GO TO 111
        IF (LEN .LT. 0) GO TO 15
        IF(KAR .EQ. 35 .AND. MM(IX-1,IY).EQ.46.AND.I.GT.1)GO TO 11
        NLARGE=LEN
C Draw part of ring here
        IF ((KAR.GE.22).AND.(KAR.LE.31)) BONDID = .TRUE.
        CALL IDENT(KAR,IX,IY,INCX,INCY,IRESET)
        RBOND = IBTYPE
        IF (BONDID) THEN
           BONDID = .FALSE.
           OPNBAR = .FALSE.
           NOCHG = 0
        ENDIF
        IF (ERR.EQ.48) THEN
           STPSZE = I
           GO TO 12
        ENDIF
        IF (K .EQ. 35) GO TO 11
        REALR(1)=K
        REALR(2)=IX
        REALR(3)=IY
        REALR(4)=NLARGE
        GO TO 11
111     BIX=IX
        IF (MM(BIX,IY) .NE.46 .AND. MM(BIX-1,IY).EQ.46)BIX=BIX-1
C WE HAVE INCORPORATED A CHAIN MARKER IN A RING
```

```
      DO 20 JJ=1,260
C DELETE IT FROM THE CHAIN MARKER TEST
      IF (LABL(JJ,1).EQ.0) GO TO 11
      IF (LABL(JJ,1).NE.BIX.OR.LABL(JJ,2).NE.IY) GO TO 20
      MRKCHN(JJ)=0
      GO TO 11
20    CONTINUE
      GO TO 11
C
C     This section retraces an existing bond - Set bondtype
C     so that existing bonds are not changed
C
15    KX=IX
      KY=IY
      IF(MM(KX,KY).NE.46 .AND. MM(KX-1,KY).EQ.46)KX=KX-1
      IBND=KAR
      CALL DELTA(IBND,INCX,INCY)
C Get existing bond
      OBND=LMM(KX+INCX,KY+INCY)
      OBND=OBND/256
      KBOND=IBTYPE
CXT
      IBTYPE = OBND
      NOCHG = 1
      BAR = .FALSE.
      CALL IDENT(KAR,IX,IY,INCX,INCY,IRESET)
C Restore bond type
      IBTYPE=KBOND
      IF (OPNBAR) THEN
         BAR = .TRUE.
      ELSE
         NOCHG = 0
      ENDIF
      IF (ERR.EQ.48) THEN
         STPSZE = I
         GO TO 12
      ENDIF
11    CONTINUE
12    CONTINUE
C SUPPRESS CURSOR DISPLAY WHEN DRAWING RING
      ICUR=0
      RBOND=IBTYPE
      IF (IBTYPE .EQ. 2 .OR. IBTYPE .EQ. 3 .OR. IBTYPE.EQ.5
     1 .OR. IBTYPE .EQ. 6 .OR. IBTYPE .EQ. 7) RBOND=1
      NLARGE=OLARGE
C     THE FOLLOWING CODE IS USED FOR ALTERNATING BONDS
C     IT SOMETIMES HAPPENS THAT 2 DOUBLE BONDS ARE
C     DRAWN TOGETHER - PARTICULARLY WHEN RINGS ARE
C     FUSED - THIS CODE EXAMINES THE LAST BOND DRAWN
C     IF IT IS A DOUBLE BOND - IT EXAMINES THE OTHER
C     BONDS AROUND THE NODE AND CHANGES THE LAST DRAWN
C     BOND TO SINGLE IF - 1 THERE IS ANOTHER DOUBLE
C     BOND FROM THAT NODE - OR 2 THE TOTAL BOND
C     COUNT EXCEEDS 4
      IF (IBTYPE .NE. 4) THEN
         OCUR = 1
         CALL INITHC(3,3,OCUR)
         ICUR = 1
         IF (ERR.EQ.48) THEN
            SIZE = STPSZE - 1
            CALL CURSOR(IX,IY)
         ELSE
            CALL CURSOR(RMXCUR,LMYCUR)
         ENDIF
         IBTYPE = OBTYPE
         RETURN
      ENDIF
      NBOND=REALR(1)
      R1 = REALR(1)
      CALL DELTA(R1,INCX,INCY)
      REALR(1) = R1
      JX=REALR(2)-1-INCX
      JY=REALR(3)-INCY
C IS THE LAST BOND A DOUBLE BOND
      MMM=LMM(JX,JY)/256
```

```
C NO - RETURN - NO PROBLEM
        IF (MMM.EQ.1) THEN
           OCUR = 1
           CALL INITHC(3,3,OCUR)
           ICUR = 1
           CALL CURSOR(RMXCUR,LMYCUR)
           RETURN
        ENDIF
        MX=REALR(2)-1
C GET BONDS AROUND NODE
        R2 = REALR(3)
        CALL LOCBND(MX,R2,BCNT)
        REALR(3) = R2
C ONLY ONE BOND - NO PROBLEM
        IF (BNCT .EQ. 1) THEN
           OCUR = 1
           CALL INITHC(3,3,OCUR)
           ICUR = 1
           CALL CURSOR(RMXCUR,LMYCUR)
           RETURN
        ENDIF
        IDOB=0
        CNT=0
        MY=REALR(3)
        DO 40 I=1,BCNT
        DIR=LBOND(I,1)
        CALL DELTA(DIR,INCX,INCY)
        MMM=LMM(MX+INCX,MY+INCY)/256
        IF (MMM .EQ. 2) IDOB=IDOB+1
        IF (MMM .GT. 3) MMM=1
        CNT=CNT+MMM
40      CONTINUE
        DO 400 I=0,2,2
        DO 4141 J=1,100
        IF (LNGBND(J,I+1) .EQ. 0) GO TO 400
        IF ((LNGBND(J,I+1) .NE. MX) .OR.
     1  (LNGBND(J,I+2) .NE. MY)) GO TO 4141
        MMM=LNGBND(J,5)
        IF (MMM .EQ. 2 ) IDOB=IDOB+1
        IF (MMM .GT. 3) MMM=1
        CNT=CNT+MMM
        GO TO 444
4141    CONTINUE
400     CONTINUE
444     IF (IDOB .LE.1 .AND. CNT .LE.4) THEN
           OCUR = 1
           CALL INITHC(3,3,OCUR)
           ICUR = 1
           CALL CURSOR(RMXCUR,LMYCUR)
           RETURN
        ENDIF
        DIR=REALR(1)+4
        IF (DIR .GT. 8) DIR = DIR -8
        DIR=DIR+21
        IF (DIR .GT. 25) DIR = DIR + 2
C REPLACE BOND
        R1 = REALR(2)
        R2 = REALR(3)
        CALL IDENT(DIR,R1,R2,INCX,INCY,IRESET)
        IBTYPE=1
        CALL IDENT(NBOND,R1,R2,INCX,INCY,IRESET)
        NOCHG = 0
        REALR(2) = R1
        REALR(3) = R2
        IBTYPE=4
        OCUR = 1
        CALL INITHC(3,3,OCUR)
        ICUR = 1
        CALL CURSOR(RMXCUR,LMYCUR)
        RETURN
        END
C
C       SUBROUTINE RNGDEL(RINGS,RCNT,IX,IY)
C
C       THIS SUBROUTINE DELETES A RING - INPUT IS THE ARRAY RINGS
C       WHICH CONTAINS THE RING GENERATING COMMAND - AND IX AND IY
```

```
C       WHICH ARE THE COORDINATES OF THE STARTING POINT FOR THE RING
C       RCNT = # OF COMMANDS IN RINGS
C
        SUBROUTINE RNGDEL(RCNT,IX,IY)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM
        LOGICAL*2 BONDEL
        COMMON /RINGY/ LBND(8,2),TSBOND(8),RHBIT(10),LAP(40,3),
     *    RINGS(16,2),RINGO(16,2)
        COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
        COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /CUR/ ICUR
        COMMON /WARN/ ERR
        COMMON /DELBND/ BONDEL
        ICUR=0
        ITYPE=0
        IF (IBTYPE .EQ. 4) ITYPE=1
        KX=IX
C INITIAL COORDINATES
        KY=IY
        DO 100 I=RCNT,1,-1
C GET COMMAND
        COM=RINGS(I,1)
        C=COM
C GO TO 200 FOR MARKER
        IF (COM .EQ. 35) GO TO 200
        IF (MM(KX,KY).NE.46 .AND. MM(KX-1,KY).EQ.46 .AND.
     *     (ERR.NE.48 .OR. I.NE.RCNT)) KX=KX-1
C GET READY TO DEL BOND
        JCHAR=1
        BOND=COM
C GET DELTAS FOR BOND
        CALL DELTA(BOND,INCX,INCY)
        JBTYPE=IBTYPE
C SET BOND DIR
        IBDIR=BOND
        JBDIR=IBDIR
C IF NEG - SKIP BOND DEL
        IF ((RINGS(I,2).LT.0).OR.(IBTYPE.EQ.0)) GO TO 300
C AND JUST SLIDE ALONG BOND TO NODE
C DEL BOND
        CALL DEL(COM,KX,KY,INCX,INCY,0)
        GO TO 100
300     LEN = IABS(RINGS(I,2))
        DO 400 K=1,LEN+1
        KX=KX-INCX
        KY=KY-INCY
400     CONTINUE
        GO TO 100
C IF NEG - SKIP DEL MARKER COMMAND
200     IF (RINGS(I,2) .LT. 0) GO TO 100
        JCHAR=2
C MOVE CURSOR JUST TO LEFT OF MARKER
        IF (MM(KX,KY).EQ. 46)KX=KX+1
        BONDEL = .FALSE.
        CALL DEL(COM,KX,KY,INCX,INCY,0)
100     CONTINUE
        IF (ICHAR .LE. 10) MCHAR=COM
        IF (ICHAR .LE. 10) JCHAR=ICHAR
C Reset to 4 if we entered with bondtype = 4
        IF (ITYPE .EQ. 1) IBTYPE=4
        JBTYPE=IBTYPE
        JBDIR=IBDIR
        ICUR=1
        CALL CURSOR(IX,IY)
        RETURN
        END
C
C       SUBROUTINE LOOK(IX,IY,ICHECK,IBADX,IBADY,LAP,LCNT,BLOB)
C
C       THIS SUBROUTINE CHECKS A 3 x 3 CELL CENTERED AT IX & IY
C
C       ICHECK = 0      THAT IS OK - IF
C
C                                         1. THE MM SUBSCRIPTS ARE GOOD
```

```
C                                     2. THE CELL IS EMPTY - OR - THE
C                                        OVERLAPS ARE VALID OVERLAPS
C                                        FOUND IN THE LAP TABLE
C       ICHECK NOT = 0 MEANS THAT BAD CONFLICTS AROSE
C
        SUBROUTINE LOOK(IX,IY,ICHECK,LCNT,BLOB)
        IMPLICIT INTEGER*2 (A-Z)
        COMMON /RINGY/ LBND(8,2),TSBOND(8),RHBIT(10),LAP(40,3),
     *    RINGS(16,2),RINGO(16,2)
        COMMON /BAD/ IBADX(9),IBADY(9)
        COMMON /FUSE/ ITIMES
C Cell is OK until proven otherwise
        ICHECK=0
C Check MM subscritps
        CALL CHECK(IX,IY,ICHECK)
C Bad subscripts - set error and return
777     IF (ICHECK .EQ.1) GO TO 10
C Space is empty - go check surrounding area
        WHAT=LMM(IX,IY)
        IF (WHAT .EQ. 0) GO TO 800
        IF (WHAT .EQ. 46 .AND. BLOB .EQ. 35) GO TO 856
        W=IABS(MOD(WHAT,256)-BLOB)
        IF (W .EQ. 0 .OR. W .EQ. 4) GO TO 856
        GO TO 851
C Novalid overlaps - set error and exit
856     IF (LCNT .EQ. 0) GO TO 10
        DO 850 I=1,LCNT
        IF (LAP(I,1) .EQ. IX .AND. LAP(I,2).EQ.IY) LAP(I,3)=1
        IF (LAP(I,1).EQ. IX .AND. LAP(I,2).EQ.IY) BLOB=-1
        IF(LAP(I,1) .EQ. IX .AND. LAP(I,2) .EQ.IY) GO TO 855
850     CONTINUE
C OK IS 2 OR MORE SIDES TO BE FUSED
        IF (ITIMES .NE. 2) GO TO 851
        IF (LCNT.GE.40) GO TO 851
        BLOB=-1
        LCNT=LCNT+1
        LAP(LCNT,1)=IX
        LAP(LCNT,2)=IY
        LAP(LCNT,3)=1
        GO TO 855
C Center of cell ocupied by valid overlap - no need to check further
851     ICHECK=1
855     CONTINUE
        RETURN
800     IF(ITIMES .EQ. 2)  RETURN
        CALL CELL(IX,IY,ICHECK)
C No problem - good cell - ICHECK=0 and return
        IF (ICHECK.EQ.0) RETURN
        DO 982 I=1,ICHECK
        DO 980  J=1,LCNT
        IF(IBADX(I).EQ.LAP(J,1) .AND. IBADY(I) .EQ. LAP(J,2)) GO TO 982
980     CONTINUE
C Overlap was not in LAP table
        BX = IBADX(I)
        BY = IBADY(I)
        A = LMM(BX,BY)
C Was it a legal overlap - i.e.
C bond - not pointing to cell
C or cell would contain bond
C and overlap is marker and cell bond
C does not pointer to marker
C A = contents of offending cell
        IF (BLOB .EQ. 35) GO TO 20
C A is a bond - is it an OK bond
        IF (A .GE. 256) GO TO 11
C A is not a bond or marker - can't be any good
        IF (A .NE. 46) GO TO 10
        B=BLOB
C       Cell will contain bond - does it point to marker
        CALL DELTA(B,INCX,INCY)
C If bond points to marker - it is no good
        IF (((IBADX(I).EQ.(IX+INCX)).AND.(IBADY(I).EQ.(IY+INCY)))
     1  .OR. ((IBADX(I).EQ. (IX-INCX)).AND.(IBADY(I).EQ.(IY-INCY))))
```

```
      2  GO TO 10
C If not - it is OK
         GO TO 982
C Not a bond - can't be OK
20       IF (A .LT. 256) GO TO 10
C Get bond direction
11       B=IDIR(A)
C Get bond deltas
         CALL DELTA(B,INCX,INCY)
         IF((((IBADX(I)+INCX).EQ. IX) .AND.((IBADY(I)+INCY).EQ.IY))
      1  .OR. (((IBADX(I)-INCX).EQ.IX).AND.((IBADY(I)-INCY).EQ.IY)))
      2  GO TO 10
C If it point to bond or marker - it is no good
982      CONTINUE
C Overlap was valid - cell OK
         ICHECK=0
C Valid overlap - return
         RETURN
10       ICHECK=1
C Bad overlap - return with error set
         RETURN
         END
C
C        SUBROUTINE MBIT(RSIZE,RHBIT)
C
C        THIS SUBROUTINE FILLS THE RHBIT ARRAY STARTING WITH CAN(SR,RSIZE)
         SUBROUTINE MBIT(RSIZE)
         IMPLICIT INTEGER*2 (A-Z)
         COMMON /RINGY/ LBND(8,2),TSBOND(8),RHBIT(10),LAP(40,3),
      *    RINGS(16,2),RINGO(16,2)
         COMMON /RCAN/ CAN(10,10)
         RSIZ=RSIZE
         IF (RSIZE .EQ. 9) RSIZ=3
         IF (RSIZE .EQ. 10) RSIZ = 5
         DO 450 K=1,RSIZ
         RHBIT(K)= CAN(K,RSIZE)
450      CONTINUE
         RETURN
         END
C
         SUBROUTINE DELTA(BOND,INCX,INCY)
         IMPLICIT INTEGER*2 (A-Z)
         COMMON/ITERM/ITER
         IF (BOND .LE. 8) GO TO 10
         BOND=BOND-21
         IF(BOND .GT. 4) BOND=BOND-2
C DETERMINE DELTA X AND DELTA Y
10       INCY = -1  * ITER
C
         IF ((BOND.GE.4).AND.(BOND.LE.6)) INCY = 1 *ITER
         IF(MOD(BOND,4) .EQ. 3) INCY = 0
         INCX=1
         IF ((BOND.GE.6) .AND.(BOND .LE.8)) INCX=-1
         IF(MOD(BOND,4) .EQ. 1) INCX=0
         RETURN
         END
C
C        SUBROUTINE MKBND(FBOND)
C
C        THIS SUBROUTINE CONVERTS A BOND DIRECTION (1-8) TO A
C        BOND COMMAND (22-25;28-31)
C
         SUBROUTINE MKBND(FBOND)
         IMPLICIT INTEGER*2 (A-Z)
         FBOND=FBOND+21
         IF (FBOND .GT. 25) FBOND=FBOND+2
         RETURN
         END
C        SUBROUTINE NEW sees if the chain is starting with a new structure.
         SUBROUTINE NEW(SUM,IX,IY)
         IMPLICIT INTEGER*2 (A-Z)
         INTEGER*4 MM
         COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
         SUM=0
         DO 10 I=-1,1
```

```
        DO 10 J=-1,1
        SUM=SUM + LMM(IX+I, IY+J)
10      CONTINUE
        RETURN
        END
C
C       SUBROUTINE FINDB finds a correct pointer bond.
        SUBROUTINE FINDB(IBDIR,KBDIR,IX,IY)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM
        LOGICAL*2 CHEK67
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /XBOND/ GOODB(2,9)
        CHEK67 = .TRUE.
        IB=0
        DO 24 J = -1,1
        DO 24 I=-1,1
        IB=IB+1
        KX=IX+I
        KY=IY+J
CIF NOT BOND - SKIP THIS ONE
        IF (LMM(KX,KY) .LT. 256) GO TO 24
        KBTYPE=LMM(KX,KY)/256
        KBDIR=LMM(KX,KY) - KBTYPE*256
21      IF (KBDIR .EQ. GOODB(1,IB)) GO TO 26
        IF ((KBTYPE.EQ.6).OR.(KBTYPE.EQ.7)) THEN
           IF (CHEK67) THEN
              KBDIR = KBDIR + 4
              IF (KBDIR.GT.8) KBDIR = KBDIR - 8
              CHEK67 = .FALSE.
              GO TO 21
           ELSE
              CHEK67 = .TRUE.
           ENDIF
        ENDIF
24      CONTINUE
CWE DID NOT FIND A BOND - SET BOND
        IBDIR=-1
CDIRECTION TO -1 AND RETURN
        RETURN
CFOUND GOOD POINTER BOND
26      IBDIR=GOODB(2,IB)
        RETURN
        END
C
C       CNTBND counts the number of bonds of a node.
C
        SUBROUTINE CNTBND(ICNT,IX,IY)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        ICNT=0
        DO 24 J=1,-1,-1
        DO 24 I=-1,1
        KX=IX+I
        KY=IY+J
        IF((I.EQ.1) .AND. (J.EQ.0) .AND.
     1  (MM(KX,KY).GE.97 .AND. MM(KX,KY).LE. 122))KX=KX+1
        IF (LMM(KX,KY).LT.256) GO TO 24
        ICNT=ICNT+1
24      CONTINUE
        RETURN
        END
C
        SUBROUTINE CHECK(IX,IY,ICHECK)
        IMPLICIT INTEGER*2 (A-Z)
        COMMON /CD/ MAXX,MAXY
        ICHECK=0
C       CHECK=0 IMPLIES INDICIES ARE OK. CHECK=1 IMPLIES INDICIES ARE BAD.
        IF(IX .LE. 0 .OR. IX .GT. MAXX .OR.
     1  IY .LE. 0 .OR. IY .GT. MAXY) ICHECK=1
        RETURN
        END
C
```

```
      SUBROUTINE SHARP(IBDIR,IX,IY,ISHARP)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*2 WHERE(8,4)
      INTEGER*4 MM
      COMMON /STRPIX/LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      DATA WHERE /-1,-1,0,0,-1,0,0,1,0,0,1,1,0,1,1,0,
     *   1,0,0,-1,1,1,0,0,0,-1,-1,0,0,0,-1,-1/
      ISHARP=0
      INBOND=IBDIR
      CALL DELTA(INBOND,KNCX,KNCY)
      KX=IX+KNCX
      KY=IY+KNCY
      WX = KX + WHERE(INBOND,1)
      WY = KY - WHERE(INBOND,2)
      K = LMM(WX,WY)
      IF(K.LT.256) GO TO 24
      GO TO 26
C
24    CONTINUE
      WX = KX + WHERE(INBOND,3)
      WY = KY - WHERE(INBOND,4)
      K = LMM(WX,WY)
      IF (K .LT. 256) GO TO  27
      GO TO 26
27    CONTINUE
      RETURN
26    CONTINUE
      ISHARP=1
      RETURN
      END
C
      SUBROUTINE GETBD(IX,IY,KBDIR,KX,KY)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      DIMENSION GETB(8,3)
      DATA GETB /-1,0,0,0,-1,-2,-2,-2,1,1,0,-1,-1,-1,0,1,
     *   5,6,7,8,1,2,3,4/
      DO 10 I=1,8
      KX=IX+GETB(I,1)
      KY = IY - GETB(I,2)
      K=LMM(KX,KY)
      KBTYPE=K/256
      KBDIR=K-KBTYPE*256
      IF(KBDIR .NE. GETB(I,3)) GO TO 10
      RETURN
10    CONTINUE
      KBDIR=-1
      END
$STORAGE:2
C
C     SUBROUTINE SITE(IX,IY,ACHAR,BCHAR,TER,ICNT)
C     ACHAR=PRIMARY TERMINATOR CHAR
C     BCHAR=ALTERNATE TERMINATOR CHAR
C     TER=TERMINATOR CHARACTER ACTUALLY RECEIVED
C     This subroutine obtains the connecting or exiting site
C     It should be a marker or a bond end
C     The type of site is not checked in this subroutine - it
C     is checked back in LIBRA
      SUBROUTINE SITE(IX,IY,ACHAR,BCHAR,TER,ICNT,REST)
      IMPLICIT INTEGER*2(A-Z)
      INTEGER*4 MM
      CHARACTER*1 HLO(3)
      CHARACTER*3 HLOE
      EQUIVALENCE (HLOE,HLO(1))
      COMMON /ISTATE/ ISTAT
      CHARACTER*1 ISTAT
      COMMON /HEAD/ MW(12),ISTATE,PAGE
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      OKAR=97
C Set last char to lc
      KAR=13
      IRESET = 0
```

```
100     CALL INPUTX(IKAR,IX,IY)
        IF (IKAR.EQ.95) THEN
           IERR = 39
           CALL MYERR(IERR,IERR,IERR)
           GO TO 100
        ELSE IF (IKAR.EQ.131) THEN
           REST = IKAR
           RETURN
        ELSE IF ((REST.EQ.1).AND.(IKAR.NE.69).AND.(IKAR.NE.83).AND.
     *     (IKAR.NE.13)) THEN
           CALL FTSIZE(2,18)
           CALL FTLOCA(6,1)
        CALL FTEXT('^Move cursor to connecting site - Type E to finalize
     * position^')
        ELSE IF ((REST.EQ.2).AND.(IKAR.NE.83).AND.(IKAR.NE.13)) THEN
           CALL FTSIZE(2,18)
           CALL FTLOCA(6,1)
        CALL FTEXT('^Move cursor to exit site - Type S to finalize posit
     *ion      ^')
        ENDIF
        PAGE = 0
        CALL FTSIZE(1,10)
        IIKAR=IKAR
C       Save char before call to IDENT because IDENT
C       may change char
C       Marker preceeded by marker or DEL = OK
        IF ((IKAR .GE. 97 .AND. IKAR .LE. 122) .AND. ((OKAR .GE. 97
     1  .AND. OKAR .LE. 122) .OR. OKAR .EQ. 127)) GO TO 1000
        IF (IKAR .GE. 48 .AND. IKAR .LE. 56) GO TO 1000
C Set bond type cmd = OK
        IF (IKAR.EQ.127.AND. (OKAR .GE. 22 .AND.OKAR .LE. 31)) GO TO 1000
C DEL preceeded by bond = OK
        IF (IKAR.GE.21 .AND. IKAR.LE.31) GO TO 1000
C Bond cmd = OK
        IF (IKAR.EQ.ACHAR.OR.IKAR .EQ. BCHAR .OR. IKAR .EQ. 13) GO TO 500
C Terminator = ACHAR or BCHAR or CR = OK = EXIT
        ICNT= ICNT+1
        CALL FTSIZE(2,18)
        CALL FTLOCA(4,1)
        CALL FTEXT('^Invalid response: ^')
        HLO(2) = CHAR(IKAR)
        CALL FTEXT(HLOE)
        CALL FTEXT('^     Enter bond, bond type, DEL(bond) or terminator
     *^')
        CALL FTSIZE(1,10)
        PAGE = 0
        GO TO 100
1000    CALL IDENT(IKAR,IX,IY,INCX,INCY,IRESET)
        IF (IKAR.EQ.21) THEN
        IF ((REST.EQ.1).AND.(IKAR.NE.69).AND.(IKAR.NE.83).AND.
     *     (IKAR.NE.13)) THEN
           CALL FTSIZE(2,18)
           CALL FTLOCA(6,1)
        CALL FTEXT('^Move cursor to connecting site - Type E to finalize
     * position^')
        ELSE IF ((REST.EQ.2).AND.(IKAR.NE.83).AND.(IKAR.NE.13)) THEN
           CALL FTSIZE(2,18)
           CALL FTLOCA(6,1)
        CALL FTEXT('^Move cursor to exit site - Type S to finalize posit
     *ion      ^')
        ENDIF
        PAGE = 0
        CALL FTSIZE(1,10)
        ENDIF
        ISTATE = 11
        CALL HEADER
        OKAR=IIKAR
C Save last command
        GO TO 100
C Go get next command
500     TER=IKAR
        IF (OKAR .GE. 48 .AND. OKAR .LE. 56)
     1  CALL IDENT(KAR,IX,IY,INCX,INCY,IRESET)
C We had an incomplete bond type - bond cycle
C Terminate it with CR
        RETURN
```

```
        END
C
C       THIS SUBROUTINE CONVERTS LUHN DOTS TO NON-CHAIN MARKERS
C       AND CHx'S TO CHAIN MARKERS
C
        SUBROUTINE REMARK(IERR)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,IDTPIX
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
        COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
        COMMON /LABELS/ NR,NJLAST,NJNEXT
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /CD/ MAXX,MAXY
C
C       ZERO MARKER ARRAYS AND POINTER NJNEXT AND ERROR FLAG IERR
C
        IERR=0
C       DEFAULT VALUE - 0 IMPLIES NO ERROR
        NJNEXT=0
        DO 50 I=1,260
           LABL(I,1)=0
           LABL(I,2)=0
           MRKCHN(I)=0
50      CONTINUE
C
C       GO THROUGH THE MM ARRAY - CHANGE LUHN DOTS (46) TO NON-CHAIN
C       MARKERS AND CHx'S TO CHAIN MARKERS
C
        DO 100 I = LOX,HIX
        DO 100 J = LOY,HIY
           IF (MM(I,J) .EQ. 46) GO TO 60
           IF (MM(I,J).NE.67 .OR. (MM(I,J).EQ.67 .AND. (MM(I+1,J).GE.
     1        97.AND.MM(I+1,J).LE.122)))  GO TO 100
C
C          CLEAR HYDROGENS AROUND CARBON
C          DELETE CARBON - INSERT MARKER - MARK MARKER AS CHAIN MARKER
C
              DO 1444 K = 1,MAXX
                 IF ((MM(I-K,J).EQ.0).OR.(LMM(I-K,J).GE.256).OR.
     *              (I-K.LE.0)) THEN
                    GO TO 1445
                 ELSE IF (MM(I-K,J).EQ.42) THEN
                    GO TO 100
                 ENDIF
1444          CONTINUE
1445          CONTINUE
        NJNEXT=NJNEXT+1
        IF (NJNEXT .GT. 260) GO TO  99
        II=I
        JJ = J
        CALL CLEARH(1,II,JJ)
        MM(I,J)=46
        LABL(NJNEXT,1)=I
        LABL(NJNEXT,2)=J
        MRKCHN(NJNEXT)=1
        GO TO 100
C
C       DELETE LUHN DOT AND ENTER MARKER HERE
C
60      NJNEXT=NJNEXT+1
        IF (NJNEXT .GT. 260) GO TO 99
C       HAVE WE RUN OUT OF MARKERS?
        LABL(NJNEXT,1)=I
        LABL(NJNEXT,2)=J
100     CONTINUE
        RETURN
99      IERR=16
        CALL MYERR(IERR,IERR,IERR)
        RETURN
        END
C
        SUBROUTINE CLEARH(WHICH,KX,KY)
        IMPLICIT INTEGER*2 (A-Z)
```

```
        INTEGER*4 MM,IDTPIX
        COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
C This subroutine clears valence hydrogens from the vicinity of nodes
C and extends bonds as needed, before re-calculation of valences.
C This is a simplified version of CLRHYD - It changes the MM array
C but it does not change the screen
C
C       Most of this code is lifted from CLRHYD
C
        IF (WHICH.EQ.1) THEN
1       IF (MM(KX-1,KY) .EQ. 46) RETURN
C       DO NOTHING IF AT A MARKER OR DOT
C       First look right for H's & subscripts & eliminate them:
        INC=1
C       Increment for looking across for H & subscripts
        MBOND=0
        IF ((MM(KX+1,KY).GE.97).AND.(MM(KX+1,KY).LE.122)) INC=2
C       2 let element
        IF (MM(KX+INC,KY).NE.72) GOTO 40
        MBOND = MAX0(MOD(MM(KX+INC+1,KY),2**13),MOD(MM(KX+INC+2,KY),
     *     2**13))
C Bond on rt of H
        LBLOB=MOD(MBOND,256)
        IF (LBLOB .NE. 3 .AND. LBLOB .NE. 7) MBOND=0
        MM(KX+INC,KY)=MBOND
C       Reinstall bond
        IF ((MM(KX+INC+1,KY).LT.50).OR.(MM(KX+INC+1,KY).GT.57))
     *     GO TO 43
        CALL CURSOR(KX+INC+1,KY)
        MM(KX+INC+1,KY)=MBOND
        GOTO 43
C       Here completh undrawing H's & subscripts on right
C       Now look on left for H & subscripts:
40      MBOND=0
        DO 42 INC=-3,-1
C       Look left for H, subscript, MBOND to copy
        IF ((MM(KX-1,KY).LT.50) .OR. (MM(KX-1,KY).GT.72)) GOTO 43
        IF (MOD(MM(KX+INC,KY),2**13).GT.256)
     *      MBOND = MOD(MM(KX+INC,KY),2**13)
        IF (MM(KX+INC,KY).NE.72) GOTO 42
        LBLOB = MOD(MBOND,256)
        IF (LBLOB.NE.3 .AND. LBLOB.NE.7) MBOND=0
        MM(KX+INC,KY)=MBOND
C       Replace H with bond
C       Look for number to right of H, on left of node
        IF ((MM(KX+INC+1,KY).LT.50) .OR. (MM(KX+INC+1,KY).GT.57))
     2     GOTO 43
C       If No number, skip out of loop: done here
        MM(KX+INC+1,KY)=MBOND
42      CONTINUE
43      CONTINUE
C       At this point, filler H's are removed
C
C       Look above and below to remove H's.
        DO 50 I = -1,1,2
           FY = KY + I
           IF (MM(KX,FY).EQ.72) THEN
              MM(KX,FY) = 0
              FX = KX + 1
              IF ((MM(FX,FY).GE.50).AND.(MM(FX,FY).LE.57))
     *           MM(FX,FY) = 0
              MBOND = LMM(KX,FY+I)
              IF ((MBOND.GE.256).AND.(MOD(IDIR(MBOND),4).EQ.1))
     *           MM(KX,FY) = MBOND
           ENDIF
50      CONTINUE
        RETURN
C
        ELSE
101     IF (IDTPIX(KX-1,KY) .EQ. 46) RETURN
C       DO NOTHING IF AT A MARKER OR DOT
C       First look right for H's & subscripts & eliminate them:
        INC=1
C       Increment for looking across for H & subscripts
        MBOND=0
```

```
      IF ((IDTPIX(KX+1,KY).GE.97).AND.(IDTPIX(KX+1,KY).LE.122)) INC=2
C     2 let element
      IF (IDTPIX(KX+INC,KY).NE.72) GOTO 140
      MBOND = MAX0(MOD(IDTPIX(KX+INC+1,KY),2**13),
   *     MOD(IDTPIX(KX+INC+2,KY),2**13))
C Bond on rt of H
      LBLOB=MOD(MBOND,256)
      IF (LBLOB .NE. 3 .AND. LBLOB .NE. 7) MBOND=0
      IDTPIX(KX+INC,KY)=MBOND
C     Reinstall bond
      IF ((IDTPIX(KX+INC+1,KY).LT.50).OR.(IDTPIX(KX+INC+1,KY).GT.57))
   *     GO TO 143
      CALL CURSOR(KX+INC+1,KY)
      IDTPIX(KX+INC+1,KY)=MBOND
      GOTO 143
C     Here completh undrawing H's & subscripts on right
C     Now look on left for H & subscripts:
140   MBOND=0
      DO 142 INC=-3,-1
C     Look left for H, subscript, MBOND to copy
      IF ((IDTPIX(KX-1,KY).LT.50) .OR. (IDTPIX(KX-1,KY).GT.72))
   *     GO TO 143
      IF (MOD(IDTPIX(KX+INC,KY),2**13).GT.256)
   *      MBOND = MOD(IDTPIX(KX+INC,KY),2**13)
      IF (IDTPIX(KX+INC,KY).NE.72) GO TO 142
      LBLOB = MOD(MBOND,256)
      IF (LBLOB.NE.3 .AND. LBLOB.NE.7) MBOND=0
      IDTPIX(KX+INC,KY)=MBOND
C     Replace H with bond
C     Look for number to right of H, on left of node
      IF ((IDTPIX(KX+INC+1,KY).LT.50).OR.(IDTPIX(KX+INC+1,KY).GT.57))
   2     GO TO 143
C     If No number, skip out of loop: done here
      IDTPIX(KX+INC+1,KY) = MBOND
142   CONTINUE
C     At this point, filler H's are removed
143   CONTINUE
C
C     Look above and below to remove H's.
      DO 150 I = -1,1,2
         FY = KY + I
         IF (IDTPIX(KX,FY).EQ.72) THEN
            IDTPIX(KX,FY) = 0
            FX = KX + 1
            IF ((IDTPIX(FX,FY).GE.50).AND.(IDTPIX(FX,FY).LE.57))
   *           IDTPIX(FX,FY) = 0
            MBOND = MOD(IDTPIX(KX,FY+I),2**13)
            IF ((MBOND.GE.256).AND.(MOD(IDIR(MBOND),4).EQ.1))
   *           IDTPIX(KX,FY) = MBOND
         ENDIF
150   CONTINUE
      RETURN
      ENDIF
      END
C
C
C     VERSION 1 - JAN 15, 1985
C
C This subroutine is called by MOVEIT and MOVEFL
C It places charges in MM - (Used by RETRIEVE)
C It does not display them
C
      SUBROUTINE ZHARGE(KAR,IX,IY,NCHRG,IERR)
      IMPLICIT INTEGER*2(A-Z)
      INTEGER*4 MM
      COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /CD/ MAXX,MAXY
      COMMON /HP/IHP
      COMMON /RANGE/ LOX,HIX,LOY,HIY
C This subroutine, called when a +,-, or = sign is entered, searches for
C a diagonal location for the charge, and types it in.
      IERR=0
      IC=0
      JJJ=IX
      IF (MM(IX,IY) .EQ. 0) GO TO 430
```

```
C This should be a delocalized charge
C Search back for the node, if any:
C look for space for charge up & to the right:
      IF ((JJJ+2.GT.MAXX).OR.(IY+2*IHP.LE.0) .OR. (IY+2*IHP .GT.MAXY))
     * GO TO 431
      IF (MM(JJJ+1,IY+IHP)+MM(JJJ+2,IY+IHP)+MM(JJJ+2,IY+2*IHP)
     * +MM(JJJ+1,IY+2*IHP) .NE.0) GO TO 431
         IF (JJJ+3.LE.MAXX) THEN
            IF (MM(JJJ+3,IY+IHP).NE.0) GO TO 431
         ENDIF
         JX=JJJ+1
         JY=IY +IHP
         IF (JX.GT.HIX) HIX = JX
      IF (IHP .EQ. 1 .AND. JY .GT. HIY) HIY=JY
      IF (IHP .NE. 1 .AND. JY .LT. LOY) LOY=JY
      IC=4
      GOTO 450
C Look down & right:
431   IF ((JJJ+2.GE.MAXX).OR.(IY-2*IHP.GE.MAXY)
     * .OR. (IY-2*IHP.LE.0)) GO TO 118
      IF (MM(JJJ+1,IY-IHP)+MM(JJJ+2,IY-IHP)+MM(JJJ+2,IY-2*IHP)
     * + MM(JJJ+1,IY-2*IHP) .NE.0) GO TO 118
         IF (JJJ+3.LE.MAXX) THEN
            IF (MM(JJJ+3,IY-IHP).NE.0) GO TO 118
         ENDIF
         JX=JJJ+1
         JY=IY - IHP
         IF (JX.GT.HIX) HIX = JX
      IF (IHP .EQ. 1 .AND. JY .LT. LOY) LOY=JY
      IF (IHP .NE. 1 .AND. JY .GT. HIY) HIY=JY
         IC=13
      GOTO 450
C Look up & left:
118   IF ((JJJ-2.LE.0).OR.(IY+2*IHP.LE.0)
     * .OR. (IY+2*IHP .GT. MAXY)) GO TO 433
      IF (MM(JJJ-2,IY+IHP)+MM(JJJ-1,IY+IHP)+MM(JJJ-1,IY+2*IHP).NE.0)
     * GO TO 433
         IF (JJJ-3.GT.0) THEN
            IF (MM(JJJ-3,IY+2*IHP)+MM(JJJ-3,IY+IHP).NE.0) GO TO 433
         ENDIF
         JX=JJJ-2
         JY=IY +IHP
         IF (JX.LT.LOX) LOX = JX
      IF (IHP .EQ. 1 .AND. JY .GT. HIY) HIY=JY
      IF (IHP .NE. 1 .AND. JY .LT. LOY) LOY=JY
         IC=1
         IF (NCHRG.LE.1) JX=JX+1
         IF (NCHRG .LE.1) IC=2
      GOTO 450
C Look down and left:
433   IF ((JJJ-2.LE.0).OR.(IY-2*IHP.GT.MAXY)
     * .OR. (IY-2*IHP .LE.0)) GO TO 434
      IF (MM(JJJ-2,IY-IHP)+MM(JJJ-1,IY-IHP)+MM(JJJ-1,IY-2*IHP)
     * +MM(JJJ-2,IY-2*IHP).NE.0) GO TO 434
         IF (JJJ-3.GT.0) THEN
            IF (MM(JJJ-3,IY-IHP)+MM(JJJ-3,IY-2*IHP).NE.0) GO TO 434
         ENDIF
         JX=JJJ-2
         JY=IY -IHP
         IF (JX.LT.LOX) LOX = JX
      IF (IHP .EQ. 1 .AND. JY .LT. LOY) LOY=JY
      IF (IHP .NE. 1 .AND. JY .GT. HIY) HIY=JY
         IC=10
         IF (NCHRG.LE.1) JX=JX+1
         IF (NCHRG.LE.1) IC=11
      GOTO 450
434   IERR=1
C     No place for charge - set error return and exit
      RETURN
C     Enter charge in MM
450   MM(JX,JY)=KAR +IC * 2**13
C     STORE LOC OF CHARGE IN HIGH ORDER PART OF MM
      IF (NCHRG.LE.1) GOTO 60
      KHAR=NCHRG
      MM(JX+1,JY)=KHAR
60    RETURN
```

```
430     JJJ=IX
C       Delocalized charge--find clear area:
493     M=0
        DO 223 I=JJJ-1,JJJ+2
        DO 223 J=IY-1,IY+1
        M=M + LMM(I,J)
223     CONTINUE
        IF (M.LE.0) GOTO 432
        JJJ=JJJ+1
        IF (JJJ .GT. MAXX) GO TO 434
C       No place for charge - bail out
        GOTO 493
432     MM(JJJ,IY)=KAR
        IF (NCHRG.LE.1) GOTO 60
        KHAR=NCHRG
        MM(JJJ+1,IY)=KHAR
        GOTO 60
        END
$STORAGE:2
C       SUBROUTINE GETIT(IX,IY,LFLAG,KAR)
C
C       This subroutine will retrieve a stand alone structure
C       or a partial structure from the disk.   The position
C       of the stand alone structure can be controlled by setting
C       the cursor to the desired location of the lower left corner of
C       the structure - Partial structures are attached to the existing
C       structure at the point indicated by the cursor. If the cursor is
C       at the end of a bond, the partial structure must be placed using
C       that bond. If that can't be done, the command is aborted. If the
C       cursor is at a node, the program will try 4 orientations of the
C       partial structure around the node before aborting the command
C       Available commands are :
C               ' - retrieve
C               V - view disk structure
C               Del - delete - delete the result of the last command
C               executed (i.e. structure, marker or bond)
C               Bond - draw a bond
C               # - enter a marker
C               lc - jump to a marker
C               | - go to NUMBER ENTRY state
C               CR - return to calling state
        SUBROUTINE GETIT(IX,IY,LFLAG,KAR)
C
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,IDTPIX,CONNEC,DELET(2000),COPYB
        INTEGER*2 LIBMAX(2)
        LOGICAL*2 EXIST,PNODE,RETR,LATEH3,VNODE,DIRECT
        LOGICAL PMESS
        CHARACTER*10 FILE,LFILE
        CHARACTER*8 LIBRET,HL08
        CHARACTER*5 KSC(2),NSC,LSC
        CHARACTER*1 NSC10(10),HALO(12),HLO(3)
        CHARACTER*12 HALOE
        CHARACTER*3 HLOE
        EQUIVALENCE (HALOE,HALO(1))
        EQUIVALENCE (HLOE,HLO(1))
        CHARACTER*1 KAN
        CHARACTER*1 ISTAT
        CHARACTER*1 NAMSTR(6)
        COMMON /HP/IHP
        COMMON /LIB/ LIBRET(640),NLIBS
        COMMON /IPLUS/ IHIGH(14,2)
        COMMON /RET/ SYM,NSC(2)
        COMMON /BAKLIB/ LSC(2)
        COMMON /ISTATE/ ISTAT
        COMMON /STRDEF/ NNODE,TABLE(255,43)
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
        COMMON /LABELS/ NR,NJLAST,NJNEXT
        COMMON /HEAD/ MW(12),ISTATE,PAGE
        COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /TEMP/ LLBOND(100,5),LLABL(260,2),MCHN(260)
        COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
        COMMON /CD/ MAXX,MAXY
```

```
      COMMON /FROM/ LCHAR
      COMMON /BAD/ IBADX(9),IBADY(9)
      COMMON /LAPE/ LAP(5,2)
      COMMON /ENTRAR/ CONNEC(2001)
      COMMON /RANGE/ LOX,HIX,LOY,HIY
      COMMON /CUR/ ICUR
      COMMON /MKSKP/ ISKIP
      COMMON /PROB/ IPROB,JPROB
      COMMON /RETLIB/OVRWRT
CXT
CXT   PNODE = TRUE is passed to SUBROUTINE VLNCE when VLNCE need only
CXT   search array MM for nodal adjacency.  DELH is assigned the attached
CXT   node's hydrogen information so it can be had for any subsequent
CXT   substructure deletion.  VNODE = TRUE indicates the substructure
CXT   is being drawn by the VIEW SECTION of SUBROUTINE GETIT.
      COMMON /VALH/ PNODE,DELH(2,3),VNODE
CXT
CXT   RETR = TRUE for calls in which SUBROUTINE REPLCE must deal with
CXT   both array MM and IDTPIX.
      COMMON /RETDRW/ RETR
      EQUIVALENCE (FILE,NSC),(NSC,NSC10),(CONNEC(2001),DELET(1))
      DIMENSION THETA(8,8)
      DATA THETA /-1,-1,2,-1,1,-1,4,-1,
     2            -1,-1,-1,1,-1,5,-1,3,
     3            2,-1,-1,-1,4,-1,3,-1,
     4            -1,1,-1,-1,-1,3,-1,5,
     5            1,-1,4,-1,-1,-1,2,-1,
     6            -1,5,-1,3,-1,-1,-1,1,
     7            4,-1,3,-1,2,-1,-1,-1,
     8            -1,3,-1,5,-1,1,-1,-1/
      DATA READS /0/, APOS /39/, IU /1/, LFILE /'          '/
C**********************************************************************
C
C     This section sets some parameters - clears the arrays IDTPIX
C     and LLBOND clears possible text from the screen and calls HEADER
C     The parameters MODE, ISTAT, and ISTATE are used by HEADER
C     LCHAR = indicates if we came from CHAIN or RING - It is used
C     to determine if we should return to CHAIN or RING instead
C     of GROUND
C     NODE will indicate whether we are at a marker or a bond or neither
C     It is used when we are trying to attach to an existing structure
C     IFLIP and IROT are used to indicate the rotation or reflection
C     operators needed
C**********************************************************************
      IF (NLIBS.EQ.0) THEN
         CALL MYERR(27,27,27)
         GO TO 6777
      ENDIF
      HALO(1) = KAN
      HALO(12) = KAN
      HLO(1) = KAN
      HLO(3) = KAN
      VNODE = .FALSE.
      ALONE = 0
      ISKIP = 1
      KCHAR = LCHAR
      COPY = 0
      XCHAR = 1
      KCHAR=LCHAR
      OCHAR=0
C     Parameter which decides when to use default origin for stand
C     alone structure
      CALL CLRPIX(2)
C     Clear IDTPIX and LLBOND
122   NODE=-1
      ISTAT=':'
      SYM = 1
C Default symmetry = 1 = axial
      MW(7)=999
C Force new heading
      MW(8)=999
      MW(9)=999
      ISTATE=12
      CALL HEADER
```

```
      IF (((FILE.NE.LFILE).OR.(OVRWRT)) .AND.(FILE.NE.'          '))
     1   THEN
      OVRWRT=.FALSE.
         DIRECT = .TRUE.
         KSC(1) = LSC(1)
         KSC(2) = LSC(2)

         DO 222 I = 1,10
            HALO(I+1) = NSC10(I)
222      CONTINUE
         GO TO 8737
      ELSE
         DIRECT = .FALSE.
      ENDIF
C Go get first file name - then await next command
C*****************************************************************
C       This section reads the next command - clears some screen dialog
C       decodes the command and goes to the appropriate section to execute
C       the command - If an invalid command is given, an error message
C       will be given and the program will wait for a valid command
C*****************************************************************
305   CONTINUE
      IF (JPROB.NE.0) GO TO 6777
      IERR = 0
      ICUR = 1
      CALL CURSOR(IX,IY)
      CALL INPUTX(KKAR,IX,IY)
      IF (KKAR.EQ.58) THEN
         IERR = 39
         CALL MYERR(IERR,IERR,IERR)
         GO TO 305
      ENDIF
      IF (KKAR.NE.127) XCHAR = 1
C
C Read command
C
C Dumb mode
      IF ((KKAR.EQ.21) .OR. (KKAR .EQ. 32) .OR. (KKAR .EQ.8)) THEN
         GO TO 4911
C Delete structure
      ELSE IF (KKAR .EQ. 127) THEN
         GO TO 650
C ' - Retrieve next structure
      ELSE IF (KKAR.EQ.39) THEN
         IF (FILE.EQ.'          ') THEN
            IERR = 58
            CALL MYERR(IERR,IERR,IERR)
            GO TO 305
         ELSE
            GO TO 87
         ENDIF
C Bond command
      ELSE IF (KKAR.GE.22 .AND. KKAR.LE.31) THEN
      COPY=0
         GO TO 793
C Enter marker command or set new enlargement factor
      ELSE IF (KKAR .EQ. 35 .OR. KKAR.EQ.38) THEN
      IF (KKAR .EQ. 35) COPY =0
         GO TO 793
C Jump to marker
      ELSE IF (KKAR.GE.97 .AND. KKAR.LE.122) THEN
         GO TO 793
C Charge (+,- or =)
      ELSE IF ((KKAR.EQ.43).OR.(KKAR.EQ.45).OR.(KKAR.EQ.61)) THEN
      COPY=0
         GO TO 793
C Set symmetry to axial
      ELSE IF (KKAR .EQ. 65) THEN
         GO TO 955
C Set symmetry to point symmetry
      ELSE IF (KKAR .EQ. 80) THEN
         GO TO 966
C Get file name
      ELSE IF (KKAR .EQ. 70) THEN
         GO TO 4923
```

```
C VIEW structure
        ELSE IF (KKAR .EQ. 86) THEN
           GO TO  4949
C Return or Quit
        ELSE IF (KKAR .EQ. 13 .OR. KKAR .EQ. 81) THEN
           GO TO 6777
C Set new bond type
        ELSE IF (KKAR.EQ.124) THEN
           GO TO 3561
        ENDIF
C LIST substructures
        IF (KKAR.NE.76) GO TO 202
201        CALL SETSCR(1)
        IF (IHP .EQ. 1) THEN
        CALL CLEAR
        CALL GRAOFF
        ENDIF
           PAGE = 1
           CALL DISPLA(1)
           CALL FTSIZE(1,10)
           IF (NLIBS.GT.320) THEN
              LIBMAX(1) = 320
              LIBMAX(2) = NLIBS - 320
              SCROLL = 2
           ELSE
              LIBMAX(1) = NLIBS
              SCROLL = 1
           ENDIF
          DO 3040 I = 1,SCROLL
              FX = 1
              FY = 1
              DO 3030 J = 1,LIBMAX(I)
                 CALL FTLOCA(FY,FX)
                 HL08 = LIBRET(J+((SCROLL-1)*320))
                 CALL FTEXT(HL08)
                 IF (FX.GE.71) THEN
                    FY = FY + 1
                    FX = 1
                 ELSE
                    FX = FX + 7
                 ENDIF
3030          CONTINUE
              CALL FTSIZE(2,18)
              FY = FY + 2
              CALL FTLOCA(FY,1)
              CALL FTEXT('^Press RETURN to continue^')
              CALL FTSIZE(1,10)
              KKAR = GETCHR()
              CALL SETCOL(0)
              CALL CLR
              CALL SETCOL(1)
3040       CONTINUE
           CALL SETSCR(2)
           PAGE = 2
           CALL DISPLA(2)
        DO 7932 I=1,12
        MW(I)=999          !Force tidy call to Header
7932    CONTINUE
        CALL HEADER
           GO TO 305
202     CONTINUE
        IF (KKAR.EQ.131) GO TO 305
        CALL FTSIZE(2,18)
        CALL FTLOCA(4,1)
        CALL FTEXT('^Invalid response: ^')
        HLO(2) = CHAR(KKAR)
        CALL FTEXT(HLOE)
        PAGE = 0
        CALL FTSIZE(1,10)
C Return to GROUND
        GO TO 305
```

```
C***********************************************************************
C       This section will (VIEW) display the last structure read into
C       memory - that is the structure whose file name was last entered
C       The view is terminated by the input of any character - At that
C       point the screen is cleared and the original structure is restored
C       to the screen and to the MM array.
C***********************************************************************
C If the picture is in MM - copy it to IDTPIX
4949    IF (COPY .EQ. 0) CALL SHIF(1,MC,LC)
        COPY = 1
C Copy = 1 implies current picture is in IDTPIX
        ICUR = 0
        SIX=IX  !Save cursor values
        SIY=IY
        CALL CURSOR(IX,IY)
        CALL SETCOL(0)
        CALL CLR
        CALL SETCOL(1)
        VLOX = LOX
        VHIX = HIX
        VLOY = LOY
        VHIY = HIY
        LOX = 1
        HIX = MAXX
        LOY = 1
        HIY = MAXY
        CALL CLRPIX(1)
C Clear MM and LNGBND
        IROT=1
        DX=0
        DY=0
C Set origin to default
        CALL MOVEIT(DX,DY,LENP,LENM,LLLEN,LENC,LEND,ABX,ABY,IROT,IERR)
C Move picture from CONNEC to MM with translation
        IF (DOT .EQ. 1) GO TO 5512
C Skip VLNCE if we have a call to DOTDIS
C       Fill in valence hydrogens
        PNODE = .TRUE.
        VNODE = .TRUE.
        IERR=0
        DO 5910 I = LOX,HIX
        DO 5910 J = LOY,HIY
        II=I
        JJ=J
        IF (MM(I,J) .GE. 65 .AND. MM(I,J) .LE. 90
     1  .AND. (MM(I,J) .NE. 72 .OR. (MM(I,J) .EQ. 72
     2  .AND. MM(I+1,J) .GE. 97 .AND. MM(I+1,J) .LE. 122)))
     3  CALL VLNCE(2,II,JJ,0,0,IERR)
        IF (IERR.EQ.12) IERR = 0
        IF (IERR .NE. 0) GO TO 5512
5910    CONTINUE
        ISWIT = 1
C Call STRDRW with markers displayed as markers
        LBLEN=LLLEN
        CALL STRDRW(ISWIT)
5512    PNODE = .FALSE.
        VNODE = .FALSE.
C View (display) the structure
        CALL FTSIZE(2,18)
        IF (JPROB.EQ.0) THEN
        IF (IHP .EQ.1) CALL CLEAR
            CALL FTLOCA(1,1)
            CALL FTEXT('^VIEW of ^')
            CALL FTEXT(HALOE)
            CALL FTEXT('^ - Enter RETURN to end VIEW^')
            PAGE = 0
            CALL FTSIZE(1,10)
            CALL INPUTX(KKAR,IX,IY)
C Await terminator character
            CALL SETCOL(0)
            CALL CLR
            CALL SETCOL(1)
        ENDIF
        ICUR = 1
        CALL CURSOR(IX,IY)
```

```
C Clear screen
      CALL SHIF(2,MC,LC)
      LOX = VLOX
      HIX = VHIX
      LOY = VLOY
      HIY = VHIY
      LBLEN=LC
      NJNEXT=MC
      ISWIT=1
      CALL STRDRW(ISWIT)
      DO 6565 I=1,12
C Force tidy call to header
         MW(I)=999
6565  CONTINUE
      CALL HEADER
      IF (IHP .EQ. 1)THEN
      IX=SIX
      IY=SIY
      ENDIF
      GO TO 305
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
C     This section accesses DUMB MODE.
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
4911  CONTINUE
         CALL SPACE(IX,IY)
         JCHAR = 2
         MCHAR = 0
         ISTATE = 12
         ISTAT = ':'
      COPY=0
         CALL HEADER
      GO TO 305
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
C     This section reserves a channel - sets some graphic switches
C     requests the file name - concatenates the extension .LIB
C     to the file name - senses the current cursor location
C     and uses that as the lower left corner of the display if the
C     structure to be retrieved is a stand alone structure
C     A file name = CR causes a return to the calling program
C     to be used again.
C     If the requested file does not exist, an error message
C     is issued and another file name is requested.
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
C
C     THIS SECTION RETRIEVES A STRUCTURE FROM THE LIBRARY
C
4923  CONTINUE
      CALL SETSCR(1)
      PAGE = 1
      CALL DISPLA(1)
      CALL FTSIZE(2,18)
4924  READS = READS + 1
C Request file name
520   CONTINUE
C
      FY = 9
      FYY = 7
      LSC(1) = NSC(1)
      LSC(2) = NSC(2)
      LFILE = FILE
565   CONTINUE
      FILE = '      '
      CALL FTLOCA(8,28)
      CALL FTEXT('^Enter 1 to 6 character file name^')
      IF (READS.GE.2) THEN
         CALL FTLOCA(9,28)
         CALL FTEXT('^or '' for previous file^')
         FY = 10
      ENDIF
C Read file name
      IF (IHP .EQ. 1) THEN
      CALL ALPCUR
      ACCEPT 691,(NAMSTR(I),I=1,6)
691   FORMAT(6A1)
      ENDIF
```

```
        CALL FTLOCA(FY,FX)
        J = 0
        DO 4445 I = 1,60
           J = J + 1
           FX = 27 + J
 1445      CONTINUE
        IF (IHP .EQ. 1) THEN
        A=ICHAR(NAMSTR(J))
        IF (A .GE. 97) A=A-32
        ELSE
           A = GETCHR()
        ENDIF
           IF (A.EQ.APOS) THEN
              IF (READS.LT.2) THEN
                 CALL FTLOCA(FYY,28)
                 CALL FTEXT('^No previous files input^')
                 GO TO 565
              ENDIF
              NSC10(1) = CHAR(A)
              HLO(2) = CHAR(A)
                IF (IHP .NE. 1) THEN
              CALL FTLOCA(FY,28)
              CALL FTEXT(HLOE)
                ENDIF
              GO TO 4447
           ENDIF
           IF (A.EQ.8) THEN
              IF (J.GT.1) J = J - 1
              FX = 27 + J
              CALL FTLOCA(FY,FX)
              CALL FTEXT('^ ^')
              NSC10(J) = ' '
              GO TO 1445
           ENDIF
           HLO(2) = CHAR(A)
        IF (IHP .NE. 1) THEN
           CALL FTLOCA(FY,FX)
           CALL FTEXT(HLOE)
        ENDIF
           IF (((A.GE.48).AND.(A.LE.57)).OR.((A.GE.65).AND.
     *        (A.LE.90)).OR.((A.GE.97).AND.(A.LE.122)).OR.
     *        ((A.EQ.34).AND.(I.EQ.1))) THEN
              NSC10(J) = CHAR(A)
           ELSE IF (A.EQ.13 .OR. A .EQ. 32) THEN
              GO TO 4447
           ELSE
              NSC10(J) = ' '
           ENDIF
           IF (J.EQ.6) GO TO 4447
 4445   CONTINUE
 4447   CONTINUE
        IF (IHP .EQ. 1) THEN
        CALL LINE4
        CALL ACLEAR
        ELSE
        CALL SETCOL(0)
        CALL CLR
        CALL SETCOL(1)
        ENDIF
        IF (NSC(1) .EQ. '     ') THEN
           CALL SETSCR(2)
           PAGE = 2
           CALL DISPLA(2)
           CALL FTSIZE(1,10)
           FILE = LFILE
           READS = READS - 1
           GO TO 305
        ELSE IF (NSC10(1).EQ.CHAR(APOS)) THEN
           IF (KSC(1).NE.'     ') THEN
              NSC(1) = KSC(1)
              NSC(2) = KSC(2)
           ELSE
              NSC(1) = LSC(1)
              NSC(2) = LSC(2)
           ENDIF
```

```
      ELSE
C     CONCATENATE .LIB EXTENSION TO FILE NAME
         NSC10(7) = '.'
         NSC10(8) = 'S'
         NSC10(9) = 'T'
         NSC10(10) = 'R'
      ENDIF
      KSC(1) = LSC(1)
      KSC(2) = LSC(2)
      DO 8334 I = 1,10
         HALO(I+1) = NSC10(I)
8334  CONTINUE
      CALL FTLOCA(7,28)
      CALL FTEXT('^Input from file: ^')
      CALL FTEXT(HALOE)
      CALL FTLOCA(8,28)
      CALL FTEXT('^Press RETURN to clear screen^')
      A = GETCHR()
      IF (IHP .EQ. 1) THEN
      CALL LINE4
      CALL ACLEAR
      ELSE
      CALL SETCOL(0)
      CALL CLR
      CALL SETCOL(1)
      ENDIF
8737  INQUIRE(FILE=FILE,EXIST=EXIST)
      IF (.NOT.EXIST) THEN
         IF (DIRECT) THEN
            CALL SETSCR(1)
            PAGE = 1
            CALL DISPLA(1)
            CALL FTSIZE(2,18)
            DIRECT = .FALSE.
         ENDIF
         CALL FTLOCA(6,28)
         CALL FTEXT('^File doesn''t exist/file empty - ^')
         CALL FTLOCA(7,28)
         CALL FTEXT('^Try another name or CR to recover^')
         FY = 9
         FYY = 10
         GO TO 565
      ENDIF
507   OPEN(IU,FILE=FILE,STATUS='OLD')
      IF (.NOT.DIRECT) THEN
         CALL SETSCR(2)
         PAGE = 2
         CALL DISPLA(2)
         CALL FTSIZE(1,10)
      ELSE
         READS = READS + 1
      ENDIF
      ICUR = 1
      CALL CURSOR(IX,IY)
      CALL HEADER
C*****************************************************************************
12    READ (IU,100,END=5777,ERR=5776) ABX,ABY,BDIR,BLEN,DOT,LBX,LBY
C     ABX ABY = coordinates of attaching bond
C     BDIR = attaching bond direction
C     BLEN = attaching bond length
C     LBX LBY = coordinates for final cursor position
100   FORMAT(7I4)
      READ(IU,100,END=5777,ERR=5776) LENP
C     LENP = # of cells used in MM
      IF (LENP .EQ. 0) GO TO 5776
      IF (3*LENP .GT. 2000) GO TO 999
C     We will be using CONNEC array temporarily to store X's, Y's, contents
C     marker coordinates and long bond info
C     This is a bounds check for CONNEC
      J=1
C     Read structure into CONNEC
      DO 51 I=1,LENP
      READ(IU,400,END=5777,ERR=5776) CONNEC(J),CONNEC(J+1),CONNEC(J+2)
C     Read X, Y and MM(X,Y)
      J=J+3
```

```
51      CONTINUE
        READ (IU,100,END=5777,ERR=5776) LENM
C       LENM = # of markers in structure
        IF (LENM .EQ. 0) GO TO 54
        IF (3*(LENM+LENP) .GT. 2000) GO TO 999
C       Bounds check
        DO 52 I=1,LENM
400     FORMAT(2I4,I10)
        READ(IU,100,END=5777,ERR=5776) CONNEC(J),CONNEC(J+1),CONNEC(J+2)
C       Read coordinates of marker and type of marker (chain or non chain)
        J=J+3
52      CONTINUE
54      READ (IU,100,END=5777,ERR=5776) LLLEN
C       LLLEN = # of long bonds
        IF (LLLEN .EQ. 0) GO TO 5666
        IF ((3*(LENP+LENM)+5*LLLEN) .GT. 2000) GO TO 999
        DO 57 I=1,LLLEN
        READ (IU,100,END=5777,ERR=5776) (CONNEC(J+K),K=0,4)
C       Read initial and final coordinates of long bond and bond type
        J=J+5
57      CONTINUE
C       LENC = # of charges
5666    READ(IU,100,END=5777,ERR=5776) LENC
        IF (LENC.EQ.0) GO TO 5611
        IF ((3*(LENP+LENM) + 5 * LLLEN + 4 * LENC).GT.2000) GO TO 999
        DO 5577 I = 1,LENC
           READ(IU,100,END=5777,ERR=5776) (CONNEC(J+K),K=0,3)
           J = J + 4
5577    CONTINUE
5611    CONTINUE
        READ(IU,100,END=5777,ERR=5776) LEND
        IF (LEND.EQ.0) GO TO 56
           IF ((3*(LENP+LENM)+5*LLLEN+4*LENC+2*LEND).GT.2000) GO TO 999
           DO 5612 I = 1,LEND
              READ(IU,100,END=5777,ERR=5776) CONNEC(J),CONNEC(J+1)
              J = J + 2
5612       CONTINUE
        GO TO 56
5776    CONTINUE
        CLOSE(IU)
        CALL FTSIZE(2,18)
        CALL FTLOCA(1,1)
        CALL FTEXT('^INPUT FILE DATA FORMAT ERROR ENCOUNTERED^')
        PAGE = 0
        CALL FTSIZE(1,10)
        GO TO 305
5777    CONTINUE
        CLOSE(IU)
        CALL FTSIZE(2,18)
        CALL FTLOCA(1,1)
        CALL FTEXT('^ERROR - END OF INPUT FILE ENCOUNTERED^')
        PAGE = 0
        CALL FTSIZE(1,10)
        GO TO 305
56      CLOSE(IU)
C       Close file
        DIRECT = .FALSE.
        GO TO 305
C Get next command
C*********************************************************************
C       Start of RETRIEVE code - Clear dialog - Save coordinates -
C       Set parameters
C*********************************************************************
87      CONTINUE
        LX=IX
C Save these coordinates in case we do a RETRIEVE followed
C by a DELETE - We will then reset the cursor to these coordinates
        LY=IY
        IROT=1
C Set rotation angle to a default of 0
        IFLIP=-1
C Set reflection code to default value 0 = equals no reflection
```

```
C*********************************************************************
C       This section shifts the current MM array to IDTPIX.
C       It also moves the marker array LABL to LLABL and
C       the long bond array LNGBND to LLBOND.
C       MC = count of markers moved.
C       LC = count of long bonds moved.
C       It also does a bounds check on the marker and long bond arrays.
C       It also determines whether we are dealing with a stand alone
C       structure (ABX and ABY = 0) or an attaching structure.
C*********************************************************************
        CALL SHIF(1,MC,LC)
        COPY = 1
        IF ((MC+LENM) .GT. 260 .OR. (LLLEN+LC) .GT. 100) GO TO 333
C       Bail out - We have too many markers or longbonds
C       This section determines whether we are dealing with a standalone
C       or attaching structure. If the cursor is at a 3X3 clear area
C       (node=-2) we have as standalone.
C       Node = -1 = error - not at bond, node or empty space
C       Node = 1 = attach group to node
C       Node = 0 = attach group to bond
C*********************************************************************
        ICUR = 0
        PNODE = .FALSE.
        FIX=IX
C       Save current cursor position because MAP could alter IX if we are
C       at a non marker node
        FIY=IY
        CALL MAP(IX,IY,NODE,OBDIR)
        IF (NODE.EQ.-2) GO TO 200
        IF (BLEN.EQ.0) GO TO 200
        IF (DOT.EQ.1) GO TO 200
        IF (NODE .NE. -1) GO TO 71
        IERR = 48
C       We are not at a marker or bond - can't attach here
        CALL MYERR(IERR,KAR,KAR)
C       Issue error message
        IX=FIX
C       Restore IX and IY
        IY=FIY
        CALL SHIF(2,MC,LC)
C       Shift old picture back to MM etc.
        COPY = 0
        GO TO 305
C       Go await new command
71      IF(NODE .EQ. 1) GO TO 711
C       If NODE = 1 go to node code
C*********************************************************************
C       This section tries to attach a structure to a pointer bond
C       It determines the direction of the dangling bond on the
C       structure on disk - If the bond directions match (i.e.
C       ABS(difference in bond directions) = 4 no rotation or reflection
C       is needed - If the difference in bond directions is odd, we can
C       not attach this group to the pointer bond, for only reflections
C       around the X and Y axes and rotations of 90, 180, and 270 degrees
C       are allowed. If the difference in bond directions is even, we
C       determine the transformation necessary. We prefer to do reflections
C       because they tend to result in fewer distorted nodes.
C       After the transformation has been performed and the picture has
C       been moved into MM, we check for collisions and for nodes that
C       have been distorted. If no collisions occur and all distorted
C       nodes can be corrected, we go to 240 to display the structure.
C       If collisions occur or distorted nodes cannot be corrected, we
C       issue an appropriate error message, restore the old picture and
C       await entry of a new command
C
C*********************************************************************
        KX=IX
        KY=IY
        PX = IX
        PY = IY
C       Get delta values for current bond
        CALL DELTA(OBDIR,INCX,INCY)
        KX=KX-INCX
        KY=KY-INCY
        IVAL=LMM(KX,KY)
        OBTYPE=IVAL/256
```

```
C       Bond type of current bond
        DO 601 I=1,MAXX
        OBLEN = I
        KX=KX-INCX
        KY=KY-INCY
        IF (LMM(KX,KY) .NE. IVAL) GO TO 602
        IF ((KX.GE.MAXX-1).OR.(KX.LE.1).OR.(KY.GE.MAXY-1).OR.(KY.LE.1))
     *     GO TO 602
601     CONTINUE
602     CONTINUE
C       OBLEN = length of bond of currently displayed structure
        DIFF = OBLEN - BLEN
C       SUB is used to calculate translation value
        PIX=KX
        PIY=KY
CXT     Use in program until VALENCED node attached end nodes are approved.
        IF (MM(PIX,PIY).NE.46) THEN
           IERR = 57
           CALL MYERR(IERR,KAR,MAR)
C          Shift old picture back to MM etc.
           IX = FIX
           IY = FIY
           CALL CURSOR(IX,IY)
           CALL SHIF(2,MC,LC)
           COPY = 0
           GO TO 305
        ENDIF
        OBX=KX+INCX
C       X coordinate for start of old bond
        OBY=KY+INCY
C       Y coordinate for start of old bond
C       Get dangling bond
        ADIR=BDIR
C       BDIR = Bond direction of stored dangling bond
        IF (IABS(BDIR-OBDIR) .EQ. 4) GO TO 78
C       Attaching bond in correct direction - No transformation other
C       than translation needed
        IF (MOD(IABS(BDIR-OBDIR),2) .EQ. 0) GO TO 79
C       Acceptable bond but transformation + translation needed
C
C       We can't attach to this bond
C       Issue an error message - shift the old picture back to MM
C       Abort command and await new command
C
        IERR = 43
C       Bad attaching bond - Bail out
        CALL MYERR(IERR,KAR,KAR)
        CALL SHIF(2,MC,LC)
        COPY = 0
        GO TO 305
C       Abort command and await new command
C
C       Determine what transformation is needed
79      NBOND=OBDIR+4
C       NBOND = dir of needed attaching bond
        IF (NBOND .GT. 8) NBOND=NBOND-8
        IF (SYM.EQ.1) GO TO 8633
        DO 862  I=1,8
        II = I
C       Calculate the rotation needed to make attaching bond right
        ADIR=ADIR+1
        IF (ADIR .GT. 8) ADIR=ADIR-8
        IF (ADIR .EQ. NBOND) GO TO 863
862     CONTINUE
863     IROT= (II / 2) + 1
        IF (IROT.EQ.2) THEN
           IROT = 4
        ELSE IF (IROT.EQ.4) THEN
           IROT = 2
        ENDIF
        IF (IROT.EQ.5) IROT = 1
C
C
C       If no rotation is needed (IROT=1) or bond direction is odd
C       and rotation is not 180  go to 78
```

```
      IF (SYM .EQ. 2) GO TO 78
C     If symmetry is point - skip next section
C     Determine needed reflection
8633  CONTINUE
      IFLIP = THETA(BDIR,NBOND)
      IF (IFLIP.EQ.2) THEN
         IFLIP = 4
      ELSE IF (IFLIP.EQ.4) THEN
         IFLIP = 2
      ENDIF
C
C     Calculate translation values
C
78    CALL DELTA(OBDIR,KNCX,KNCY)
      OX = ABX + BLEN*KNCX
      OY = ABY + BLEN*KNCY
      DX=OX-IX
      DY=OY-IY
C     Move picture into MM after performing necessary transformations
C
      CALL CLRPIX(1)
      IF ((IFLIP.EQ.-1).AND.(SYM.EQ.1)) IROT = 1
     IF ((SYM.EQ.1).AND.(IFLIP.NE.-1))
    1 CALL MOVEFL(DX,DY,LENP,LENM,LLLEN,LENC,LEND,ABX,ABY,IFLIP,IERR)
C     Move picture from CONNEC to MM with translation and reflection
      IF ((SYM.EQ.2).OR.((SYM.EQ.1).AND.(IFLIP.EQ.-1)))
    * CALL MOVEIT(DX,DY,LENP,LENM,LLLEN,LENC,LEND,ABX,ABY,IROT,IERR)
C     Move picture from CONNEC to MM with translation to new origin
C
C     If IERR=1 we have a bounds problem and we will go to 546
      IF (IERR.NE.0) GO TO 546
C
C     Erase the old bond in IDTPIX
C     Erase the old bond from the screen
C     Copy the new bond into MM
      COPYB=MM(ABX-DX,ABY-DY)
      LE = 0
      DO 605 I=1,OBLEN+1
         MX = OBX + (I-1)*INCX
         MY = OBY + (I-1)*INCY
         IF (IDTPIX(MX,MY).EQ.0) GO TO 605
         IF (MOD(IDTPIX(MX,MY),2**13).LT.256) GO TO 805
         LE = I
C        Erase old bond in IDTPIX
         IDTPIX(MX,MY)=0
         MM(MX,MY)=COPYB
605   CONTINUE
805   CONTINUE
      IF (DIFF.LT.0) THEN
C     Erase excess bond if bond on disk was longer than bond on screen
         IEND=-DIFF
         DO 123 I=1,IEND
            MX=OBX-(I*INCX)
            MY=OBY-(I*INCY)
            IF (MM(MX,MY).GT.256) MM(MX,MY)=0
123      CONTINUE
      ENDIF
      IF (OBLEN.LT.BLEN) THEN
         MX = PX - (OBLEN*INCX)
         MY = PY - (OBLEN*INCY)
      ELSE
         MX = ABX - DX
         MY = ABY - DY
      ENDIF
      DO 504 I = 1,LE
         MX = MX + INCX
         MY = MY + INCY
         IF (LMM(MX,MY).LT.256) THEN
            FX = MX
            FY = MY
            MX = MX - INCX
            MY = MY - INCY
            GO TO 515
         ENDIF
504   CONTINUE
      FX = MX + INCX
```

```
      FY = MY + INCY
515   CONTINUE
      IBDIR = OBDIR + 4
      IF (IBDIR.GT.8) IBDIR = IBDIR - 8
      IBTYPE = 0
      MBTYPE = COPYB / 256
      LNCX = -1 * INCX
      LNCY = -1 * INCY
      RETR = .TRUE.
      CALL REDRAW(MX,MY,LNCX,LNCY,MBTYPE)
      IBTYPE = 1
      IF (IABS(INCX*INCY).EQ.0) THEN
         IF (IDTPIX(MX,MY).EQ.0) THEN
            CALL FTLOCA(MY,MX)
            CALL FTEXT('^ ^')
         ELSE
            CALL REPLCE(MX,MY,0,0,0,0,0)
         ENDIF
         IF (IDTPIX(FX,FY).EQ.0) THEN
            CALL FTLOCA(FY,FX)
            CALL FTEXT('^ ^')
          ELSE
             CALL REPLCE(FX,FY,0,0,0,0,0)
          ENDIF
       ELSE
          LATEH3 = .FALSE.
          DO 607 JY = MY,FY,INCY
             DO 606 J = -3,4
                IF ((J.EQ.0).AND.(JY.NE.MY).AND.(JY.NE.FY))
     *             GO TO 606
                JX = MX + J
                IF ((IDTPIX(JX,JY).EQ.0).AND.(MM(JX,JY).NE.0)) THEN
                   CALL FTLOCA(JY,JX)
                   CALL FTEXT('^ ^')
                   IF (MOD((JY*10),40).EQ.0) THEN
                      IF ((JY.EQ.8).OR.(JY.EQ.28).OR.(JY.EQ.16)) THEN
                         FYY = ((JY * 10) / 11) + 1
                         CALL FTSIZE(1,11)
                      ELSE
                         FYY = ((JY * 10) / 9) + 1
                         CALL FTSIZE(1,9)
                      ENDIF
                   ELSE
                      FYY = ((JY * 10) / 8) + 1
                      CALL FTSIZE(1,8)
                   ENDIF
       IF (IHP .EQ. 1) FYY=JY
                   CALL FTLOCA(FYY,JX)
                   CALL FTEXT('^ ^')
                   CALL FTSIZE(1,10)
                ELSE IF (IDTPIX(JX,JY).NE.0) THEN
                   CALL REPLCE(JX,JY,0,0,0,0,0)
                   IF (LATEH3) MM(JX-1,JY) = 0
                   IF (((IDTPIX(JX+1,JY).LT.50).OR.(IDTPIX(JX+1,JY)
     *               .GT.57)).OR.(JX+1.GT.MX+3)) THEN
                      LATEH3 = .FALSE.
                   ELSE
                      MM(JX,JY) = IDTPIX(JX,JY)
                      LATEH3 = .TRUE.
                   ENDIF
                ENDIF
606          CONTINUE
             MX = MX + INCX
607       CONTINUE
      ENDIF
      RETR = .FALSE.
      IF ((MBTYPE.EQ.6).OR.(MBTYPE.EQ.7)) THEN
          IF (((BDIR.EQ.3).AND.((OBDIR.EQ.3).OR.(OBDIR.EQ.5))).OR.
     *       (BDIR.EQ.2).OR.(BDIR.EQ.4).OR.((BDIR.EQ.5).AND.
     *       ((OBDIR.EQ.5).OR.(OBDIR.EQ.7).OR.(OBDIR.EQ.3)))) THEN
             IF (MBTYPE.EQ.6) THEN
                MBTYPE = 7
             ELSE
                MBTYPE = 6
             ENDIF
             COPYB = MBTYPE * 256 + OBDIR
```

```
            ENDIF
            IF (((BDIR.EQ.1).AND.((OBDIR.EQ.7).OR.(OBDIR.EQ.1)))
     *         .OR.((BDIR.EQ.5).AND.(OBDIR.EQ.7))
     *         .OR.((BDIR.EQ.7).AND.((OBDIR.EQ.1).OR.(OBDIR.EQ.7)))
     *         .OR.(((BDIR.EQ.2).OR.(BDIR.EQ.4)).AND.((OBDIR.EQ.6).OR.
     *         (OBDIR.EQ.8)))
     *         .OR.((BDIR.EQ.6).AND.((OBDIR.EQ.6).OR.(OBDIR.EQ.8)))
     *         .OR.((BDIR.EQ.8).AND.((OBDIR.EQ.6).OR.(OBDIR.EQ.8))))
     *          THEN
               CBDIR = OBDIR + 4
               IF (CBDIR.GT.8) CBDIR = CBDIR - 8
               IF (MBTYPE.EQ.6) THEN
                  COPYB = 7 * 256 + CBDIR
               ELSE
                  COPYB = 6 * 256 + CBDIR
               ENDIF
            ENDIF
         ENDIF
         DO 609 I = 1,LE
            MX = PX - I*INCX
            MY = PY - I*INCY
            IF (MM(MX,MY).GT.0) GO TO 610
            MM(MX,MY) = COPYB
609      CONTINUE
610      CONTINUE
C
C        See if there are collisions between the new group and old
C        structure
C        Erase excess bond if bond on disk was longer than bond on screen
1234     CALL FIXUP(IERR)
C Fix up any bad node caused by rotations and reflections
         IF (IERR .EQ. 0 ) GO TO 2401
C If FIXUP OK -then go add valence hydrogens
2403     IERR=17
C We have a distorted node problem - bail out
         GO TO 173
C
C        Fill in valence hydrogens
2401     ierr=0
         DO 2402 I = LOX,HIX
         DO 2402 J = LOY,HIY
         ii=i
         jj=j
         LL = LMM(I,J)
         IF ((LL.EQ.46).OR.((LL.GE.65).AND.(LL.LE.90)).OR.
     *      ((LL.GE.95).AND.(LL.LE.122)).OR.((LL.GE.50).AND.
     *      (LL.LE.57).AND.(MM(I-1,TY).EQ.72))) THEN
            DO 1012 X = -1,1
               MX = I + X
               IF ((MX.LE.0).OR.(MX.GT.MAXX)) GO TO 1012
               DO 1122 Y = -1,1
                  MY = J + Y
                  IF ((MY.LE.0).OR.(MY.GT.MAXY)) GO TO 1122
                  L = MOD(IDTPIX(MX,MY),2**13)
                  IF ((L.EQ.0).OR.(L.GE.256)) GO TO 1122
                  IF ((L.EQ.34).OR.(L.EQ.43).OR.(L.EQ.45).OR.
     *               (((L.GE.50).AND.(L.LE.57)).AND.((MOD(IDTPIX(MX-1,
     *               MY),2**13).EQ.43).OR.(MOD(IDTPIX(MX-1,MY),2**13)
     *               .EQ.45).OR.((IABS(X+Y).NE.1).AND.(IDTPIX(MX-1,MY)
     *               .EQ.72))).AND.(MX-1.GT.0))) GO TO 1122
                     IERR = 48
                     GO TO 5663
1122              CONTINUE
1012           CONTINUE
               if ((MM(I,J).EQ.46).OR.(mm(i,j).ge.65.and.mm(i,j).le.90
     1         .and. (mm(i,j).ne.72 .or. (mm(i,j).eq.72
     2         .and. mm(i+1,j).ge.97 .and. mm(i+1,j).le.122)))
     3         call vlnce(2,ii,jj,0,0,ierr)
          ENDIF
5663      IF (IERR.EQ.12) THEN
             IERR = 0
             EX = II
             EY = JJ
          ELSE if (ierr .ne. 0) THEN
             DO 2705 L = 1,260
```

```
            IF (LABL(L,1).EQ.0) THEN
               LOW =  L - LENM
               DO 2703 LL = LOW,L-1
                  LABL(LL,1) = 0
                  LABL(LL,2) = 0
 2703          CONTINUE
               GO TO 546
            ENDIF
 2705    CONTINUE
         GO TO 546
      ENDIF
 2402 continue
C     See if there are collisions between the new group and the old
C     structure.
      LAP(1,1)=PIX
      LAP(1,2)=PIY
      LCNT=1
      CALL CURSOR(LOX,LOY)
      DO 710 I = LOX,HIX
      DO 710 J = LOY,HIY
      II = I
      JJ = J
      IF (MM(I,J).EQ.0) GO TO 710
      IF ((I.EQ.PIX).AND.(J.EQ.PIY)) GO TO 710
C     Empty space - no collision worry
      BLOB=LMM(I,J)
C     This is used to see if a possible collision is acceptable
      CALL LOOKR(II,JJ,ICHECK,LCNT,BLOB)
C     Check for conflicts
C
      IF (ICHECK .NE. 0) THEN
         DO 705 L = 1,260
            IF (LABL(L,1).EQ.0) THEN
               LOW =  L - LENM
               DO 703 LL = LOW,L-1
                  LABL(LL,1) = 0
                  LABL(LL,2) = 0
 703           CONTINUE
               GO TO 546
            ENDIF
 705     CONTINUE
         GO TO 546
      ENDIF
C     ICHECK not = 0 indicate collision - bail out
 710  CONTINUE
      GO TO 240
C
C     We have a problem - bounds, collision or irreparably distorted node
C     Issue error message - shift old picture back to MM etc.
C     Then we go to 683 to redraw the pointer bond and go await
C     new command
 546  IERR=48
 173  IF (JPROB.EQ.0) CALL MYERR(IERR,KAR,KAR)
C     Issue message
      CALL CLRPIX(1)
C     Clear picture array
      CALL SHIF(2,MC,LC)
      COPY = 0
C     Restore old picture
      GO TO 683
C     Go to redraw pointer bond
C
C
C
C*****************************************************************************
C     This section handles attaching a structure to a node
C*****************************************************************************
 711  NIX=IX
C     Save node coordinates
      LY=IY
      NIY=IY
      LX=IX-1
      LAP(1,1)=NIX
      LAP(1,2)=NIY
      LCNT=1
      IF (LMM(NIX,NIY) .EQ. 46) GO TO 306
```

```
C       If we are at a marker go to 306
        IERR = 57
C       Not at marker or bond - exit to calling state
        CALL MYERR(IERR,KAR,MAR)
C       Shift old picture back to MM etc.
        IX = FIX
        IY = FIY
        CALL CURSOR(IX,IY)
        CALL SHIF(2,MC,LC)
        COPY = 0
        GO TO 305
306     ITRY = 1
C       We will try 4 orientations of the attaching group before
C       we give up - We will try the unrotated and unreflected
C       group first because it is likely to look the best
        ADIR=BDIR
        IFLIP=-1
        IROT=1
310     CALL DELTA(ADIR,INCX,INCY)
C Get delta values so you can calculate where to attach the bond
        DX=ABX-NIX+INCX
        DY=ABY-NIY+INCY
        IF (ITRY .GT. 1) CALL FIXMRK(1,MC)
C Eliminate debris from LABL and MRKCHN
        CALL CLRPIX(1)
C Clear the MM array
        IF (SYM .EQ. 2 .OR. (SYM .EQ. 1 .AND. IFLIP .EQ. -1))
     1 CALL MOVEIT(DX,DY,LENP,LENM,LLLEN,LENC,LEND,ABX,ABY,IROT,IERR)
C Move picture from CONNEC to MM with translation to new origin plus rotation
        IF (IHP .NE. 1) THEN
        IF (IROT.EQ.4) THEN
           IROT = 2
        ELSE IF (IROT.EQ.2) THEN
           IROT = 4
        ENDIF
        ENDIF
        IF (SYM .EQ.1 .AND. IFLIP .NE. -1)
     1  CALL MOVEFL(DX,DY,LENP,LENM,LLLEN,LENC,LEND,ABX,ABY,IFLIP,IERR)
C Move picture from CONNEC to MM with translation and reflection
        IF (IERR .NE. 0) GO TO 300
C If the move didn't work - bail out
        CALL FIXUP(IERR)
C Fix up any bad node caused by rotations or reflections
        IF (IERR .EQ. -1) GO TO 300
C Irreparable node - bail out or try new orientation
        ierr=0
        DO 3402 I = LOX,HIX
        DO 3402 J = LOY,HIY
        ii=i
        jj=j
        LL = LMM(I,J)
        IF ((LL.EQ.46).OR.((LL.GE.65).AND.(LL.LE.90)).OR.
     *     ((LL.GE.95).AND.(LL.LE.122)).OR.((LL.GE.50).AND.
     *     (LL.LE.57).AND.(MM(I-1,TY).EQ.72))) THEN
           DO 112 X = -1,1
              MX = I + X
              IF ((MX.LE.0).OR.(MX.GT.MAXX)) GO TO 112
              DO 1212 Y = -1,1
                 MY = J + Y
                 IF ((MY.LE.0).OR.(MY.GT.MAXY)) GO TO 1212
                 L = MOD(IDTPIX(MX,MY),2**13)
                 IF ((L.EQ.0).OR.(L.GE.256)) GO TO 1212
                 IF ((L.EQ.34).OR.(L.EQ.43).OR.(L.EQ.45).OR.
     *              (((L.GE.50).AND.(L.LE.57)).AND.((MOD(IDTPIX(MX-1,
     *              MY),2**13).EQ.43).OR.(MOD(IDTPIX(MX-1,MY),2**13)
     *              .EQ.45).OR.((IABS(X+Y).NE.1).AND.(IDTPIX(MX-1,MY)
     *              .EQ.72))).AND.(MX-1.GT.0))) GO TO 1212
                 IERR = 48
                 GO TO 3033
1212          CONTINUE
112         CONTINUE
            if ((MM(I,J).EQ.46).OR.(mm(i,j).ge.65 .and. mm(i,j).le.90
     1         .and. (mm(i,j).ne.72 .or. (mm(i,j).eq.72
     2         .and. mm(i+1,j).ge.97 .and. mm(i+1,j).le.122)))
     3         call vlnce(2,ii,jj,0,0,ierr)
          ENDIF
```

```
3033     IF (IERR.EQ.12) THEN
            IERR = 0
            EX = II
            EY = JJ
         ELSE if (ierr.ne. 0) THEN
            DO 3705 L = 1,260
               IF (LABL(L,1).EQ.0) THEN
                  LOW =  L - LENM
                  DO 3703 LL = LOW,L-1
                     LABL(LL,1) = 0
                     LABL(LL,2) = 0
3703              CONTINUE
                  GO TO 300
               ENDIF
3705       CONTINUE
           go to 300
        ENDIF
3402    continue
        CALL CURSOR(LOX,LOY)
        DO 301 I = LOX,HIX
        DO 301 J = LOY,HIY
        II = I
        JJ = J
        IF (MM(I,J) .EQ. 0) GO TO 301
        IF ((I.EQ.NIX).AND.(J.EQ.NIY)) GO TO 301
C Spot is empty - no collision problem
C       Not is empty - no collision problem
        BLOB=LMM(I,J)
C       This is used to see if a possible collision is acceptable
        CALL LOOKR(II,JJ,ICHECK,LCNT,BLOB)
C       Check for conflicts
C
        IF (ICHECK .NE. 0) THEN
           DO 1705 L = 1,260
              IF (LABL(L,1).EQ.0) THEN
                 LOW =  L - LENM
                 DO 1703 LL = LOW,L-1
                    LABL(LL,1) = 0
                    LABL(LL,2) = 0
1703             CONTINUE
                 GO TO 300
              ENDIF
1705       CONTINUE
           GO TO 300
        ENDIF
C       Bad conflict - bail out or try new orientation
301     CONTINUE
        MX = ABX - DX
        MY = ABY - DY
        MBTYPE = MM(MX,MY) / 256
        IF ((MBTYPE.EQ.6).OR.(MBTYPE.EQ.7)) THEN
           IF (((BDIR.EQ.1).AND.((ADIR.EQ.1).OR.(ADIR.EQ.5))).OR.
     *        (BDIR.EQ.6).OR.(BDIR.EQ.8).OR.
     *        ((BDIR.EQ.1).AND.(ADIR.EQ.3)).OR.
     *        ((BDIR.EQ.7).AND.((ADIR.EQ.3).OR.(ADIR.EQ.5)))) THEN
              IF (MBTYPE.EQ.6) THEN
                 MBTYPE = 7
              ELSE
                 MBTYPE = 6
              ENDIF
              COPYB = MBTYPE * 256 + ADIR
              DO 2998 I = 1,BLEN
                 IF (LMM(MX,MY).LT.256) GO TO 2999
                 MM(MX,MY) = COPYB
                 MX = MX - INCX
                 MY = MY - INCY
2998          CONTINUE
2999          CONTINUE
           ENDIF
           MX = ABX - DX
           MY = ABY - DY
           IF (((BDIR.EQ.1).AND.(ADIR.EQ.1))
     *        .OR.((BDIR.EQ.5).AND.((ADIR.EQ.7).OR.(ADIR.EQ.1)))
     *        .OR.((BDIR.EQ.3).AND.((ADIR.EQ.7).OR.(ADIR.EQ.1)))
     *        .OR.((BDIR.EQ.6).AND.((ADIR.EQ.6).OR.(ADIR.EQ.8)))
     *        .OR.((BDIR.EQ.8).AND.((ADIR.EQ.6).OR.(ADIR.EQ.8)))
     *        .OR.((BDIR.EQ.2).AND.((ADIR.EQ.6).OR.(ADIR.EQ.8)))
     *        .OR.((BDIR.EQ.4).AND.((ADIR.EQ.6).OR.(ADIR.EQ.8))))
```

```
*           THEN
            CBDIR = ADIR + 4
            IF (CBDIR.GT.8) CBDIR = CBDIR - 8
            IF (MBTYPE.EQ.6) THEN
               COPYB = 7 * 256 + CBDIR
            ELSE
               COPYB = 6 * 256 + CBDIR
            ENDIF
            DO 8998 I = 1,BLEN
               IF (LMM(MX,MY).LT.256) GO TO 8999
               MM(MX,MY) = COPYB
               MX = MX - INCX
               MY = MY - INCY
8998        CONTINUE
8999        CONTINUE
         ENDIF
      ENDIF
C     Irreparable node - bail out or try new orientation
      IF (IOP .EQ. 1) IFLIP=0
C     Prepare for possible delete and go draw group
      IF (IHP .NE. 1) THEN
      IF (IROT.EQ.2) THEN
         IROT = 4
      ELSE IF (IROT.EQ.4) THEN
         IROT = 2
      ENDIF
      ENDIF
      GO TO 240
C     No collisions - go draw it
300   ITRY=ITRY+1
      IF (ITRY .GT. 4) GO TO 5460
      JPROB = 0
C     Bail out - we can't do it
      IROT=IROT+1
      ADIR=BDIR + (IROT-1)*2
      IF (IHP .EQ. 1 .AND. IROT .EQ. 2) ADIR = ADIR + 4
      IF (IHP .EQ. 1 .AND. IROT .EQ. 4) ADIR=ADIR-4
C     Halo y axis direction is opposite HP and requires rotational
C     substitution.
      IF (IHP .NE. 1) THEN
      IF (IROT.EQ.2) THEN
         IROT = 4
      ELSE IF (IROT.EQ.4) THEN
         IROT = 2
      ENDIF
      ENDIF
      IF (ADIR .GT. 8) ADIR=ADIR-8
C
      IFLIP = THETA(BDIR,ADIR)
      IF (IFLIP.EQ.2) THEN
         IFLIP = 4
      ELSE IF (IFLIP.EQ.4) THEN
         IFLIP = 2
      ENDIF
C Get reflection value
      GO TO 310
C Try next orientation
C     Try next orientation
5460  IERR=48
C     No space or distorted node - issue error message
      IF (JPROB.EQ.0) CALL MYERR(IERR,KAR,KAR)
      CALL SHIF(2,MC,LC)
      COPY = 0
      GO TO 305
C     Await new command
```

```
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
C       This section tries to display a stand alone structure
C       It defines the origin for the new structure - Determines the
C       minimum X and Y coordinates in the new structure - Calculates
C       the translation values needed and checks to see if the new
C       structure collides with the current structure. If no collision
C       occurs, the MM and LNGBND arrays are cleared and the new picture
C       is moved (with the necessary translation to the new origin)
C       into MM. If there is a bounds problem encountered while copying
C       the picture to MM, an error message is issued, the old picture
C       array is copied back into MM and the program awaits entry of a
C       new command.
CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
200     ALONE = 1
        IF (OCHAR .NE. 68) GO TO 211
C       Set new origin to 0 if KAR = D
        DX=0
        DY=0
        GO TO 212
211     OX=IX
C       We are doing a stand alone structure
        OY=IY
C       Set new origin
C       Find min X and min Y in structure we're going to retrieve
        MX=10000
        MY=10000
        J=1
        DO 13 I=1,LENP
        IF (CONNEC(J) .LT. MX) MX=CONNEC(J)
        IF (CONNEC(J+1) .LT. MY) MY=CONNEC(J+1)
        J=J+3
13      CONTINUE
C
C       Calculate translation value
C
        DX=MX-OX
        DY=MY-OY
C
C       See if new structure at new origin collides with current structure
C
212     J=1
        DO 261  I=1,LENP
        JX=CONNEC(J)-DX
        JY=CONNEC(J+1)-DY
        CALL CELL2(JX,JY,IGOOD)
        IF (IGOOD .NE. 0) GO TO 480
C       IGOOD .NE. 0 implies there is a collision
        J=J+3
261     CONTINUE
        GO TO 260
C
C       We have a collision - issue error messages  - go to await
C       entry of new command
C
480     CONTINUE
C       Type error message
        CALL FTSIZE(2,18)
        CALL FTLOCA(4,1)
        CALL FTEXT('^New structure collides with old structure - ^')
        PMESS=.TRUE.
        GO TO 491
C
C       No collision - clear MM and LNGBND
C
260     CALL CLRPIX(1)
250     IROT=1
C Set rotation to 0 degree rotation
        IFLIP=-1
        CALL MOVEIT(DX,DY,LENP,LENM,LLLEN,LENC,LEND,ABX,ABY,IROT,IERR)
C Move picture from CONNEC to MM with translation to new origin
        IF (IERR .NE. 0) GO TO 490
C If there is a bounds problem - bail out
C       Fill in valence hydrogens
        IF (DOT .EQ. 1) GO TO 6512
```

```
C Skip valence call if we have a DOTDIS
        IERR=0
        DO 4910 I = LOX,HIX
        DO 4910 J = LOY,HIY
        II=I
        JJ=J
        LL = LMM(I,J)
        IF ((LL.EQ.46).OR.((LL.GE.65).AND.(LL.LE.90)).OR.
     *     ((LL.GE.95).AND.(LL.LE.122)).OR.((LL.GE.50).AND.
     *     (LL.LE.57).AND.(MM(I-1,TY).EQ.72))) THEN
           DO 113 X = -1,1
              MX = I + X
              IF ((MX.LE.0).OR.(MX.GT.MAXX)) GO TO 113
              DO 1313 Y = -1,1
                 MY = J + Y
                 IF ((MY.LE.0).OR.(MY.GT.MAXY)) GO TO 1313
                 L = MOD(IDTPIX(MX,MY),2**13)
                 IF ((L.EQ.0).OR.(L.GE.256)) GO TO 1313
                 IF ((L.EQ.34).OR.(L.EQ.43).OR.(L.EQ.45).OR.
     *              (((L.GE.50).AND.(L.LE.57)).AND.((MOD(IDTPIX(MX-1,
     *              MY),2**13).EQ.43).OR.(MOD(IDTPIX(MX-1,MY),2**13)
     *              .EQ.45).OR.((IABS(X+Y).NE.1).AND.(IDTPIX(MX-1,MY)
     *              .EQ.72))).AND.(MX-1.GT.0))) GO TO 1313
                 IERR = 48
                 GO TO 4040
 1313         CONTINUE
 113       CONTINUE
           if ((MM(I,J).EQ.46).OR.(mm(i,j).ge.65 .and. mm(i,j).le.90
     1        .and. (mm(i,j).ne.72 .or. (mm(i,j).eq.72
     2        .and. mm(i+1,j).ge.97 .and. mm(i+1,j).le.122)))
     3        call vlnce(2,ii,jj,0,0,ierr)
        ENDIF
 4040   IF (IERR.EQ.12) THEN
           IERR = 0
           EX = II
           EY = JJ
        ELSE IF (IERR.NE.0) THEN
           DO 4705 L = 1,260
              IF (LABL(L,1).EQ.0) THEN
                 LOW =  L - LENM
                 DO 4703 LL = LOW,L-1
                    LABL(LL,1) = 0
                    LABL(LL,2) = 0
 4703            CONTINUE
                 GO TO 3305
              ENDIF
 4705      CONTINUE
           GO TO 3305
        ENDIF
 4910   CONTINUE
        GO TO 6512
 3305   CALL CLRPIX(1)
        CALL SHIF(2,MC,LC)
        COPY = 0
        GO TO 305
 6512   CONTINUE
        DO 492 I = LOX,HIX
        DO 492 J = LOY,HIY
        II = I
        JJ = J
        IF (MM(I,J) .EQ. 0) GO TO 492
        CALL CELL2(I,J,IGOOD)
        IF (IGOOD .NE. 0 ) THEN
           DO 5705 L = 1,260
              IF (LABL(L,1).EQ.0) THEN
                 LOW =  L - LENM
                 DO 5703 LL = LOW,L-1
                    LABL(LL,1) = 0
                    LABL(LL,2) = 0
 5703            CONTINUE
                 GO TO 490
              ENDIF
 5705      CONTINUE
           GO TO 490
```

```
        ENDIF
492     CONTINUE
        GO TO 240
C       If there is no bounds problem - go to 240 where we will display
C       the picture.  If we have a bounds problem, shift old picture back
C       to MM etc.  Type error message - and go to await new command.
C
490     CONTINUE
491     CALL SHIF(2,MC,LC)
        CALL FTSIZE(2,18)
        IF (IHP .EQ. 1 .AND. PMESS .EQ. .TRUE.) THEN
                        PMESS=.FALSE.
                        ELSE
        CALL FTLOCA(4,1)
        ENDIF
        COPY = 0
C       Type error message
        CALL FTEXT('^Bad origin requested ^')
        PAGE = 0
        IF (OCHAR.EQ.68) THEN
           CALL FTEXT('^                                              ^')
           CALL FTSIZE(1,10)
           GO TO 9222
        ENDIF
C Have we tried default origin
        OCHAR=68
        IF (IHP .EQ. 1) CALL FTLOCA(5,1)
        CALL FTEXT('^- Will try default origin.^')
        IF (IHP .EQ. 1) THEN
                CALL DELAY
                CALL DELAY
                CALL FTLOCA(5,1)
                CALL FTEXT('^                                ^')
                ENDIF
        CALL FTSIZE(1,10)
        GO TO 200
9222    OCHAR=0
C We've tried default - give up
        GO TO 305
C***********************************************************************
C       This section displays the retrieved structure.
C       It defines the parameters LBLEN (# of long bonds) and
C       NJNEXT (last marker index used) - displays the structure -
C       Sets XCHAR = 0 (This indicates that we just did a retrieve)
C       Sets OCHAR = 0 (This indicates that the origin is not the
C       default origin.
C       It then adds the old picture back to the new picture (MM) and
C       adds the old long bonds to the new long bonds (LNGBND).
C       It then clears screen dialog and moves the cursor to the
C       requested final cursor position. The cursor position is
C       adjusted by SYNCH if it is not at a valid position.
C***********************************************************************
240     CONTINUE
        NJNEXT=LENM+MC
        ISWIT=1
C       Call STRDRW with markers displayed as markers
        LBLEN=LLLEN
        do 2562,ii=1,maxx
        do 2562,jj=1,maxy
2562    continue
        CALL STRDRW(ISWIT)
        ICUR = 1
C       Display retrieved structure
C
C       Move the structure back to CONNEC - We may have called FIXUP
C       which may have moved nodes - thus we need a good copy in
C       CONNEC in case we have to do a delete
C
        K=1
        DO 94 I = LOX,HIX
        DO 94 J = LOY,HIY
        IF (MM(I,J) .EQ. 0) GO TO 94
        DELET(K)=I
        DELET(K+1)=J
```

```
        DELET(K+2)=MM(I,J)
        K=K+3
94      CONTINUE
        DENP = K / 3
        XCHAR=0
C       XCHAR = 0 implies that we just did a retrieve
        OCHAR=0
C       Reset origin character to not default
        CALL ADDBCK
C       Add old picture to new picture
        CALL ADDLNG(LC,LLLEN)
C       Add old long bonds to new long bonds
        COPY=0
C Current picture is in MM
C Erase dialog
        SSYM = SYM
        CALL FINDXY(IX,IY,LBX,LBY,DX,DY,ABX,ABY,IROT,IFLIP,SSYM)
        SYM = SSYM
C Calculate final cursor values
        IF (ALONE .EQ. 0 ) GO TO 5687
        ALONE=0
        IF (BLEN .EQ. 0) GO TO 5687
        CALL DELTA(BDIR,KNCX,KNCY)
C Delete dangling bond if structure is stand alone and has dangling bond.
        KX=ABX-DX+KNCX
        KY=ABY-DY+KNCY
        JCHAR=1
        ICHAR=1
        CALL DEL(KAR,KX,KY,KNCX,KNCY,IWHICH)
CXT
CXT     The valence hydrogens of the attached node are computed.
        PNODE = .TRUE.
        DELH(1,3) = 0
        DELH(2,3) = 0
        SXX = KX - 1
        CALL CLRHYD(SXX,KY)
        CALL VLNCE(1,SXX,KY,0,0,IERR)
        PNODE = .FALSE.
CXT     The valence hydrogens of the attached node are made deletable.
        DO 5369 I = 1,2
           IF (DELH(I,3).NE.0) THEN
              DELET(K) = DELH(I,1)
              DELET(K+1) = DELH(I,2)
              DELET(K+2) = DELH(I,3)
              DENP = DENP + 1
              K = K + 3
           ENDIF
5369    CONTINUE
CXT
C Delete bond
        IF (IERR.EQ.12) THEN
           IX = EX
           IY = EY
        ENDIF
        IF (IABS(ABX-LBX).GT.1 .OR. IABS(ABY-LBY).GT.1) GO TO 4568
C If beginning site
C equals leaving site equals bond and we have deleted bond
C set cursor to node at end of erased bond
        IX=KX
        IY=KY
5687    IF (IERR.EQ.12) THEN
           IX = EX
           IY = EY
        ENDIF
        IF (NODE .NE. 0 ) GO TO 4567
        IF (DIFF .GE. 0) GO TO 4567
        IF (IABS(ABX-LBX).GT.1 .OR. IABS(ABY-LBY).GT.1) GO TO 4567
        IX=OBX
C The bond on disk is longer than the bond on screen
        IY=OBY
C Adjust the final cursor position so that it is really
C at the end of the screen bond
4567    IF (DOT .NE. 1) GO TO 4568
```

```
        IX=IX-1
C Skip SYNCH call if this is a DOTDIS
        GO TO 305
4568        CALL SYNCH(KAR,IX,IY)
C Adjust and display final cursor position
        GO TO 305
C
C**********************************************************************
C       This section will call IDENT to handle bond entry commands -
C       marker entry commands and jump to marker commands
C       It then sets XCHAR to 1 to indicate that we just called IDENT
C       and did not just do a retrieve - This parameter is used by the delete sect
C**********************************************************************
793     CALL IDENT(KKAR,IX,IY,INCX,INCY,IRESET)
        IF ((KKAR.GE.22).AND.(KKAR.LE.31)) NOCHG = 0
C       Do bond-enter marker-or-jump to marker
        XCHAR=1
C       XCHAR=1 implies that we just did a call to IDENT - not a retrieve
        IF (KKAR.NE.38) GO TO 305
        ISTATE = 12
        MW(7) = 999
        MW(8) = 999
        MW(9) = 999
        CALL HEADER
        GO TO 305
C       Go get next command
C**********************************************************************
C       This section sets the type of symmetry to axial
C**********************************************************************
955     SYM=1
        CALL HEADER
        GO  TO 305
C**********************************************************************
C       This section sets the symmetry to point
C**********************************************************************
966     SYM=2
        CALL HEADER
        GO TO 305
C**********************************************************************
C       This section sets a bondtype and does a bond command or
C       sets a charge value and enters a charge.
C**********************************************************************
3561    CALL CURSOR(IX,IY)
        CALL NUMBER(KKAR,IX,IY)
        IF (KKAR.EQ.81) GO TO 6777
        MW(7) = 999
        MW(8) = 999
        MW(9) = 999
        ISTAT = ':'
        ISTATE = 12
        CALL HEADER
        GO TO 305
C**********************************************************************
C       This section deletes the result of the last operation
C       If XCHAR = 0, we delete the last retrieved structure
C       If XCHAR = 1, we delete the last bond or marker entered
C**********************************************************************
650     IF (XCHAR .NE. 0) GO TO 728
C       If XCHAR = 1 we will go delete a bond or marker
C
C       We will be deleting the structure just drawn
C
        J=1
        BX=KX
        BY=KY
C       This loop picks up the X and Y coordinates from DELETE
C       ZAP is called to erase from the screen the character or bond at KX,KY
C
        ICUR = 0
        CALL CURSOR(KX,KY)
        DO 527 I=1,DENP
        KX=DELET(J)
        KY=DELET(J+1)
528     CALL ZAP(KX,KY)
C       Erase the character or bond at KX,KY
```

```
529     J=J+3
527     CONTINUE
C
C       Erase current pointer bond
        IF (NODE.NE.0) GO TO 7529
        DO 545 I=1,OBLEN
           MX=OBX + (I-1)*INCX
           MY=OBY + (I-1)*INCY
           CALL ZAP(MX,MY)
545     CONTINUE
        SXX = MX - INCX
        SYY = MY - INCY
        CALL CLRHYD(SXX,SYY)
        CALL VALNCE(2,SXX,SYY,0,0)
C
C       Now delete the long bonds from the new structure
C
7529    IF (LLLEN .EQ. 0) GO TO 980
        OCHAR=JCHAR
C       Save old JCHAR
        JCHAR=8
C       Set JCHAR so that we will delete longbond
        DO 64 I=1,LLLEN
        CALL DEL(KAR,IX,IY,INCX,INCY,0)
C       Del last longbond drawn
64      CONTINUE
C
C       Delete the last LLLEN longbonds from LLBOND before SHIFT is
C       called.
        DO 984 I = LLLEN+LC,LC+1,-1
        DO 984  J=1,5
        LLBOND(I,J)=0
984     CONTINUE
        LBLEN = LC
C
C       Now move old picture back to MM etc.
C
980     CONTINUE
        CALL SHIF(2,MC,LC)
        COPY = 0
        NJNEXT=MC
        LABL(NJNEXT+1,1) = 0
C       Index of last used label
        JCHAR=OCHAR
C       Restore JCHAR
        ICUR = 1
        CALL CURSOR(IX,IY)
C
C       Redraw pointer bond if we were attaching to bond not node
C
        IF (NODE .NE. 0) GO TO 444
683     OTYPE=IBTYPE
C       Save old bond type and enlarge factor
        OLARGE=NLARGE
        NOCHG = 1
        IBTYPE = OBTYPE
C       Set bond type for pointer bond
        NLARGE=OBLEN
C       Set bond length for pointer bond
        ICHAR=2
        JCHAR=2
C       Set JCHAR to 'just entered a node'
        CMD=OBDIR+21
C       Set CMD to bond command
        IF (CMD .GT. 25) CMD=CMD+2
        PPIX = PIX + 1
        PPIY = PIY
        CALL IDENT(CMD,PPIX,PPIY,INCX,INCY,IRESET)
C       Redraw bond
        NLARGE=OLARGE
C       Reset NLARGE and IBTYPE
        NOCHG=0
        IBTYPE=OTYPE
444     IX=LX
C       Reset coordinates as they were when we started RETRIEVE
        IY=LY
```

```
      CALL SYNCH(KAR,IX,IY)
      XCHAR = 1
C     Adjust and display cursor position
      GO TO 305
C     Delete last bond or marker
728   COPY=0

      CALL IDENT(KKAR,IX,IY,INCX,INCY,IRESET)
      GO TO 305
C*************************************************************************
C
C     We found too many markers or longbonds - Issue error message
C     Shift old picture back to MM etc.  -  Then exit
C
C*************************************************************************
333   CONTINUE
      CALL FTSIZE(2,18)
      CALL FTLOCA(4,1)
      CALL FTEXT('^Command aborted - Too many markers or longbonds^')
      PAGE = 0
      CALL FTSIZE(1,10)
C
C     Shift old picture back to MM etc.
C
      CALL SHIF(2,MC,LC)
      COPY = 0
      GO TO 6777
C*************************************************************************
C     We found a bounds problem in CONNEC - Close the file
C     Release the channel - Issue an error message and prepare
C     to exit.
C*************************************************************************
999   IERR = 54
      CALL MYERR(IERR,KAR,MAR)
C     Bounds problem with CONNEC
67    CLOSE(IU)
C     Close file
      GO TO 305
C*************************************************************************
C     This section prepares to exit from GETIT
C     The screen dialog is erased.
C     If we came from Ground level - call HEADER to display
C     Ground level heading and return to Ground level
C     If we came from RING or CHAIN, then display the
C     appropriate heading and return to RING or CHAIN
C     respectively
C*************************************************************************
6777  CONTINUE
      IF (FILE.NE.'            ') LFILE = FILE
      LCHAR=KCHAR
      KAR=KKAR
      ISTATE=0
      IF ((LCHAR .EQ. 12 .OR. LCHAR .EQ.13).and.kkar.ne.81) GO TO 2000
      LFLAG=0
      IF (KKAR .EQ. 81) LFLAG=1
      LEVEL=0
      DO 6789 I=1,12
6789  MW(I)=999
C FORCE A COMPLETE NEW HEADING
      ISKIP = 0
      CALL HEADER
C     SET LEVEL AND ISTATE TO GROUND AND CALL HEADER
      RETURN
2000  LFLAG=1
      LEVEL=1
      ICHAR=LCHAR
      IF (ICHAR .EQ. 12) KAR = 94

      IF (ICHAR .EQ. 13) KAR = 33
      DO 9898 I = 1,12
9898  MW(I) = 999
      ISKIP = 0
      CALL HEADER
      RETURN
      END
$STORAGE:2
C
```

```
C       SUBROUTINE MAP(IX,IY,NODE,BDIR)
C
C       This subroutine examines the neighborhood of point MM(IX,IY)
C       to determine if the point is a node or a bond or neither
C
C       NODE = 0 implies that we are at the end of a bond
C       NODE = 1 implies that we are at a node
C       NODE = -1 implies that we are not at a node or a bond or a
C           3*3 clear space
C       NODE = -2 implies we are at a 3*3 clear space
C       BDIR = bond direction of bond if NODE = 0
C       Beware - MAP may change IX - If IX,IY is near a node -
C       i.e. at 2 or H of CH2 - IX will be altered so that it
C       is at the C
        SUBROUTINE MAP(IX,IY,NODE,BDIR)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
C
C       Determine if we are at a 3X3 blank space
C
        NODE = -2
        CALL NEW(SUM,IX,IY)
C       SUM = 0  implies we are at a 3*3 blank space - i.e. not bond or node
        IF (SUM .EQ. 0) THEN
        RETURN
        ENDIF
C
C       We are not at a 3X3 blank area - See if we are at a bond
C
        IF (MM(IX,IY) .NE. 0) GO TO 12
C       MM(IX,IY) not equal 0 implies we are not at the end of a bond
C       because the cursor is positioned at empty cell just
C       beyond bond after a bond is entered
        CALL FINDB(IBDIR,KBDIR,IX,IY)
C       See if there is a bond around MM(IX,IY)
        IF (IBDIR .EQ. -1) GO TO 12
C       IBDIR=-1 implies that we are not at a bond
        NODE = 0
C       We are at the end of a bond - Set NODE=0 and BDIR to bond direction
        BDIR=KBDIR
        GO TO 13
C
C       Determine if we are at a node
C
12      KX=IX
        DO 30 I=0,5
C       See if we are at a node - Node = marker, ?, or upper case
        MX=KX-I
        LL=LMM(MX,IY)
        IF ((LL .NE. 46) .AND. (LL .NE. 63) .AND. ((LL .LT. 65) .OR.
     1  (LL .GT. 90))) GO TO 30
        IF (LL .EQ. 72 .AND. ((MM(MX+1,IY) .LE. 97 .OR. (MM(MX+1,IY))
     1   .GE. 122))) GO TO 30
        IX=MX
        CALL CURSOR(IX,IY)
        NODE=1
C       We are at a node
        GO TO 13
30      CONTINUE
C
C       We are not at a node or a bond
C
11      NODE=-1
C       We aren't at a bond or a node
13      CONTINUE
        RETURN
        END
C
C       SUBROUTINE MOVEIT(DX,DY,LENP,LENM,LLLEN,LENC,LEND,ABX,ABY,IROT,
C          IERR)
C       THIS SUBROUTINE MOVES THE PICTURE FROM ITS TEMPORARY STORAGE
C       PLACE IN CONNEC TO MM - IN THE PROCESS IT TRANSLATES THE
C       PICTURE TO THE NEW ORIGIN BY USING THE DELTA VALUES DX AND DY
C       IF NECESSARY (IN THE CASE OF AN ATTACHING GROUP) IT ALSO ROTATES
```

```
C       THE GROUP AROUND THE GROUPS ATTACHING BOND AT ABX,ABY
C       THE ANGLE OF ROTATION IS SPECIFIED BY IROT
C       IROT=1 = ANGLE 0    IROT=2 = ANGLE 90    IROT=3 = ANGLE 180
C       IROT=4 = ANGLE 270
C
        SUBROUTINE MOVEIT(DX,DY,LENP,LENM,LLLEN,LENC,LEND,ABX,ABY,IROT,
     *     IERR)
        IMPLICIT INTEGER*2(A-Z)
        INTEGER*4 MM,IDTPIX,CONNEC,LL
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /CD/ MAXX,MAXY
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /ENTRAR/ CONNEC(2001)
        DIMENSION KSIN(4),KCOS(4)
        DATA KSIN /0,1,0,-1/
        DATA KCOS /1,0,-1,0/
        IERR=0
C       Return code - IERR will be set to 1 if we have bounds problems
        IF (IROT.EQ.2) THEN
           ROT = 4
        ELSE IF (IROT.EQ.4) THEN
           ROT = 2
        ELSE
           ROT = IROT
        ENDIF
        DELT = (ROT - 1) * 2
        J=1
        DO 200 I=1,LENP
        TX=((CONNEC(J)-ABX)*KCOS(IROT)+(CONNEC(J+1)-ABY)*KSIN(IROT))
     1  +ABX-DX
        TY=-(CONNEC(J)-ABX)*KSIN(IROT)+(CONNEC(J+1)-ABY)*KCOS(IROT)
     1  +ABY-DY
        IF (TX .GT. 0 .AND. TX .LE. MAXX .AND. TY .GT. 0
     1  .AND. TY .LE. MAXY) GO TO 201
225     IF (TX .GT. 0 .AND. TX .LE. MAXX .AND. TY .GT. 0
     1  .AND. TY .LE. MAXY) GO TO 201
55      IERR = 48
C       We found a bounds problem
        RETURN
201     CONTINUE
        IF (TX.LT.LOX) THEN
           LOX = TX
        ELSE IF (TX.GT.HIX) THEN
           HIX = TX
        ENDIF
        IF (TY.LT.LOY) THEN
           LOY = TY
        ELSE IF (TY.GT.HIY) THEN
           HIY = TY
        ENDIF
        LL=CONNEC(J+2)
C       Translate values to new origin and store in MM
        MM(TX,TY)=LL
        IF (LMM(TX,TY).LT.256) GO TO 203
C
C       If LL is a bond - rotate it and then store in MM
C
        BDIR=IDIR(LL)
C       Extract bond dir from bond
        LL=LL-BDIR
        BDIR=BDIR+DELT
C       Rotate bond
        IF (BDIR .GT. 8) BDIR=BDIR-8
        LL=LL+BDIR
        MM(TX,TY)=LL
C       Store rotated bond in MM
203     J=J+3
200     CONTINUE
        IF (LENM .EQ. 0) GO TO 207
        DO 40 I=1,260
        II = I
        IF (LABL(I,1) .EQ. 0) GO TO 50
40      CONTINUE
50      LABLEN = II-1
```

```
C       Find end of LABL ARRAY
        IF (LABLEN+LENM .GT. 260) THEN
           IERR = 48
           RETURN
        ENDIF
C       Bounds problem with LABL array
        DO 206  I=LABLEN+1,LABLEN+LENM
C       Copy markers to end of present marker array
        LABL(I,1)=((CONNEC(J)-ABX)*KCOS(IROT)+(CONNEC(J+1)-ABY)
     1  *KSIN(IROT))+ABX-DX
        LABL(I,2)=-(CONNEC(J)-ABX)*KSIN(IROT)+(CONNEC(J+1)-ABY)
     1  *KCOS(IROT)+ABY-DY
        MRKCHN(I)=CONNEC(J+2)
        J=J+3
206     CONTINUE
207     IF (LLLEN.EQ.0) GO TO 2088
C       Set up
        DO 209 I=1,LLLEN
        LNGBND(I,1)=((CONNEC(J)-ABX)*KCOS(IROT)+
     1  (CONNEC(J+1)-ABY)*KSIN(IROT))+ABX-DX
        LNGBND(I,2)=-(CONNEC(J)-ABX)*KSIN(IROT)+
     1  (CONNEC(J+1)-ABY)*KCOS(IROT)+ABY-DY
        LNGBND(I,3)=((CONNEC(J+2)-ABX)*KCOS(IROT)+
     1  (CONNEC(J+3)-ABY)*KSIN(IROT))+ABX-DX
        LNGBND(I,4)=-(CONNEC(J+2)-ABX)*KSIN(IROT)+
     1  (CONNEC(J+3)-ABY)*KCOS(IROT)+ABY-DY
        LNGBND(I,5)=CONNEC(J+4)
        J=J+5
209     CONTINUE
C
2088    IF (LENC .EQ. 0) GO TO 2081
C Handle charges if there are any
        DO 1200 I=1,LENC
        TX=((CONNEC(J)-ABX)*KCOS(IROT)+(CONNEC(J+1)-ABY)*KSIN(IROT))
     1  +ABX-DX
        TY=-(CONNEC(J)-ABX)*KSIN(IROT)+(CONNEC(J+1)-ABY)*KCOS(IROT)
     1  +ABY-DY
        IF (TX .GT. 0 .AND. TX .LE. MAXX .AND. TY .GT. 0
     1  .AND. TY .LE. MAXY) GO TO 1201
5555    IERR=48
C We found a bounds problem
        RETURN
1201    CONTINUE
        KAR=CONNEC(J+2)
C Get sign of charge
        NCHRG=CONNEC(J+3)
C Get digit associated with charge
        CALL ZHARGE(KAR,TX,TY,NCHRG,IERR)
C Position charge
        IF (IERR .NE. 0) GO TO 5555
C Couldn't place charge - bail out
1203    J=J+4
1200    CONTINUE
2081    IF (LEND.EQ.0) GO TO 208
        DO 1205 I = 1,LEND
           TX = ((CONNEC(J)-ABX)*KCOS(IROT)+(CONNEC(J+1)-ABY)*
     *        KSIN(IROT)) + ABX - DX
           TY = -(CONNEC(J)-ABX)*KSIN(IROT)+(CONNEC(J+1)-ABY)*
     *        KCOS(IROT) + ABY - DY
           IF ((TX.GT.0).AND.(TY.LE.MAXX).AND.(TY.GT.0).AND.(TY.LE.
     *        MAXY)) GO TO 1202
5556       IERR = 1
           RETURN
1202       KAR = 34
           IDRAW = 1
           CALL IND1(KAR,TX,TY,IDRAW,IERR)
           IF (IERR.NE.0) GO TO 5556
           J = J + 2
1205    CONTINUE
208     CONTINUE
        RETURN
        END
C
C       SUBROUTINE MOVEFL(DX,DY,LENP,LENM,LLLEN,LENC,LEND,ABX,ABY,IFLIP,
C          IERR)
```

```
C
C       THIS SUBROUTINE MOVES THE PICTURE FROM ITS TEMPORARY STORAGE
C       PLACE IN CONNEC TO MM - IN THE PROCESS IT TRANSLATES THE
C       PICTURE TO THE NEW ORIGIN BY USING THE DELTA VALUES DX AND DY
C       AND REFLECTS THE PICTURE AROUND THE X AND/OR Y AXIS ACCORDING TO
C       THE VALUE OF IFLIP
C       IFLIP=1 (REFLECT AROUND X AXIS)
C       IFLIP=2 (REFLECT AROUND LINE MAKING 45 DEGREE ANGLE WITH X AXIS
C       IFLIP=3 (REFLECT AROUND Y AXIS)
C       IFLIP=4 (REFLECT AROUND LINE MAKING 135 DEGREE ANGLE WITH X AXIS
C       IFLIP=5 (REFLECT AROUND X AND Y AXES)
C
        SUBROUTINE MOVEFL(DX,DY,LENP,LENM,LLLEN,LENC,LEND,ABX,ABY,
     *     IFLIP,IERR)
        IMPLICIT INTEGER*2(A-Z)
        INTEGER*4 MM,IDTPIX,CONNEC,LL
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /CD/ MAXX,MAXY
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /ENTRAR/ CONNEC(2001)
        DIMENSION FLIPBD(8,5),KSIN(4),KCOS(4)
        DATA FLIPBD /5,4,3,2,5,8,7,6,
     *              7,6,5,4,3,6,1,8,
     *              1,8,7,6,5,4,3,2,
     *              3,2,1,8,7,6,5,4,
     *              5,6,7,8,1,2,3,4/
        DATA KSIN /0,1,0,-1/, KCOS /1,0,-1,0/
C
        IERR=0
C       Return code - IERR will be set to 1 if we have bounds problems
        J=1
        DO 200 I=1,LENP
        IF (IFLIP.NE.5) GO TO 219
           TX = -CONNEC(J) + 2 * ABX - DX
           TY = -CONNEC(J+1) + 2 * ABY - DY
           GO TO 225
219     CONTINUE
           TX = ((CONNEC(J)-ABX) * KCOS(IFLIP) + (CONNEC(J+1)-ABY) *
     *        KSIN(IFLIP)) + ABX - DX
           TY = ((CONNEC(J)-ABX) * KSIN(IFLIP) - (CONNEC(J+1)-ABY) *
     *        KCOS(IFLIP)) + ABY - DY
225     IF ((TX.GT.0).AND.(TX.LE.MAXX).AND.(TY.GT.0).AND.(TY.LE.
     *     MAXY)) GO TO 201
55      IERR=48
C       We found a bounds problem
        RETURN
201     CONTINUE
        IF (TX.LT.LOX) THEN
           LOX = TX
        ELSE IF (TX.GT.HIX) THEN
           HIX = TX
        ENDIF
        IF (TY.LT.LOY) THEN
           LOY = TY
        ELSE IF (TY.GT.HIY) THEN
           HIY = TY
        ENDIF
        LL=CONNEC(J+2)
C       Translate values to new origin and store in MM
        MM(TX,TY)=LL
        IF (LMM(TX,TY).LT. 256) GO TO 203
C
C       If LL is a bond - flip it and then store in MM
C
        BDIR=IDIR(LL)
C       Extract bond dir from bond
        LL=LL-BDIR
        BDIR=FLIPBD(BDIR,IFLIP)
C       Flip bond as necessary
        IF (BDIR .GT. 8) BDIR=BDIR-8
        LL=LL+BDIR
C       Store flipped bond in MM
        MM(TX,TY)=LL
203     J=J+3
```

```
200     CONTINUE
        IF (LENM .EQ. 0) GO TO 207
        DO 40 I=1,260
        II = I
        IF (LABL(I,1) .EQ. 0) GO TO 50
40      CONTINUE
50      LABLEN = II-1
C       Find end of LABL ARRAY
        IF (LABLEN+LENM .GT. 260) THEN
           IERR = 49
           RETURN
        ENDIF
C       Bounds problem with LABL array
        DO 206  I=LABLEN+1,LABLEN+LENM
C       Copy markers to end of present marker array
        IF (IFLIP .NE. 5 ) GO TO 406
        LABL(I,1)=-CONNEC(J)+2*ABX-DX
        LABL(I,2)=-CONNEC(J+1)+2*ABY-DY
        MRKCHN(I)=CONNEC(J+2)
        GO TO 407
406     LABL(I,1)=((CONNEC(J)-ABX)*KCOS(IFLIP)+(CONNEC(J+1)-ABY)
     1  *KSIN(IFLIP))+ABX-DX
        LABL(I,2)=((CONNEC(J)-ABX)*KSIN(IFLIP)-(CONNEC(J+1)-ABY)
     2  *KCOS(IFLIP))+ABY-DY
        MRKCHN(I)=CONNEC(J+2)
407     J=J+3
206     CONTINUE
207     IF (LLLEN .EQ. 0) GO TO 2088
C Set up LNGBND
        DO 209 I=1,LLLEN
        IF (IFLIP .NE. 5) GO TO 607
        LNGBND(I,1)=-CONNEC(J)+2*ABX-DX
        LNGBND(I,2)=-CONNEC(J+1)+2*ABY-DY
        LNGBND(I,3)=-CONNEC(J+2)+2*ABX-DX
        LNGBND(I,4)=-CONNEC(J+3)+2*ABY-DY
        GO TO 608
607     LNGBND(I,1)=((CONNEC(J)-ABX)*KCOS(IFLIP)+
     1  (CONNEC(J+1)-ABY)*KSIN(IFLIP))+ABX-DX
        LNGBND(I,2)=(CONNEC(J)-ABX)*KSIN(IFLIP)-
     1  (CONNEC(J+1)-ABY)*KCOS(IFLIP)+ABY-DY
        LNGBND(I,3)=((CONNEC(J+2)-ABX)*KCOS(IFLIP)+
     1  (CONNEC(J+3)-ABY)*KSIN(IFLIP))+ABX-DX
        LNGBND(I,4)=(CONNEC(J+2)-ABX)*KSIN(IFLIP)-
     1  (CONNEC(J+3)-ABY)*KCOS(IFLIP)+ABY-DY
608     LNGBND(I,5)=CONNEC(J+4)
        J=J+5
209     CONTINUE
2088    IF (LENC .EQ. 0) GO TO 2081
C Do charges if there are any
        DO 2000 I=1,LENC
        IF (IFLIP .NE. 5) GO TO 309
        TX=-CONNEC(J)+2*ABX-DX
        TY=-CONNEC(J+1)+2*ABY-DY
        GO TO 310
309     TX=((CONNEC(J)-ABX)*KCOS(IFLIP)+(CONNEC(J+1)-ABY)*KSIN(IFLIP))
     1  +ABX-DX
        TY=((CONNEC(J)-ABX)*KSIN(IFLIP)-(CONNEC(J+1)-ABY)*KCOS(IFLIP))
     1  +ABY-DY
310     IF (TX .GT. 0 .AND. TX .LE. MAXX .AND. TY .GT. 0
     1  .AND. TY .LE. MAXY) GO TO 2011
5555    IERR=48
C We found a bounds problem
        RETURN
2011    CONTINUE
        KAR=CONNEC(J+2)
C Get sign of charge
        NCHRG=CONNEC(J+3)
C Get digit associated with charge
        CALL ZHARGE(KAR,TX,TY,NCHRG,IERR)
        IF (IERR .NE. 0) GO TO 5555
        J=J+4
2000    CONTINUE
2081    IF (LEND.EQ.0) GO TO 208
        DO 1205 I = 1,LEND
```

```
         IF (IFLIP.EQ.5) THEN
            TX = -CONNEC(J)+ 2*ABX - DX
            TY = -CONNEC(J+1) + 2*ABY - DY
         ELSE
            TX = ((CONNEC(J)-ABX)*KCOS(IFLIP)+(CONNEC(J+1)-ABY)*
     *         KSIN(IFLIP)) + ABX - DX
            TY = -((CONNEC(J)-ABX)*KSIN(IFLIP)+(CONNEC(J+1)-ABY)*
     *         KCOS(IFLIP)) + ABY - DY
         ENDIF
         IF ((TX.GT.0).AND.(TY.LE.MAXX).AND.(TY.GT.0).AND.(TY.LE.
     *      MAXY)) GO TO 1202
5556     IERR = 1
         RETURN
1202     KAR = 34
         IDRAW = 1
         CALL IND1(KAR,TX,TY,IDRAW,IERR)
         IF (IERR.NE.0) GO TO 5556
         J = J + 2
1205  CONTINUE
208   CONTINUE
      RETURN
      END
C
C     SUBROUTINE CLRPIX(A,LB)
C
C     THIS WILL CLEAR THE PICTURE ARRAYS - MM &  LNGBND
C                               OR  - IDTPIX & LLBOND
      SUBROUTINE CLRPIX(WHICH)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM,IDTPIX
      COMMON /CD/ MAXX,MAXY
      COMMON /RANGE/ LOX,HIX,LOY,HIY
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
      COMMON /TEMP/ LLBOND(100,5),LLABL(260,2),MCHN(260)
C
      IF (WHICH.EQ.1) THEN
         DO 10 I = LOX,HIX
         DO 10 J = LOY,HIY
10       MM(I,J)=0
         DO 12 I=1,100
         IF (LNGBND(I,1).EQ.0) GO TO 30
         DO 12 J=1,5
12       LNGBND(I,J)=0
      ELSE IF (WHICH.EQ.2) THEN
      DO 20 I = LOX,HIX
      DO 20 J = LOY,HIY
20       IDTPIX(I,J)=0
         DO 22 I=1,100
         IF (LLBOND(I,1).EQ.0) GO TO 30
         DO 22 J=1,5
22       LLBOND(I,J)=0
      ENDIF
30    CONTINUE
      RETURN
      END
C
C     SUBROUTINE ADDLNG(MCNT,LLLEN)
C
C     Move the new longbonds to the end of the temporary longbond
C     array LLBOND - Then copy LLBOND back to LNGBND
C     This must be done because the new longbonds must be at the
C     end for longbond delete to work correctly
C
      SUBROUTINE ADDLNG(MCNT,LLLEN)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /TEMP/ LLBOND(100,5),LLABL(260,2),MCHN(260)
      IF (LLLEN .EQ. 0) GO TO 100
      FIRST=MCNT+1
      K=1
      DO 10 I=FIRST,FIRST+LLLEN-1
         DO 11 J=1,5
            LLBOND(I,J)=LNGBND(K,J)
```

```
11          CONTINUE
            K=K+1
10       CONTINUE
100      IF ((MCNT + LLLEN) .EQ. 0) RETURN
         K=1
         DO 13 I=1,MCNT+LLLEN
            DO 12 J=1,5
               LNGBND(I,J)=LLBOND(K,J)
12       CONTINUE
         K=K+1
13       CONTINUE
         LBLEN = MCNT + LLLEN
         RETURN
         END
C
C        SUBROUTINE ADDBCK
C
C        Add old picture (stored in IDTPIX) to new picture (stored in MM)
         SUBROUTINE ADDBCK
         IMPLICIT INTEGER*2 (A-Z)
         INTEGER*4 MM,IDTPIX
         COMMON /CD/ MAXX,MAXY
         COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
         COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
         COMMON /RANGE/ LOX,HIX,LOY,HIY
         DO 10 I = LOX,HIX
         DO 10 J = LOY,HIY
10       MM(I,J)=MM(I,J)+IDTPIX(I,J)
         RETURN
         END
C
C        SUBROUTINE SHIFT(A,B,C,D,E,F,G,H,MCNT,LCNT)
C
C        THIS SUBROUTINE SHIFTS ARRAYS A TO B
C                          C TO D AND E TO F UNTIL 0 ENTRY IS FOUND IN C
C                          G TO H UNTIL 0 ENTRY FOUND
C        MCNT = COUNT OF MARKERS MOVED
C        LCNT = COUNT OF LONGBONDS MOVED
C
         SUBROUTINE SHIF(WHICH,MCNT,LCNT)
         IMPLICIT INTEGER*2 (A-Z)
         INTEGER*4 MM,IDTPIX
         COMMON /CD/ MAXX,MAXY
         COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
         COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
         COMMON /TEMP/ LLBOND(100,5),LLABL(260,2),MCHN(260)
         COMMON /RANGE/ LOX,HIX,LOY,HIY
         IF (WHICH.EQ.1) THEN
         DO 10 I = LOX,HIX
         DO 10 J = LOY,HIY
10          IDTPIX(I,J) = MM(I,J)
C           Move A to B
            DO 11 I=1,260
               IF (LLABL(I,1).EQ.0) GO TO 14
               DO 12 J=1,2
12             LLABL(I,J)=0
C              Clear D and F
               MCHN(I)=0
11          CONTINUE
14          CONTINUE
            DO 13 I=1,260
               II = I
               IF (LABL(I,1) .EQ. 0) GO TO 20
C              Move C to D and E to F until 0 entry is found in C
               LLABL(I,1) = LABL(I,1)
               LLABL(I,2) = LABL(I,2)
               MCHN(I) = MRKCHN(I)
13          CONTINUE
20          MCNT = II-1
C           MCNT = # of markers moved
            DO 50 I=1,100
            IF (LLBOND(I,1).EQ.0) GO TO 51
            DO 50 J=1,5
50          LLBOND(I,J)=0
51          CONTINUE
```

```
C         Move G to H until 0 entry is found in G
          DO 35 I=1,100
          II = I
          IF (LNGBND(I,1) .EQ. 0) GO TO 40
          DO 35 J=1,5
             LLBOND(I,J) = LNGBND(I,J)
35        CONTINUE
40        LCNT = II - 1
C         LCNT = # of longbonds moved
       ELSE IF (WHICH.EQ.2) THEN
          DO 100 I = LOX,HIX
          DO 100 J = LOY,HIY
100       MM(I,J) = IDTPIX(I,J)
C         Move A to B
          DO 110 I=1,260
             IF (LABL(I,1).EQ.0) GO TO 111
             DO 120 J=1,2
120          LABL(I,J)=0
C            Clear D and F
             MRKCHN(I)=0
110       CONTINUE
111       CONTINUE
          DO 130 I=1,260
             II = I
             IF (LLABL(I,1) .EQ. 0) GO TO 200
C            Move C to D and E to F until 0 entry is found in C
             LABL(I,1) = LLABL(I,1)
             LABL(I,2) = LLABL(I,2)
             MRKCHN(I) = MCHN(I)
130       CONTINUE
200       MCNT = II - 1
C         MCNT = # of markers moved
          DO 500 I=1,100
          IF (LNGBND(I,1).EQ.0) GO TO 501
          DO 500 J=1,5
500       LNGBND(I,J)=0
501       CONTINUE
C         Move G to H until 0 entry is found in G
          DO 350 I = 1,100
             II = I
             IF (LLBOND(I,1) .EQ. 0) GO TO 400
             DO 350 J=1,5
                LNGBND(I,J) = LLBOND(I,J)
350       CONTINUE
400       LCNT = II - 1
C         LCNT = # of longbonds moved
       ENDIF
       RETURN
       END
C
C
C      SUBROUTINE ZAP(IX,IY)
C
C      THIS SUBROUTINE WILL ERASE SCREEN LOCATION IX,IY
       SUBROUTINE ZAP(IX,IY)
       IMPLICIT INTEGER*2 (A-Z)
       INTEGER*4 MM,IDTPIX
       COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
       COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
       COMMON /HP/IHP
       COMMON /CUR/ ICUR
          ICUR = 0
          CALL CURSOR(IX,IY)
          LL = LMM(IX,IY)
          IF ((LL.GE.256).AND.(MOD(IDIR(LL),4).NE.3)) THEN
             FX = IX - 1
       IF (IHP .EQ. 1) THEN
   CALL BERASE(IX,IY)
   ELSE
        CALL FTLOCA(IY,FX)
        CALL FTEXT('^   ^')
   ENDIF
        IF ((MM(FX,IY).NE.0).OR.(IDTPIX(FX,IY).NE.0))
*          CALL REPLCE(FX,IY,1,1,0,0,0)
```

```
         FX = IX + 1
         IF ((MM(FX,IY).NE.0).OR.(IDTPIX(FX,IY).NE.0))
*           CALL REPLCE(FX,IY,1,1,0,0,0)
      ELSE
         CALL FTLOCA(IY,IX)
         CALL FTEXT('^ ^')
      ENDIF
      IF ((MM(IX,IY).EQ.46).OR.(LL.GE.256).OR.
*        ((MM(IX,IY).GE.50).AND.(MM(IX,IY).LE.57).AND.
*        (LMM(IX-1,IY).NE.43).AND.(LMM(IX-1,IY).NE.45)).OR.
*        (MM(IX,IY).EQ.103).OR.(MM(IX,IY).EQ.106).OR.(MM(IX,IY).EQ
*        .112).OR.(MM(IX,IY).EQ.113).OR.(MM(IX,IY).EQ.121).OR.
*        (MM(IX,IY).EQ.95)) THEN
         IF (MOD((IY*10),40).EQ.0) THEN
            IF ((IY.EQ.8).OR.(IY.EQ.28).OR.(IY.EQ.16)) THEN
               FY = ((IY * 10) / 11) + 1
               CALL FTSIZE(1,11)
            ELSE
               FY = ((IY * 10) / 9) + 1
               CALL FTSIZE(1,9)
            ENDIF
         ELSE
            FY = ((IY * 10) / 8) + 1
            CALL FTSIZE(1,8)
         ENDIF
         IF ((LL.GE.256).AND.(MOD(IDIR(LL),4).NE.3)) THEN
            FX = IX - 1
          IF (IHP .EQ. 1) THEN
          CALL BERASE(IX,IY)
          ELSE

            CALL FTLOCA(FY,FX)
            CALL FTEXT('^    ^')
            CALL FTSIZE(1,10)
          ENDIF
            FY = IY - IHP
            IF ((MM(FX,FY).NE.0).OR.(IDTPIX(FX,FY).NE.0))
*              CALL REPLCE(FX,FY,1,1,0,0,0)
            IF ((MM(IX,FY).NE.0).OR.(IDTPIX(IX,FY).NE.0))
*              CALL REPLCE(IX,FY,1,1,0,0,0)
            FX = IX + 1
            IF ((MM(FX,FY).NE.0).OR.(IDTPIX(FX,FY).NE.0))
*              CALL REPLCE(FX,FY,1,1,0,0,0)
         ELSE
   IF (IHP .EQ. 1) THEN
   CALL ERASE(IX,IY)
   ELSE
            CALL FTLOCA(FY,IX)
            CALL FTEXT('^ ^')
            CALL FTSIZE(1,10)
   ENDIF
            FY = IY - IHP
            IF ((MM(IX,FY).NE.0).OR.(IDTPIX(IX,FY).NE.0))
    *                CALL REPLCE(IX,FY,0,0,0,0,0)
              ENDIF
           ENDIF
           IF ((LL.GE.256).AND.(MOD(IDIR(LL),4).NE.3)) THEN
              MM(IX,IY) = 0
              FY = IY - 1
              CALL REPLCE(IX,FY,1,1,0,0,1)
              FY = IY + 1
              CALL REPLCE(IX,FY,1,1,0,0,1)
           ELSE
              MM(IX,IY) = 0
           ENDIF
         RETURN
         END
C
C
C        SUBROUTINE FIXMRK(A,B,C,D,MCNT)
C
C        This subroutine will zero array B and D and copy A to B
C        and C to D until a zero entry is found in A
C        It is used to tidy up the LABL and MRKCHN so that spurious
C        markers are not left in them after an unsuccessful RETRIEVE
C        attempt
```

```
      SUBROUTINE FIXMRK(WHICH,MCNT)
      IMPLICIT INTEGER*2(A-Z)
      INTEGER*4 IDTPIX
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
      COMMON /TEMP/ LLBOND(100,5),LLABL(260,2),MCHN(260)
      IF (WHICH.EQ.1) THEN
         DO 10 I=1,260
            LLABL(I,1) = 0
            LLABL(I,2) = 0
            MCHN(I)=0
10       CONTINUE
         DO 11 I=1,260
            II = I
            IF (LABL(I,1) .EQ. 0) GO TO 20
            LLABL(I,1) = LABL(I,1)
            LLABL(I,2) = LABL(I,2)
            MCHN(I) = MRKCHN(I)
11       CONTINUE
20       MCNT= II - 1
      ELSE
         DO 100 I=1,260
            LABL(I,1) = 0
            LABL(I,2) = 0
            MRKCHN(I)=0
100      CONTINUE
         DO 110 I=1,260
            II = I
            IF (LABL(I,1) .EQ. 0) GO TO 200
            LABL(I,1) = LLABL(I,1)
            LABL(I,2) = LLABL(I,2)
            MRKCHN(I) = MCHN(I)
110      CONTINUE
200      MCNT = II-1
      ENDIF
      RETURN
      END
C
C     SUBROUTINE SYNCH(KAR,KX,KY)
C
C     This subroutine adjusts the cursor (initially positioned at KX,KY) so
C     positioned at a node or at the end of a bond. It sets the
C     argument variable KAR and the COMMON variables ICHAR and JCHAR to refl
C     (just drew a bond - or - just entered a node) If cursor
C     can't be positioned at a nearby node or bond, the cursor
C     position will be moved to a 3X3 empty space  and JCHAR and ICHAR,
C     will be set to 0 and KAR will be set to 13 (i.e. CR)
      SUBROUTINE SYNCH(KAR,KX,KY)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
      COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
      COMMON /CD/ MAXX,MAXY
      COMMON /RANGE/ LOX,HIX,LOY,HIY
C
      KAR=13
      ICHAR=0
      JCHAR=0
C     First check that X and Y are in bounds
      IF (KX .GT. 0 .AND. KX .LE. MAXX .AND. KY .GT. 0 .AND. KY
     1  .LE. MAXY) GO TO 710
C     Bounds problems
      KX=10
C     Set X and Y to valid coordinates and then move cursor
      KY=10
C     to clear area and exit
710   CALL NEW(IGOOD,KX,KY)
C     See if we are at A 3x3 empty area
      IF (IGOOD .NE. 0) GO TO 70
      CALL CURSOR(KX,KY)
      RETURN
C     If so return with  KAR=13 ICHAR=0 JCHAR=0
70    L=LMM(KX,KY)
      IF (L .NE. 0) GO TO 10
C
C     Cell is empty
```

```
C
      IIBDIR = IBDIR
      CALL FINDB(IIBDIR,KBDIR,KX,KY)
      IBDIR = IIBDIR
C     Are we at the end of a bond?
      IF (IBDIR .EQ. -1) GO TO 20
C
C     We're at the end of a bond
C
      ICHAR = 1
      CALL MKBND(KBDIR)
C     Convert bond direction to bond command
      KAR=KBDIR
C              (22-25;28-31)
      GO TO 100
C
C     Cell was empty, but we weren't at a bond
C     Look alternately left and right 3 times for non empty cell
C     Then give up and RETURN with parameters ICHAR & JCHAR set to zero & cursor at
C     a 3X3 empty area and KAR=13
20    IX=KX
          DO 30 I=1,3
          DO 35 J=1,2
          IF (J .EQ. 1) THEN
             EDIR = -1
          ELSE
             EDIR = 1
          ENDIF
          KX = IX + EDIR * I
CXT
          IF ((KX.LE.0).OR.(KX.GT.MAXX)) GO TO 35
CXT
          L=LMM(KX,KY)
          IF ( L .NE. 0) GO TO 10
35        CONTINUE
30        CONTINUE
C         Cells to left are empty and cells to right are empty - give up
C         Set cursor to 3X3 empty area and exit
          GO TO 500
C
C         Cell was not empty - What kind is it?
C
10        IF (L .GE. 256 .AND. (MM(KX-1,KY) .NE. 0) .AND.
     1    (LMM(KX-1,KY) .LT. 256)) KX=KX-1
C         If cell holds bond and cell to left is not empty and not a bond
C         shift pointer to left for it is likely to be our node
          IF (LMM(KX,KY) .LT. 256) GO TO 25
C        It should be a node - go see if it is
C         Cell to left of bond is empty or a bond - trace bond to end
C
          IIBDIR = IBDIR
          CALL BSLIDE(KX,KY,IIBDIR)
          IBDIR = IIBDIR
C
C         If we couldn't find the end of the bond - give up
C         Return with cursor at 3X3 empty area and parameters
C         set to zero
C
          IF (IBDIR .EQ. -1) GO TO 500
C
C         If we traced bond to end and found a blank at the end - then
C         set parameters and ICHAR and KAR and prepare to exit
C
          IF (MM(KX,KY) .NE. 0) GO TO 25
          ICHAR=1
          IIBDIR = IBDIR
          CALL MKBND(IIBDIR)
          IBDIR = IIBDIR
          KAR=IBDIR
C         KAR = bond command
          GO TO 100
C
C         We are near a node  -  Find correct X position for cursor
C
25        CALL FNODEB(KX,KY,JX)
```

```
        IF (JX .EQ. 0) GO TO 500
C       Can't find X position for node - give up
        KX=JX
C       KX = correct X position for cursor
        KAR=LMM(KX-1,KY)
        ICHAR=2
C       Set ICHAR to "we just entered a node"
C
C       We found node or bond - set cursor and parameters and RETURN
C
100     CALL CURSOR(KX,KY)
        JCHAR=ICHAR
        MCHAR=KAR
        RETURN
C
C       We couldn't find the node or bond so we are going to
C       place the cursor at an empty 3X3 area
C
500     I1=MIN0(KX,(MAXX-1))
        J1=MIN0(KY,(MAXY-1))
        DO 501 I=I1,MAXX-1
        II = I
C       NOTE - I LOOK FOR A 3x3 EMPTY CELL
        DO 501 J=J1,MAXY-1
        JJ = J
C       NEAR THE CURRENT X,Y POSITION
        CALL NEW(IGOOD,II,JJ)
        IF (IGOOD .EQ. 0) GO TO 502
501     CONTINUE
502     KX=II
        KY=JJ
        CALL CURSOR(KX,KY)
        RETURN
        END
C
C       SUBROUTINE FNODE(IX,IY,KX,IDIR)
C
C
C       This subroutine will look for a node in the MM array
C       starting with loc IX, IY and looking left 3 spaces if IDIR = -1
C       and looking right 3 spaces if IDIR = 1
C       Output is KX which is the proper X coordinate for the node
        SUBROUTINE FNODE (IX,IY,KX,EDIR)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        IEND = EDIR * 3
        IDELTA = EDIR
        KX=0
C
C       An empty cell or a bond containing cell causes ABORT with KX = 0
C
        IF (MM(IX,IY) .EQ. 0 .OR. LMM(IX,IY) .GT. 256) RETURN
        DO 10 I=0,IEND,IDELTA
        II = I
        M=LMM(IX+I,IY)
        MP1=LMM(IX+I+1,IY)
        IF (M .EQ. 63 .OR. M .EQ. 46) GO TO 11
C       Is it a ? or a FAT DOT?
        IF (M .GE. 65 .AND. M .LE. 90 .AND. M .NE. 72) GO TO 11
C       Is it a non-H UC letter?
        IF (M.EQ.72 .AND.(MP1.GE.97 .AND. MP1.LE.122)) GO TO 11
C       Is it a H followed by a lower case letter?
10      CONTINUE
        RETURN
C       Didn't find it - Return with KX = 0
11      KX = IX + II + 1
C       Position X correctly
        RETURN
        END
C
C       Subroutine FNODEB(IX,IY,KX)
C
C       This subroutine will look for a node by first looking in the 3 spaces to th
C       left of MM(IX,IY) - If that is not successful - it will then
```

```
C       look in the 3 spaces to the right
C       If that is not successful - it will abort with KX=0
        SUBROUTINE FNODEB(IX,IY,KX)
        IMPLICIT INTEGER*2 (A-Z)
        EDIR = -1
        CALL FNODE(IX,IY,KX,EDIR)
        IF (KX .NE. 0) RETURN
        EDIR = 1
        CALL FNODE(IX,IY,KX,EDIR)
        RETURN
        END
C
C       SUBROUTINE BSLIDE(IX,IY,IBDIR)
C
C       This subroutine finds the end of the bond passing through MM(IX,IY)
C       Inputs to this subroutine are the X and Y coordinates of the bond in MM
C       If the end of the bond is found IX and IY are set to the cell
C       just beyond the end of the bond in the bond direction
C       If not, IX and IY are not changed
C       If the end of the bond can't be found IBDIR is set to -1
C       If the end is found, IBDIR is set to the bond direction
        SUBROUTINE BSLIDE(IX,IY,IBDIR)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /CD/ MAXX,MAXY
C
        KX=IX
        KY=IY
        L=LMM(IX,IY)
        IBDIR=IDIR(L)
C       L=bond direction
        CALL DELTA(IBDIR,INCX,INCY)
C       Get deltas for bond
        DO 10 I=1,100
        IX=IX+INCX
        IY=IY+INCY
        IF (IX.LE.0 .OR. IX.GT.MAXX .OR. IY.LE.0 .OR. IY.GT.MAXY)
      1 GO TO 100
C       Are coordinates out of bounds?
        IF (LMM(IX,IY) .LT. 256) RETURN
C       Found end of bond - RETURN
10      CONTINUE
100     IBDIR=-1
C       Couldn't find end of bond - Set coordinates to 0 and RETURN
        IX=KX
C       Reset X and Y to their values at time of input
        IY=KY
        RETURN
        END
C
C       SUBROUTINE FINDXY(IX,IY,KX,KY,DX,DY,ABX,ABY,IROT,IFLIP,SYM)
C
C       This subroutine calculates the appropriate X and Y values
C       using the appropriate translation, rotation and reflection
C       operators
C
C       Input is KX and KY - the unoperated coordinates
C             DX and DY - the translation values
C             ABX & ABY - the coordinates of the end of the attaching bond
C             IROT      - indicates what rotation, if any, is necessary
C             IFLIP     - indicates what reflection, if any, is necessary
        SUBROUTINE FINDXY(IX,IY,KX,KY,DX,DY,ABX,ABY,IROT,IFLIP,SYM)
        IMPLICIT INTEGER*2  (A-Z)
        DIMENSION KSIN(4),KCOS(4)
        DATA KSIN/0,1,0,-1/
        DATA KCOS/1,0,-1,0/
C
        IF ((SYM.EQ.2).OR.((SYM.EQ.1).AND.(IFLIP.EQ.-1))) GO TO 100
        IF (IFLIP .NE. 5) GO TO 200
        IX=-KX+2*ABX-DX
        IY=-KY+2*ABY-DY
        RETURN
C
C       We need to do a reflection
C
```

```
 200    IX=(KX-ABX)*KCOS(IFLIP)+(KY-ABY)*KSIN(IFLIP)+ABX-DX
 .      IY=(KX-ABX)*KSIN(IFLIP)-(KY-ABY)*KCOS(IFLIP)+ABY-DY
        RETURN
 C
 C      We need to do a rotation
 C
 100    IX=(KX-ABX)*KCOS(IROT) + (KY-ABY)*KSIN(IROT) + ABX-DX
        IY=-(KX-ABX)*KSIN(IROT)+(KY-ABY) * KCOS(IROT) + ABY -DY
        RETURN
        END
 C
 C      SUBROUTINE LOOKR(IX,IY,MM,ICHECK,IBADX,IBADY,LAP,LCNT,BLOB)
 C
 C      THIS SUBROUTINE CHECKS A 3 x 3 CELL CENTERED AT IX & IY
 C      ICHECK = 0      THAT IS OK - IF
 C
 C                                       1. THE MM SUBSCRIPTS ARE GOOD
 C                                       2. THE CELL IS EMPTY - OR - THE
 C                                          COLLISIONS ARE VALID COLLISIONS
 C      ICHECK NOT = 0 MEANS THAT BAD CONFLICTS AROSE
 C
        SUBROUTINE LOOKR(IX,IY,ICHECK,LCNT,BLOB)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,IDTPIX,WHAT,A
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /BAD/ IBADX(9),IBADY(9)
        COMMON /LAPE/ LAP(5,2)
        COMMON /CD/ MAXX,MAXY
        ICHECK=0
 C      Cell is OK until proven otherwise
        CALL CHECK(IX,IY,ICHECK)
 C      Check IDTPIX subscripts
 777    IF (ICHECK .EQ.1) GO TO 10
 C      Bad subscripts - set error and return
        WHAT = IDTPIX(IX,IY)
        IF (WHAT .NE. 0) GO TO 10
 C      Space is occupied - set error and return
        CALL CELL2(IX,IY,ICHECK)
 C      Space is empty - check surrounding area
        IF (ICHECK .EQ. 0) RETURN
 C      No problem - good cell - ICHECK = 0 and return
        DO 982 I=1,ICHECK
        DO 980 J=1,LCNT
        IF (IBADX(I).EQ.LAP(J,1) .AND. IBADY(I).EQ.LAP(J,2)) GO TO 982
 980    CONTINUE
        A = IDTPIX(IBADX(I),IBADY(I))
 C      Was it a legal collision?  Was it a legal overlap - i.e.
 C      bond - not pointing to cell or cell would contain bond
 C      and overlap is node and cell bond does not point to node
 C      A = contents of offending cell
        IF ((BLOB.EQ.43).OR.(BLOB.EQ.45).OR.(A.EQ.43).OR.(A.EQ.45))
      *    GO TO 10
 C      If it is a collision with a charge - it is bad
        IF (BLOB .LT. 46) GO TO 20
 C      Blob is a node
        IF (A .GE. 256) GO TO 11
 C      A is a bond - is it an OK bond
        B=BLOB
        CALL DELTA(B,INCX,INCY)
 C      Cell will contain bond - does it point to node
        IF (((IBADX(I).EQ.(IX+INCX)).AND.(IBADY(I).EQ.(IY+INCY)))
      1 .OR.((IBADX(I).EQ.(IX-INCX)).AND.(IBADY(I).EQ.(IY-INCY))))
      2 GO TO 10
 C      If bond points to node - it is no good
        GO TO 982
 C      If not - it is OK
 20     IF (A .LT. 256) GO TO 10
 C      Not a bond - can't be OK
 11     B=IDIR(A)
 C      Get bond direction
        CALL DELTA(B,INCX,INCY)
```

```
C       Get bond deltas
        IF((((IBADX(I)+INCX).EQ. IX) .AND.((IBADY(I)+INCY).EQ.IY))
     1  .OR. (((IBADX(I)-INCX).EQ.IX).AND.((IBADY(I)-INCY).EQ.IY)))
     2  GO TO 10
C       If it points to bond or node - it is no good
982     CONTINUE
        ICHECK=0
C       Overlap was valid - cell OK
        RETURN
C       Valid overlap - return
10      ICHECK=1
        RETURN
C       Bad overlap - return with error set
        END
C
        SUBROUTINE CKNOD2(I,J,IVAL,IERR)
        IMPLICIT INTEGER*2(A-Z)
        INTEGER*4 MM
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        IERR=0
        IVAL=LMM(I,J)
        IF (IVAL .LT. 97 .OR. IVAL .GT. 122) RETURN
        IVALL=LMM(I-1,J)
        IF (IVALL .GE. 65 .AND. IVALL .LE. 90) RETURN
        IERR=1
        RETURN
        END
C
        SUBROUTINE VLNCE(II,IX,IY,INCX,INCY,IERR)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,IDTPIX
        LOGICAL*2 PNODE,VNODE
        CHARACTER*1 HALO(3)
        CHARACTER*1 KAN
        COMMON /ELECHR/ IELEM(126,5)
        COMMON /CD/ MAXX,MAXY
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
C       MM(I,J) CONTAINS BOND OR ATOM TYPE, & BOND DIRECTION
C       FOR EACH OF MAXX * MAXY LOCATIONS.
        COMMON /CHARS/IES, IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /PARAMS/ JBDIR,NOCHG,LASTN,MCHAR,JCHAR,NLARGE,LEVEL
        COMMON /MODES/ JBTYPE,ICHAR,IBDIR,IBTYPE,ISMART,MODE,ISKILL,ISP
        COMMON /PROB/ IPROB,JPROB
        COMMON /IPLUS/ IHIGH(14,2)
        COMMON /LABELS/ NR,LJLAST,NJNEXT
        COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
        COMMON /QTVLNC/ OERR,CHER
        COMMON /HP/IHP
CXT
CXT     PNODE = TRUE is passed by SUBROUTINE GETIT if only array MM need
CXT     be searched for nodal adjacency.  DELH is assigned the attached
CXT     node's hydrogen information so it can be had for any subsequent
CXT     substructure deletion.  VNODE = TRUE indicates the substructure
CXT     is being drawn by the VIEW SECTION of SUBROUTINE GETIT.
        COMMON /VALH/ PNODE,DELH(2,3),VNODE
        COMMON /CUR/ ICUR
C
        ICUR = 0
        HALO(1) = KAN
        HALO(3) = KAN
        MAR=0
C Filler atoms not triggered by bond.
        IF (II.GT.2) GO TO 1000
C Look at grid space BEFORE bond.
        JX=IX-(NLARGE+1)*INCX
C (NLARGE+1) removes incrementing done in DRAW.
        JY=IY-(NLARGE+1)*INCY
        IF (II.LT.2) GOTO 23
C If overdrawing an existing bond, II=2.
        JX=IX-INCX
        JY=IY-INCY
C If to right of element, skip back over lower case second letter:
23      IF ((MM(JX,JY).GT.96) .AND. (MM(JX,JY).LT.123)) JX=JX-1
C If bond didn't originate at a (non-dot) node (i.e. cap letter), return
```

```
      IF(MM(JX,JY).EQ.46) GO TO 63
      IF ((MM(JX,JY).LT.65) .OR. (MM(JX,JY).GT.90)) RETURN
      GO TO 87
C IS THIS A MARKER OR FAT DOT
63    DO 64 I=1,NJNEXT
      IF(JX .EQ. LABL(I,1) .AND. JY .EQ. LABL(I,2))RETURN
64    CONTINUE
      MAR=1
C IF FAT DOT SET PARAMS FOR CARBON
      LET1=67
      LET2=0
      IELT=1
      GO TO 800
C First letter of symbol
87    LET1=LMM(JX,JY)
      LET2=0
C Second letter, if 2-letter symbol
      IF ((MM(JX+1,JY).GE.97) .AND. (MM(JX+1,JY).LE.122))
     2         LET2=MM(JX+1,JY)
C Dont check H2,ETC
      IF((LET1.EQ.72) .AND. (LET2.EQ.0)) RETURN
C Count of OCCUPIED valence positions
      IVALNC=0
C Element number of node at JX,JY
      IELT=0
C
C Search for element in element table
            DO 1 I=1,125
            IF ((LET1.NE.IELEM(I,1)) .OR. (LET2.NE.IELEM(I,2)))
     2               GOTO 1
C Records row number of correct element
            IELT=I
C No valence in table
            IF (IELEM(IELT,3).EQ.0) RETURN
            GOTO 2
1           CONTINUE
C
2     IF (IELT.NE.0) GO TO 800
C ELEMENT NOT FOUND - ISSUE MESSAGE AND CONTINUE
      IERR=11
      CALL MYERR(IERR,LET1,LET2)
C BEWARE I DON'T KNOW ALL THE IMPLICATIONS OF THIS RETURN
      RETURN
C
C Now search around node for bonds, charges, for 'valence users'.
C
800   CONTINUE
C           where to put filler H's if there is room on both sides.
C     BEWARE - VAA MODIFIED LOOP 3 - THE MODIFICATION IS TO DETECT
C     CHARGES ON THE RIGHT DIAGONALS OF THE SECOND LETTER OF A 2
C     LETTER ELEMENT NAME
C Count of bonds 'used'.
      IVALNC=0
C search around node - LOOP CHANGED TO 2 BY VAA
      DO 3 IDIRX=-1,2
      DO 3 IDIRY=-1,1
      IF ((IDIRX.EQ.0) .AND. (IDIRY.EQ.0)) GOTO 3
      IF((IDIRX .EQ. 2) .AND. (IDIRY .EQ.0)) GO TO 3
C WE DON'T NEED TO CHECK THIS ONE
C WE WILL CATCH A CHARGE AT THIS LOCATION
C WHEN X=1 AND Y=0
C Nearby array location to look for bonds
      NEWX=JX + IDIRX
      NEWY=JY + IDIRY
C Off the edge
7     IF ((NEWX.LT.1) .OR. (NEWX.GT.MAXX)) GOTO 3
      IF ((NEWY.LT.1) .OR. (NEWY.GT.MAXY))  GOTO 3
C Blank space
      IF (MM(NEWX,NEWY).EQ.0) GOTO 3
C Bonds are >256
      IF (LMM(NEWX,NEWY).LT.256)  GOTO 4
C WE ARE ONLY LOOKING FOR CHARGES AT THIS PLACE - NOT BONDS
      IF (IDIRX .EQ. 2) GO TO 3
C Bond extracted for type
      JBOND=LMM(NEWX,NEWY)/2**8
C Following 5 lines skip bonds not pointed to node being analyzed:
```

```
C Direction of bond
        JDIR=LMM(NEWX,NEWY)-JBOND*2**8
        IF ((IDIRX*IDIRY.EQ.-1).AND.(MOD(JDIR,4).NE.2)) GOTO 3
        IF ((IDIRX*IDIRY.EQ.1).AND.(MOD(JDIR,4).NE.0)) GOTO 3
        IF ((IDIRX.EQ.0) .AND. (MOD(JDIR,4).NE.1)) GOTO 3
        IF ((IDIRY.EQ.0) .AND. (MOD(JDIR,4).NE.3)) GOTO 3
C Useful for bondtypes 1-3 others revised below
        IVAL = JBOND
C Stereo bonds are single.
        IF (JBOND.GT.3) IVAL=1
        IVALNC = IVALNC + IVAL
C Only if a valence-using bond is on this side.
        GOTO 3
C Charges
4       IF ((LMM(NEWX,NEWY).NE.43) .AND. (LMM(NEWX,NEWY).NE.45))GOTO 5
4444    LOC=IHMM(NEWX,NEWY)
        IFX=NEWX-IHIGH(LOC,1)
        IFY=NEWY+IHP*IHIGH(LOC,2)
C IS CHARGE ASSOCIATED WITH THIS NODE
        IF(JX.NE.IFX .OR.JY.NE.IFY) GO TO 5
C Set the sign from ASCII char
        ISIGN = 44 - LMM(NEWX,NEWY)
        IF ((MM(NEWX+1,NEWY).LT.50).OR.(MM(NEWX+1,NEWY).GT.57)) GOTO 6
C       Number of charges>1
        ISIGN = ISIGN * (LMM(NEWX+1,NEWY) - 48)
C       Correct # of valencies used for chg
6       IVALNC=IVALNC + IABS(ISIGN)
        ISIGN=0
C Only if a valence-using bond is on this side.
        GOTO 3
C
C H, lowercase, numerals, etc, keep looking
5       NEWX = NEWX + IDIRX
C H, lc, OR NUMERAL CAN'T
        IF (IDIRX .EQ. 0) GO TO 3
C CONTRIBUTE TO VALENCE IN THIS LOC
C BEWARE CHANGED BY VAA - TO FIX
C ENDLESS LOOP FOUND BY GREG
        GOTO 7
C Close loop of looking around each node.
3       CONTINUE
C
C Following code (through label 200) adds to IVALNC those bonds 'used'
C by long bonds:
C Beginning & ending nodes of long bond
        DO 200 I=0,2,2
C Up to 100 long bonds stored
        DO 201 J=1,100
C Done with this column of node
        IF (LNGBND(J,I+1).EQ.0) GOTO 200
C Check if current nodeJX,JY is listed as a node of a long bond:
        IF ((LNGBND(J,I+1).NE.JX) .OR. (LNGBND(J,I+2).NE.JY)) GOTO 201
C Use of valence from this long bond
        IVAL = 1
        IF (LNGBND(J,5).EQ.2) IVAL=2
        IF (LNGBND(J,5).EQ.3) IVAL=3
        IVALNC = IVALNC + IVAL
201     CONTINUE
200     CONTINUE
C
C Number of H's required at this node. Neg no for test
        IHYD=-7
C Elect smallest valence from IELEM which would satisfy all existing bonds.
                DO 10 M=3,5
C
                IF(IELEM(IELT,M).LT.IVALNC) GOTO 10
                IHYD = IELEM(IELT,M) - IVALNC
                GOTO 11
10              CONTINUE
C Now draw hydrogens
11      CONTINUE
        IF (IHYD.GE.0 .AND. MAR .EQ. 0)  GO TO 1000
        IF(IHYD .GE. 0 .AND. MAR .EQ. 1) RETURN
C TOO MANY BONDS FOR VALENCY
        IERR=12
        OERR = IERR
```

```
      CALL MYERR(IERR,IVALNC,KAR)
1000  CONTINUE
      IF (MM(JX,JY).EQ.46) RETURN
C
C Now look left & right to determine where filler atoms can fit:
C
C Done if no filler atoms needed.
      IF (IHYD) 111,111,30
C =1 means there IS room for H('s) on left
30    ILEFT=1
C similarly
      IRIGHT=1
C
C Look right to see if there is room for H('s):
C MX is first position to right of node.
      MX=JX+1
C Two-letter symbol
      IF (LET2.GT.0) MX=JX+2
C Number of chars needed for H('s):=1 or 2
      KHYD=1
      IF (IHYD.GT.1) KHYD = 2
CXT
C
C Edge of screen problems are checked.
      IF (MX+1.GT.MAXX) THEN
         DG = LMM(JX-KHYD,JY)
         IF (((DG.LT.256).AND.(DG.GT.0)).OR.((DG.GE.256).AND.
     *      (MOD(IDIR(DG),4).NE.3))) GO TO 9394
         IF (.NOT.PNODE) THEN
            DG = MOD(IDTPIX(JX-KHYD,JY),2**13)
            IF (((DG.LT.256).AND.(DG.GT.0)).OR.((DG.GE.256).AND.
     *         (MOD(IDIR(DG),4).NE.3))) GO TO 9394
         ENDIF
         GO TO 42
      ELSE IF (JX-2.LT.1) THEN
         DG = LMM(JX+KHYD,JY)
         IF (((DG.LT.256).AND.(DG.GT.0)).OR.((DG.GE.256).AND.
     *      (MOD(IDIR(DG),4).NE.3))) GO TO 9394
         IF (.NOT.PNODE) THEN
            DG = MOD(IDTPIX(JX+KHYD,JY),2**13)
            IF (((DG.LT.256).AND.(DG.GT.0)).OR.((DG.GE.256).AND.
     *         (MOD(IDIR(DG),4).NE.3))) GO TO 9394
         ENDIF
         GO TO 43
      ENDIF
C
C     If CHER = 1, SUBROUTINE QUIT is converting chain markers to "C"s.
C     Check for bad bonds coming in on the left diagonals.
      L1 = LMM(MX-1,JY-1)
      L2 = LMM(MX-1,JY+1)
      IF (((L1.EQ.0).OR.((L1.GT.256).AND.(MOD(IDIR(L1),4).NE.0)))
     *   .AND.((L2.EQ.0).OR.((L2.GT.256).AND.(MOD(IDIR(L2),4).NE.
     *   2)))) GO TO 522
      IF (.NOT.PNODE) THEN
         L3 = LMM(MX-1,JY-1)
         L4 = LMM(MX-1,JY+1)
         IF (((L3.EQ.0).OR.((L3.GT.256).AND.(MOD(IDIR(L3),4).NE.0)))
     *      .AND.((L4.EQ.0).OR.((L4.GT.256).AND.(MOD(IDIR(L4),4).NE.
     *      2)))) GO TO 522
       ENDIF
       IRIGHT = 0
       GO TO 34
C
C The actual search-right algorithm loop.
522          DO 33 I=0,KHYD
                IF (((PNODE).AND.(MM(MX+I,JY).EQ.0)).OR.((.NOT.PNODE)
     *             .AND.(MM(MX+I,JY).EQ.0).AND.(IDTPIX(MX+I,JY).EQ.0)))
     *             THEN
                   GO TO 330
                ELSE IF ((LMM(MX+I,JY).LT.256).OR.((IDTPIX(MX+I,JY)
     *             .NE.0).AND.(.NOT.PNODE))) THEN
                   GO TO 400
                ENDIF
```

```
                ITEST=LMM(MX+I,JY)/256
                ITEST=LMM(MX+I,JY)-ITEST*256
C               CHECK FOR BOND IN LEFT OR RIGHT DIR
                IF (ITEST.EQ.3 .OR. ITEST.EQ.7) GO TO 330
C If non-blank or non-bond on right within
400             IRIGHT=0
C KHYD+1 to right of node, can't put H('s)there
                GOTO 34
330           CONTINUE
              L1 = LMM(MX+I,JY-1)
              L2 = LMM(MX+I,JY+1)
              L3 = LMM(MX+I,JY-1)
              L4 = LMM(MX+I,JY+1)
              IF ((PNODE).AND.(L1.EQ.0).AND.(L2.EQ.0)) GO TO 33
              IF ((.NOT.PNODE).AND.(L1.EQ.0).AND.(L2.EQ.0).AND.(L3.EQ.0)
     *          .AND.(L4.EQ.0)) GO TO 33
              IF (I.LE.2) THEN
                 IF ((L1.EQ.46).OR.((L1.GE.65).AND.(L1.LE.90))) GO TO 400
                 IF ((L2.EQ.46).OR.((L2.GE.65).AND.(L2.LE.90))) GO TO 400
              ENDIF
              IF ((I.EQ.KHYD).AND.(((L1.GT.256).AND.
     *           (MOD(IDIR(L1),4).EQ.2)).OR.((L2.GT.256)
     *           .AND.(MOD(IDIR(L2),4).EQ.0)))) GO TO 400
              IF ((KHYD.EQ.1).AND.(I.EQ.0).AND.((
     *           (L1.GE.256).AND.(MOD(IDIR(L1),4).EQ.1)).OR.(
     *           (L2.GT.256).AND.(MOD(IDIR(L2),4).EQ.1)))) GO TO 400
              IF ((KHYD.EQ.2).AND.(I.EQ.0).AND.((
     *           (L1.GE.256).AND.((MOD(IDIR(L1),4).EQ.1).OR.
     *           (MOD(IDIR(L1),4).EQ.0))).OR.(
     *           (L2.GT.256).AND.((MOD(IDIR(L2),4).EQ.1).OR.
     *           (MOD(IDIR(L2),4).EQ.2))))) GO TO 400
              IF ((KHYD.EQ.2).AND.(I.EQ.1).AND.((
     *           (L1.GE.256).AND.((MOD(IDIR(L1),4).EQ.1).OR.
     *           (MOD(IDIR(L1),4).EQ.2))).OR.(
     *           (L2.GT.256).AND.((MOD(IDIR(L2),4).EQ.1).OR.
     *           (MOD(IDIR(L2),4).EQ.0))))) GO TO 400
              IF (.NOT.PNODE) THEN
                 IF (I.LT.2) THEN
                    IF ((L3.EQ.46).OR.((L3.GE.65).AND.(L3.LE.90)))
     *                 GO TO 400
                    IF ((L4.EQ.46).OR.((L4.GE.65).AND.(L4.LE.90)))
     *                 GO TO 400
                 ENDIF
                 IF ((I.EQ.KHYD).AND.(((L3.GT.256).AND.
     *              (MOD(IDIR(L3),4).EQ.2)).OR.((L4.GT.256)
     *              .AND.(MOD(IDIR(L4),4).EQ.0)))) GO TO 400
                 IF ((KHYD.EQ.1).AND.(I.EQ.0).AND.((
     *              (L3.GE.256).AND.(MOD(IDIR(L3),4).EQ.1)).OR.(
     *              (L4.GT.256).AND.(MOD(IDIR(L4),4).EQ.1)))) GO TO 400
                 IF ((KHYD.EQ.2).AND.(I.EQ.0).AND.((
     *              (L3.GE.256).AND.((MOD(IDIR(L3),4).EQ.1).OR.
     *              (MOD(IDIR(L3),4).EQ.0))).OR.(
     *              (L4.GT.256).AND.((MOD(IDIR(L4),4).EQ.1).OR.
     *              (MOD(IDIR(L4),4).EQ.2))))) GO TO 400
                 IF ((KHYD.EQ.2).AND.(I.EQ.1).AND.((
     *              (L3.GE.256).AND.((MOD(IDIR(L3),4).EQ.1).OR.
     *              (MOD(IDIR(L3),4).EQ.2))).OR.(
     *              (L4.GT.256).AND.((MOD(IDIR(L4),4).EQ.1).OR.
     *              (MOD(IDIR(L4),4).EQ.0))))) GO TO 400
              ENDIF
33          CONTINUE
              IF (IRIGHT.EQ.1) GO TO 36
C Now look left to see if filler atoms can be put there:
C Look left for non-blank,non-bonds.
34            L1 = LMM(JX,JY-1)
              L2 = LMM(JX,JY+1)
              L3 = LMM(JX,JY-1)
              L4 = LMM(JX,JY+1)
              IF (((L1.EQ.0).OR.((L1.GT.256).AND.(MOD(IDIR(L1),4).NE.2)))
     *           .AND.((L2.EQ.0).OR.((L2.GT.256).AND.(MOD(IDIR(L2),4)
     *           .NE.0)))) GO TO 3441
              IF (.NOT.PNODE) THEN
                 L3 = LMM(JX,JY-1)
                 L4 = LMM(JX,JY+1)
```

```
          IF (((L3.EQ.0).OR.((L3.GT.256).AND.(MOD(IDIR(L3),4).NE.
     *       2))).AND.((L4.EQ.0).OR.((L4.GT.256).AND.(MOD(IDIR(L4)
     *       ,4).NE.0)))) GO TO 3441
        ENDIF
        ILEFT = 0
        GO TO 36
3441    DO 35 I=1,KHYD+1
          IF ((PNODE).AND.(MM(JX-I,JY).EQ.0)) GO TO 3555
          IF ((.NOT.PNODE).AND.(MM(JX-I,JY).EQ.0).AND.
     *       (IDTPIX(JX-I,JY).EQ.0)) GO TO 3555
          IF ((LMM(JX-I,JY).LT.256).OR.((IDTPIX(JX-I,JY).NE.0)
     *       .AND.(.NOT.PNODE))) GO TO 401
          ITEST=LMM(JX-I,JY)/256
          ITEST=LMM(JX-I,JY)-ITEST*256
          IF (ITEST.EQ.3 .OR. ITEST.EQ.7) GO TO 3555
401       ILEFT=0
          GOTO 36
3555    L1 = LMM(JX-I,JY-1)
        L2 = LMM(JX-I,JY+1)
        L3 = LMM(JX-I,JY-1)
        L4 = LMM(JX-I,JY+1)
        IF ((PNODE).AND.(L1.EQ.0).AND.(L2.EQ.0)) GO TO 35
        IF ((.NOT.PNODE).AND.(L1.EQ.0).AND.(L2.EQ.0).AND.(L3.EQ.0)
     *     .AND.(L4.EQ.0)) GO TO 35
        IF ((L1.EQ.46).OR.((L1.GE.65).AND.(L1.LE.90))) GO TO 401
        IF ((L2.EQ.46).OR.((L2.GE.65).AND.(L2.LE.90))) GO TO 401
        IF ((I.EQ.KHYD+1).AND.(((L1.GT.256).AND.
     *     (MOD(IDIR(L1),4).EQ.0)).OR.((L2.GT.256)
     *     .AND.(MOD(IDIR(L2),4).EQ.2)))) GO TO 401
        IF ((KHYD.EQ.1).AND.(I.EQ.1).AND.((
     *     (L1.GE.256).AND.(MOD(IDIR(L1),4).EQ.1)).OR.(
     *     (L2.GT.256).AND.(MOD(IDIR(L2),4).EQ.1)))) GO TO 401
        IF ((KHYD.EQ.2).AND.(I.EQ.2).AND.((
     *     (L1.GE.256).AND.((MOD(IDIR(L1),4).EQ.1).OR.
     *     (MOD(IDIR(L1),4).EQ.0))).OR.(
     *     (L2.GT.256).AND.((MOD(IDIR(L2),4).EQ.1).OR.
     *     (MOD(IDIR(L2),4).EQ.2))))) GO TO 401
        IF ((KHYD.EQ.2).AND.(I.EQ.1).AND.((
     *     (L1.GE.256).AND.((MOD(IDIR(L1),4).EQ.1).OR.
     *     (MOD(IDIR(L1),4).EQ.2))).OR.(
     *     (L2.GT.256).AND.((MOD(IDIR(L2),4).EQ.1).OR.
     *     (MOD(IDIR(L2),4).EQ.0))))) GO TO 401
        IF (.NOT.PNODE) THEN
        IF ((L3.EQ.46).OR.((L3.GE.65).AND.(L3.LE.90))) GO TO 401
        IF ((L4.EQ.46).OR.((L4.GE.65).AND.(L4.LE.90))) GO TO 401
        IF ((I.EQ.KHYD+1).AND.(((L3.GT.256).AND.
     *     (MOD(IDIR(L3),4).EQ.0)).OR.((L4.GT.256)
     *     .AND.(MOD(IDIR(L4),4).EQ.2)))) GO TO 401
        IF ((KHYD.EQ.1).AND.(I.EQ.1).AND.((
     *     (L3.GE.256).AND.(MOD(IDIR(L3),4).EQ.1)).OR.(
     *     (L4.GT.256).AND.(MOD(IDIR(L4),4).EQ.1)))) GO TO 401
        IF ((KHYD.EQ.2).AND.(I.EQ.2).AND.((
     *     (L3.GE.256).AND.((MOD(IDIR(L3),4).EQ.1).OR.
     *     (MOD(IDIR(L3),4).EQ.0))).OR.(
     *     (L4.GT.256).AND.((MOD(IDIR(L4),4).EQ.1).OR.
     *     (MOD(IDIR(L4),4).EQ.2))))) GO TO 401
        IF ((KHYD.EQ.2).AND.(I.EQ.1).AND.((
     *     (L3.GE.256).AND.((MOD(IDIR(L3),4).EQ.1).OR.
     *     (MOD(IDIR(L3),4).EQ.2))).OR.(
     *     (L4.GT.256).AND.((MOD(IDIR(L4),4).EQ.1).OR.
     *     (MOD(IDIR(L4),4).EQ.0))))) GO TO 401
        ENDIF
35    CONTINUE
C
C See if ILEFT, IRIGHT, or both equal 1. If one is, insert H('s) there.
C If both equal 1, use criteria to decide which side to put H('s) on.
C If neither equals 1, call error message that there is no room for H.
C
36    CONTINUE
      IF (ILEFT+IRIGHT.NE.0) THEN
         IF (IRIGHT.EQ.0) THEN
            GO TO 42
         ELSE
            GO TO 43
         ENDIF
```

```
        ENDIF
CXT
CXT     Placement attached hydrogens vertical to the node is attempted.
9394    CONTINUE
        DO 9395 IN = IHP,-IHP,-IHP*2
           FY = JY + IN
           IF (((PNODE).AND.((MM(JX,FY).EQ.0).OR.(LMM(JX,FY).GE.256)))
     *        .OR.((.NOT.PNODE).AND.((MM(JX,FY).EQ.0).OR.
     *        (LMM(JX,FY).GE.256)).AND.(IDTPIX(JX,FY).EQ.0))) THEN
              DO 939 KK = -1,2
                 IF ((KK.EQ.2).AND.(KHYD.LE.1)) GO TO 939
                 DO 938 JJ = 0,1
                    IL = JX + KK
                    JL = FY + (JJ * IN)
                    IF ((MM(IL,JL).GT.0).AND.(LMM(IL,JL).LT.256).AND.
     *                 (MM(IL,JL).NE.34).AND.(LMM(IL,JL).NE.43).AND.
     *                 (LMM(IL,JL).NE.45)) GO TO 9395
                    IF ((.NOT.PNODE).AND.(IDTPIX(IL,JL).GT.0).AND.
     *                 (MOD(IDTPIX(IL,JL),2**13).LT.256).AND.
     *                 (IDTPIX(IL,JL).NE.34).AND.(MOD(IDTPIX(IL,JL),
     *                 2**13).NE.43).AND.(MOD(IDTPIX(IL,JL),2**13)
     *                 .NE.45)) GO TO 9395
938              CONTINUE
939           CONTINUE
              IF (KHYD.GT.1) THEN
                 FX = JX + 1
                 IF (((PNODE).AND.(MM(FX,FY).EQ.0)).OR.
     *              ((.NOT.PNODE).AND.(MM(FX,FY).EQ.0).AND.
     *              (IDTPIX(FX,FY).EQ.0))) THEN
                    MM(JX,FY) = 72
                    MM(FX,FY) = IHYD + 48
                    IF ((PNODE).AND.(.NOT.VNODE)) THEN
                       IF (MM(JX,FY).GE.256) THEN
                          CALL FTLOCA(FY,JX)
                          CALL FTEXT('^ ^')
                       ENDIF
                       CALL CURSOR(JX,FY)
                       HALO(2) = 'H'
                       CALL TEXT(HALO)
                       CALL CURSOR(FX,FY)
                       IF (MM(FX,FY).GE.256) THEN
                          CALL FTLOCA(FY,FX)
                          CALL FTEXT('^ ^')
                       ENDIF
                       IJ = IHYD + 48
                       HALO(2) = CHAR(IJ)
                       CALL MOVTCR(0,2)
                       CALL TEXT(HALO)
                       CALL MOVTCR(0,-2)
                       DELH(1,1) = JX
                       DELH(1,2) = FY
                       DELH(1,3) = 72
                       DELH(2,1) = FX
                       DELH(2,2) = FY
                       DELH(2,3) = IJ
                    ENDIF
                    IF (FX.GT.HIX) HIX = FX
                    GO TO 9396
                 ELSE
                    GO TO 9395
                 ENDIF
              ELSE
                 MM(JX,FY) = 72
                 IF ((PNODE).AND.(.NOT.VNODE)) THEN
                    DELH(1,1) = JX
                    DELH(1,2) = FY
                    DELH(1,3) = 72
                    IF (MM(JX,FY).GE.256) THEN
                       CALL FTLOCA(FY,JX)
                       CALL FTEXT('^ ^')
                    ENDIF
                    CALL CURSOR(JX,FY)
                    HALO(2) = 'H'
                    CALL TEXT(HALO)
                 ENDIF
```

```
            GO TO 9396
          ENDIF
        ENDIF
9395    CONTINUE
        GO TO 9397
9396    CONTINUE
        IF (FY.LT.LOY) THEN
          LOY = FY
        ELSE IF (FY.GT.HIY) THEN
          HIY = FY
        ENDIF
        CALL CURSOR(JX,JY)
        RETURN
9397    IERR=14
        JPROB=1
C ERROR IN DECIDING WHERE TO PUT H'S
        CHER = 2
        CALL MYERR(IERR,KAR,KAR)
        CHER = 0
        RETURN
C
C       Draw H on left:
C Saved for possible extension of bond
42      MBOND=LMM(JX-1,JY)
C Move to H location
        CALL CURSOR(JX-KHYD,JY)
C ASCII H into array
        MM(JX-KHYD,JY)=72
        IF ((PNODE).AND.(.NOT.VNODE)) THEN
          IF (MM(JX-KHYD,JY).GE.256) THEN
            FX = JX  - KHYD
            CALL FTLOCA(JY,FX)
            CALL FTEXT('^ ^')
          ENDIF
          HALO(2) = 'H'
          CALL TEXT(HALO)
          DELH(1,1) = JX - KHYD
          DELH(1,2) = JY
          DELH(1,3) = 72
        ENDIF
C Insert H here
        IF ((JX-2).LT.LOX) LOX = MIN0(JX-2,1)
C Skip subscript if not necessary.
        IF (KHYD.LE.1) GOTO 45
C Move to cursor position: one left of node.
        CALL CURSOR(JX-1,JY)
C ASCII for typing
        IJ=IHYD+48
C backspace
        IBACK=8
C ASCII of numeral into array
        MM(JX-1,JY)=IJ
        IF ((PNODE).AND.(.NOT.VNODE)) THEN
          IF (MM(JX-1,JY).GE.256) THEN
            FX = JX - 1
            CALL FTLOCA(JY,FX)
            CALL FTEXT('^ ^')
          ENDIF
          HALO(2) = CHAR(IJ)
          CALL MOVTCR(0,2)
          CALL TEXT(HALO)
          CALL MOVTCR(0,-2)
          DELH(2,1) = JX - 1
          DELH(2,2) = JY
          DELH(2,3) = IJ
        ENDIF
C
C If blank now to the left of H, extend whatever bond was covered over
C by the H and/or subscript,if any.(If MBOND=0,there was no bond there):
45      IF (MM(JX-KHYD-1,JY).NE.0) GOTO 111
C Move cursor
        IF ((IBDIR.EQ.7) .AND. (ILEFT.EQ.1)) IX=JX-KHYD-2
        IF (MBOND.GT.256) ICHAR=1
C beyond the end of the extended bond.
C Done with valence after left insertion.
        CALL CURSOR (IX,IY)
```

```
111     CONTINUE
        RETURN
C
C  Insert (H's) on right:
C Position for H on right of node
43      MX = JX + 1
        IF (LET2.GT.0) MX=JX+2
C Save for possible bond extension.
        MBOND = LMM(MX,JY)
        CALL CURSOR(MX,JY)
C Insert H.
        IF ((JX+2).GT.HIX) HIX = MAX0(JX+2,MAXX)
C ASCII H into array
        MM(MX,JY)=72
        IF ((PNODE).AND.(.NOT.VNODE)) THEN
           IF (MM(MX,JY).GE.256) THEN
              CALL FTLOCA(JY,MX)
              CALL FTEXT('^ ^')
           ENDIF
           HALO(2) = 'H'
           CALL TEXT(HALO)
           DELH(1,1) = MX
           DELH(1,2) = JY
           DELH(1,3) = 72
        ENDIF
C No subscript needed
        IF (KHYD.LE.1) GOTO 44
C Position of subscript
        CALL CURSOR(MX+1,JY)
C ASCII for subscript
        IJ=IHYD+48
        IBACK=8
C ASCII of numeral into array
        MM(MX+1,JY)=IJ
        IF ((PNODE).AND.(.NOT.VNODE)) THEN
           IF (MM(MX+1,JY).GE.256) THEN
              FX = MX + 1
              CALL FTLOCA(JY,FX)
              CALL FTEXT('^ ^')
           ENDIF
           HALO(2) = CHAR(IJ)
           CALL MOVTCR(0,2)
           CALL TEXT(HALO)
           CALL MOVTCR(0,-2)
           DELH(2,1) = MX+1
           DELH(2,2) = JY
           DELH(2,3) = IJ
        ENDIF
C If H and subscript covered over all of bond (if any), replace with one length
C of bond, using DRAW2:
44      IF(MM(MX+KHYD,JY).NE.0) GOTO 115
        IF ((IBDIR.EQ.3) .AND. (IRIGHT.EQ.1)) IX=MX+KHYD+1
115     CONTINUE
        CALL CURSOR(IX,IY)
C Completed with insertion of H on right
        RETURN
        END
$STORAGE:2
C       SUBROUTINE NSEW(I,J,ORIENT)
C       This subroutine determines if we are dealing with groups that
C       are vertically bonded or horizontally. Vertically bonded groups
C       are defined as groups in which the components H, digits, or lower
C       case letters are bracketed on the left and right by blanks
C       or by diagonal bonds.
C       Inputs are I and J - the coordinates of the element in MM
C       Output is the variable ORIENT - ORIENT = 1 = vertically bonded
C                                              = 0 = horizontally bonded
      SUBROUTINE NSEW(I,J,ORIENT)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      ORIENT=0
C
C     Set to default 'horizontally bonded'
      IVAL1=LMM(I-1,J)
```

```
      IVAL1A = LMM(I-1,J-1)
      IVAL1B = LMM(I-1,J+1)
      IVAL2=LMM(I+1,J)
      IVAL2A = LMM(I+1,J-1)
      IVAL2B = LMM(I+1,J+1)
      IF ((IVAL1.EQ.0 .OR. (IVAL1A.GE.256 .AND. MOD(IDIR(IVAL1A),2)
     2   .EQ.0) .OR. (IVAL1B.GE.256 .AND. MOD(IDIR(IVAL1B),2).EQ.0))
     3   .AND. (IVAL2.EQ.0 .OR. (IVAL2A.GE.256 .AND.
     4   MOD(IDIR(IVAL2A),2).EQ.0) .OR. (IVAL2B.GE.256 .AND.
     5   MOD(IDIR(IVAL2B),2).EQ.0))) ORIENT=1
C     If there is a blank or a diagonal bond
C     on the left and right
C     then the component is 'vertically bonded'
      RETURN
      END
C
C
C       SUBROUTINE GLEN(I,J,ORIENT,LEN,START)
C
C
C       This subroutine determines the X or Y coordinate of the start
C       Inputs are I and J - the coordinates of the element in MM
C                 ORIENT = the parameter which indicates vertical
C                          or horizontal bonds
C       Outputs are LEN (the length of the group) and START
C       START = minimum X coordinate in a horizontally bonded group
C             = minimum Y coordinate in a vertically bonded group
C       If there is a problem finding the ends of the group LEN is set to -1
      SUBROUTINE GLEN(I,J,ORIENT,LEN,START)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
C
      IF (ORIENT .EQ. 1) GO TO 20
C
C     We are dealing with a horizontal node.
      DO 40 L=0,5
         LL = L
         IF (MM(I-L,J) .EQ. 0 .OR. LMM(I-L,J) .GE. 256) GO TO 41
40    CONTINUE
      GO TO 99
C     Something is wrong - set LEN = -1 and abort
41    START = I - LL + 1
      DO 60 L=1,5
         LL = L
         IF (MM(START+L,J).EQ.0.OR.LMM(START+L,J).GE.256) GO TO 61
60    CONTINUE
      GO TO 99
C     Something is wrong - set LEN = -1 and abort
61    LEN=LL
      RETURN
C     We are dealing with a vertical node
20    DO 10 L=0,5
         LL = L
         IF (MM(I,J-L) .EQ. 0 .OR. LMM(I,J-L) .GE. 256) GO TO 11
CXT      IF (MM(I,J+L).EQ.0.OR.LMM(I,J+L).GE.256) GO TO 11
10    CONTINUE
      GO TO 99
C     Something is wrong - set LEN = -1 and abort
11    START=J-L+1
CXT11    START = J + LL - 1
      DO 12 L=1,5
         LL = L
         IF (MM(I,START+L).EQ.0.OR.LMM(I,START+L).GE.256) GO TO 130
CXT      IF (MM(I,START-L).EQ.0.OR.LMM(I,START-L).GE.256) GO TO 130
12    CONTINUE
      GO TO 99
C     Something is wrong - set LEN = -1 and abort
130   LEN = LL
      RETURN
99    IERR=-1
      RETURN
      END
C
C       SUBROUTINE BRANCH(I,J,LEN,ORIENT,RESULT)
```

```
C
C       This subroutine determines if the node starting at MM(I,J) is
C       branched
C       Inputs are I, J, LEN and ORIENT
C       I & J = coordinates of the start of the node
C       LEN = the length of the node
C       ORIENT = indicates if the node is horizontally or vertically bonded
C
C       OUTPUT = RESULT
C            = 0 = no horizontal bonds on a vertically bonded group
C                    or no vertical bonds on a horizontally bonded group
C              = 1 if a horizontally bonded group has a bond coming in
C                from below or if a vertically bonded group has a bond
C                coming in from the left
C              = 2 if a horizontally bonded group has a bond coming in
C                from above or if a vertically bonded group has a bond
C                coming in from the right
C              = 3 if a horizontally bonded group has a bond coming in
C                from below AND above or if a vertically bonded group
C                has a bond coming in from the right AND from the left
      SUBROUTINE BRANCH(I,J,LEN,ORIENT,RESULT)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
C
      LOW=0
      HIGH=0
      IF (ORIENT .EQ. 1) GO TO 100
C
C     Here we deal with horizontally bonded groups
      DO 10 II=-1,LEN
C!!         IVAL1=LMM(I+II,J-1)
C!!         IVAL2=LMM(I+II,J+1)
         IVAL1 = LMM(I+II,J+1)
         IVAL2 = LMM(I+II,J-1)
         IF (II .NE. -1 .AND. II .NE. LEN) GO TO 2
         IF (II .EQ. -1.AND.(IVAL1.GE.256.AND.(IDIR(IVAL1).EQ.2
     1      .OR. IDIR(IVAL1) .EQ. 6))) LOW = 1
         IF (II.EQ.-1.AND.(IVAL2.GE.256.AND.(IDIR(IVAL2).EQ.4
     1      .OR. IDIR(IVAL2) .EQ. 8))) HIGH=1
         IF (II.EQ.LEN.AND.(IVAL1 .GE.256.AND.(IDIR(IVAL1).EQ.4
     1      .OR. IDIR(IVAL1) .EQ. 8))) LOW=1
         IF (II.EQ.LEN.AND.(IVAL2.GE.256.AND.(IDIR(IVAL2).EQ.2
     1      .OR. IDIR(IVAL2) .EQ. 6))) HIGH=1
        GO TO 10
2       IF (IVAL1 .GE. 256) LOW=1
        IF (IVAL2 .GE. 256) HIGH=1
10      CONTINUE
        GO TO 200
C
C       Here we deal with vertically bonded groups
C
100     DO 20 JJ=-1,LEN
           IVAL1=LMM(I-1,J+JJ)
           IVAL2=LMM(I+1,J+JJ)
           IF (JJ .NE. -1 .AND. JJ .NE. LEN) GO TO 4
CXT         IF (JJ .NE. 1 .AND. JJ .NE. -LEN) GO TO 4
CXT         IF (JJ.EQ.1.AND.(IVAL1.GE.256.AND.(IDIR(IVAL1).EQ.2
C!!            IF (JJ.EQ.-1.AND.(IVAL1.GE.256.AND.(IDIR(IVAL1).EQ.2
C!!    1          .OR. IDIR(IVAL1) .EQ. 6))) LOW=1
            IF (JJ.EQ.-1.AND.(IVAL1.GE.256.AND.(IDIR(IVAL1).EQ.4
     1        .OR. IDIR(IVAL1) .EQ. 8))) LOW=1
CXT         IF (JJ.EQ.1.AND.(IVAL2.GE.256.AND.(IDIR(IVAL2).EQ.4
C!!         IF (JJ.EQ.-1.AND.(IVAL2.GE.256.AND.(IDIR(IVAL2).EQ.4
C!!   1        .OR.IDIR(IVAL2).EQ.8))) HIGH=1
            IF (JJ.EQ.-1.AND.(IVAL2.GE.256.AND.(IDIR(IVAL2).EQ.2
     1        .OR.IDIR(IVAL2).EQ.6))) HIGH=1
CXT        IF (JJ.EQ.-LEN.AND.(IVAL2.GE.256.AND.(IDIR(IVAL1).EQ.4
C!!        IF (JJ.EQ.LEN.AND.(IVAL2.GE.256.AND.(IDIR(IVAL1).EQ.4
C!!  1       .OR.IDIR(IVAL2).EQ.8))) LOW=1
           IF (JJ.EQ.LEN.AND.(IVAL2.GE.256.AND.(IDIR(IVAL1).EQ.2
     1       .OR.IDIR(IVAL2).EQ.6))) LOW=1
CXT        IF (JJ.EQ.-LEN.AND.(IVAL2.GE.256.AND.(IDIR(IVAL2).EQ.2
C!!           IF (JJ.EQ.LEN.AND.(IVAL2.GE.256.AND.(IDIR(IVAL2).EQ.2
C!!    1         .OR.IDIR(IVAL2).EQ.6))) HIGH=1
```

```
          IF (JJ.EQ.LEN.AND.(IVAL2.GE.256.AND.(IDIR(IVAL2).EQ.4
     1      .OR.IDIR(IVAL2).EQ.8))) HIGH=1
          GO TO 20
4       IF(IVAL1 .GE. 256) LOW=1
        IF (IVAL2 .GE. 256) HIGH=1
20      CONTINUE
200     RESULT = LOW + 2*HIGH
        RETURN
        END
C
C       SUBROUTINE BRAKIT(I,J,LEN,ORIENT,LOW,HIGH)
C
C       This subroutine returns the bracketing values of the group
C       (i.e. the values at the ends of the group)
C       Inputs are I, J, LEN, and ORIENT
C       I & J are the coordinates of the start of the group
C       LEN = length of the group
C       ORIENT = indicates whether the group is vertically or horizontally bonded
C
C       Outputs are LOW and HIGH
C
C       LOW = array value to the left of a horizontally bonded group
C             or below vertically bonded group
C       HIGH = array value to the right of a horizontally bonded group
C              or above a vertically bonded group
      SUBROUTINE BRAKIT(I,J,LEN,ORIENT,LOW,HIGH)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
C
      IF (ORIENT .EQ. 1) GO TO 200
C
C        Here we handle horizontally bonded groups
C
         LOW=LMM(I-1,J)
         HIGH=LMM(I+LEN,J)
         RETURN
C
C       Here we handle vertically bonded groups
C
200     LOW=LMM(I,J-1)
        HIGH=LMM(I,J+LEN)
CXT200     LOW=LMM(I,J+1)
CXT     HIGH=LMM(I,J-LEN)
      RETURN
      END
C
C       SUBROUTINE COPY(I,J,LEN,ORIENT,NODE)
C
C
C       This subroutine copies the node in MM to the vector NODE
C
C
C       Inputs are I, J, LEN, and ORIENT
C       I & J = coordinates of the group in MM
C       LEN = length of the group
C       ORIENT = indicates if the group is a horizontally or vertically bonded gr
C       Output is the vector NODE
      SUBROUTINE COPY(I,J,LEN,ORIENT)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM,NODE
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /KNOD/ NODE(4)
C     Zero NODE
C
      DO 5 K=1,4
5        NODE(K)=0
         IF (ORIENT .EQ. 1) GO TO 100
C
C        Here we handle a horizontally bonded group
C
         DO 10 K=1,LEN
            NODE(K)=MM(I+K-1,J)
10       CONTINUE
         RETURN
```

```
C
C         Here we handle vertically bonded groups
C
100       DO 30 K=1,LEN
          NODE(K)=MM(I,J+K-1)
CXT       NODE(K)=MM(I,J-K+1)
30        CONTINUE
          RETURN
       END
C
C        SUBROUTINE RORDER(NODE,LEN,LC,DIG)
C
C        This subroutine will reorder the NODE so that the characters
C        appear in the following order
C                        UC - lc - H - digit
C        Inputs are NODE (the 4 element array) and LEN (the # of Characters in NODE)
C        Outputs are the reordered NODE, LC, and DIG
C        LC = the lower case char in NODE if there is one
C           = 0 if the NODE contains no lower case character
C        DIG = the digit in NODE if there is one
C            = 0 if the NODE contains no digit
       SUBROUTINE RORDER(LEN,LC,DIG)
       IMPLICIT INTEGER*2 (A-Z)
       INTEGER*4 MM,NODE
       COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
       COMMON /KNOD/ NODE(4)
C
       H=0
       LC=0
       DIG=0
       UC=0
       DO 10 K=1,LEN
          IF (NODE(K) .EQ. 72) H=72
          IF ((NODE(K).GE.65.AND.NODE(K).LE.90).AND.NODE(K).NE.72)
      1      UC=NODE(K)
          IF (NODE(K) .GE. 49 .AND. NODE(K) .LE. 57) DIG=NODE(K)
          IF (NODE(K) .GE. 97 .AND. NODE(K) .LE. 122) LC=NODE(K)
 10    CONTINUE
       FULL=0
       IF (H .NE. 0) FULL=FULL+1
       IF (LC .NE. 0) FULL=FULL+1
       IF (DIG .NE. 0) FULL=FULL+1
       IF (UC .NE. 0) FULL=FULL+1
       IF (UC .EQ. 0) UC=72
 C     UC = H if no other UC found
       IF (FULL .GT. LEN) H=0
       I=1
       NODE(I)=UC
       I=I+1
       IF (LC .EQ. 0) GO TO 500
       NODE(I)=LC
       I=I+1
 500   IF (H .EQ. 0) GO TO 600
         NODE(I)=H
         I=I+1
         IF (DIG .EQ. 0) GO TO 600
         NODE(I)=DIG
 600   RETURN
       END
C
C        SUBROUTINE ORDER2(NODE,LEN,IERR)
C
C        This subroutine is used to reorder the NODE if we are trying
C        to copy the node to the left not the right
C        Consider NODE=CH3 - ORDER2 will change it so that NODE=C3H
C        Then when node is copied to the right (in reverse) it will appear as H3C
C        Inputs are NODE and LEN - LEN is the length of NODE
C
C        Outputs are the reordered NODE and the error return IERR
C        This reordering can't be done if the NODE includes a 2 letter element
C        In that case IERR=1  -  If the reordering is successful IERR=0
       SUBROUTINE ORDER2(LEN,IERR)
       IMPLICIT INTEGER*2 (A-Z)
       INTEGER*4 NODE
       COMMON /KNOD/ NODE(4)
```

```
      IERR=1
C
C     Bail out if we find a lower case char
      DO 10 I=1,LEN
         IF (NODE(I) .GE. 97 .AND. NODE(I) .LE. 122) RETURN
10    CONTINUE
      IERR=0
C
C       If there is no digit - just return
C
        IF (NODE(LEN) .LT. 49 .OR. NODE(LEN) .GT. 57) RETURN
        HOLD=NODE(LEN)
        NODE(LEN)=NODE(LEN-1)
        NODE(LEN-1)=HOLD
        RETURN
        END
C
C       SUBROUTINE MOVE1(I,J,LEN,NODE)
C
C
C       This subroutine copies the contents of NODE into the horizontally
C       bonded node of length LEN starting at MM(I,J)
      SUBROUTINE MOVE1(I,J,LEN)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM,NODE
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /RANGE/LOX,HIX,LOY,HIY
      COMMON /KNOD/ NODE(4)
      DO 10 K=0,LEN-1
         MM(I+K,J)=NODE(K+1)
10    CONTINUE
        IF (HIX .LT.(I+LEN-1)) HIX=I+LEN-1
      RETURN
      END
C
C       SUBROUTINE MOV2(I,J,LEN1,K,M,LEN,NODE,REP)
C
C       This subroutine will replace LEN1 chars of the vertically bonded node
C       starting at MM(I,J) with the value in REP (REP will be a 0
C       or a bond) It will then copy the node of length LEN stored in NODE into
C       MM starting at coordinates K and L and continuing to the right
        SUBROUTINE MOV2(I,J,LEN1,K,M,LEN,REP)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,NODE
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /RANGE/LOX,HIX,LOY,HIY
        COMMON /KNOD/ NODE(4)
        IF (LEN1 .EQ. 0) GO TO 15
        DO 10 N=0,LEN1-1
        MM(I,J+N)=REP
CXT        MM(I,J-N) = REP
10      CONTINUE
15      DO 11 N=0,LEN-1
           MM(K+N,M) = NODE(N+1)
11      CONTINUE
        IF (HIX .LT. (K+LEN-1)) HIX=K+LEN-1
        RETURN
        END
C
C       SUBROUTINE MOV3(I,J,LEN1,K,M,LEN,NODE,REP)
C
C
C       This subroutine will replace LEN1 chars of the vertically bonded node
C       starting at MM(I,J) with the value in REP (REP will be a 0
C       or a bond) It will then copy the node of length LEN stored in NODE into
C       MM starting at coordinates K and L and continuing to the left
        SUBROUTINE MOV3(I,J,LEN1,K,M,LEN,REP)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,NODE
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /KNOD/ NODE(4)
        COMMON /RANGE/LOX,HIX,LOY,HIY
C
        IF (LEN1 .EQ. 0) GO TO 15
        DO 10 N=0,LEN1-1
```

```
      MM(I,J+N)=REP
CXT   MM(I,J-N) = REP
10    CONTINUE
15    DO 11 N=0,LEN-1
         MM(K-N,M) = NODE(N+1)
11    CONTINUE
      IF (LOX .GT. (K-(LEN-1))) LOX=K-(LEN-1)
      RETURN
      END
C
C     SUBROUTINE MOV4(I,J,K,M,LEN,NODE,REP)
C
C     This subroutine will replace the horizontally bonded node of length
C     LEN starting at MM(I,J) with the value in REP (REP will be a 0
C     or a bond) It will then copy the node stored in NODE into
C     MM starting at coordinates K and L and continuing to the right
      SUBROUTINE MOV4(I,J,K,M,LEN,REP)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM,NODE
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /KNOD/ NODE(4)
      COMMON /RANGE/LOX,HIX,LOY,HIY
      DO 10 N=1,LEN
         MM(I+N-1,J)=REP
10    CONTINUE
      DO 11 N=0,LEN-1
         MM(K+N,M)=NODE(N+1)
11    CONTINUE
      IF (HIX .LT. (K+LEN-1)) HIX=K+LEN-1
      RETURN
      END
C
C     SUBROUTINE SCAN(I,J,IERR)
C
C     This subroutine will scan IDTPIX and MM for space conflicts
C
C     This subroutine will scan MM(I,J), MM(I,J-1) and MM(I,J+1)
C     and the corresponding elements in IDTPIX.
C     It will return IERR = 0 if IDTPIX(I,J) is empty and MM(I,J)
C     is empty or contains a horizonal bond and
C     MM(I,J-1), IDTPIX(I,J-1), IDTPIX(I,J+1) and MM(I,J+1)
C     are empty or contain a diagonal bond
C     Else it will return IERR = 1.
C
      SUBROUTINE SCAN(I,J,IERR)
      IMPLICIT INTEGER*2 (A-Z)
      INTEGER*4 MM,IDTPIX
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
C
      IERR=1
      IVAL1=MM(I,J-1)
      IVAL2=MM(I,J+1)
      IVAL3=IDTPIX(I,J-1)
      IVAL4=IDTPIX(I,J+1)
C     IF ((MM(I,J) .EQ. 0  .AND. (IVAL1 .EQ. 0 .OR. (IVAL1 .GE. 256
C    1   .AND. (MOD(IDIR(IVAL1),2) .EQ. 0))) .AND. (IVAL2 .EQ.0 .OR.
C    2   (IVAL2 .GE. 256 .AND. (MOD(IDIR(IVAL2),2) .EQ.0))))
      IF (((MM(I,J).EQ.0 .OR. IDIR(LMM(I,J)).EQ.3 .OR. IDIR(LMM(I,J))
     1  .EQ.7) .AND. (IVAL1.EQ.0 .OR. (IVAL1.GE.256 .AND.
     2  (MOD(IDIR(IVAL1),2).EQ.0))) .AND. (IVAL2 .EQ.0 .OR.
     2  (IVAL2 .GE. 256 .AND. (MOD(IDIR(IVAL2),2) .EQ.0))))
     3  .AND.
     4  (IDTPIX(I,J) .EQ. 0 .AND. (IVAL3 .EQ. 0 .OR. (IVAL3 .GE.256
     5  .AND. (MOD(IDIR(IVAL3),2).EQ.0))) .AND. (IVAL4 .EQ. 0 .OR.
     6  (IVAL4 .GE. 256 .AND. (MOD(IDIR(IVAL4),2) .EQ. 0)))))
     7  IERR=0
        RETURN
        END
C
C     SUBROUTINE FINDX(I,J,IVAL,LEN,INODE)
C
C     This subroutine will search LEN cells of the array MM for the
C     value IVAL starting at coordinates I & J and looking to the right
C     It will return the X coordinate in INODE if the value is found
```

```
C       If the value is not found INODE will be set to -1
C
        SUBROUTINE FINDX(I,J,IVAL,LEN,INODE)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        DO 10 K=0,LEN-1
           KK = K
           IF (IVAL .EQ. MM(I+K,J)) GO TO 25
10      CONTINUE
        INODE=-1
        RETURN
25      INODE = I + KK
        RETURN
        END
C
C       SUBROUTINE BLEN(I,J,IVAL,LEN)
C
C       There should be a horizontal bond of type IVAL starting at MM(I,J)
C       This subroutine will determine the length of the bond and
C       return it in LEN - If the bond is not found the LEN will be 0
        SUBROUTINE BLEN(I,J,IVAL,LEN)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        LEN=0
        DO 10 K=0,100
           IF (MM(I+K,J) .NE. IVAL) GO TO 100
           LEN=LEN+1
10      CONTINUE
100     CONTINUE
        RETURN
        END
C
C       SUBROUTINE FINDY(I,J,IVAL,LEN,INODE)
C
C       This subroutine will search LEN cells of the array MM for the
C       value IVAL starting at coordinates I & J and looking up
C       It will return the Y coordinate in INODE if the value is found
C       If the value is not found INODE will be set to -1
C
        SUBROUTINE FINDY(I,J,IVAL,LEN,INODE)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        DO 10 K=0,LEN-1
           KK = K
        IF (IVAL .EQ. MM(I,J+K)) GO TO 25
CXT     IF (IVAL .EQ. MM(I,J-K)) GO TO 25
10      CONTINUE
        INODE=-1
        RETURN
25      INODE = J + KK
        RETURN
        END
C
C       SUBROUTINE FIXUP(IERR)
C
C       This subroutine will examine nodes in MM - If the node is not
C       in the proper order due to rotations or reflections, FIXUP
C       will try to reorder the node - If it can, the node will be reordered
C       and IERR will be set to 0 - If it can't, IERR will be set to -1
C
        SUBROUTINE FIXUP(IERR)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 MM,NODE
        COMMON /CD/ MAXX,MAXY
        COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
        COMMON /KNOD/ NODE(4)
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /CUR/ ICUR
C
C       Start looking through the array
C
        DO 10 I = LOX,HIX
```

```
         DO 10 J = LOY,HIY
               IF (MM(I,J).EQ.0) GO TO 10
               II = I
               JJ = J
               ICUR = 0
               CALL CURSOR(II,JJ)
               CALL CKNOD2(II,JJ,IVAL,IERR)
C              Is there a problem with this node.
               IF (IERR .EQ. 0) GO TO 10
C              IERR=0 means node is OK
C
C              Node is bad - See if we can fix it
C
               CALL NSEW(II,JJ,ORIENT)
C              Get node orientation
               CALL GLEN(II,JJ,ORIENT,LEN,START)
C              Get length of node and starting location of node
               IF (ORIENT .EQ. 0) GO TO 500
C
C         Here we handle vertical nodes
          CALL COPY (II,START,LEN,ORIENT)
C         Copy node in MM into NODE
          CALL RORDER(LEN,LC,DIG)
C         Reorder the node
          CALL BRAKIT(II,START,LEN,ORIENT,LOW,HIGH)
C         Get the values above and below the node
          NOD = NODE(1)
          CALL FINDY(II,START,NOD,LEN,INODE)
          NODE(1) = NOD
C         Find Y coordinate for start of UC element of node
          L=INODE-START
          LEND=LEN-L-1
          IF (LEND .EQ. 0) GO TO 22
          DO 20 K=1,LEND
C            Extend bond value or blank value from above the node downward.
20        MM(I,INODE+K)=HIGH
CXT20        MM(I,INODE-K)=HIGH
C
C            Try to extend node to the right
22       DO 61 K=1,LEN
C           See if room for node on the right
            M=I + K
            CALL SCAN(M,INODE,IERR)
            IF (IERR .EQ. 1) GO TO 80
C           No room on this side but we can try other side
61       CONTINUE
         CALL MOV2(II,START,L,II,INODE,LEN,LOW)
C        Copy node to MM
         GO TO 10
80       DO 75 K=1,LEN
            M=I - K
C           Do we have room on the left
            CALL SCAN(M,INODE,IERR)
            IF (IERR .EQ. 1) GO TO 900
C           No room - bail out
75       CONTINUE
         CALL ORDER2(LEN,IERR)
C        Reorder node for left side
         IF (IERR .EQ. -1) GO TO 900
C        Can't reorder - bail out
C
C        Extend node to the left
C
         CALL MOV3(II,START,L,II,INODE,LEN,LOW)
C        Copy node to MM
         GO TO 10
C
C        We are dealing with a horizontal node
500      CALL BRANCH(START,JJ,LEN,ORIENT,RESULT)
C        Determine if the node is branched
         CALL COPY(START,JJ,LEN,ORIENT)
C        Copy node in MM into NODE
         CALL RORDER(LEN,LC,DIG)
C        Reorder the node
         CALL BRAKIT(START,JJ,LEN,ORIENT,LOW,HIGH)
```

```
C       Get the values to the left and right of the node
        IF (RESULT .NE. 0) GO TO 600
C
C       We are dealing with an unbranched node
C
        CALL MOVE1(START,JJ,LEN)
C       Copy node into MM
        GO TO 10
C
C       We are dealing with a branched node
C
600        NOD = NODE(1)
              CALL FINDX(II,JJ,NOD,LEN,INODE)
        NODE(1) = NOD
C       Find position where node should start
        IF (INODE .EQ. -1) GO TO 900
C       Can't find starting char - abort
        IVAL=HIGH
C       IVAL = value of bond to right of node
        IF (IVAL .EQ. 0) GO TO 800
C       If IVAL=0 - call SCAN to see if we have room to extend
C       node on the right
        END=START+LEN
C       END = X coordinate just beyond end of node
        CALL BLEN(END,JJ,IVAL,BONDL)
C       Get bond length of bond to right of node
        IF (BONDL .EQ. 0) GO TO 900
C       Bad bond - abort
        IF (BONDL .LT. LEN) GO TO 900
C       Bond too short - abort
        GO TO 700
800     DO 83 K=1,LEN
           M=INODE+K
           CALL SCAN(M,JJ,IERR)
C          SCAN to right to see if we have room for node
           IF (IERR .EQ. 1) GO TO 900
83      CONTINUE
700     CALL MOV4(START,JJ,INODE,JJ,LEN,LOW)
C       Move node into MM and pad to the left of the new node with value
C       LOW (from BRAKIT)
10      CONTINUE
        IERR=0
C       Set error code IERR to 0 = OK
        RETURN
900     IERR=-1
        RETURN
        END

$STORAGE:2
        SUBROUTINE BOND(IERR,IX,IY)
C  This program converts the 90x31 arrays which contain graphic
C  structures of chemical compounds to connection tables.
C  In addition, long bond information is read from a separate file
C  and merged with the bond information from the standard data to form
C  a complete connection table.
C
C
        IMPLICIT INTEGER*2 (A-Z)
        COMMON /NDE/ NODE(255,3),IATOM
C       SET ERROR FLAG = 0 = OK FOR NOW
        IERR=0
        CALL READD(IERR,IX,IY)
C       RETURN TO STRINP IF BAD RETURN FROM READ
        IF (IERR .NE. 0 ) RETURN
        CALL NOD(IERR,IX,IY)
C       RETURN TO STRINP ON BAD RETURN FROM NOD
        IF (IERR .NE. 0) RETURN
        CALL CONNET(IERR,IX,IY)
C       RETURN TO STRINP ON BAD RETURN FROM CONNET
        IF (IERR .NE. 0) RETURN
        CALL CHGHYD(IERR,IX,IY)
        IF (IERR.NE.0) RETURN
        IF(IATOM .NE. 0) GO TO 40
        IERR=18
C       NULL CONNECTION TABLE - RETURN TO DIS WITH NO DATA
```

```
        CALL MYERR(IERR,KAR,KAR)
        RETURN
 40     CONTINUE
        CALL TBLOUT(IERR,IX,IY)
        RETURN
        END
C
C
        SUBROUTINE READD(IERR,JX,JY)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 IARRAY
        COMMON /CD/ MAXX,MAXY
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /STRPIX/ LPIX,IARRAY(90,38),LBLEN,LNGBND(100,5)
        COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
        COMMON /CUR/ ICUR
C
C       Variable MNUM contains the number of *M structures and array
C       IMS contains the following items for each *M structure:
C          1 - The multiplier of the structure.
C          2 - The M1 identifying ordinal value.
C          3,4 - The x and y coordinates of the *M.
C          5 - The length of the *M conection table entry.
C          6 - The length of the formula to follow.
C          7 - The divisor of the multiplier (if fractional).
C          8 thru 90 - The molecular formula of the M1 structure.
        COMMON /M1/ MNUM,IMS(90,5)
        COMMON /DTDS/ DTN,DTX(30),DTY(30),DTN1(30),DTN2(30)
C       # of D1's - coordinates - multiplier-1 and node #
        DIMENSION ISTRNG(20),ISTRUC(7,5),JSTRUC(5)
C         READS IN ARRAY OF GRAPHICAL INFORMATION
C         Each element of IARRAY(IX,IY) contains a part
C          of the graph of the chemical compound.  An integer
C          less than 256 indicates an ASCII character (Cap or l.c.)
C         --symbol of an element {O, Ca, etc or a dot[Carbon]},
C         a numeral, + or - sign). An integer >256 indicates a bond.
C         IARRAY(IX,IY) Mod 256 indicates the direction (0--3), while
C         the greatest integer in IARRAY(IX,IY)/256 indicates
C         the bond type, according to a code.
        DATA ISTRUC/72,78,78,67,67,72,0,67,97,97,
     *     108,108,43,0,108,0,43,0,45,0,0,0,0,0,0,0,0,0,
     *     0,0,0,0,0,0,0/
C structures:  HCl,Na,Na+,Cl,Cl-,H+
C
        MNUM = 0
        M1MAX = 14
        DTN = 0
        DO 21 I= LOX,HIX
        DO 21 J= LOY,HIY
        IF (IARRAY(I,J).NE.42) GOTO 2211
        JX = I
        JY = J
        DTN = DTN + 1
        IF (DTN.GT.30) THEN
           CALL FTSIZE(2,18)
           CALL FTLOCA(1,1)
           CALL FTEXT('^DOTDIS STRUCTURES EXCEED MAXIMUM OF 30^')
           IERR = 200
           PAGE = 0
           DTN = 30
           CALL FTSIZE(1,10)
           GO TO 37
        ENDIF
        DTX(DTN) = I
        DTY(DTN) = J
        NUMTOR = 0
        K=0
C Routine to handle dot_disconnects;K=no of char in number or fraction
        M=1
        IDIGIT=0
        IFRAC=0
C Set fraction indicator to no
C *=dot-disconn struc follows
        IF (IARRAY(I+M,J).EQ.0) GOTO 56
C blank after *: skip
```

```
CXT     IARRAY(I,J)=0
C Eliminate '*' from array
        IF (ILRRAY(I+M,J).EQ.43 .OR. ILRRAY(I+M,J).EQ.45) GO TO 56
C Not a + or - so go on
C We found a + or - so erase the entire dot-disconnected structure
CXT     IEND=MAXX - I
CXT     DO 61 L=1,IEND
CXT     IF (IARRAY(I+L,J) .EQ. 0) GO TO 21
CXT     IARRAY(I+L,J)=0
C Erase all dot-disconnect until space is found
CXT61      CONTINUE
CXT     GO TO 21
        IF (IARRAY(I+M,J).GE.97 .AND. IARRAY(I+M,J).LE.122) GO TO 56
C Do we have a lower case letter
C Dot disconnect is of the form nHCl - Eliminate the n
CXT     IARRAY(I+M,J)=0
CXT     M=M+1
C Get next character
70      CONTINUE
        VAL = 1
        IF (IARRAY(I+M,J).LT.48 .OR. IARRAY(I+M,J).GT.57) GO TO 80
C Is it a digit?
C We found a digit
        IDIGIT=M+I
        VAL = ILRRAY(IDIGIT,J) - 48
        DTN1(DTN) = VAL
C Location of first digit in number
        K=K+1
C # of characters in # or fraction
        M=M+1
75      IF (IARRAY(I+M,J) .LT. 48 .OR. IARRAY(I+M,J) .GT. 57) GO TO 80
C We found another digit
        VAL = (VAL * 10) + IARRAY(I+M,J) - 48
        IF (VAL.GE.1000) GO TO 56
        IF (IFRAC.EQ.0) THEN
           DTN1(DTN) = VAL
        ELSE IF (IFRAC.EQ.1) THEN
           DTN1(DTN) = NUMTOR
           DTN2(DTN) = VAL
        ENDIF
        K=K+1
C Increase character count
        M=M+1
C Get next character
C M+I>103 implies we went off the edge
        IF ((M+I).LE.MAXX) GO TO 75
        GO TO 56
C Issue error message and return
80      IF (IARRAY(I+M,J) .NE. 47) GO TO 85
C 47 = /
C We found a /  We have a fraction
        IFRAC = IFRAC + 1
        IF (IFRAC.GT.1) GO TO 56
        NUMTOR = VAL
        VAL = 0
C Set fraction indicator to yes
        K=K+1
C Increase character count
        M=M+1
C Get next character
        IF ((I+M).LE.MAXX) GO TO 75
        GO TO 56
C We went off the edge - issue msg and return
85      CONTINUE
        IF ((IFRAC.EQ.1).AND.(VAL.EQ.0)) GO TO 56
        IF (IARRAY(I+M,J).NE.77.OR.IARRAY(I+M+1,J).LT.112.OR.
     *     IARRAY(I+M+1,J).GT.120) GO TO 88
C Is it a D1 or M1 structure
C We found an M1 or D1
        DTX(DTN) = 0
        DTY(DTN) = 0
        DTN1(DTN) = 0
        DTN2(DTN) = 0
        DTN = DTN - 1
        MNUM = MNUM + 1
```

```
      IF ((MNUM.GT.5).OR.(IARRAY(I+M+2,J).NE.58)) GO TO 56
      IF (IFRAC.EQ.0) THEN
         IMS(1,MNUM) = VAL
      ELSE IF (IFRAC.EQ.1) THEN
         IMS(7,MNUM) = VAL
         IMS(1,MNUM) = NUMTOR
      ENDIF
      IMS(2,MNUM) = ILRRAY(I+M+1,J)
      IMS(3,MNUM) = I + M
      IMS(4,MNUM) = J
C     If more than of the same M1 structure definitions exist,
C     differing only in the multiplication factor, the duplicate
C     definitions are not entered into the connection table.
      DO 6350 KK = 1,MNUM-1
         IF (IMS(2,KK).EQ.IMS(2,MNUM)) THEN
            JX = IMS(3,MNUM)
            JY = IMS(4,MNUM)
            IERR = 46
            CALL MYERR(IERR,IERR,IERR)
            ICUR = 1
            CALL CURSOR(JX,JY)
            RETURN
         ENDIF
6350  CONTINUE
C     It is a M1 - Count its length and erase it all for it should
C     not appear in the connection table
      IEND = MAXX - I
      DO 6351 KK = 2,IEND
         IF (IARRAY(I+M+KK,J).EQ.0) GO TO 6352
         IMS(5,MNUM) = IMS(5,MNUM) + 1
         IMS(6+KK,MNUM) = ILRRAY(I+M+KK,J)
6351  CONTINUE
6352  CONTINUE
      IMS(6,MNUM) = IMS(5,MNUM)
C
C      Length of formula including multiplier, x and y coordinates,
C      and their delimiters is computed and assigned.
       IF (IMS(1,MNUM).GT.1) THEN
          IMS(5,MNUM) = IMS(5,MNUM) + 2
          IF (IMS(1,MNUM).GE.10) THEN
             IMS(5,MNUM) = IMS(5,MNUM) + 1
             IF (IMS(1,MNUM).GE.100) IMS(5,MNUM) =
     *          IMS(5,MNUM) + 1
          ENDIF
       ENDIF
       IF (IMS(7,MNUM).GT.0) THEN
          IMS(5,MNUM) = IMS(5,MNUM) + 2
          IF (IMS(7,MNUM).GE.10) THEN
             IMS(5,MNUM) = IMS(5,MNUM) + 1
             IF (IMS(7,MNUM).GE.100) IMS(5,MNUM) = IMS(5,MNUM) + 1
          ENDIF
       ENDIF
       IMS(5,MNUM) = IMS(5,MNUM) + 6
       IF (IMS(3,MNUM).GE.10) THEN
          IMS(5,MNUM) = IMS(5,MNUM) + 1
          IF (IMS(3,MNUM).GE.100) IMS(5,MNUM) = IMS(5,MNUM) + 1
       ENDIF
       IF (IMS(4,MNUM).GE.10) THEN
          IMS(5,MNUM) = IMS(5,MNUM) + 1
          IF (IMS(4,MNUM).GE.100) IMS(5,MNUM) = IMS(5,MNUM) + 1
       ENDIF
      M1MAX = M1MAX + IMS(5,MNUM) + 2
      IF (M1MAX.GT.160) THEN
         JX = IMS(3,MNUM)
         JY = IMS(4,MNUM)
         IERR = 22
         CALL MYERR(IERR,IERR,IERR)
         ICUR = 1
         CALL CURSOR(JX,JY)
         RETURN
      ENDIF
      DO 89 KK=0,IEND
      IF (IARRAY(I+KK,J) .EQ. 0) GO TO 21
      IARRAY(I+KK,J)=0
89    CONTINUE
```

```
      GO TO 21
C
C
C We found a D1
CXT90     IF (IFRAC .EQ. 1) GO TO 56
C D1 with fractional multiplier not allowed
C No multiplier = no problem
CXT       IF (K .GT. 5) GO TO 56
C Multiplier with > 5 digits is not allowed
C Convert numeric characters to integer
C Multiplier = 1 implies no problem
CXT       IDNUM=IDNUM+1
C # of D1 structures found
CXT       IF (IDNUM .GT. 9) GO TO 56
C No more than 9 D1's allowed
CXT       IDS(IDNUM,1)=I+M
C X coordinate of D1
CXT       IDS(IDNUM,2)=J
C Y coordinate of D1
CXT       IDS(IDNUM,3) = VAL
C # of additional times D1 will have to be copied into connection table
CXT       IDS(IDNUM,4)=0
C Will eventually be set to node #
CXT       GO TO 21
C Regular dot-disconnect - See if it is allowed
88              M=M-1
                DO 32 L=1,5
                JSTRUC(L)=0
C used to match structure to library file
32              CONTINUE
                DO 33 L=1,5
                IF (IARRAY(I+M+L,J).EQ.74) IARRAY(I+M+L,J) = 72
                IF (IARRAY(I+M+L,J).EQ.0 ) GOTO 34
                JSTRUC(L)=ILRRAY(I+M+L,J)
C Copy structure from array to JSTRUC
33              CONTINUE
34      CONTINUE
                DO 35 K=1,7
                DO 36 L=1,5
                IF (JSTRUC(L).NE.ISTRUC(K,L)) GOTO 35
36              CONTINUE
                GOTO 21
C Successful match to library in ISTRUC
35              CONTINUE
39      IERR=20
C SET ERROR FLAG
      CALL MYERR(IERR,KAR,KAR)
37      CONTINUE
      JX = I + M
      JY = J
      ICUR = 1
      CALL CURSOR(JX,JY)
C TYPE DOT-DISCONNECTED UNIT NOT ON FILE IN SUB READ
      RETURN
2211    IF (IARRAY(I,J).GT.0) THEN
          IF (ILRRAY(I,J).LT.256) THEN
            IF (IARRAY(I,J).NE.46) THEN
              IF ((IARRAY(I,J).LT.65).OR.(IARRAY(I,J).GT.90)) THEN
                IF ((IARRAY(I,J).LT.48).OR.(IARRAY(I,J).GT.57)) THEN
                  IF ((IARRAY(I,J).LT.97).OR.(IARRAY(I,J).GT.122))
     *              THEN
                    IF ((ILRRAY(I,J).NE.43).AND.(ILRRAY(I,J)
     *                .NE.45))THEN
                      IF ((IARRAY(I,J).NE.63).AND.
     *                  (IARRAY(I,J).NE.34)) THEN
                        IF (IARRAY(I,J).NE.47) THEN
                          IERR = 10
                          CALL MYERR(IERR,IERR,IERR)
                          JX = I
                          JY = J
                          RETURN
                        ENDIF
                      ENDIF
                    ENDIF
                  ENDIF
```

```
                    ENDIF
                 ENDIF
              ENDIF
           ENDIF
        ENDIF
21      CONTINUE
C Search  thru array
        GOTO 57
C To end
56      IERR=21
        CALL MYERR(IERR,KAR,KAR)
        ICUR = 1
        CALL CURSOR(JX,JY)
C Problem handling dot disconnected structure
57      RETURN
        END
C
C
        SUBROUTINE NOD(IERR,JX,JY)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 IARRAY
        COMMON /CD/ MAXX,MAXY
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /HP/IHP
        COMMON /NDE/ NODE(255,3),IATOM
C       NODE(255,3) stores the X, Y, and chem element code for up to 255
C       nodes (junctions of bonds) for the compound under study.
        COMMON /STRPIX/ LPIX,IARRAY(90,38),LBLEN,LNGBND(100,5)
C       IARRAY(I,J) CONTAINS BOND OR ATOM TYPE, & BOND DIRECTION
C       FOR EACH OF MAXX * MAXY LOCATIONS.
C       DNUM is the # of D1 structures found
        COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
C       IDS(1) = x-coordinate of D1 structure
C       IDS(2) = y-coordinate of of D1 structure
C       IDS(3) = multiplier - 1 (i.e. # of additional times D1 must be
C          copied into connection table)
C       IDS(4) = NODE # for the node
C       IDS(5) = NODE # for the last node in the fragment
C       IDS(6) = NNODE = # of nodes before fragment was replicated in
C          connection table.
        COMMON /ELECHR/ IELEM(126,5)
        COMMON /CUR/ ICUR
        COMMON /M1/ MNUM,IMS(90,5)
        COMMON /LNGOUT/ LNGNDE(100,2)
        COMMON /WARN/ ERR
        COMMON /QTVLNC/ OERR,CHER
        COMMON /HEAD/ MW(12),ISTATE,PAGE
        COMMON /DTDS/ DTN,DTX(30),DTY(30),DTN1(30),DTN2(30)
        COMMON /GPRNT/ KHAR
        COMMON /ELENOD/ IELT
C
        IATOM=0
C       Fill NODE by searching through IARRAY:
        DO 999 I= LOX,HIX
        DO 999 J= LOY,HIY
C       Lowercase and non'.' are not nodes.
        IF(((IARRAY(I,J).LE.62).OR.(IARRAY(I,J).GE.91))
     2     .AND.(IARRAY(I,J).NE.46)) GO TO 999
C  H's not followed by a lowercase letter are not nodes.
        IF ((IARRAY(I,J).EQ.72).AND.(((IARRAY(I+1,J).LT.97).OR.
     2     (IARRAY(I+1,J).GT.122)).AND.(((IARRAY(I-1,J).NE.42).AND.
     3     (IARRAY(I-1,J).LT.48).AND.(IARRAY(I-1,J).GT.57)).OR.
     3     (ILRRAY(I+1,J).NE.43)))) GOTO 999
        IATOM=IATOM + 1
CXT     M = 33
        IF (IATOM.GT.255) THEN
C Too many nodes - i.e. greater than 255
           IERR=35
           CALL MYERR(IERR,KAR,KAR)
           RETURN
        ENDIF
C X,Y of node are equal to I,J
        NODE(IATOM,1)=I
        NODE (IATOM,2)=J
C       Dot (ASCII 46) is a Carbon atom.
```

```
         IF (IARRAY(I,J).EQ.46) GO TO 921
CXT      IF (IARRAY(I,J).NE.46) GOTO 950
C LTR1, LTR2 are ASCII codes for first, second letter of chem element.
C Blank second characters are set to ASCII zero.
CXT950      CONTINUE
         LTR1=ILRRAY(I,J)
         LTR2=0
         IF ((IARRAY(I+1,J).LT.123).AND.(IARRAY(I+1,J).GT.96))
     2     LTR2=ILRRAY(I+1,J)
         IF ((LTR1.EQ.77).AND.(LTR2.GE.112).AND.(LTR2.LE.120)) GO TO 945
         IF ((LTR1.EQ.68).AND.(LTR2.GE.112).AND.(LTR2.LE.120)) GO TO 943
C Search element array to find element code from node's ASCII code.
            DO 444 JJ = 1,MAXX
               IF ((IARRAY(I-JJ,J).EQ.0).OR.(ILRRAY(I-JJ,J).GE.256).OR.
     *            (I-JJ.EQ.0)) THEN
                  GO TO 921
               ELSE IF (IARRAY(I-JJ,J).EQ.42) THEN
                  DO 1 KK = 1,107
                     IF ((LTR1.NE.IELEM(KK,1)).OR.
     *                  (LTR2.NE.IELEM(KK,2))) GO TO 1
                     M = KK
                     GO TO 930
1                 CONTINUE
                  IERR = 11
                  CALL MYERR(LTR1,LTR2,IERR)
                  ICUR = 1
                  JX = I + 1
                  JY = J
                  CALL CURSOR(JX,JY)
                  RETURN
               ENDIF
444         CONTINUE
921      CONTINUE
         JX = I
         JY = J
         ERR = 0
         PAGE = 2
         ICUR = 0
         CALL CURSOR(JX,JY)
         CALL CLRHYD(JX,JY)
         CHER = 1
         CALL VALNCE(3,JX,JY,0,0)
         M = IELT
         IF (ERR.NE.0) THEN
            IERR = ERR
            P = 0
            IF (IERR.EQ.12) THEN
               ICUR = 1
               CALL CURSOR(JX,JY)
               CALL FTSIZE(2,18)
               CALL FTLOCA(1,37)
               CALL FTEXT('^-Enter "C" to edit structure -or- "S" ^')
               CALL FTEXT('^to continue.^')
               CALL FTSIZE(1,10)
               PAGE = 0
               CALL INPUTX(P,JX,JY)
            ENDIF
            IF ((P.NE.83).AND.(P.NE.115)) THEN
               IF (IERR.NE.12) THEN
                  CHER = 2
                  CALL MYERR(IERR,IERR,IERR)
               ELSE
                  CHER = 0
                  CALL REMARK(DIERR)
                  CALL SETCOL(0)
                  CALL CLR
                  CALL SETCOL(1)
                  ISWIT = 1
                  CALL STRDRW(ISWIT)
                  IF (IERR.EQ.11) THEN
                     ICUR = 1
                     JX = I + 1
                     JY = J
                     CALL CURSOR(JX,JY)
                  ELSE
```

```
               IERR = 12
            ENDIF
         ENDIF
         RETURN
      ELSE
         IERR = 0
      ENDIF
   ENDIF
   CHER = 2
   GO TO 930
C
945   CONTINUE
C     The *M node is prepared for entry into the connection table.
      DO 9466 POS = 117,125
         IF (IELEM(POS,2).EQ.LTR2) THEN
            M = POS
            DO 3036 KK = 1,MNUM
               IF (IMS(2,KK).EQ.LTR2) GO TO 930
3036        CONTINUE
            ICUR = 1
            JX = I + 1
            JY = J
            CALL CURSOR(JX,JY)
            IERR = 46
            CALL MYERR(IERR,IERR,IERR)
            RETURN
         ENDIF
9466  CONTINUE
      GO TO 930
C     Convert D1's to atom type 33 - i.e. unkn - store Node # in IDS(*,4)
C
943   CONTINUE
C     Dummy atom code
      DO 946 POS = 108,116
         IF (IELEM(POS,2).EQ.LTR2) M = POS
946   CONTINUE
C     No D1's with multiplier in this structure
      IF (IDNUM.EQ.0) GO TO 930
      DO 942 K = 1,IDNUM
         IF ((IDS(K,1).NE.I).OR.(IDS(K,2).NE.J)) GO TO 942
         IDS(K,4) = IATOM
         GO TO 930
942   CONTINUE
C     D1 not in table because it has no multiplier - ok - go on
930   NODE(IATOM,3)=M
999   CONTINUE
C
      ICUR = 0
      CALL CURSOR(JX,JY)
      IF (LBLEN.GT.0) CALL RELONG
      IF (KHAR.EQ.71) THEN
         CALL GPRINT
      IF (IHP .EQ. 1) THEN
      CALL FTLOCA(1,1)
      CALL FTEXT('^    ^')
      ENDIF
         CALL FTSIZE(2,18)
         CALL FTLOCA(3,1)
         CALL FTEXT('^CONNECTION TABLE IS BEING PROCESSED^')
         CALL FTSIZE(1,10)
      ENDIF
C
      DO 1910 I = 1,MNUM
         DO 1905 J = 1,IATOM
            IF ((IMS(2,I).EQ.IELEM(NODE(J,3),2)).AND.
     *         (IELEM(NODE(J,3),1).EQ.77)) GO TO 1910
1905     CONTINUE
         JX = IMS(3,I)
         JY = IMS(4,I)
         ICUR = 1
         CALL CURSOR(JX,JY)
         IERR = 46
         CALL MYERR(IERR,IERR,IERR)
         RETURN
1910  CONTINUE
```

```
C
C Zero fill balance of NODE
        DO 920 I=IATOM+1,255
        NODE(I,1)=0
        NODE(I,2)=0
        NODE(I,3)=0
920     CONTINUE
C
C Now that node table is available, the XY's in the long bond table
C can be converted to node numbers.  The node number for X1,Y1 is
C placed in the first column of the row; that for X2,Y2 is placed in
C column 3.  Columns 2 and 4 are zeroed out, while column 5, the bond
C type, is not changed:
C
C Rows of LNGBND
        DO 20 I=1,LBLEN
           II = I
C Beginning node, ending node
        DO 20 J=1,3,2
           JJ = J
           IF (J.EQ.3) THEN
              PLC = 2
           ELSE
              PLC = 1
           ENDIF
C All long bonds analyzed
C Search thru node table
                DO 22 K=1,IATOM
                IF (NODE(K,1).LE.0) GO TO 25
C Check for XY match
                IF ((NODE(K,1).NE.LNGBND(I,J)) .OR. (NODE(K,2).NE.
     2            LNGBND(I,J+1))) GOTO 22
C NODE # of XY is row # within array NODE
                LNGNDE(I,PLC) = K
C Go from beginning node to end node of longbd,
                GOTO 20
C                  or from end node to next long bond
22              CONTINUE
20      CONTINUE
21      RETURN
25      IERR = 9
C LONG BOND NODE NOT IN NODE
        CALL MYERR(IERR,KAR,KAR)
        JX = LNGBND(II,JJ)
        JY = LNGBND(II,JJ+1)
        ICUR = 1
        CALL CURSOR(JX,JY)
        RETURN
        END
C
C
        SUBROUTINE CHGHYD(IERR,JX,JY)
        IMPLICIT INTEGER*2 (A-Z)
        INTEGER*4 IARRAY
        LOGICAL*2 LOCH
        COMMON /H/ MOBILE(255,2)
        COMMON /NDE/ NODE(255,3),IATOM
        COMMON /STRPIX/ LPIX,IARRAY(90,38),LBLEN,LNGBND(100,5)
        COMMON /CONNCT/ IBOND(255,16),KBOND(255,16)
        COMMON /KHARGE/ ICHRGE(50,4),NCHG
        COMMON /IPLUS/ IHIGH(14,2)
        COMMON /CD/ MAXX,MAXY
        COMMON /RANGE/ LOX,HIX,LOY,HIY
        COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
        COMMON /CUR/ ICUR
        COMMON /HP/IHP
C
C  Counts the number of potentially mobile hydrogens and - charges
C  for each node.  Used only for tautomer analysis.
C
C  Now search IARRAY for H, D, T, -, +, ":
C       SITES OF INDETERMINATE LINK TO A 'D' STRUCTURE SYMBOLS (").
C       ARE IDENTIFIED.
           DO 111 I = 1,IATOM
```

```
            IF ((NODE(I,3).GE.108).AND.(NODE(I,3).LE.116).AND.
     *         (NBD1.NE.0)) GO TO 113
            IF ((NODE(I,3).GE.108).AND.(NODE(I,3).LE.116).AND.
     *         (NBD1.EQ.0)) THEN
               JX = NODE(I,1) + 1
               JY = NODE(I,2)
               GO TO 112
            ENDIF
 111      CONTINUE
          IF (NBD1.EQ.0) GO TO 113
          JX = DSCNC(3,1)
          JY = DSCNC(4,1)
 112      IERR = 8
          CALL MYERR(IERR,IERR,IERR)
          ICUR = 1
          CALL CURSOR(JX,JY)
          GO TO 7777
 113      CONTINUE
          DO 3333 I = 1,NBD1
            DO 2222 J = 1,IATOM
              IF ((NODE(J,1).EQ.DSCNC(3,I)).AND.(NODE(J,2).EQ.
     *           DSCNC(4,I))) THEN
                IF (IARRAY(DSCNC(5,I),DSCNC(6,I)).EQ.34) THEN
                  DSCNC(1,I) = J
                  DO 1111 K = 1,I-1
                    IF (DSCNC(1,K).EQ.J) THEN
                      IERR = 47
                      CALL MYERR(IERR,IERR,IERR)
                      ICUR = 1
                      JX = DSCNC(3,K)
                      JY = DSCNC(4,K)
                      GO TO 7777
                    ENDIF
 1111             CONTINUE
                  GO TO 3333
                ELSE
                  GO TO 2223
                ENDIF
              ENDIF
 2222       CONTINUE
 2223       CONTINUE
            DSCNC(1,I) = 0
 3333     CONTINUE
C
        NCHG = 0
        DO 3 I = LOX,HIX
        DO 3 J = LOY,HIY

        ISIGN = 1
        IF ((IARRAY(I,J).NE.72) .AND. (IARRAY(I,J).NE.68) .AND.
     2      (IARRAY(I,J).NE.84) .AND. (ILRRAY(I,J).NE.45) .AND.
     3      (ILRRAY(I,J).NE.43))    GOTO 3
C
C If first letter is H, D, T, but second is lowercase, you have a node,
C not a hydrogen--mobile group:
        IF ((IARRAY(I+1,J).GT.96).AND.(IARRAY(I+1,J).LT.128)) GOTO 3
        IF ((IARRAY(I,J).EQ.72).AND.((IARRAY(I-1,J).EQ.42).OR.
     *      ((IARRAY(I-1,J).GE.48).AND.(IARRAY(I-1,J).LE.57))).AND.
     *      (ILRRAY(I+1,J).EQ.43)) GO TO 3
C Take care of + sign (ISIGN=-1) and NUM:
        IF (ILRRAY(I,J).EQ.45) ISIGN = -1
        NUM = 1
        IF ((IARRAY(I+1,J).GE.50) .AND. (IARRAY(I+1,J).LE.57))
     2      NUM = IARRAY(I+1,J) - 48
        IF ((ILRRAY(I,J).NE.43).AND.(ILRRAY(I,J).NE.45))GO TO 60
C
C       WE HAVE A CHARGE - NOW FIND ITS NODE
C
        ICRNR = 0
        LINE=0
C       CHARGE IS DELOCALIZED
        IGH = IARRAY(I,J) / 2**13
        IF (IGH.EQ.0) THEN
        DO 15 IK = I-1,I+2
        DO 14 JK = J-1,J+1
```

```
      IF ((IARRAY(IK,JK) .EQ. 46).OR.((IARRAY(IK,JK).GE.65)
     *        .AND. (IARRAY(IK,JK).LE.90)).OR.((IARRAY(IK,JK).GE.
     *        97) .AND.(IARRAY(IK,JK).LE.122))) THEN
      IF ((K .EQ. I+2).AND.((IARRAY(IK+1,JK).LT.50).AND.
     *        (IARRAY(IK+1,JK).LE.57))) GO TO 14
      IERR=60
      CALL MYERR(IERR,IERR,IERR)
      JX=I
      JY=J
      GO TO 7777
      ENDIF
14    CONTINUE
15    CONTINUE
      GO TO 133
      ENDIF
      IX = I - IHIGH(IGH,1)
      IY = J +IHP* IHIGH(IGH,2)
C
    DO 17 K=1,IATOM
C       THE RELATIVE POSITON OF THE CHARGE IS NOTED FOR THE CONNECTION
C       TABLE. THE 8 CORNER POSITIONS ARE U=1, UR=2, R=3,
C       DR=4, D=5, DL=6, L=7, UL=8.
        IF ((IX.EQ.NODE(K,1)).AND.(IY.EQ.NODE(K,2))) THEN
           LINE = K
           IF (IGH.EQ.3) THEN
              ICRNR = 1
           ELSE IF (IGH.EQ.4) THEN
              ICRNR = 2
           ELSE IF (IGH.EQ.5) THEN
              ICRNR = 12
           ELSE IF (IGH.EQ.8) THEN
              ICRNR = 3
           ELSE IF (IGH.EQ.9) THEN
              ICRNR = 13
           ELSE IF (IGH.EQ.13) THEN
              ICRNR = 4
           ELSE IF (IGH.EQ.14) THEN
              ICRNR = 14
           ELSE IF (IGH.EQ.12) THEN
              ICRNR = 5
           ELSE IF (IGH.EQ.10) THEN
              ICRNR = 16
           ELSE IF (IGH.EQ.11) THEN
              ICRNR = 6
           ELSE IF (IGH.EQ.6) THEN
              ICRNR = 17
           ELSE IF (IGH.EQ.7) THEN
              ICRNR = 7
           ELSE IF (IGH.EQ.1) THEN
              ICRNR = 18
           ELSE IF (IGH.EQ.2) THEN
              ICRNR = 8
           ENDIF
           DO 16 L = 1,NCHG
              IF (LINE.EQ.ICHRGE(L,1)) THEN
                 IERR = 38
                 CALL MYERR(IERR,IERR,IERR)
                 ICUR = 1
                 JX = IX
                 JY = IY
                 CALL CURSOR(JX,JY)
                 GO TO 7777
              ENDIF
16         CONTINUE
           GO TO 133
        ENDIF
17  CONTINUE
C
C  The relative positions of attached hydrogens are noted for
C  the connection table.
C  First look left for node associated with IARRAY(I,J):
60    CONTINUE
      LOCH = .FALSE.
      IX = I - 1
      IF ((IX.LT.1).OR.(IARRAY(IX,J).LT.65).OR.(IARRAY(IX,J).GE.122))
```

```
     *     GO TO 4
C  If its lower case, move one more to left:
        IF (IARRAY(IX,J).GT.96) IX = IX -1
        LINE = 0
        DO 5 K=1,IATOM
        IF ((IX.EQ.NODE(K,1)) .AND. (J.EQ.NODE(K,2))) LINE = K
        IF (LINE.GT.0) GOTO 7
5       CONTINUE
        IF(LINE.EQ.0) GOTO 4
7       MOBILE(LINE,1) = NUM
        MOBILE(LINE,2) = 3
        LOCH = .TRUE.
C
C   Try looking on the right of the sign for a node:
C
4       IX = I + 1
        IF (NUM.GT.1) IX = IX + 1
        IF ((IARRAY(IX,J).LT.65).OR.(IARRAY(IX,J).GT.90).OR.(IX.GT.
     *     MAXX)) GO TO 10
        IF (IARRAY(IX,J).EQ.72) GO TO 10
        IF (LOCH) THEN
           IERR = 42
           CALL MYERR(IERR,IERR,IERR)
           JX = IX
           JY = J
           GO TO 7777
        ENDIF
        LINE = 0
        DO 8 K=1,IATOM
        IF ((IX.EQ.NODE(K,1)).AND.(J.EQ.NODE(K,2))) LINE = K
        IF (LINE.GT.0) GOTO 9
8       CONTINUE
        IF (LINE.EQ.0) GOTO 10
9       MOBILE(LINE,1) = NUM
        MOBILE(LINE,2) = 7
10      CONTINUE
C
C       Up
        IY = J + IHP
        IF ((IY.LE.1).OR.(ILRRAY(I,IY).LT.65).OR.(ILRRAY(I,IY).GT.90))
     *     GO TO 500
           IF (IARRAY(I,IY).EQ.72) GO TO 500
           IF (LOCH) THEN
              IERR = 42
              CALL MYERR(IERR,IERR,IERR)
              JX = I
              JY = IY
              GO TO 7777
           ENDIF
           DO 410 LINE = 1,IATOM
              IF ((I.EQ.NODE(LINE,1)).AND.(IY.EQ.NODE(LINE,2))) THEN
                 MOBILE(LINE,1) = NUM
                 MOBILE(LINE,2) = 5
                 LOCH = .TRUE.
                 GO TO 500
              ENDIF
410        CONTINUE
500     CONTINUE
C
C       Down
        IY = J - IHP
        IF ((IY.GE.MAXY).OR.(ILRRAY(I,IY).LT.65).OR.
     *     (ILRRAY(I,IY).GT.90)) GO TO 3
           IF (LOCH) THEN
              IERR = 42
              CALL MYERR(IERR,IERR,IERR)
              JX = I
              JY = IY
              GO TO 7777
           ENDIF
           DO 710 LINE = 1,IATOM
              IF ((I.EQ.NODE(LINE,1)).AND.(IY.EQ.NODE(LINE,2))) THEN
                 MOBILE(LINE,1) = NUM
                 MOBILE(LINE,2) = 1
                 GO TO 3
```

```
              ENDIF
710         CONTINUE
          IERR = 15
          CALL MYERR(IERR,IERR,IERR)
          JX = I
          JY = J
          GO TO 7777
133       CONTINUE
C
          IF ((ILRRAY(I,J).NE.45).AND.(ILRRAY(I,J).NE.43)) GOTO 3
          NCHG = NCHG + 1
C         CHARGE NODE NUMBER AND VALUE IS ASSIGNED.
125       ICHRGE(NCHG,1) = LINE
          ICHRGE(NCHG,2) = ISIGN*NUM
C         NONLOCAL CHARGE X & Y COORDINATES ARE
C         ASSIGNED.
          IF ((ICRNR.EQ.0).AND.(LINE.EQ.0)) THEN
              ICHRGE(NCHG,3) = I
              ICHRGE(NCHG,4) = J
              GO TO 3
          ENDIF
C         LOCAL CHARGE RELATIVE POSITION IS ASSIGNED.
          ICHRGE(NCHG,3) = ICRNR
3         CONTINUE
          GO TO 8888
C**       DO 991 I = 1,IATOM
C**          WRITE(10,444) (NODE(I,J),J=1,3),(MOBILE(I,J),J=1,2)
C**991     CONTINUE
C**       DO 888 I=1,20
C**          WRITE(10,444) I,ICHRGE(I,1),ICHRGE(I,2),ICHRGE(I,3)
C**444    FORMAT(10I8)
C**888       CONTINUE
7777      CONTINUE
          DO 8004 I = 1,IATOM
             DO 8002 J = 1,16
                IBOND(I,J) = 10000
                KBOND(I,J) = 10000
8002         CONTINUE
8004      CONTINUE
8888      RETURN
          END
C
C
          SUBROUTINE CONNET(IERR,JX,JY)
          IMPLICIT INTEGER*2 (A-Z)
          INTEGER*4 IARRAY
          COMMON /NDE/ NODE(255,3),IATOM
          COMMON /STRPIX/ LPIX,IARRAY(90,38),LBLEN,LNGBND(100,5)
C   IBOND lists up to 16 node numbers to which a given node is bonded.  The
C   row of IBOND is the node under consideration, while the contents of
C   the array elements 1-->10 are the numbers of those nodes to which it
C   is bonded.  Unused spaces are filled with integer 10000.
C   KBOND contains bond types associated with same element of IBOND.
          COMMON /CONNCT/ IBOND(255,16),KBOND(255,16)
          COMMON /CD/ MAXX,MAXY
          COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
          COMMON /M1/ MNUM,IMS(90,5)
          COMMON /CUR/ ICUR
          COMMON /LNGOUT/ LNGNDE(100,2)
C
          DO 999 I=1,IATOM
C         Search for bonds around each node. Search direction is:
C         IDIRX  left, center, right
C         IDIRY  below, center, above
             DO 990 IDIRX=-1,1
             DO 990 IDIRY=-1,1
             IF ((IDIRX.EQ.0) .AND. (IDIRY.EQ.0)) GOTO 990
C    NEWX & NEWY are nearby array elements to search for bondings.
             NEWX=NODE(I,1)
             NEWY=NODE(I,2)
234           NEWY=NEWY + IDIRY
             IF((NEWY.LT.1).OR.(NEWY.GT.MAXY))  GOTO 990
             NEWX=NEWX + IDIRX
             IF ((NEWX.LT.1) .OR. (NEWX.GT.MAXX)) GOTO 990
C            Blank, +, and - signs cannot be in bonding direction. Try
```

```
C          next direction.
C
C  JDIR is the direction a bond must have if it attaches at NODE(I,*)
           IF (IDIRX*IDIRY.EQ.1) THEN
              IF (IDIRX.GT.0) THEN
                 JDIR = 4
              ELSE
                 JDIR = 8
              ENDIF
           ELSE IF (IDIRX*IDIRY.EQ.-1) THEN
              IF (IDIRX.GT.IDIRY) THEN
                 JDIR = 2
              ELSE
                 JDIR = 6
              ENDIF
           ELSE IF (IABS(IDIRX).GT.IABS(IDIRY)) THEN
              IF (IDIRX.GT.IDIRY) THEN
                 JDIR = 3
              ELSE
                 JDIR = 7
              ENDIF
           ELSE
              IF (IDIRX.GT.IDIRY) THEN
                 JDIR = 1
              ELSE
                 JDIR = 5
              ENDIF
           ENDIF
C  If direction is ok and it is a bond, assume a link and follow it:
           IF ((MOD(JDIR,4).EQ.MOD(MOD(ILRRAY(NEWX,NEWY),2**8),4)).AND.
     2         (ILRRAY(NEWX,NEWY).GT.255)) GOTO 1000
C    A SYMBOL must have been found. LOOK FURTHER one link at line 234:
              IF (((IARRAY(NEWX,NEWY).EQ.72).OR.((IARRAY(NEWX,NEWY)
     *           .GE.49).AND.(IARRAY(NEWX,NEWY).LE.57)).AND.
     *           (IDIRY.EQ.0)).OR.((IARRAY(NEWX,NEWY).EQ.72).AND.
     *           (IDIRX.EQ.0)).OR.((IARRAY(NEWX,NEWY).GE.97).AND.
     *           (IARRAY(NEWX,NEWY).LE.122).AND.(IDIRX.EQ.1).AND.
     *           (IDIRY.EQ.0))) THEN
                 GOTO 234
              ELSE
                 GO TO 990
              ENDIF
C     Follow an acceptable bond to its other node & save bondtype:
1000          IBDTYP=ILRRAY(NEWX,NEWY)/2**8
              IBDT = IARRAY(NEWX,NEWY)
              DIR = IDIR(IBDT)
              DO 1010 K=1,MAXX
                 NEWX=NEWX+IDIRX
                 IF ((NEWX.GT.MAXX).OR.(NEWX.LT.1)) GOTO 990
                 NEWY= NEWY + IDIRY
                 IF ((NEWY.GT.MAXY).OR.(NEWY.LT.1)) GOTO 990
C  Search through node table to find second node of this bond:
                 IF (ILRRAY(NEWX,NEWY).GE.256) GO TO 1010
                 IF (((ILRRAY(NEWX,NEWY).LE.48).AND.(IARRAY(NEWX,NEWY)
     *              .NE.46)).OR.((ILRRAY(NEWX,NEWY).GE.256).AND.
     *              (IARRAY(NEWX,NEWY).NE.IBDT).AND.
     *              (IABS(IARRAY(NEWX,NEWY)-IBDT).NE.4)).OR.
     *              ((IARRAY(NEWX,NEWY).GE.49).AND.(IARRAY(NEWX,NEWY)
     *              .LE.57).AND.((MOD(DIR,4).NE.3).OR.(IARRAY(NEWX-1,
     *              NEWY).NE.72)))) GO TO 1111
                 IF ((IARRAY(NEWX,NEWY).GE.97).AND.
     *              (IARRAY(NEWX,NEWY).LE.122).AND.((MOD(DIR,4).NE.3).OR.
     *              (IARRAY(NEWX-1,NEWY).LT.65).OR.(IARRAY(NEWX-1,NEWY)
     *              .GT.90))) GOTO 1111
                    GO TO 2222
1111                CONTINUE
                    IERR = 41
                    CALL MYERR(IERR,IERR,IERR)
                    ICUR = 1
                    JX = NEWX
                    JY = NEWY
                    CALL CURSOR(JX,JY)
                    GO TO 777
2222             CONTINUE
                 DO 1020 L=1,IATOM
```

```
                    M=L
C                   Skip hanging (open) bond.
                    IF ((NODE(L,1).EQ.NEWX).AND.(NODE(L,2).EQ.NEWY))
     *                 GO TO 1101
1020               CONTINUE
1010             CONTINUE
C  There is a connection between nodes I & M.
C  Store M on next available column of Ith row of IBOND.
1101             DO 666 J = 1,16
                 IF (IBOND(I,J).NE.10000) GOTO 666
                 IBOND(I,J)=M
                 KBOND(I,J)=IBDTYP
                 GOTO 990
666            CONTINUE
C FOUND TOO MANY CONNECTIONS / NODE - ABORT
             IERR=26
             CALL MYERR(IERR,KAR,KAR)
             ICUR = 1
             CALL CURSOR(NEWX,NEWY)
777          CONTINUE
             DO 1004 L1 = 1,I
                DO 1002 L2 = 1,16
                   IBOND(L1,L2) = 10000
                   KBOND(L1,L2) = 10000
1002            CONTINUE
1004         CONTINUE
             RETURN
990            CONTINUE
999          CONTINUE
C
C Next piece of code (thru label 29) takes long bonds in LNGBND (which
C have beginning and ending node numbers in column 1 and 3 respecively,
C and bond type in column 5; columns 2 & 4 and unused rows zero-filled)
C and incorporates them into the bond tables IBOND and KBOND:
C for reversing "to" and "from"
       DO 29 M=1,2
C      Rows of LNGBND
          DO 20 I=1,LBLEN
             IF (M.GT.1) GOTO 25
C            Node# becomes line# in IBOND
                LINE = LNGNDE(I,1)
C               "to" node

                ITO = LNGNDE(I,2)
                GOTO 26
C               Reverse of above: both directions must be added to bond tables
25              LINE = LNGNDE(I,2)
                ITO = LNGNDE(I,1)
C
C               Now, put "to" node in numerical order on the LINE'th
C               line of IBOND; similarly for KBOND.  Skip across the
C               row of IBOND until ITO > IBOND(LINE,J); move the balance
C               up one column and insert the new one.
C
26             JJ=0
               DO 21 J = 1,16
               IF (ITO.GT.IBOND(LINE,J)) GOTO 21
                  IF (ITO.EQ.IBOND(LINE,J)) THEN
                     IERR = 33
                     CALL MYERR(IERR,IERR,IERR)
                     ICUR = 1
                     JX = LNGBND(I,1) + 1
                     JY = LNGBND(I,2)
                     CALL CURSOR(JX,JY)
                     DO 1008 L1 = 1,IATOM
                        DO 1006 L2 = 1,16
                           IBOND(L1,L2) = 10000
                           KBOND(L1,L2) = 10000
1006                    CONTINUE
1008                 CONTINUE
                     RETURN
                  ENDIF
                  JJ=J
C                 Move higher ones up
                  DO 22 K = 16,JJ+1,-1
                     IBOND(LINE,K) = IBOND (LINE,K-1)
```

```
                  KBOND(LINE,K) = KBOND (LINE,K-1)
 22             CONTINUE
                GOTO 23
 21           CONTINUE
 C            Fill in nodes of long bonds in place
 23           IBOND(LINE,JJ)=ITO
 C            Fill in bond type
              KBOND(LINE,JJ) = LNGBND(I,5)
 20         CONTINUE
 29       CONTINUE
 C At this point in Subroutine CONNET, INODE contains IX, IY, Element type of
 C each node (connecting atom, excluding H).  IBOND contains list of
 C connections between nodes.  The row in IBOND corresponds to the row
 C in INODE for the 'primary' end of each bond, the contents of each column
 C (up to ten columns) contains the 'other' node which the bond
 C is attached to.  At this point, each bond is represented twice.
 C KBOND contains the numerical bondtype for each bond in IBOND.
 C Unused matrix elements of K- and IBOND have been filled with 10000.
 C Note also that rows of IBOND are already sorted in numerical order
 C of node number, due to direction of node numbering, and careful
 C placing of long bonds in K- and IBOND rows.
 C
 C        The bond elements are duplicated with 2 way pointers.
          DO 8000 I = 1,IATOM
             DO 7000 J = 1,16
                IF (IBOND(I,J).LT.10000) THEN
                   IF (IBOND(I,J).LT.I) THEN
                      DO 6000 K = 1,16
                         IF (IBOND(IBOND(I,J),K).EQ.I) GO TO 6100
                         IF (IBOND(IBOND(I,J),K).EQ.10000) THEN
                            IBOND(IBOND(I,J),K) = I
                            IF ((KBOND(I,J).LT.6).OR.(KBOND(I,J).GT.7))
     *                         THEN
                               KBOND(IBOND(I,J),K) = KBOND(I,J)
                            ELSE
                               IF (KBOND(I,J).EQ.6) THEN
                                  KBOND(IBOND(I,J),K) = 7
                               ELSE
                                  KBOND(IBOND(I,J),K) = 6
                               ENDIF
                            ENDIF
                            GO TO 6100
                         ENDIF
 6000                 CONTINUE
 6100                 CONTINUE
                   ENDIF
                ENDIF
 7000        CONTINUE
 8000     CONTINUE
 C
 CXT      DEBUG DUMP WRITES
 C**      DO 1234 I=1,IATOM
 C**        WRITE(10,444) I,NODE(I,1),NODE(I,2),NODE(I,3)
 C**1234     CONTINUE
 C**444      FORMAT (16I5)
 C**      WRITE(10,444) IATOM
 C**      DO 1235 I = 1,IATOM
 C**         WRITE(10,444) I,(IBOND(I,J),J=1,8)
 C**         WRITE(10,444) I,(KBOND(I,J),J=1,8)
 C**1235     CONTINUE
 C**        WRITE(10,444) IDNUM
 C**        DO 1236 I = 1,IDNUM
 C**           WRITE(10,444) (IDS(I,J),J=1,6)
 C**1236     CONTINUE
 C**      WRITE(10,444) NBD1
 C**        DO 1237 I = 1,NBD1
 C**           WRITE(10,444) (DSCNC(J,I),J=1,2)
 C**1237     CONTINUE
 C**        WRITE(10,444) MNUM
 C**        DO 1238 I = 1,MNUM
 C**          WRITE(10,444) (IMS(J,I),J=1,16)
 C**1238     CONTINUE
 C
 C        Bonds of types 5-8 are changed to bond types 4-7 respectively.
          DO 5000 I = 1,IATOM
```

```
         DO 4500 J = 1,16
            IF (KBOND(I,J).GE.5) KBOND(I,J) = KBOND(I,J) - 1
 4500    CONTINUE
 5000 CONTINUE
      RETURN
      END
$STORAGE:2
C     SUBROUTINE TBLOUT creates the connection table according
C     to the output format developed for IBM XT preprocessing.
C
C     ORI   Paul Broderick   July, 1984
C
      SUBROUTINE TBLOUT(IERR,JX,JY)
      IMPLICIT INTEGER*2 (A-Z)
      DIMENSION CA(16),CB(16)
C
C     Array MOBILE contains each node's number of attached
C     hydrogens and the code for the graphic position of the
C     hydrogen value. The positional code used for the hydrogen
C     as well as for the charge and indeterminate bond site marker is:
C     U=1; UR=2; R=3; LR=4; DR=5; D=6; DL=7; L=8; UL=8.
      COMMON /H/ MOBILE(255,2)
C
C     The following variables are the output of SUBROUTINE
C     TBLOUT.  NNODE contains the number of nodes in the
C     chemical structure. Array TABLE comprises the connection
C     table.
      COMMON /STRDEF/ NNODE,TABLE(255,43)
C
C     Array NODE contains 3 columns: column 3 contains the
C     numeric element code that maps to the chemical symbol
C     array. Columns 1 and 2 contain the x and y graphic coordinates,
C     respectively. Variable IATOM contians the number of nodes.
      COMMON /NDE/ NODE(255,3),IATOM
C
C     Array IBOND contains, for each node, the sequence numbers of
C     up to 16 connected nodes.  Array KBOND contains the
C     corresponding bond types.
      COMMON /CONNCT/ IBOND(255,16),KBOND(255,16)
C
C     Array IELEM contains the chemical symbols for 106
C     elements plus lower case c to be output for luhn dots.
      COMMON /ELECHR/ IELEM(126,5)
C
C     Array ICHRGE contains 4 columns: column 1 contains the
C     node number to which the entry is attached. If the charge is
C     nonlocalized, the value in column 1 is 0. Column 2 contains
C     the charge value. Column 3 contains either the charge's
C     positional code relative to its node, or if the charge is
C     nonlocalized, the graphic x-coordinate of the charge. If the
C     charge is nonlocalized, column 4 contains the y-coordinate;
C     otherwise column 4 is valueless.
      COMMON /KHARGE/ ICHRGE(50,4),NCHG
C
C     Variable NBD1 contains the number of nodes which may be bonded
C     to *D structures.
      COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
      COMMON /M1/ MNUM,IMS(90,5)
      COMMON /DTDS/ DTN,DTX(30),DTY(30),DTN1(30),DTN2(30)
C
      COMMON /CUR/ ICUR
      DATA NODENO,EL,XCOOR,YCOOR,CHG,RELCGP,NHYD,RLHYDP,MASS,
     *     NCON/1,2,4,5,6,7,8,9,10,11/, MULT /6/
      DATA CA /12,14,16,18,20,22,24,26,28,30,32,34,36,38,40,42/
      DATA CB /13,15,17,19,21,23,25,27,29,31,33,35,37,39,41,43/
C
C     SUBROUTINE OUD1 is called to provide bond information arrays
C     information at the nodes of uncertain connection.  This
C     information constists of pointers to all *D structures, and
C     relative positions of graphical uncertain bond markers.
      IF (NBD1.GT.0) CALL OUD1
C
C
      DO 100 I = 1,DTN
         TABLE(I,NODENO) = I
```

```
         TABLE(I,EL) = 42
         TABLE(I,EL+1) = 32
         TABLE(I,XCOOR) = DTX(I)
         TABLE(I,YCOOR) = DTY(I)
         TABLE(I,CHG) = DTN1(I)
         TABLE(I,RELCGP) = DTN2(I)
100   CONTINUE
C
C     The number of nodes in the structure is assigned to the table.
      NNODE = IATOM + DTN
C
C     Assignments are made for each node.
      DO 500 I = DTN+1,NNODE
C
         II = I - DTN
C        The node's sequence number is assigned to the table.
         TABLE(I,NODENO) = I
C
C        The element's chemical symbol is assigned to the table.
         TABLE(I,EL) = IELEM(NODE(II,3),1)
         TABLE(I,EL+1) = IELEM(NODE(II,3),2)
         IF (TABLE(I,EL+1).EQ.0) TABLE(I,EL+1) = 32
         IF (TABLE(I,EL).EQ.74) TABLE(I,EL) = 72
C
C        The element's graphic coordinates are assigned to the table.
         TABLE(I,XCOOR) = NODE(II,1)
         TABLE(I,YCOOR) = NODE(II,2)
C
C        The connections between nodes are searched and each
C        bond to a node of higher sequence number is entered
C        into the table.  The corresponding bond types are
C        also entered.  The number of connections added to the
C        table is counted.
         NUMCON = 0
         N = 1
         IF ((TABLE(I,EL).EQ.68).AND.((TABLE(I,EL+1).GE.112).AND.
     *      (TABLE(I,EL+1).LE.120))) THEN
            SUB = 4
         ELSE IF ((TABLE(I,EL).EQ.77).AND.((TABLE(I,EL+1).GE.112)
     *      .AND.(TABLE(I,EL+1).LE.120))) THEN
            SUB = 5
         ELSE
            SUB = 0
         ENDIF
         DO 200 J = 1,16
            IF ((IBOND(II,J).EQ.10000).OR.(IBOND(II,J).LE.II))
     *         THEN
               TABLE(I,CA(J)-SUB) = 0
               TABLE(I,CB(J)-SUB) = 0
            ELSE
               TABLE(I,CA(N)-SUB) = IBOND(II,J) + DTN
               TABLE(I,CB(N)-SUB) = KBOND(II,J)
               NUMCON = NUMCON + 1
               N = N + 1
            ENDIF
200      CONTINUE
C
C        The number of connections entered into the table is
C        assigned to the table.
         TABLE(I,NCON-SUB) = NUMCON
C
C        The node's charge value and graphic relative position are
C        initialized to 0.
         IF (SUB.NE.5) THEN
            TABLE(I,CHG) = 0
            IF (SUB.NE.4) TABLE(I,RELCGP) = 0
         ENDIF
         IF (SUB.EQ.0) THEN
C
C           The node's number of attached hydrogens and their graphic
C           relative position are assigned to the table.
            TABLE(I,NHYD) = MOBILE(II,1)
            TABLE(I,RLHYDP) = MOBILE(II,2)
C
C           The abnormal mass value is set to 0.
```

```
            TABLE(I,MASS) = 0
         ELSE IF (SUB.EQ.4) THEN
C
C           The D1 structure multiplication factor is assigned.
            DO 450 J = 1,IDNUM
               IF (IDS(J,4).EQ.II) THEN
                  TABLE(I,MULT) = IDS(J,3)
                  GO TO 460
               ENDIF
450         CONTINUE
460         CONTINUE
         ENDIF
500   CONTINUE
C
C     With chemical symbol lengths convenient, a search for adjacent
C     nodes is made.
      DO 600 I = DTN+1,NNODE
         DO 550 J = I+1,NNODE
            DY = IABS(TABLE(I,YCOOR)-TABLE(J,YCOOR))
            DX = TABLE(I,XCOOR) - TABLE(J,XCOOR)
            IF (DY.LE.1) THEN
               IF (DX.EQ.0) THEN
                  OFFSET = 0
               ELSE IF (IABS(DX).LE.2) THEN
                  IF ((TABLE(I,EL+1).EQ.32).OR.(DX.GT.0)) THEN
                     OFFSET = DX / IABS(DX)
                  ELSE
                     OFFSET = 2 * DX / IABS(DX)
                  ENDIF
               ENDIF
               IF ((OFFSET.EQ.2).AND.(TABLE(I,XCOOR)-TABLE(J,XCOOR)
     *            .EQ.1)) GO TO 525
               IF ((OFFSET.EQ.-2).AND.(TABLE(I,XCOOR)-TABLE(J,XCOOR)
     *            .EQ.-1)) GO TO 525
               IF (TABLE(I,XCOOR)-TABLE(J,XCOOR).EQ.OFFSET) GO TO 525
               DX = TABLE(J,XCOOR) - TABLE(I,XCOOR)
               IF (DX.EQ.0) THEN
                  OFFSET = 0
               ELSE IF (IABS(DX).LE.2) THEN
                  IF ((TABLE(J,EL+1).EQ.32).OR.(DX.GT.0)) THEN
                     OFFSET = DX / IABS(DX)
                  ELSE
                     OFFSET = 2 * DX / IABS(DX)
                  ENDIF
               ENDIF
               IF ((OFFSET.EQ.2).AND.(TABLE(J,XCOOR)-TABLE(I,XCOOR)
     *            .EQ.1)) GO TO 525
               IF ((OFFSET.EQ.-2).AND.(TABLE(J,XCOOR)-TABLE(I,XCOOR)
     *            .EQ.-1)) GO TO 525
               IF (TABLE(J,XCOOR)-TABLE(I,XCOOR).NE.OFFSET) GO TO 550
            ELSE
               GO TO 550
            ENDIF
525         CONTINUE
               ICUR = 1
               JX = TABLE(I,XCOOR)
               JY = TABLE(I,YCOOR)
               CALL CURSOR(JX,JY)
               IERR = 40
               CALL MYERR(IERR,IERR,IERR)
               DO 540 K = 1,NNODE
                  DO 530 L = 1,16
                     IBOND(K,L) = 10000
                     KBOND(K,L) = 10000
530               CONTINUE
540            CONTINUE
               RETURN
550      CONTINUE
600   CONTINUE
C
C     All node values have been assigned except for possible
C     charge values and their graphic positions or possible
C     connection pointers to D structures and the relative graphic
C     position of the marker. Any such values are now sought and,
C     if found, are assigned to their node's table entry. If a
```

```
C       a nonlocalized charge is found, a node is created for it as
C       the last node and the number of nodes is adjusted.
        DO 700 I = 1,NCHG
           IF (ICHRGE(I,1).EQ.0) THEN
              NNODE = NNODE + 1
              TABLE(NNODE,NODENO) = NNODE
C
C             Nonlocalized charge value is assigned.
              IF (ICHRGE(I,2).GT.0) THEN
                 TABLE(NNODE,EL) = 43
              ELSE
                 TABLE(NNODE,EL) = 45
              ENDIF
              TABLE(NNODE,EL+1) = IABS(ICHRGE(I,2)) + 48
C
C             Nonlocalized graphic x and y locations are assigned.
              TABLE(NNODE,XCOOR) = ICHRGE(I,3)
              TABLE(NNODE,YCOOR) = ICHRGE(I,4)
           ELSE
C
C             Either the localized charge and relative position or
C             the identifying value of the bonded D structure and
C             the marker's relative position are assigned.
              TABLE(ICHRGE(I,1)+DTN,CHG) = ICHRGE(I,2)
              TABLE(ICHRGE(I,1)+DTN,RELCGP) = ICHRGE(I,3)
           ENDIF
700     CONTINUE
C
C       The connection table is passed to SUBROUTINE TBLCHR to be
C       converted to character strings for transmission.
        CALL TBLCHR(IERR)
C
        RETURN
        END
C
C      SUBROUTINE OUD1 places bond information for nodes which are
C      potentially, but uncertainly bonded with *D structures.  For each
C      such node, the node number representation of the *D site pointed
C      to is placed in the next available 2nd cell of array ICHRGE, the
C      relative position of its uncertain location bond marker is placed
C      in the corresponding 3rd cell, while the nod number of the node
C      itself is placed in the 1st cell.
C
C      ORI   Paul Broderick   August, 1984
C
       SUBROUTINE OUD1
       IMPLICIT INTEGER*2 (A-Z)
       COMMON /D1/ IDNUM,IDS(9,6),NBD1,DSCNC(6,50)
       COMMON /KHARGE/ ICHRGE(50,4),NCHG
C
       IDN = 1
       DO 500 I = 1,NBD1
          IF (DSCNC(1,I).NE.0) THEN
             NCHG = NCHG + 1
             ICHRGE(NCHG,1) = DSCNC(1,I)
             ICHRGE(NCHG,2) = IDN + 100
             IF (IDN.LT.IDNUM) IDN = IDN + 1
             ICHRGE(NCHG,3) = DSCNC(2,I)
          ENDIF
500    CONTINUE
       RETURN
       END
C
C   SUBROUTINE NUMCHR assigns the ASCII representation of a passed
C   decimal integer value of 1 - 3 digits to the transmission string.
C
C   ORI   Paul Broderick   July, 1984
C
       SUBROUTINE NUMCHR(VALUE,RET,NDGT)
       IMPLICIT INTEGER*2 (A-Z)
       CHARACTER*1 DIGIT(3),RET(3)
C
       IF ((VALUE.GT.999).OR.(VALUE.LT.-99)) THEN
          NDGT = 0
          RETURN
```

```
      ENDIF
      VAL = IABS(VALUE)
      DO 100 I = 1,3
         DIVD = MOD(VAL,10)
         VAL = VAL / 10
         DIGIT(I) = CHAR(DIVD + 48)
         NDGT = I
         IF (VAL.EQ.0) GO TO 110
100   CONTINUE
110   CONTINUE
C
      IF (VALUE.LT.0) THEN
         NDGT = NDGT + 1
         DIGIT(NDGT) = '-'
      ENDIF
      N = 1
      DO 200 I = NDGT,1,-1
         RET(N) = DIGIT(I)
         N = N + 1
200   CONTINUE
C
      RETURN
      END
C
C   SUBROUTINE CHKGEN computes the check digit for each transmission
C   string.
C
C   ORI   Paul Broderick   July, 1984
C
      SUBROUTINE CHKGEN(POS,CHK)
      IMPLICIT INTEGER*2 (A-Z)
      CHARACTER*1 TRANS,CHK,CHR,TMP,MSK
      COMMON /TRNS/ TRANS(80)
      EQUIVALENCE (CHR,ICHR),(TMP,ITMP),(MSK,IMSK)
      DATA ADD /32/, IMSK /63/
      ICHR = 0
      ITMP = 0
C
      DO 100 I = 1,POS
         CHR = TRANS(I)
C
         ITMP = IEOR(ITMP,ICHR)
C
100   CONTINUE
C
      ITMP = IAND(ITMP,IMSK)
C
      ITMP = ITMP + ADD
      IF (ITMP.EQ.32) ITMP = 33
      CHK = TMP
C
      RETURN
      END


!       This file contains the DUMMY files which replace some of
!       Paul's FASTTEXT files.

!       It also contains the terminal dependent graphic routines
!       needed for the HP terminal


!       Subroutine SETSCR(IARG)

!       This is a dummy subroutine - In Paul's version this sets
!       the screen number where 1 = interactive screen used for
!       prompts and 2 = graphic screen where molecules are displayed

        SUBROUTINE SETSCR(IARG)
        RETURN
        END
!       Subroutine SETCOL(IARG)

!       This is a dummy subroutine - In Paul's version this sets
!       the color of screen to black (0) or white (1)
```

```
        SUBROUTINE SETCOL(IARG)
        RETURN
        END

!       Subroutine FTSIZE(IARG1,IARG2)

!       This is a dummy subroutine - In Paul's version this
!       sets the size of the character used

        SUBROUTINE FTSIZE(IARG1,IARG2)
        RETURN
        END

!       This subroutine sets the Y and X locations for subsequent
!       calls to FTEXT

        SUBROUTINE FTLOCA(IY,IX)
        COMMON /FTLOC/IFTY,IFTX,IOFTY,IOFTX
        COMMON /CHARS/ IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        IFTY=IY-1
        IFTX=IX-1
        IOFTY=-1
        TYPE 100,IES
100     FORMAT('+',R1,'*dR',$)
        RETURN
        END

!       This subroutine sets IndHNDSHK(G) = Yes
!                            IndDC2(H) = Yes
!                            Compatibility = Off

        SUBROUTINE HNDOFF
        COMMON /CHARS/ IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        TYPE 21, IES
21      FORMAT('+',r1,'&s1g1h0p0Q',$)
        RETURN
        END

!       This subroutine gets the device ID

        SUBROUTINE DEVICE (MODEL)
        COMMON /CHARS/ IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        TYPE 22,IES
22      FORMAT('+',R1,'*s1^',$)
        ACCEPT 33,MODEL
33      FORMAT(A5)
        RETURN
        END

!       This is terminal dependent code
!       This subroutine downloads the special function keys F1 to F8

        SUBROUTINE DOWNLO
        COMMON/KEYS/ICODE(8)
        COMMON/CHARS/IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON/MOD/MODEL
        TYPE 1999,IES ! DC1,DC2 off
1999    FORMAT('+',R1,'&s1g1h0p0Q',$)

        IF (MODEL.EQ.'2647A') GOTO 3
C *** The following sequence is required for the HP-2623A
        TYPE 11,IES
11      FORMAT('+',R1,'&ja')

        TYPE 112,IES,ICODE(8)
112     FORMAT('+',R1,'&f0a1k6d1L   UP ',R1,$)
        TYPE 113,IES,ICODE(4)
113     FORMAT ('+',R1,'&f0a2k14d1L UP  &   RIGHT',R1,$)
        TYPE 114,IES,ICODE(3)
114     FORMAT ('+',R1,'&f0a3k14d1L         RIGHT',R1,$)
        TYPE 115,IES,ICODE(2)
115     FORMAT ('+',R1,'&f0a4k14d1L DOWN &  RIGHT',R1,$)
        TYPE 116,IES,ICODE(1)
116     FORMAT ('+',R1,'&f0a5k6d1L  DOWN',R1,$)
        TYPE 117,IES,ICODE(5)
```

```
117     FORMAT ('+',R1,'&f0a6k14d1L DOWN &   LEFT',R1,$)
        TYPE 118,IES,ICODE(6)
118     FORMAT ('+',R1,'&f0a7k14d1L          LEFT',R1,$)
        TYPE 119,IES,ICODE(7)
119     FORMAT ('+',R1,'&f0a8k14d1L  UP &    LEFT',R1,$)
        TYPE 22,IES
22      FORMAT('+',R1,'&jB')
        RETURN
3       ICR=13 ! Carriage return
C    Following code to download keys onto 2647A terminal:

        TYPE 112,IES,ICODE(8)
        TYPE 213,IES,ICODE(4)
213     FORMAT('+',R1,'&f0a2k8d1LUP&RIGHT',R1,$)
        TYPE 214,IES,ICODE(3)
214     FORMAT('+',R1,'&f0a3k6d1L RIGHT',R1,$)
        TYPE 215,IES,ICODE(2)
215     FORMAT('+',R1,'&f0a4k8d1LDN&RIGHT',R1,$)
        TYPE 116,IES,ICODE(1)
        TYPE 217,IES,ICODE(5)
217     FORMAT('+',R1,'&f0a6k8d1LDN &LEFT',R1,$)
        TYPE 218,IES,ICODE(6)
218     FORMAT('+',R1,'&f0a7k6d1L  LEFT',R1,$)
        TYPE 219,IES,ICODE(7)
219     FORMAT('+',R1,'&f0a8k8d1LUP &LEFT',R1,$)
        TYPE 220,IES,ICR ! Display labels on 2647A terminal+
220     FORMAT('+',R1,',cDIsplay Window #7',R1,$)
        RETURN
        END

!       This is terminal dependent code
!       This subroutine gets a character (in I3 form - i.e. if A
!       is typed on the keyboard, KAR=065) from the keyboard
!       and the X and Y coordinates

        SUBROUTINE GETCR(KAR,IX,IY)
        COMMON /CHARS/IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /SIZZE/MULTX,MULTY
        COMMON/OLD/IOX,IOY
        TYPE 20,IES
20      FORMAT('+',R1,'&k0C',$) !Caps lock off
        TYPE 21,IES
21      FORMAT('+',R1,'&k0P',$) !Caps mode disabled
        TYPE 5,IES
5       FORMAT('+',R1,'*dK',$) ! Graphics cursor on
106     TYPE 1,IES
1       FORMAT('+',R1,'b',$) ! Enable keyboard
        TYPE 2,IES
2       FORMAT('+',R1,'*s4^') ! Read cursor position & wait for kbd input
        IREADU=5          !Set read unit
        READ(IREADU,3,ERR=100)NX,NY,KAR  ! Read cursor coordinates, keystoke.i
C                      (KAR=decimal # of ASCII char)
3       FORMAT (I6,1XI6,1XI3)
c       TYPE 4,IES
4       FORMAT('+',R1,'c',$)  ! Disable keyboard
C    CLEAR PREVIOUS ERROR MESSAGE(formats 10-13)
        TYPE 10,IES
        TYPE 11,IES
        TYPE 12,IES
        TYPE 13,IES
10      FORMAT ('+',R1,'m',$) ! memory lock off
11      FORMAT('+',R1,'&a4r1C',$) ! Alpha cursor to 4th line
12      FORMAT('+',R1,'K',$)  ! Clear line
13      FORMAT('+',R1,'l',$)  ! Memory lock on
        IX=NX/MULTX  ! Scale to array coordinates
        IY=NY/MULTY  !  from graphic coordinates.
        IF ((IX*MULTX.NE.NX) .OR. (IY*MULTY.NE.NY))
      2  CALL CURSOR(IX,IY) ! Move cursor to corner if moved
        TYPE 14,IES
14      FORMAT('+',R1,'*dL',$) ! Graphics cursor off
        IF (KAR .EQ. 27) KAR=131        !Set KAR = 131 if KAR = ESC
        RETURN
100     IERR=59
        CALL MYERR(IERR,KAR,KAR)
        TYPE 5, IES
```

```
      ACCEPT 9,A
      GO TO 106
9     FORMAT(R1)
      END
!     FUNCTION GETCHR

!     This function will return the character entered from the
!     keyboard using a Fortran ACCEPT statement with an A1 FORMAT.

      INTEGER FUNCTION GETCHR()
      CHARACTER*1 KAR
      COMMON /FTLOC/IFTY,IFTX,IOFTY,IOFTX
      DATA IES/"33/
      IF (IOFTY .EQ. -1) THEN
                      IFFTY=IFTY
                      IFFTX=IFTX
      ELSE
                      IFFTY=IOFTY
                      IFFTX=IOFTX
      ENDIF
      IFFTX=IFFTX+1
      TYPE 50, IES,IFFTY,IFFTX
50    FORMAT('+',R1,'&a',I3,'r',I3,'C',$)

      ACCEPT 100,KAR
100   FORMAT(A1)
      GETCHR=ICHAR(KAR)
      IF (GETCHR .EQ. 32) GETCHR = 13 !Set GETCHR to CR if it is blank
      RETURN
      END

!     Subroutine CLOSEG

!     This is a dummy subroutine - In Paul's version this terminates
!     HALO environment and restores 'host' environment.

      SUBROUTINE CLOSEG
      RETURN
      END

!     Subroutine SETTCL(IARG1,IARG2)

!     This is a dummy subroutine - In Paul's version this defines
!     stroke text line and internal color.

      SUBROUTINE SETTCL(IARG1,IARG2)
      RETURN
      END

!     INITTC

!     This is a dummy subroutine. In Paul's version it initializes
!     the text cursor

      SUBROUTINE INITTC
      RETURN
      END

!     INITHC

!     This is a dummy subroutine. In Paul's version it initializes
!     the cross hair cursor.
      SUBROUTINE INITHC
      RETURN
      END

!     SETTEX

!     This is a dummy subroutine. In Paul's version this sets some
!     text attributes.

      SUBROUTINE SETTEX(I1,I2,I3,I4)
      RETURN
      END
```

```
!       SETDEG

!       This is a dummy subroutine. In Paul's version this sets the
!       angle definition to degrees or radians.

        SUBROUTINE SETDEG(I1)
        RETURN
        END

!       SETIEE

!       This is a dummy subroutine. In Paul's version this sets the
!       floating font format

        SUBROUTINE SETIEE(I1)
        RETURN
        END

!       FTCOLO

!       This is a dummy routine. In Paul's version this sets the character
!       and box colors for FASTTEXT

        SUBROUTINE FTCOLO(IARG1,IARG2)
        RETURN
        END

!       This is a set of graphics routines for the HP

!       SETMOD(IARG)

!       This routine sets the drawing mode
!       Input is IARG. It must be in the range 1-4
!       Values out of range are ignored

        SUBROUTINE SETMOD(IARG)
        IMPLICIT INTEGER(A-Z)
        COMMON /DRAWIT/DRWMOD
        DATA IES/"33/
        IF (IARG .LE. 0 .OR. IARG .GE. 5) RETURN        !Do nothing
                                                        !if IARG is out
                                                        !of range
        IF (IARG .EQ. 1) TYPE 10, IES   !MODE = CLEAR
        IF (IARG .EQ. 2) TYPE 20, IES   !MODE = SET
        IF (IARG .EQ. 3) TYPE 30, IES   !MODE = COMPLEMENT
        IF (IARG .EQ. 4) TYPE 40, IES   !MODE = JAM
        DRWMOD=IARG     !Save drawing mode
10      FORMAT('+',R1,'*m1A',$)
20      FORMAT('+',R1,'*m2A',$)
30      FORMAT('+',R1,'*m3A',$)
40      FORMAT('+',R1,'*m4A',$)
        RETURN
        END

!       SETLNS(IARG)

!       This subroutine sets the line type.
!       Input is IARG.Currently it must be in the range 1-3.
!       If IARG is outside the range, line type will be set
!       to 1 (solid).

        SUBROUTINE SETLNS(IARG)
        DATA IES/"33/
        IF (IARG .EQ. 2) THEN
                TYPE 20,IES             !Dashed line
        ELSE IF (IARG .EQ. 3) THEN
                TYPE 30, IES            !Dotted line
        ELSE
                TYPE 10,IES             !Solid line
                ENDIF

10      FORMAT('+',R1,'*m1B',$)
20      FORMAT('+',R1,'*m 170 2 c 2 B',$)
30      FORMAT('+',R1,'*m 85 1 c 2 B',$)
```

```
        RETURN
        END

!       MOVABS(INITX,INITY)

!       This subroutine replaces Paul's MOVABS. It does not cause an
!       actual move with PEN UP to (INITX,INITY). It merely save the
!       X and Y coordinates in INX and INY. This subroutine must
!       be used in conjunction with LNABS(IFINX,IFINY). A call to
!       MOVABS followed by a call to LNABS results in the drawing of
!       a vector from (INITX,INITY) to (IFINX,IFINY) in the mode
!       last set by SETMOD and in the line style last set by SETLNS.

        SUBROUTINE MOVABS(INITX,INITY)
        COMMON /VECT/INX,INY
        INX=INITX
        INY=INITY
        RETURN
        END

!       LNABS(IFINX,IFINY)

!       This subroutine will cause a vector to be drawn from
!       (INX,INY) - set by MOVABS - to (IFINX,IFINY) in the mode last
!       set by SETMOD and in the line style last set by SETLNS.

        SUBROUTINE LNABS(IFINX,IFINY)
        COMMON /VECT/INX,INY
        DATA IES/"33/
        TYPE 10, IES, INX,INY, IFINX,IFINY
10      FORMAT('+',R1,'*pa',4I4,'A',$)
        RETURN
        END

!       HOME

!       This subroutine moves the alpha cursor home. The 'home'
!       command is different depending on the HP model we are
!       using. Therefore MODEL in the named COMMON MOD must be
!       set to '2623A' or '2647A' before HOME is called. It can
!       be set by calling the subroutine DEVICE

        SUBROUTINE HOME
        COMMON /MOD/MODEL
        DATA IES/"33/

        IF (MODEL .EQ. '2623A' ) THEN
                        TYPE 10, IES
                        ELSE
                        TYPE 20,IES
                        ENDIF
10      FORMAT('+',R1,'H')
20      FORMAT('+',R1,'h',$)
        RETURN
        END

!       ACLEAR

!       This subroutine will clear the alpha display from the current
!       location of the alpha cursor to the end of memory

        SUBROUTINE ACLEAR
        DATA IES/"33/
        TYPE 10,IES
10      FORMAT('+',R1,'J')
        RETURN
        END

!       INITGR(IARG)

!       This substitutes for Paul's version of INITGR. This does not
!       really do all that INITGR does. It turns graphic display on,
!       turns alpha display on, turns graphic text mode off and clears
```

```
!       graphic memory. It unlocks alpha memory and moves alpha cursor
!       to HOME position. It clears the alpha screen. IARG is a dummy
!       argument.

        SUBROUTINE INITGR(IARG)
        COMMON /MOD/ MODEL
        DATA IES/"33/
        CALL MEMOFF
        CALL HOME
        CALL ACLEAR
        TYPE 10, IES
10      FORMAT('+',R1,'*dcetA')
        RETURN
        END

!       SETGPR
!       This is a dummy subroutine. In Paul's version this sets
!       the hard copy output device

        SUBROUTINE SETGPR(I1)
        RETURN
        END

!       FTINIT

!       This is a dummy subroutine. In Paul's version this initializes
!       FASTTEXT

        SUBROUTINE FTINIT
        RETURN
        END

!       GPRINT

!       This subroutine makes a hard copy of the current graphic display
        SUBROUTINE GPRINT
        COMMON/CHARS/IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /MOD/MODEL
        CALL CLEAR        !Clear alpha display
722     FORMAT(A5)
        IF (MODEL.EQ.'2623A') TYPE 724,IES ! Print graphics on 2623A
724     FORMAT('+',R1,'&p7s6dF', $)
        IF (MODEL.EQ.'2623A') ACCEPT 722,MD ! S U or F sent by term
        ICR=13 ! Carriage return
        IF (MODEL.EQ.'2647A') TYPE 726,IES,ICR !Print graphics on 2647A
726     FORMAT('+',R1,',c TRansfer File from Graphics to Hp-ib#1',R1,$)
        RETURN
        END

!       MEMOFF

!       This subroutine unlocks the memory

        SUBROUTINE MEMOFF
        COMMON/CHARS/IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        TYPE 4,IES
4       FORMAT('+',R1,'m',$)
        RETURN
        END

!       CLEAR

!       This subroutine clears all the alpha memory including the
!       first few lines which are usually locked

        SUBROUTINE CLEAR
        CALL MEMOFF       !Unlock memory
        CALL HOME         !Move alpha cursor to home position
        CALL ACLEAR       !Clear screen
        RETURN
        END

!       BAR

!       This replaces Paul's version of BAR. His version draws a
```

```
!       fat dot with borders defined by JX JY J3X J3Y.

        SUBROUTINE BAR(JX,JY,J3X,J3Y)
        IMPLICIT INTEGER(A-Z)
        COMMON /DRAWIT/DRWMOD
        COMMON /CHARS/IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        JJX=JX+8          !TEST FOR OFFSET
        JJY=JY+8
        OLDMOD=DRWMOD     !Save current drawing mode
        CALL SETMOD(4)    !Set JAM mode
        TYPE 15,IES,JJX,JJY
15      FORMAT('+',R1,'*pa',2i4,'g 0 2 2 0 0 -2 -1 0 0 1 aZ',$)
        CALL SETMOD(OLDMOD)      !Reset old drawing mode
        RETURN
        END

!       CLR

!       This clears the alpha display if IDIS=<1. If not,
!       it clears graphics memory

        SUBROUTINE CLR
        IMPLICIT INTEGER(A-Z)
        COMMON/HEAD/ MW(12),ISTATE,PAGE
        COMMON /DISPL/IDIS
        COMMON/CHARS/IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        IF (IDIS .LE. 1) THEN
                CALL CLEAR      !Clear alpha display

                ELSE
                TYPE 100,IES    !Clear graphics memory
100             FORMAT('+',R1,'*dA',$)
                ENDIF
        RETURN
        END

!       FTEXT

!       This program will display the message in the string S
!       (without the terminator characters) The first and last characters
!       are assumed to be the terminator characters. If the message is
!       a-blank-a where a's are terminators, ERASE is called to erase
!       a single graphics pixel.

!       The message is comprised of all characters encountered after
!       the first delimiter character and before the next delimiter
!       character. The string will be displayed starting at row IFTY
!       and col IFTX. This are set by the subroutine FTLOCA.

        SUBROUTINE FTEXT(S)
        CHARACTER S*(*)
        CHARACTER SS(98)*1
        CHARACTER*1 LIM,DELIM
        COMMON /FTLOC/ IFTY,IFTX,IOFTY,IOFTX
        COMMON /CHARS/IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        DATA IES/"33/
        IF (IOFTY .EQ. -1 ) THEN
                        IFFTY=IFTY
                        IFFTX=IFTX
        ELSE
                        IFFTY=IOFTY
                        IFFTX=IOFTX
        ENDIF
        DELIM = S(1:1)
        DO 10 I=2,98
        LIM=S(I:I)
        IF (LIM .EQ. DELIM) GO TO 12
10      CONTINUE
        I=98
12      L=I
        DO 90 I=2,L-1
        SS(I-1)=S(I:I)
90      CONTINUE
        IF (L .EQ. 3 .AND. SS(1) .EQ. ' ') THEN !We are really trying to
                        ITX=IFFTX+1
```

```
                    ITY=IFFTY+1
                    CALL ERASE(ITX,ITY)     !erase a pixel
        ELSE
        TYPE 80,IES
80      FORMAT('+',R1,'m',$)    !Memory lock off
        TYPE 134,IES,IFFTY,IFFTX,(SS(I),I=1,L-2)
134     FORMAT('+',R1,'&a',I3,'r',I3,'C',98A1,$)
        ENDIF
        IOFTX=IFFTX+L-2 !This shifts the X value to end of message
        IOFTY=IFFTY
                        !just typed
        RETURN
        END

!       MEMDSK

!       This is a dummy subroutine. At the moment it sets the variables
!       BPSECT, SPCLUS and CPDISK to 1 and CLUSTS to 50,000.

        SUBROUTINE MEMDSK(CLUSTS,CPDISK,BPSECT,SPCLUS)
        IMPLICIT INTEGER (A-Z)
        CLUSTS=50000
        CPDISK=1
        BPSECT=1
        SPCLUS=1
        RETURN
        END

!       MOVTCA

!       This subroutine positions the text cursor (graphics cursor)
!       absolutely.

        SUBROUTINE MOVTCA(INTX,INTY)
        DATA IES/"33/
!
!       Graphics text mode off - Position graphics cursor absolutely
!       Turn off graphics cursor
!
        TYPE 111, IES,INTX,INTY
111     FORMAT('+',R1,'*dt',I4,',',I4,'oL',$)
        RETURN
        END

!       MOVTCR
!       This subroutine positions the graphics cursor relatively.

        SUBROUTINE MOVTCR(INTX,INTY)
        DATA IES/"33/

!       Turn off graphic text mode - Position graphic cursor relatively
!       It changes the sign of the Y coordinate to account
!       for the difference in Y addressing.
!       Turn off graphic cursor

        MINTY=-INTY
        TYPE 111, IES,INTX,MINTY
111     FORMAT('+',R1,'*dt',I4,',',I4,'pL',$)
        RETURN
        END

!       MOVHCA

!       This is a dummy subroutine

        SUBROUTINE MOVHCA(INTX,INTY)
        RETURN
        END

!       STARTG(IARG)

!       This substitutes for Paul's version of STARTG. This does not
!       really do all that STARTG does. It turns graphic display on,
!       turns alpha display on and turns graphic text mode off. IARG is
!       a dummy argument.
```

```
        SUBROUTINE STARTG(IARG)
        DATA IES/"33/
        TYPE 10, IES
10      FORMAT('+',R1,'*dceT')
        RETURN
        END

!       DISPLA

!       This subroutine will turn on the display. If IARG is 1, the
!       alpha display will be turned on. If IARG is 2, the graphics
!       display will be turned on.

        SUBROUTINE DISPLA(IARG)
        COMMON /DISPL/IDIS
        DATA IES/"33/
        IDIS=IARG
        IF (IARG .EQ. 1) THEN
        TYPE 10,IES
10      FORMAT('+',R1,'*dE',$)  !Turn on alpha display
        ELSE
        TYPE 20,IES
20      FORMAT('+',R1,'*dcT',$) !Turn on graphics display and
                                !turn off graphics text mode
        ENDIF
        RETURN
        END
!       TEXT

!       This subroutine will display a single character at the current
!       graphics cursor position

        SUBROUTINE TEXT(A)
        IMPLICIT INTEGER (A-Z)
        COMMON /DRAWIT/DRWMOD

        CHARACTER A(3)*1
        COMMON/CUR/ICUR
        DATA IES/"33/
        OLDMOD=DRWMOD     !Save old drawing mode
        CALL SETMOD(4)    !Set JAM mode
                IF (ICUR .EQ. 0) THEN
                        TYPE 12,IES,A(2),IES
12              FORMAT('+',R1,'*dkS',A1,R1,'*dlT',$)     !Graphic text on
                        !graphics cursor on - type character - graphic
                        !text off

                ELSE
                TYPE 122, IES,A(2),IES
122             FORMAT('+',R1,'*dS',A1,R1,'*dlT',$)      !Graphic text on
                        !type character - graphics text off
                ENDIF
        CALL SETMOD(OLDMOD)     !Reset drawing mode
        RETURN
        END

!       MEMON

!       This subroutine locks the memory

        SUBROUTINE MEMON
        COMMON/CHARS/IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        TYPE 4,IES
4       FORMAT('+',R1,'l',$)
        RETURN
        END

!       LINE4

!       This subroutine moves the alpha cursor to X=1 Y=4

        SUBROUTINE LINE4
        COMMON /CHARS/IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
```

```
        TYPE 50,IES       !Graphics text mode off
 50     FORMAT('+',R1,'*dT',$)
        TYPE 100,IES      !Memory lock off
 100    FORMAT('+',R1,'m',$)
        TYPE 87,IES
 87     FORMAT('+',R1,'&a4r1C',$)        !Alpha cursor to 4th line
        TYPE 200, IES
 200    FORMAT('+',R1,'l',$)      !Memory lock on
        RETURN
        END
!       ERASE

!       This will erase a pixel. If the pixel has address IX,IY,
!       this subroutine will erase area with diagonals defined
!       by (IX*MULTX,IY*MULTY)(IX*MULTX+7,IY*MULTY+10)

        SUBROUTINE ERASE(IX,IY)
        IMPLICIT INTEGER(A-Z)
        COMMON /DRAWIT/DRWMOD
        COMMON /CHARS/ IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /SIZZE/MULTX,MULTY
        KX=IX*MULTX
        KY=IY*MULTY
        TYPE 30,IES,KX,KY         !Erase block - See HP manual p10-10
 30     FORMAT('+',R1,'*m1a1b',2I4,'j 0 0 7 10 F',$)
        CALL SETMOD(DRWMOD)       !Reset drawing mode
        RETURN
        END


!       ALPOFF

!       This subroutine turns off the ALPHA display

        SUBROUTINE ALPOFF
        DATA IES/"33/
        TYPE 100,IES
 100    FORMAT('+',R1,'*dF',$)
        RETURN
        END

!       GRAOFF

!       This subroutine turns off the GRAPHIC display

        SUBROUTINE GRAOFF
        DATA IES/"33/
        TYPE 100,IES
 100    FORMAT('+',R1,'*dD',$)
        RETURN
        END

!       ALPCUR

!       This subroutine moves the alpha cursor to
!       (IFTX+1,IFTY) if IOFTY is -1
!       and sets it to
!       (IOFTX+1,IOFTY) if IOFTY is not -1
!       NOTE: These variables are set by FTLOCA

        SUBROUTINE ALPCUR
        COMMON /FTLOC/IFTY,IFTX,IOFTY,IOFTX
        DATA IES/"33/
        IF (IOFTY .EQ. -1) THEN
                        IFFTY=IFTY
                        IFFTX=IFTX
        ELSE
                        IFFTY=IOFTY
                        IFFTX=IOFTX
        ENDIF
        IFFTX=IFFTX+1
        TYPE 50, IES,IFFTY,IFFTX
 50     FORMAT('+',R1,'&a',I3,'r',I3,'C',$)
        RETURN
        END
```

```
!       This subroutine causes a 1 second delay

        SUBROUTINE DELAY
        DATA IES/"33/
        TYPE 100,IES
100     FORMAT('+',R1,'a')
        RETURN
        END


!       This subroutine turns on the Alpha cursor

        SUBROUTINE ALPCON
        DATA IES/"33/
        TYPE 100, IES
100     FORMAT('+',R1,'*dQ',$)
        RETURN
        END

!       ISENSE

!       This subroutine will sense the location of the grpahics cursor
!       It will return the coordinates in IX and IY.

        SUBROUTINE ISENSE(IX,IY)
        COMMON/CHARS/IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /SIZZE/MULTX,MULTY

        TYPE 1,IES
1       FORMAT('+',R1,'&s1g1h0p0Q',$)
C       TYPE 112,IES
112     FORMAT('+',R1,'*dT')
5       TYPE 111,IES
111     FORMAT('+',R1,'*s3^',$)
        continue
        IREADU=5
        READ(IREADU,3,ERR=100) NX,NY     !Sense cursor position
3       FORMAT(I6,1X,I6)
        IX=NX/MULTX
        IY=NY/MULTY
        RETURN
100     GO TO 5          !Bad read of cursor - try again
        RETURN
        END


        !This subroutine will move the graphics cursor to IX,IY

        SUBROUTINE GRACUR(IX,IY)
        COMMON/CHARS/IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
        COMMON /SIZZE/MULTX,MULTY

C       CONVERT COORDINATES TO RASTER
        INTX=IX*MULTX
        INTY=IY*MULTY
        TYPE 111,IES,INTX,INTY
111     FORMAT('+',R1,'*dt',I4,',',I4,'oL',$)
C       (Cursor will not position correctly unless graphic text mode is
C       turned off)
        RETURN
        END


!
!       HPLONG(LB)
!
!       This subroutine contains the HP code for deleting a LONGBOND
!       It deletes long bond with index HP in the LNGBND table

      SUBROUTINE HPLONG(LB)
      IMPLICIT INTEGER*2 (A-Z)
      REAL THETA,DTHETA,THETA2,DELX,DELY,SLOPE,DX,DY
      INTEGER*4 MM,IDTPIX
```

```
      COMMON /SIZZE/ MULTX,MULTY
        COMMON/DRAWIT/DRWMOD
      COMMON /CD/ MAXX,MAXY
      COMMON /STRPIX/ LPIX,MM(90,38),LBLEN,LNGBND(100,5)
      COMMON /STRED/ IDTPIX(90,38),LABL(260,2),MRKCHN(260)
C
        OLDDRW=DRWMOD
        CALL SETMOD(1)  !Set mode to clear
            IX1 = LNGBND(LB,1)
            IY1 = LNGBND(LB,2)
            IX2 = LNGBND(LB,3)
            IY2 = LNGBND(LB,4)
            KBTYPE = LNGBND(LB,5)
C           Now calculate bond endpoints, based on circle of rad 6
C           surrounding node.
            DX=MULTX*(IX2-IX1)
            DY=MULTY*(IY2-IY1)
            SLOPE = 0.0
        IF (DX .EQ. 0) THEN
        IF (IY2 .GT. IY1) THEN
        DELV1=6
        DELV2=-6
        THETA=1.571
        ELSE
        DELV1=-6
        DELV2=6
        THETA=-1.571
        ENDIF
        DELX=0
        DELY=0
        ELSE
        DELV1=0
        DELV2=0
           SLOPE = DY/DX
           THETA=ATAN(SLOPE)
           IF ((THETA.LE.0.) .AND. (DX.LT.0)) THETA = THETA - 3.14159265
C          Principal value problem
           IF ((THETA.GT.0.) .AND. ((DX.LT.0) .OR. (DY.LT.0)))
     2        THETA = THETA + 3.14159265
C          Bond connects to circle of rad 6 pixels from center of node
           DELX=6*COS(THETA)
           DELY=6*SIN(THETA)
        ENDIF
        JX1=IX1*MULTX+4+DELX
        JY1=IY1*MULTY+5+DELY+DELV1
        JX2=IX2*MULTX+4-DELX
        JY2=IY2*MULTY+5-DELY+DELV2
C
C           Now determine bond type to draw.
            IBOND=1
            IF (KBTYPE.LE.3) IBOND=KBTYPE
C           Set mode, solid line
            CALL SETLNS(1)
C           WIGGLY LINE - BOND TYPE 8
            IF (KBTYPE.EQ.5) CALL SETLNS(2)
C           Single or triple: draw central line:
            IF ((IBOND.EQ.1).OR.(IBOND.EQ.3)) THEN
               CALL MOVABS(JX1,JY1)
               CALL LNABS(JX2,JY2)
            ENDIF
            IF (KBTYPE .EQ. 8) GO TO 70
C           No more lines to draw
            IF (IBOND.EQ.1) GOTO 100
C
C           Calculate side lines for double or triple bonds:
C           Use angle of +-.6 radians from center for side lines for triple;
C           .3 for double
70          CONTINUE
            IF (IBOND.EQ.2) THEN
               DTHETA = .2
            ELSE IF ((KBTYPE.EQ.8).OR.(IBOND.EQ.3)) THEN
               DTHETA = .6
            ENDIF
C           Change sign
            DO 55 I=1,-1,-2
```

```
            IF ((KBTYPE.EQ.8).AND.(I.EQ.1)) CALL SETLNS(2)
            IF ((KBTYPE.EQ.8).AND.(I.EQ.-1)) CALL SETLNS(3)
      THETA2 = THETA + DTHETA*I
      DELX= (6*COS(THETA2))
      DELY=(6*SIN(THETA2))
      JX1 = IX1 * MULTX + 4 + DELX
      JY1 = IY1 * MULTY + 5 + DELY
      THETA2 = 3.14159265 + THETA - I*DTHETA
      DELX=(6*COS(THETA2))
      DELY=(6*SIN(THETA2))
      JX2 = IX2 * MULTX + 4 + DELX
      JY2 = IY2 * MULTY + 5 + DELY
         CALL MOVABS(JX1,JY1)
         CALL LNABS(JX2,JY2)
55       CONTINUE
100      CONTINUE
         CALL SETLNS(1)
C        Solid line
1000  CONTINUE
      CALL SETMOD(OLDDRW)     !Restore old drawing mode
     RETURN
     END
!     BERASE

!     This will erase a pixel. If the pixel has address IX,IY,
!     this subroutine will erase area with diagonals defined
!     by (IX*MULTX-2,IY*MULTY-3)(IX*MULTX+10,IY*MULTY+12)
      SUBROUTINE BERASE(IX,IY)
      IMPLICIT INTEGER(A-Z)
      COMMON /DRAWIT/DRWMOD
      COMMON /CHARS/ IES,IDOT,ITAG,JUMP,LBOND,KAN,ISPACE
      COMMON /SIZZE/MULTX,MULTY
      KX=IX*MULTX
      KY=IY*MULTY
      TYPE 30,IES,KX,KY         !Erase block - See HP manual p10-10
30    FORMAT('+',R1,'*m1a1b',2I4,'j -2 -3 10 12 F',$)
      CALL SETMOD(DRWMOD)      !Reset drawing mode
      RETURN
      END
```

What is claimed is:

1. A computer-operated method for minimizing the number of keystrokes required to be entered at a data entry keyboard to display two-dimensional figures on a display controlled by a computer, which display is subdivided into multiple two-dimensionally arrayed grid locations, said figures being made up of plural individual segments to be entered from said keyboard and displayed in individual display grid locations, some of said segments taking the form of alphanumeric characters corresponding to keys of said keyboard, others of said segments taking the form of directional symbols having forward and rearward ends and which, when displayed, link displayed alphanumeric characters and extend in respective horizontal, vertical and diagonal directions on said display, the method comprising the steps of:

(a) entering into the computer signals representing individual graphic figure segments actuated in succession on said keyboard;

(b) storing within said computer a stored array of entered characters with locations corresponding to respective grid locations on said display;

(c) establishing a movable cursor grid location on said display;

(d) providing a plurality of selectable operating states for said computer, in each of which said plural operating states said component will interpret key entries on said keyboard differently;

(e) for each of said plural operating states, providing a protocol of preferred display element orientations each having an order of preference;

(f) storing within said computer a plurality of display elements each having a plurality of permissible orientations;

(g) in response to the entry of a display element recall code, examining in said computer said entered display element recall code and determining the identity of a corresponding stored display element to be recalled;

(h) recalling said identified stored display element;

(i) applying said respective protocol of permissible display element orientations to said identified recalled display element; and

(j) orienting the recalled display element relative to a grid location on said display according to said respective protocol.

2. A computer-operated method as claimed in claim 1, wherein said plural operating states comprise a ring state corresponding to the displaying of ringed chemical structural symbols and a chain state corresponding to the displaying of chained chemical structural symbols.

3. The computer-operated method according to claim 1, wherein said display element recall code further comprises a connection code.

4. The computer-operated method according to claim 3, further comprising the steps of:

specifying markers for each said display element for indicating the location of atoms of chemical structures represented by said display elements; and

identifying the location of each marker in each said recalled display element according to a predetermined sequence, said predetermined sequence beginning at a point therealong determined from the marker most recently used on said display prior to recall of each said stored display element.

5. The computer-operated method according to claim 1, wherein said display element recall code selectively contains a connection code;

and further comprising the step of examining said display element recall code to determine the presence of a connection code;

in response to the presence of a connection code, connecting said display element in accordance with said connection code; and

if the absence of a connection code is detected, applying a default connection code to determine connection of said display element.

6. The computer-operated method according to claim 5, wherein said connection code selectively specifies a connection by a joined bond attachment between chemical structures to be displayed, a connection by fusion of one side between chemical structures to be displayed, and a connection by fusion of two sides between chemical structures to be displayed.

7. The computer-operated method according to claim 1, wherein the recalled said display element, once oriented, can be re-oriented in accordance with the respective said protocol by entry of a re-orientation command.

8. The computer-operated method according to claim 7, further comprising the step of entering a flip command to provide a mirror-image orientation of a recalled asymmetrical display element about a predetermined point.

9. The computer-operated method according to claim 1, wherein at least some of said stored display elements have a specified merging bond attachment site associated therewith at which merging bond attachment sites said respective display elements may be connected to other display elements on said display.

10. A computer-operated method for data-entry at a keyboard to display two-dimensional figures on a display controlled by said computer, comprising the steps of:

(a) storing within a computer a plurality of stored display elements, each said stored display element corresponding to a respective system operating state in each which respective system operating state key entries are differently interpreted by said computer to cause graphic figures to be displayed in corresponding different ways on said display;

(b) establishing a movable cursor grid location on said display;

(c) entering into the computer signals representing individual graphic figure segments actuated in succession at said keyboard;

(d) in response to entry at said keyboard of a display element recall code, recalling one of said plurality of stored display elements corresponding thereto; and

(e) orienting said recalled display element according to a connection code protocol corresponding to a respective said system operating state.

11. A computer-operated method as claimed in claim 10, wherein said respective system operating state includes a chain state for displaying of chained chemical structural symbols and a ring state for displaying of ringed chemical structural symbols.

12. A computer-operated method as claimed in claim 11, wherein said connection code protocol includes spiro, hinged and jointed chemical bond attachment interfaces having specified predetermined permissible display orientations.

13. A computer-operated method of claim 10, wherein a plurality of system operating states are provided, including a chain state for displaying of chained chemical structural symbols, a ring state for displaying of ringed chemical structural symbols, a ground state for displaying display elements on said display as entered at said keyboard, and a retrieve state for retrieving from said computer stored user-defined graphic figures.

14. The computer-operated method of claim 10, further comprising the step just prior to step (a) of specifying a connecting site on at least some of said plurality of stored display elements.

15. The computer-operated method of claim 10, wherein said connection code protocol includes a preferred, ordered set of angle-pairs, and of preferred angles of rotation.

16. A computer-operated method for data entry at a keyboard to display two-dimensional figures at a display controlled by said computer, comprising the steps of:

(a) storing within said computer a plurality of stored display elements, each display element having nodes;

(b) establishing a predetermined marker sequence and ;

(c) in response to recall of a display element, recalling one of said plurality of figures and determining the position in said predetermined sequence of a last marker used for designating an atom;

said figure having markers arranged according to said predetermined sequence beginning from said last marker used.

17. The computer-operated display of claim 16, further including the steps of:

in response to the presence of an alphanumeric character in the present cursor display grid location and to an entered figure segment corresponding to a directional symbol: moving the cursor grid location under computer control to a new cursor grid location one grid space in the direction of the entered directional symbol segment.

18. The computer-operated method according to claim 16, further comprising the steps of:

in response to the presence of two alphanumeric characters supplied from a data-input means, supplying a directional symbol between the two alphanumeric characters.

19. The computer-operated method of claim 16, further comprising the steps of:

supplying a signal by an input means to said computer to indicate completion of a diagram;

wherein in response to said completion symbol, supplying under computer control all remaining markers with a symbol most commonly occurring in diagrams.

20. The computer-operated method of claim 18, wherein said symbol is the chemical symbol for a carbon atom.

21. The computer-operated method of claim 16, wherein said predetermined sequence is permitted to repeat;

further comprising the steps of:

in response to inputting a symbol when the present cursor display grid location corresponds to a marker location, replacing said marker with said symbol;

in response to inputting a marker symbol, moving the cursor grid location under computer control to a new cursor grid location corresponding to the last said marker used; and

in response to input of a command signal which indicates that another marker in a previous sequence was to have been identified, moving the cursor grid location under computer control to a new cursor grid location corresponding to an immediately preceding said marker in an immediately preceding said predetermined sequence.

* * * * *