DOCUMENTATION OF A MULTIPLE-TECHNIQUE COMPUTER PROGRAM FOR PLOTTING MAJOR-ION COMPOSITION OF NATURAL WATERS

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Documentation of a Multiple-Technique Computer Program for Plotting Major-Ion Composition of Natural Waters

By L.I. Briel

Abstract

This report is a user's manual for a new computer program that incorporates six different graphical techniques to produce diagrams for displaying data on water analyses. A multiple-technique approach to water-quality diagrams improves the display of data, because relations among variables that are not obvious on one type of diagram may be obvious on another. Piper, Stiff, pie, X–Y, boxplot, and three-dimensional (3–D) Piper diagrams can be generated from the same file of input data. The Piper 3–D diagram is a new method that projects data from the surface of a 2–D Piper plot into a triangular prism to show how variations in chemical composition can be related to variations in other water-quality variables. The modular structure of this program makes it possible to incorporate additional graphical techniques in the future.

This computer program is menu-driven, and program output can be modified in many different ways. From a menu, the user can select the type of diagram generated and a large number of individual features of the plot. These choices can also be placed in the data file if needed, which reduces the amount of information that must be entered from the terminal.

The program writes plot output to a file, and seven different formats are available from a menu: four types of device-independent metafiles, Adobe PostScript graphics files, and two Hewlett-Packard graphics language formats (7475 and 7586). In addition to the plot file, the program generates an ASCII data-table file that documents the values computed for each sample plotted. The data-table file can be omitted if needed.

This program is written in Fortran '77 and uses graphics routines from the PRIOR Advanced Graphics Toolkit reference library (PRIOR AGTK is a product of PRIOR Data Sciences, Ltd.). Currently, the program has been implemented on Prime series 50 and Data General Aviion computers; portability to other systems is limited by the availability of the graphics library. The program is intended as an analytical tool to aid in the interpretation of water-quality data; the program does not provide a means for generating camera-ready illustrations for publication by the U.S. Geological Survey.

CHAPTER 1.—INTRODUCTION

The physical and chemical properties of natural waters are used to determine water quality. Physical properties are called water-quality characteristics, whereas dissolved substances are called water-quality constituents. Because both types of water-quality data can include hundreds of different variables, the determination of the quality of a water is commonly limited to specific characteristics and constituents that best suit the needs of an investigation. Systems of classification of waters are commonly based on relations among water-quality characteristics and the concentrations of the most abundant (major) ions, and a number of different numerical and graphical techniques have been developed to display and identify these relations.

Background

Diagrams that are used for classification, correlation, and analysis of water-quality data have been introduced over the years by Palmer (1911), Rogers (1917), Hill (1940), Piper (1944), Stiff (1951), and Tukey (1977). Extended discussions of graphical methods for displaying water-quality data can be found in Zaporozec (1972), Matthess (1982), Hem (1985), and Helsel and Hirsch (1992). Digital computers have been used to produce water-quality diagrams for about 30 years. Morgan and others (1966) showed that computer methods for generating these diagrams provided the advantages of speed and reliability. Since that time, the quality of computer graphics has improved dramatically: Modern equipment can produce high-resolution color images of complex diagrams that can be rotated in three dimensions if needed. Computer-generated diagrams can be displayed rapidly on terminal screens, and permanent copies can be made on plotters, laser printers, and photographic film. Some of these advantages have been included in a new computer program that can produce six different types of water-quality diagrams.

The new computer program described in this report incorporates methodology that was used in three earlier computer programs written by others in the U.S. Geological Survey (USGS). These three unrelated programs were designed to produce Piper and Stiff diagrams (Scott Bartholoma, U.S. Geological Survey, written commun., 1987), and boxplot diagrams (Dennis Helsel, U.S. Geological Survey, written commun., 1987). Fundamental differences in the internal mechanics of these programs have been resolved, so that all three diagrams can now be produced by a single program. The new program also produces three additional types of water-quality diagrams: (1) pie diagrams that show the proportions of major ions, (2) X–Y diagrams that show relations between user-selected pairs of water-quality variables, and (3) three-dimensional (3–D) projections of Piper diagrams that show how variations in chemical composition can be related to variations in other water-quality characteristics and constituents.

Purpose and Scope

This report is a user's manual for a new multiple-technique computer program that can generate Piper, Stiff, pie, X–Y, boxplot, and Piper 3–D diagrams from the same set of water-quality data. The scope of the report is limited to techniques that are a part of the program. Each of these techniques emphasizes different aspects of the data set; relations among variables that are not obvious on one type of diagram may be obvious on another. A multiple-technique approach improves the display of data.

This program is an analytical tool that is intended as an aid in the interpretation of water-quality data. Diagrams generated by the program do not conform to all of the publication standards of the USGS, and the program is not a means for generating camera-ready illustrations for publication by the USGS. The machine figures shown in this report were generated in HPGL–7475 graphics format and have been further processed with CorelDRAW software. CorelDRAW is a product of

the Corel Systems Corporation, Ottawa, Ontario. These figures have been reduced in size and enclosed in a frame. Original output from the program is drawn to fill an 11 by 8.5-inch page (landscape orientation), and no frame is shown on the plot.

General Features

This program can be run in either interactive or batch mode. In the interactive mode, the program is menu-driven, and many features of the output can be selected from screen menus. In the batch mode, these features can be selected either by the use of program defaults, or by indicating the preferred option in the data file. Batch mode reduces the amount of information that needs to be entered from the terminal during a run.

In either interactive or batch mode, this program always reads water-quality data from an input file and writes the graphics to an output file. The program does not display the plot; plots can be displayed after a run is completed by additional processing of the output file. The type of processing that is needed to display the plot depends on the format of the plot file; seven different formats are available from the program. Plot files can be generated (1) as device-independent metafiles—including AGTK compressed-binary and three types of CGM metafiles—which require post-processor software to display the plot; (2) as Adobe PostScript graphics files, which require a laser PostScript printer to display the plot; or (3) in either of two Hewlett-Packard Graphics Language (HPGL) formats (HPGL 7475 and HPGL 7586). Plot files written in HPGL formats can be displayed on several kinds of graphics devices, including terminal screens, pen plotters, and photographic film.

In addition to the plot file, the program can produce an ASCII[1] file that lists the computed values for each sample plotted. This data table can be displayed on a terminal screen or sent to a line printer. The data-table file is an optional feature of the output and can be disabled if needed.

Portability of the Program

A portable program is one that can be easily interchanged among different computing systems. For a graphics program, the two most important factors that determine portability are the programming language and the method used to generate the graphics. The computer program described in this report is written in Fortran '77—a widely supported programming language—and uses graphics subroutines from either the PRIOR Advanced Graphics Toolkit (PRIOR AGTK) or the CA–DISSPLA graphics library. PRIOR AGTK is a product of PRIOR Data Sciences, Ltd., Kanata, Ontario, Canada; CA–DISSPLA is a product of Computer Associates International, Inc., San Diego, Calif. Either library can be used, because the graphics subroutines that are needed by the program are contained in both libraries.

The new computer program has been implemented on Prime series 50 and Data General Aviion computers within the USGS. The portability of this program to other computing systems depends primarily on the availability of the library. Versions of these libraries are available for many mainframe computers, and this program should work on any machine which supports both Fortran '77 and the required library. These libraries are not currently available for most microcomputers.

Organization of this Report

This report is divided into chapters so that a user can quickly locate specific information that is needed to run the program. Chapter numbering facilitates cross-referencing of related material. Because each of the six plotting techniques is run independently, each is discussed in a separate chapter. If a technique is not used, that chapter does not have to be read.

In this report, the term "technique" refers to the theoretical principles on which a diagram is based, whereas the term "procedure" refers to a

[1]ASCII is an acronym that represents the American Standard Code for Information Interchange. This standard assigns specific 7-bit codes to each of 128 characters, including letters, numerals, and control characters. ASCII files are also called compressed or flat files.

section of the computer program that deals with a particular technique. In chapters 2–7, the graphical technique is presented first, and this information is followed by a discussion of diagrams generated by the program. The advantages, limitations, and other features of each type of diagram are shown in figures taken from the literature and diagrams generated by the program. Comparisons are made of similarities and differences in the information that is shown on each type of diagram, and examples are shown of various user modifications that can be made to the graphics output.

Sources of program input required by all procedures are presented in chapter 8. The most important source of input is the data file; its contents and structure are described in detail. All users should read chapter 8, because a data file is needed before the program can be run. An example data file can be produced by the program if needed. A different source of required input comes from the terminal. The main menu for each of the procedures is described at the end of chapter 8.

The two principal output files, the plot file and the data-table file, are discussed in chapter 9. The formats of these files, the conventions used by the program to generate filenames, and the different means for displaying these files are described in detail. Users should study chapter 9 carefully, before the program is run for the first time. A summary of the report is presented in chapter 10. Three appendixes provide additional information on symbols and patterns (appendix A), the structure of auxiliary files (appendix B), and the different options of the program (appendix C). Numeric codes for each of the options used to produce the machine-generated figures are shown in table C–8 (appendix C).

Acknowledgments

The author acknowledges the significant contributions of John W. Atwood (computer specialist, U.S. Geological Survey, Bismarck, N.D.). Several utility subroutines written by Mr. Atwood have been incorporated into the program. His time, patience, and many helpful suggestions are greatly appreciated.

CHAPTER 2. —TRILINEAR DIAGRAMS

Trilinear diagrams have been used in chemistry and engineering disciplines for many years to express relations among three components in a system. The most common use of trilinear diagrams shows the possible phases that can exist at equilibrium when three components are mixed. Because natural waters are a single homogeneous liquid phase, trilinear diagrams are used to display composition relations that are possible among three groups of constituent ions. Units on trilinear diagrams are generally expressed as percentages of the total milliequivalents per liter for each ion in a sample, and the assumption is always made that the sum of these percentages is equal to 100.

Piper's Technique

Natural waters commonly contain 8 to 10 major dissolved ionic constituents. If ions that have similar chemical properties are grouped together, the composition of most samples can be closely approximated by three cationic and three anionic groups and represented on a compound trilinear diagram by a technique introduced by Piper (1944) and revised by him (1953). Piper's trilinear diagram (fig. 1) contains three distinct fields for plotting major ionic constituents—two equilateral triangular fields at the lower left and lower right corners of the diagram and an intervening diamond-shaped field between the triangles. Usually, a gap is left between these fields for annotation. The width of this gap has not been standardized and can differ from one presentation to another; but the three fields are always aligned so that the two upper sides of the diamond are extensions of the lines forming the outer sides of the triangles, and the upper corner of the diamond always forms a larger equilateral triangle with the outer corners of the lower triangles. Each side of each of the plotting fields has a scale reading in 100 parts.

In the cation field at the lower left, percentages of total milliequivalents per liter for three groups of cations: (1) calcium (plus barium and strontium, when needed), (2) magnesium, and (3) sodium plus potassium (plus lithium, cesium, rubidium, and ammonium, when needed) are plotted as a single point according to conventional trilinear coordinates. In the anion field at the lower right, percentages of total milliequivalents per liter for three groups of anions: (1) chloride (plus other halides, nitrates, and phosphates, when needed), (2) bicarbonate (plus carbonate), and (3) sulfate are plotted as a single point. These two points on the diagram—one in each of the triangular fields—indicate the relative concentrations of many different dissolved constituents in a sample.

A third point on the diagram in the diamond field is used to show the overall chemical character of the water. This third point is the intersection of rays projected from each of the other two points and parallel to the outer edges of the triangles (fig. 1). The position of each point in the diamond field indicates the relative composition of a sample in terms of the cation-anion pairs that correspond to the four vertices of the diamond. When the midpoints of opposite sides of the diamond are connected, each of the four smaller diamonds represents a distinct type of water composition: (1) calcium magnesium bicarbonate waters plot in the leftmost subarea, (2) calcium magnesium sulfate waters plot in the top subarea, (3) sodium potassium chloride waters (brines) plot in the rightmost subarea, and (4) sodium potassium carbonate waters plot in the bottom subarea. This classification of chemical composition represents the predominant cation and anion in the water, expressed in milliequivalents per liter. If no cation or anion constitutes as much as 50 percent of the totals, the water is classified as a mixed type, which plots near the center of the large diamond. Waters plotting within 10 percent of a boundary between types are commonly regarded as mixed types Matthess (1982).

The fields of a Piper diagram show the essential chemical character of a water according to the relative concentration of its constituents, but not according to the absolute concentration of dissolved ionic constituents in the sample. Because a knowledge of the total concentration of dissolved ions is commonly needed to compare different

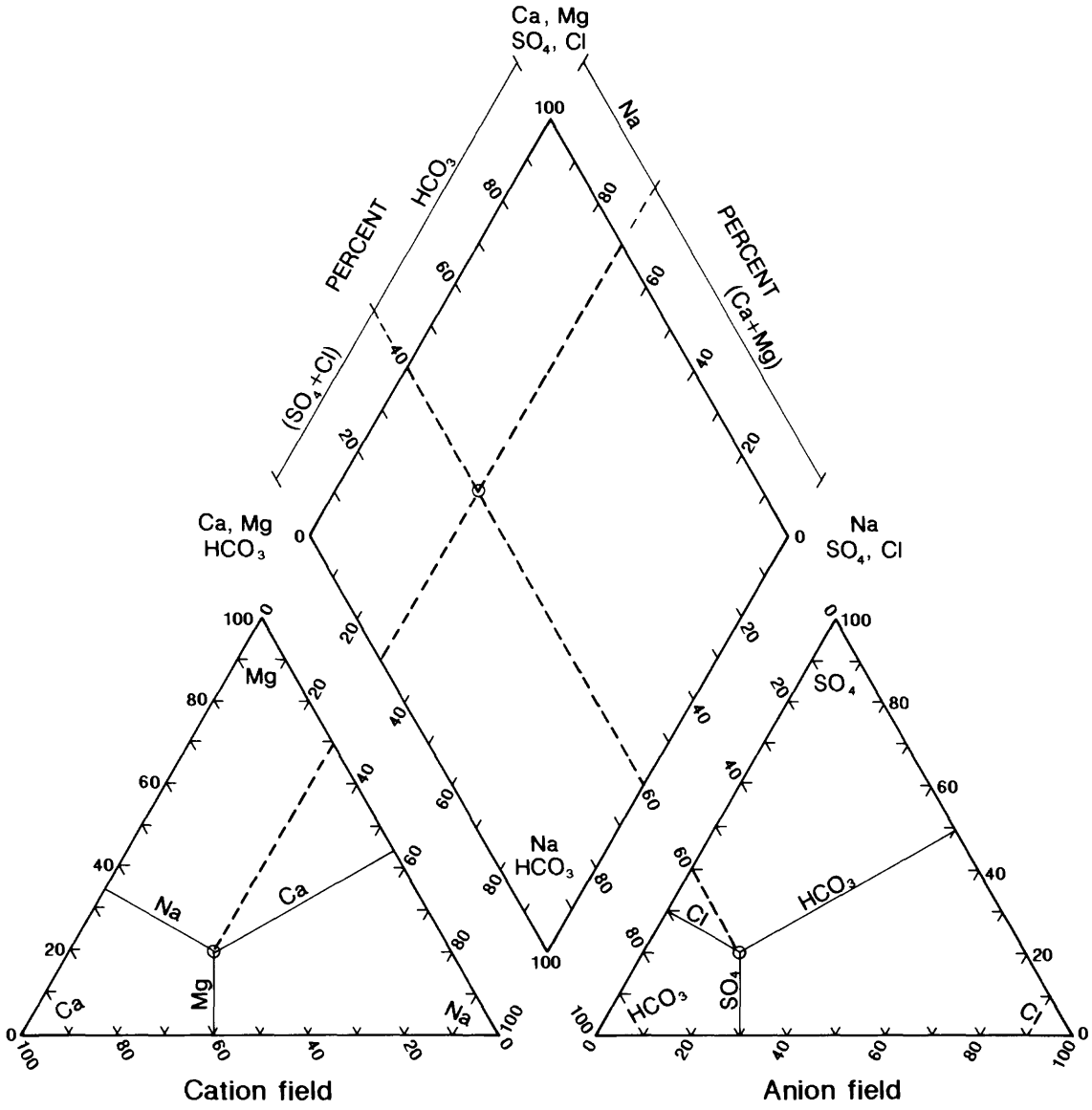

Figure 1. Piper's trilinear diagram showing the location of a water analysis in the cation and anion triangles and his method for projecting the analysis into the diamond-shaped field (modified from Piper, 1953).

waters, Piper represented the total concentration of dissolved ions for each sample in the diamond field by circles of different sizes, the area of each circle being proportional to the total ionic concentration of the sample (Piper, 1953).

Analysis of Mixtures

One advantage of the trilinear plotting technique is the ability to analyze conservative-component mixtures of waters from two or three different sources. A conservative-component mixture is one in which the total mass of each of the dissolved constituents remains unchanged after mixing has occurred; that is, no chemical reactions occur which add to or remove dissolved constituents from the system. For the remainder of this report, the term "mixture" refers to a conservative-component mixture.

On a Piper diagram, all possible mixtures of two different source waters plot on a straight line that joins the compositions of the two sources; this is true in each of the three fields of the diagram (fig. 2). To calculate the fractional volume of each of two sources in a mixture, one can treat the line joining the three points as a lever with its fulcrum at the composition of the mixture and the composition of each source acting at its respective end. A mixture of equal volumes from two different source waters always plots at the midpoint of the lever line, whereas a mixture of unequal volumes is shifted proportionally closer to the composition of the larger contributor (Rhines, 1956). The volume fraction for each source in a two-component mixture can be calculated from the following two inverse proportionalities:

$$V_A = b \times C_B / (a \times C_A + b \times C_B)$$

$$V_B = a \times C_A / (a \times C_A + b \times C_B)$$

where V_A and V_B are the volume fractions of the two sources, A and B, in the mixture; C_A and C_B are the concentration in milliequivalents per liter of any particular ion in each of the two sources; and a and b are the lengths of the two lever arms between the composition of the mixture and the composition of each of the sources (fig. 2). Lever arms can be measured in any convenient unit and in any of the three fields of the diagram. If the mixed water is a simple binary, both equations will yield the same mixing proportions for any constituent. Piper diagrams are commonly used to test the appropriateness of a binary-mixing model. If a sample does not plot on the line connecting two hypothetical source waters, calculation of binary mixing proportions is not justified.

Ternary-mixing models can also be evaluated on Piper diagrams. For three-source mixing, the compositions of the three sources form a triangle on the diagram, and all possible mixtures plot within that triangle. To calculate the proportions of a ternary mixture, one can still apply the lever principle: The source triangle becomes a lever plane supported on a fulcrum at the composition of the mixture. There is a unique combination of mixing proportions from three source waters that will balance the lever plane, and this is true in each of the three fields of the diagram (fig. 3). A mixture of equal volumes from three source waters plots at the geometric center of the triangle, whereas a mixture of unequal volumes is shifted proportionally closer to the composition of the larger contributors. The volume fraction of each source in a three-source mixture can be calculated from the relative length of the lever arms formed by a line drawn from each of the sources through the mixture to its intersection with the opposite side of the source triangle. The volume fraction is equal to the ratio of the more distant lever arm to the total length of the two arms (Rhines, 1956), as shown in figure 3:

$$V_A = a_2 / (a_1 + a_2)$$

$$V_B = b_2 / (b_1 + b_2)$$

$$V_C = c_2 / (c_1 + c_2)$$

where V_A, V_B, and V_C are the volume fractions of each of the three sources, A, B, and C, in the mixture; a_1 and a_2 are the lengths of two lever arms formed by a line from the location of source A through the location of the mixture to the opposite side of the triangle; b_1 and b_2 and c_1 and c_2 have similar relations to source B and source C, respectively. The lever arms can be measured in any convenient unit and in any field of the diagram. For ternary mixtures, it is not necessary to know the ionic concentration of any particular constituent, but two of the lever equations must be applied to determine the proportions of the mixture. If the composition of a sample does not

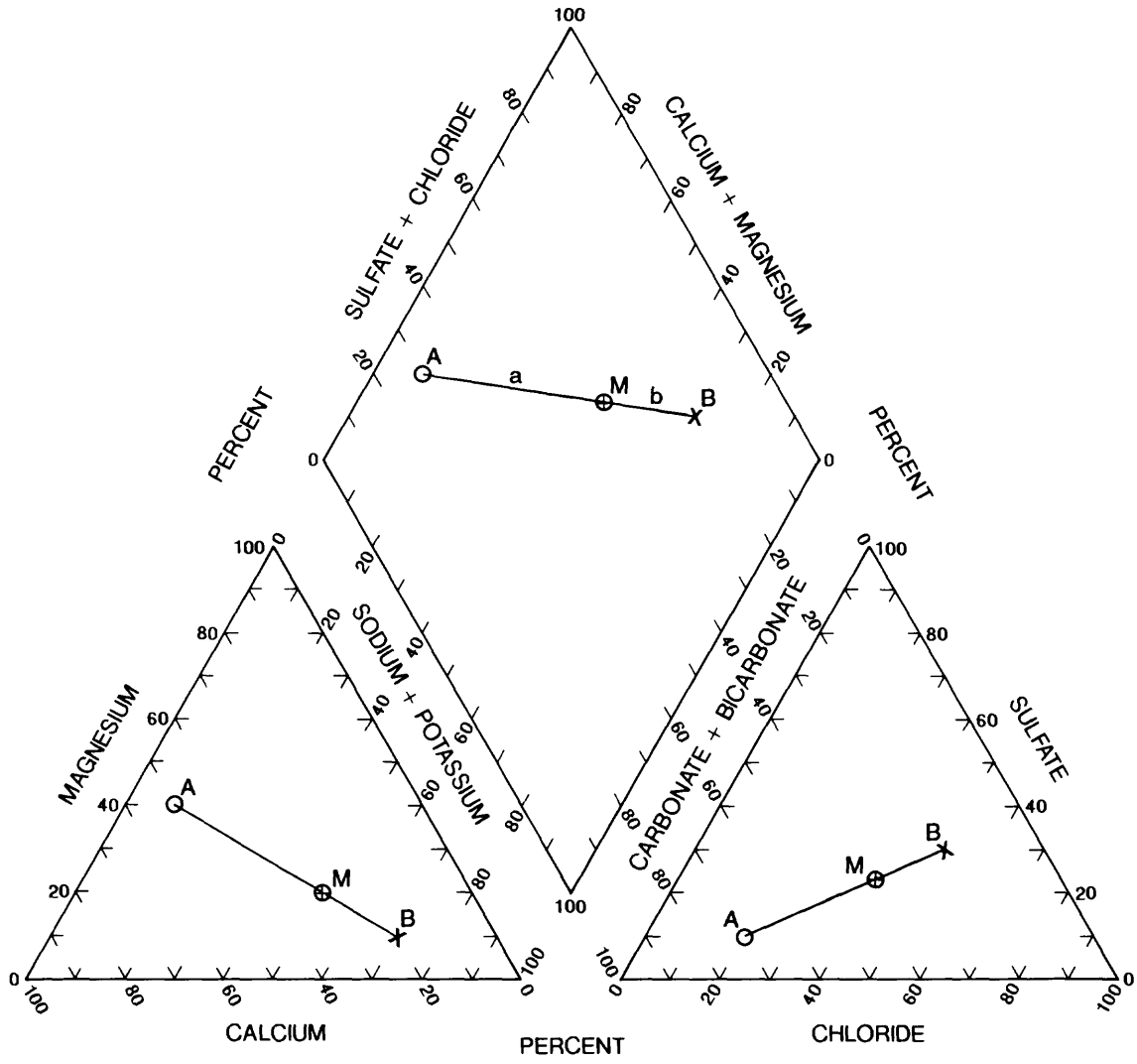

Figure 2. Piper diagram used to test the hypothesis of a binary-mixing model. If a water having a composition represented by point **M** is a binary mixture of two source waters represented by points **A** and **B**, then **M** must lie on the line connecting **A** and **B**. The fractional contributions of sources **A** and **B** in mixture **M** are inversely proportional to the lengths of the line segments a and b.

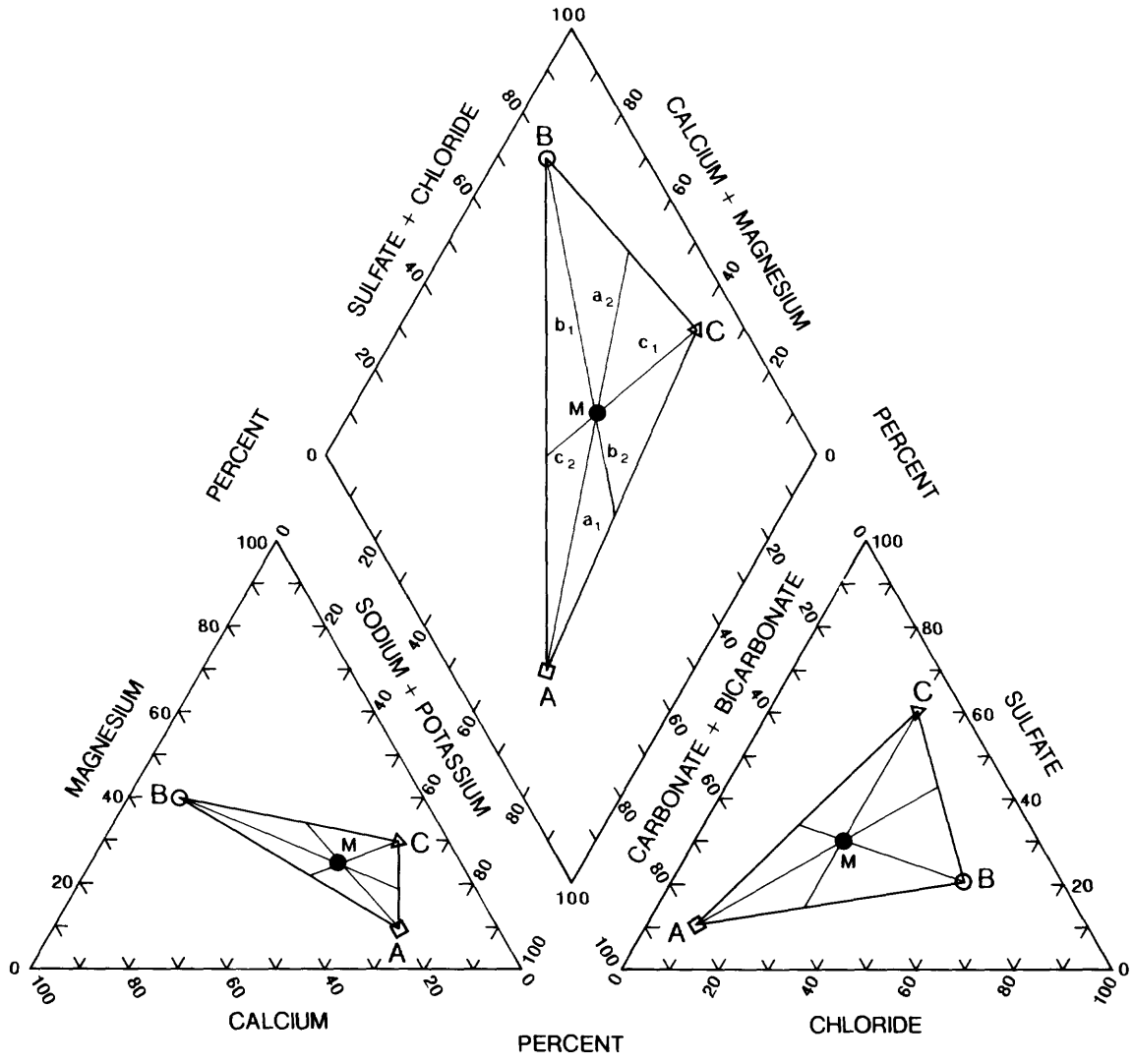

Figure 3. Piper diagram used to test the hypothesis of a ternary-mixing model. If a water having a composition represented by point **M** is a ternary mixture of three source waters represented by points **A**, **B**, and **C**, then **M** must lie inside the triangle formed by connecting **A**, **B**, and **C**. The fractional contribution of source **A** to mixture **M** is proportional to the length of the more distant line segment a_2 divided by the total distance from point **A** through mixture **M** to the opposite side of the triangle. Similar relations exist for sources **B** and **C**.

plot within the area of the source triangle, calculation of simple ternary mixing proportions for that sample is not justified.

If four or more source waters are mixed, a unique solution for the proportions of the mixture cannot be obtained without imposing additional assumptions. Ternary-mixing models can be used to estimate the proportions of sources in higher-order mixing systems by selecting three source waters that seem to be the most important contributors to a mixture and calculating the relative proportions of these sources in the mixture. Then, each of the source waters can be treated as a mixture of three other sources, and the process can be repeated until all potential sources have been considered. The final result is a succession of mixing proportions for the original mixture that is distributed among all the sources. The result, however, depends on the assumptions used to assemble the hierarchy of sources, and it is not a unique solution for that mixture.

Piper-Diagram Output from the Program

The conversion factors given in the table at the front of this report are used to calculate concentrations in milliequivalents per liter for 10 ionic constituents. Next, total milliequivalents per liter of cations and anions are calculated, and then milliequivalent percentages are calculated for each of the individual ions within its respective group. The sequence of calculations can not impose the constraint of ionic charge balance, and this is one of the limitations of the Piper procedure. For balance, milliequivalents of cations must be equal to milliequivalents of anions. The program plots samples in the trilinear fields of the diagram whether or not the ionic charges are balanced. It is left to the user to screen samples in a data set for charge balance. This screening can be done by use of the Stiff (chap. 3), pie (chap. 4), or X–Y diagram (chap. 5) procedures of the program. These procedures can indicate which samples are too far out of balance to be included on a Piper diagram.

The Piper 2–D diagrams generated by this program give no indication of the total ionic concentration of individual samples, because it is not practical to extend Piper's technique of different-sized circles to irregularly shaped plotting symbols. On these diagrams, dilute samples (rain water) can appear in the same locations as concentrated samples (brines). A user should understand that although adjacent points on Piper diagrams can indicate similar water compositions, individual variations in other important water-quality constituents and characteristics, notably, dissolved solids, specific conductance, and pH, are not being shown. The Piper procedure uses pH in a rather subtle way: The maximum pH found in a data set is used to select an appropriate label for the carbonate-bicarbonate axis. Unless a sample is strongly alkaline, the carbonate ion ($CO_3^{=}$) concentration represents only a small fraction of the total concentration of carbonate ion plus bicarbonate ion (HCO_3^{-}); if the pH of a sample is less than 7.3, the $CO_3^{=}$ concentration represents less than 1 percent of this total. Therefore, if the maximum pH for a set of samples is less than 7.3, the axis label on the Piper diagram is shown as **BICARBONATE**; otherwise, this label is shown as **CARBONATE + BICARBONATE**. Although the absolute concentration of individual samples is not shown on Piper 2–D diagrams generated by this program, diagrams from the other five procedures can show absolute concentration in different ways (chaps. 3–7).

Examples of trilinear plots generated by the program are shown in figures 4–6. Figure 4 shows the default output for the Piper procedure: A file of samples is identified by a plot title at the top of the page. The composition of each sample is represented by the location of a distinctive plotting symbol, which appears in each of the three fields of the diagram and in the explanation field at the right. In the explanation field, symbols are paired with sample-identification labels taken from the data file. Consecutive samples in the file with the same sample-identification label are plotted with the same symbol, and only one entry per group of samples appears in the explanation field (see The Label Variable, chap. 8). Supplementary information on median dissolved-solids concentration, median specific conductance, median pH, ionic-charge balance, and dates of sample collection is shown in five subtitles at the upper left. The user-date-time tag at the lower left corner of the page shows when the plot was generated and by whom.

Figure 5 shows some user-selected modifications to the Piper plot: The subtitles have been omitted, and the explanation field has been expanded to accommodate a maximum of 48 labels. The PRIOR AGTK graphics library contains a total of 18 different symbol shapes (appendix A, fig. A–1). If the number of samples (or groups of samples) exceeds 18, symbols must be used more than once on a diagram to represent different samples. In this situation, the program changes the color of each plotting symbol, and the 18 shapes are used again in the same order. The order of symbol selection can be changed if needed (see appendix B). If more than 36 samples are in a data set, the symbol color is changed again, and so on. If PostScript is selected for the plot format, there are subtle changes in the appearance of plotting symbols that are attributable to changes in the color variable. Symbols of different colors are drawn with differences in density of shading, but some of these changes are not particularly obvious.

To identify a larger number of labels, the program provides an alternative symbol set that contains 60 different shapes (appendix A, fig. A–2). The choice of symbol set is left to the user; the alternative set, however, is the default for the program. If a single symbol is used to plot all samples (fig. 6), that symbol can be chosen from either set.

A distinct advantage of Piper's technique is that one diagram can display information on the composition of a large group of individual samples. In figure 6, the explanation field has been omitted, symbol shape and color do not change from sample to sample, and symbol size has been reduced to one-half of the default size. This diagram shows the composition of 366 different samples. Any number of samples can be plotted, but the resolution of adjacent points becomes difficult to see as a diagram becomes crowded.

Most of the annotation on the Piper diagram including the main title, the five additional subtitles, the axis labels, and the user-date-time tag can be omitted selectively. The axis numbering, however, is always on. When a subtitle is omitted, all remaining subtitles are automatically moved upward, so that large gaps are not left on the plot.

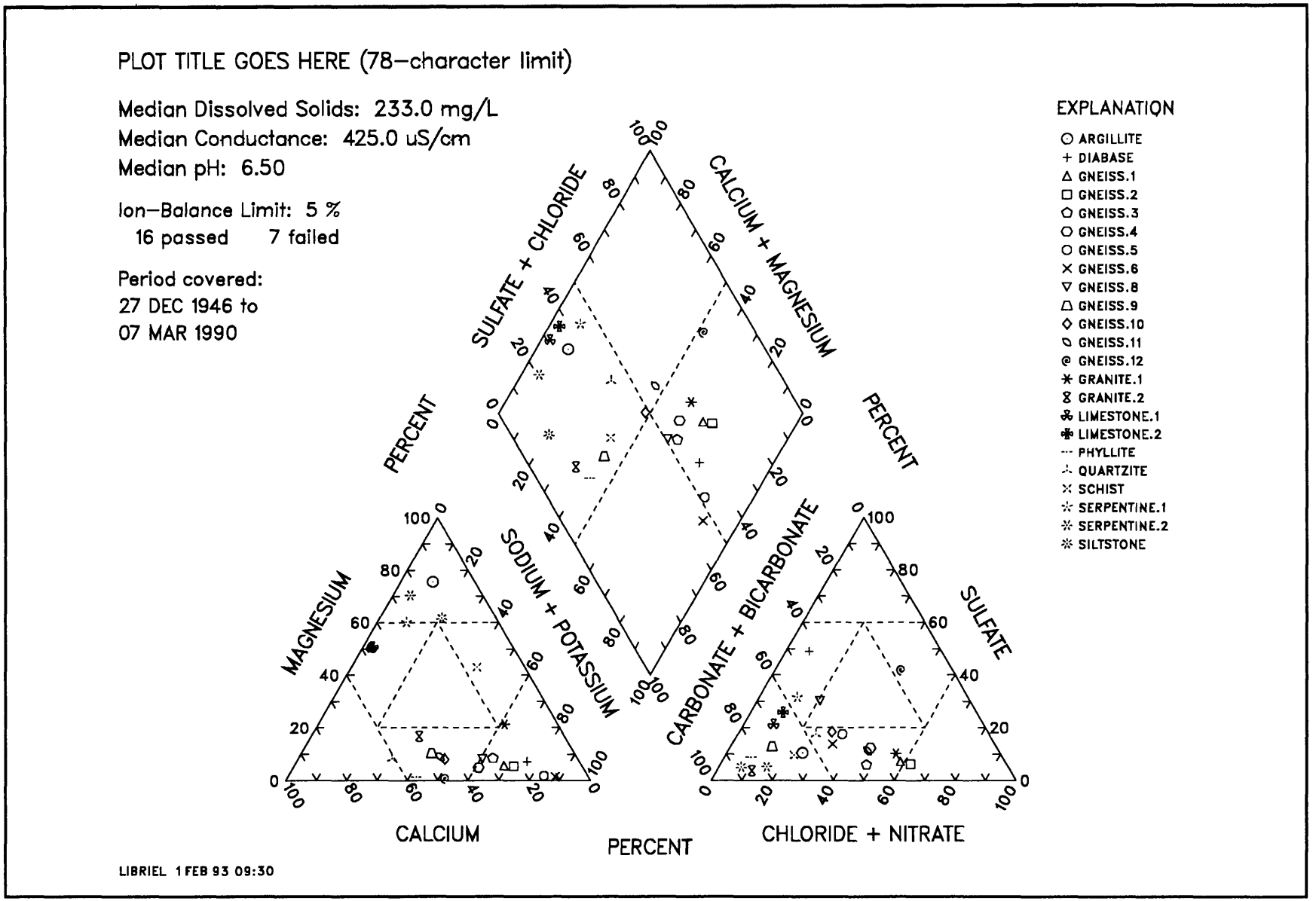

Figure 4. Piper diagram generated by the program from test data showing standard features of the diagram for a group of 23 water analyses.

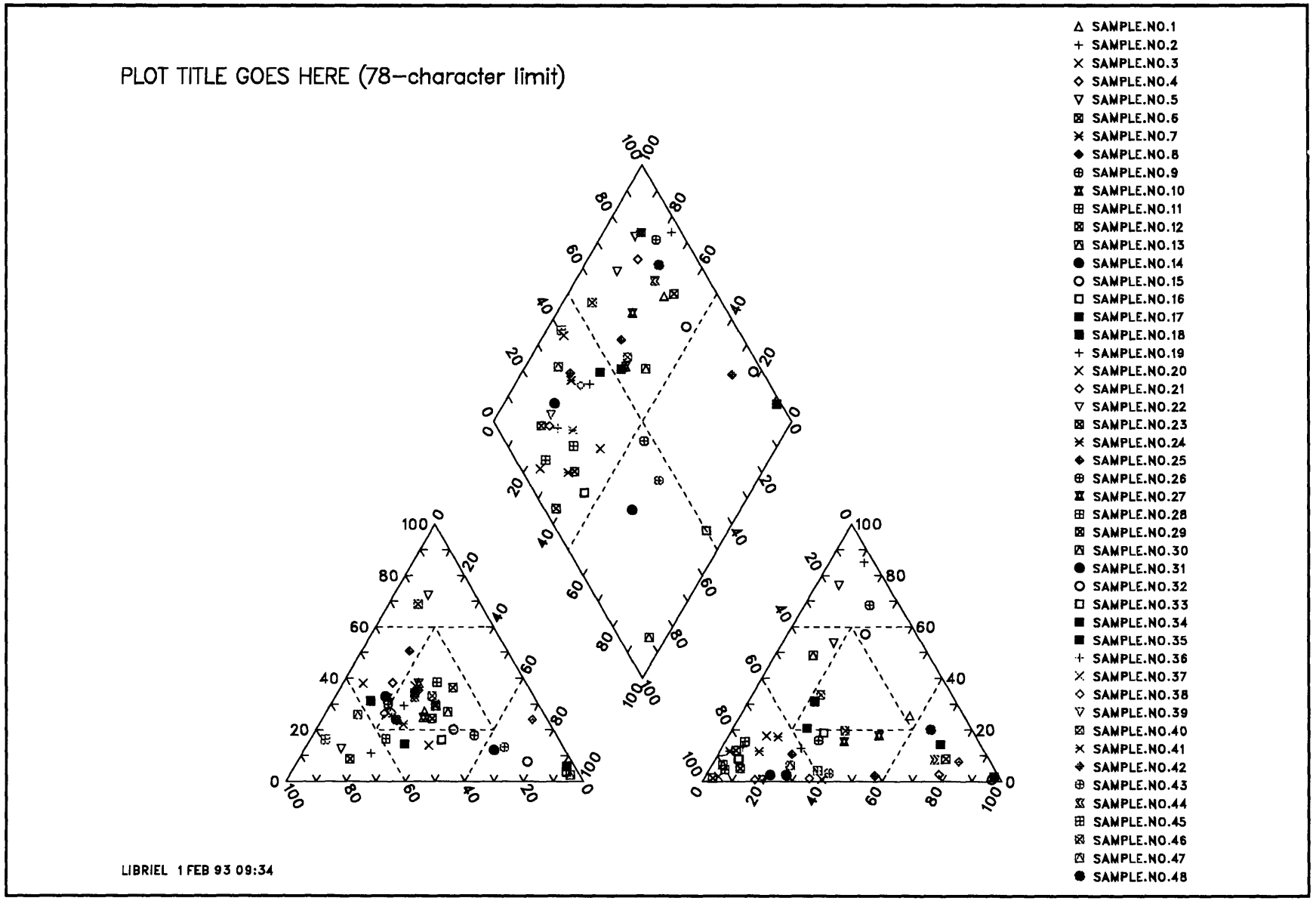

Figure 5. Piper diagram generated by the program from test data showing maximum expansion of the symbol-explanation field to identify 48 symbols and reduced annotation around the diagram.

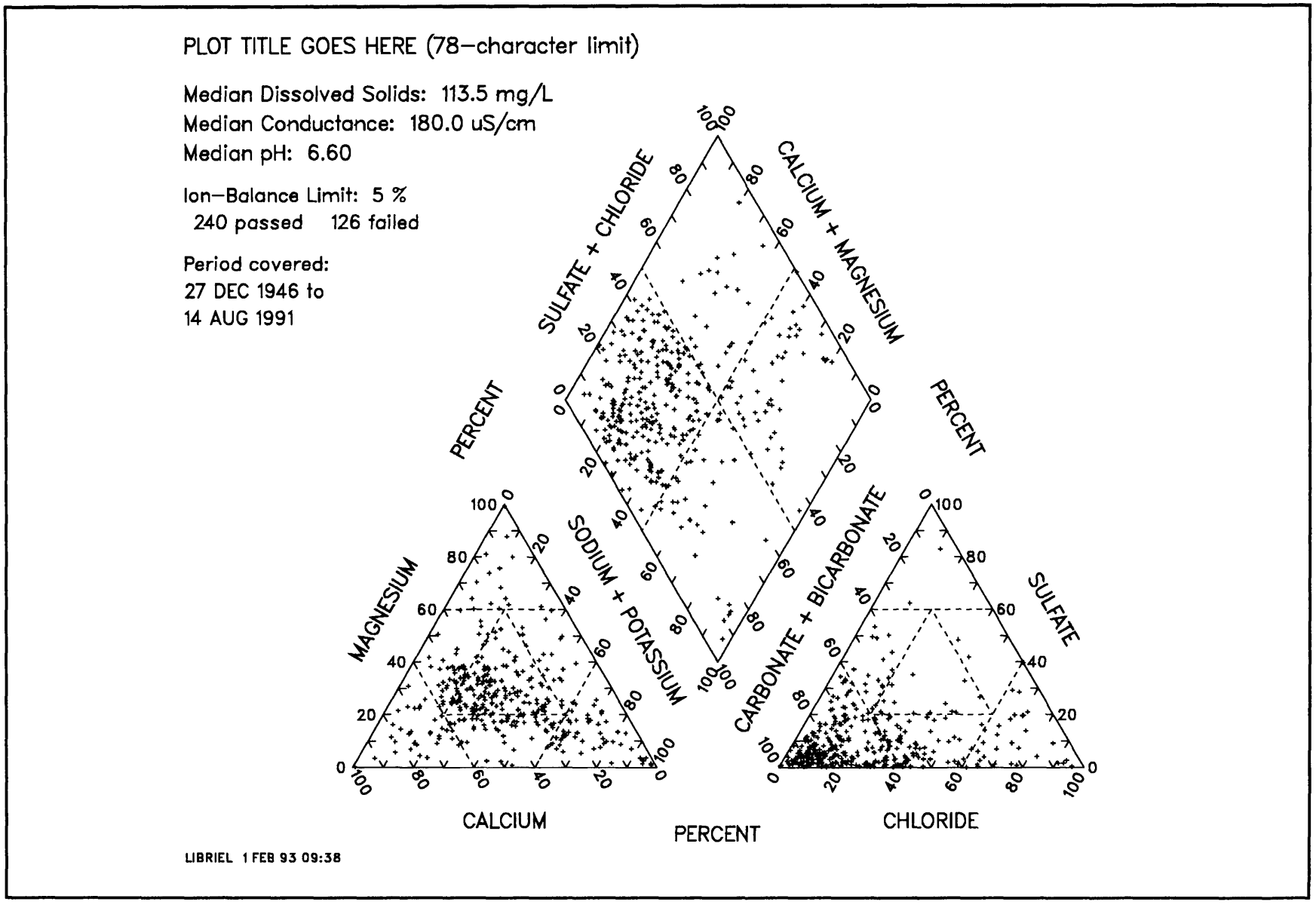

Figure 6. Piper diagram generated by the program from test data showing the use of the diagram to display the composition of a large number of water analyses.

CHAPTER 3.—DISTINCTIVE-PATTERN DIAGRAMS

A number of methods have been proposed for constructing distinctive-pattern diagrams to show the composition of water samples. These diagrams generally involve vectors radiating from a common point or line, the length of each vector being proportional to the concentration (in milli-equivalents per liter) of various cations and anions in the water. Distinctive-pattern diagrams can be drawn in any convenient size, and they are particularly useful for showing similarities and differences in water composition as symbols on a map (Hem, 1985). Distinctive-pattern diagrams display data with much greater perceptual precision than pie diagrams, and distinctive-pattern diagrams are preferred when it is important to show small differences among water samples (Helsel and Hirsch, 1992). An irregularly-shaped polygonal pattern diagram introduced by Stiff (1951) for analyzing oilfield waters is perhaps the most widely used of the distinctive-pattern water-quality diagrams.

Stiff's Technique

Stiff's distinctive-pattern diagram (fig. 7a–b) uses four parallel horizontal axes extending on each side of a vertical (zero) axis. Milliequivalent concentrations of four cations (sodium, calcium, magnesium, and iron) are plotted to the left of zero, one on each horizontal axis; likewise, milli-equivalent concentrations of four anions (chloride, bicarbonate, sulfate, and carbonate) are plotted to the right of zero (fig. 7a). The ions are always plotted in the same sequence. Any system of suitable scales can be used for plotting ionic concentrations on the horizontal axes, but for fresh waters, Stiff (1951) suggested that the same scale should be used for all four axes. Adjacent points on the diagram are connected to form an irregular polygonal shape (fig. 7b) that is characteristic of a distinct type of water composition.

One advantage of Stiff's technique is the tendency of a polygon to retain its characteristic shape as a sample becomes diluted. Stiff showed that an analysis of the shape of a polygon can be used to trace the movement of ground water in an area, and to detect mixing of ground waters (leakage) of different characteristic types. The Stiff diagram, however, does not allow the precise determination of mixing volumes, which can be determined on trilinear diagrams.

Another advantage of Stiff's technique is the ability to show the total ionic concentration of each sample. If all horizontal axes are drawn to the same scale, the width of each polygon, as measured from the maximum cation concentration to the maximum anion concentration, is an approximate indication of total ionic concentration. Stiff polygons for very dilute samples (rain water) are narrow, whereas Stiff polygons for concentrated samples (brines) are broad. Therefore, even if Stiff polygons for two different samples happen to have the same characteristic shape, these samples cannot be mistaken for one another.

Stiff-Diagram Output from the Program

Stiff diagrams generated by the program depart from Stiff's model in several ways: (1) The diagrams are drawn with less detail than is shown in figure 7b. The polygon and the vertical axis are shown on each diagram, but the horizontal axes are not shown. A uniform scale is used for all of the horizontal axes, and this scale is shown along a horizontal line which lies at the base of the diagram. This line is not one of the horizontal axes of the polygon, but it is parallel to them. (2) Stiff diagrams generated by the program have a different system of axes than the one shown in figure 7b. These diagrams show the same constituents that appear on Piper diagrams generated by the program. Stiff diagrams have only three cation axes on the left side of the vertical axis and three or four anion axes on the right side. The fourth axis can be created if a user needs to display nitrogen and phosphorous; this is an advantage in the analysis of waters that contain unusually large amounts of nitrogen and phosphorous. (3) Stiff diagrams generated by the program use a scheme for grouping the constituents shown on the

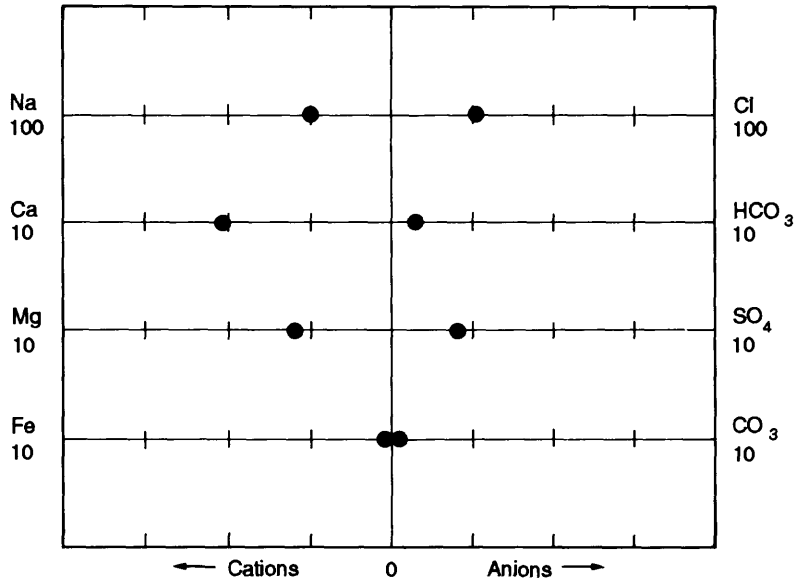

Figure 7a. Stiff's pattern diagram for displaying water-quality data on a system of four parallel horizontal axes and one vertical (zero) axis. This diagram shows the concentration of four cations and four anions.

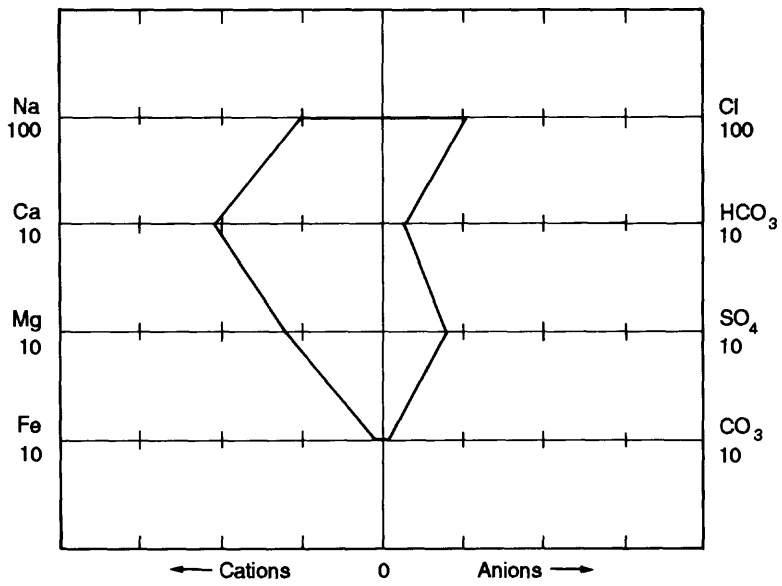

Figure 7b. Stiff figure formed by connecting the eight points plotted in figure 7a. Individual points on the diagram are not emphasized in Stiff's technique. (Modified from Stiff, 1951).

horizontal axes: Sodium is combined with potassium (**NA+ K**); chloride is combined with fluoride (**CL + F**); bicarbonate is combined with carbonate ($\mathbf{HCO_3 + CO_3}$); and nitrogen is combined with phosphorous (**N + P**), if both are present.

Piper's technique allows many samples to appear on a single diagram; Stiff's technique plots each sample on a separate diagram. The program draws as many as 12 Stiff diagrams on a page, each diagram in a separate field. If more than 12 samples are in a file, a new plot page is generated to accommodate each set of 12 diagrams. All multiple pages have the same plot title and user-date-time tag, and each page has a unique tag in the upper right corner. The page tag is automatically moved to the lower left corner, if the length of the plot title exceeds 67 characters. Examples of Stiff diagrams generated by the program are shown in figures 8 and 9.

Figure 8 shows the default output for the Stiff procedure: A file of samples is identified by a plot title at the top of the page. The composition of each sample is represented by a Stiff polygon drawn in a separate area of the page. A sample-identification label from the input file is shown at the upper left of each diagram, and a sequential sample number is shown at the upper right. Sequential sample numbers on the plot pages provide a means of cross-reference between each Stiff polygon and its data in the data table (chap. 9). The ends of the horizontal axes are labeled with standard chemical notation to indicate which cations and anions are shown on the axis.

The pH of each sample is used to select an appropriate label for the carbonate-bicarbonate axis: If pH is less than 7.3, the label is shown as $\mathbf{HCO_3}$; otherwise, the label is shown as $\mathbf{HCO_3 + CO_3}$. The ion-balance value in percent shown at the bottom of each Stiff diagram is an indication of charge balance for the sample.

Ion balance is calculated from total concentrations of cations and anions by use of the following equation:

$$\text{ion balance} = \frac{(\text{cations} - \text{anions})}{(\text{cations} + \text{anions})} \times 100.$$

If the concentrations of cations and anions are equal, the ion-balance value is equal to zero. If the ion-balance value is greater than zero, the concentration of cations exceeds the concentration of anions by the percentage shown, and if the ion-balance value is less than zero, the opposite is true. For convenience, the Stiff diagrams show only the absolute value of the ion-balance. If the ion-balance value is placed on the cation (left) side of the diagram, the concentration of cations exceeds the concentration of anions; if the value is placed on the right side of the diagram, anions exceed cations.

The default scaling option for the Stiff procedure draws each diagram to a concentration scale suitable for that sample, which maximizes the size of each polygon within its field. For purposes of comparison, a user may prefer a uniform scale for all diagrams. At the beginning of each run, the program reports the largest concentration found in the data, which aids in the selection of a uniform scale. The diagram scale can be either entered from the terminal or placed in the data file. Figure 9 shows a Stiff plot in which all diagrams are drawn to the same scale.

The Stiff-diagram procedure deals with samples in the data file one at a time; no data are stored, and the procedure does not limit the number of diagrams that can be drawn during a run. Because Stiff diagrams do not use different colors and shade patterns, Stiff plot files are generated faster and occupy less disk space than plot files from the other procedures.

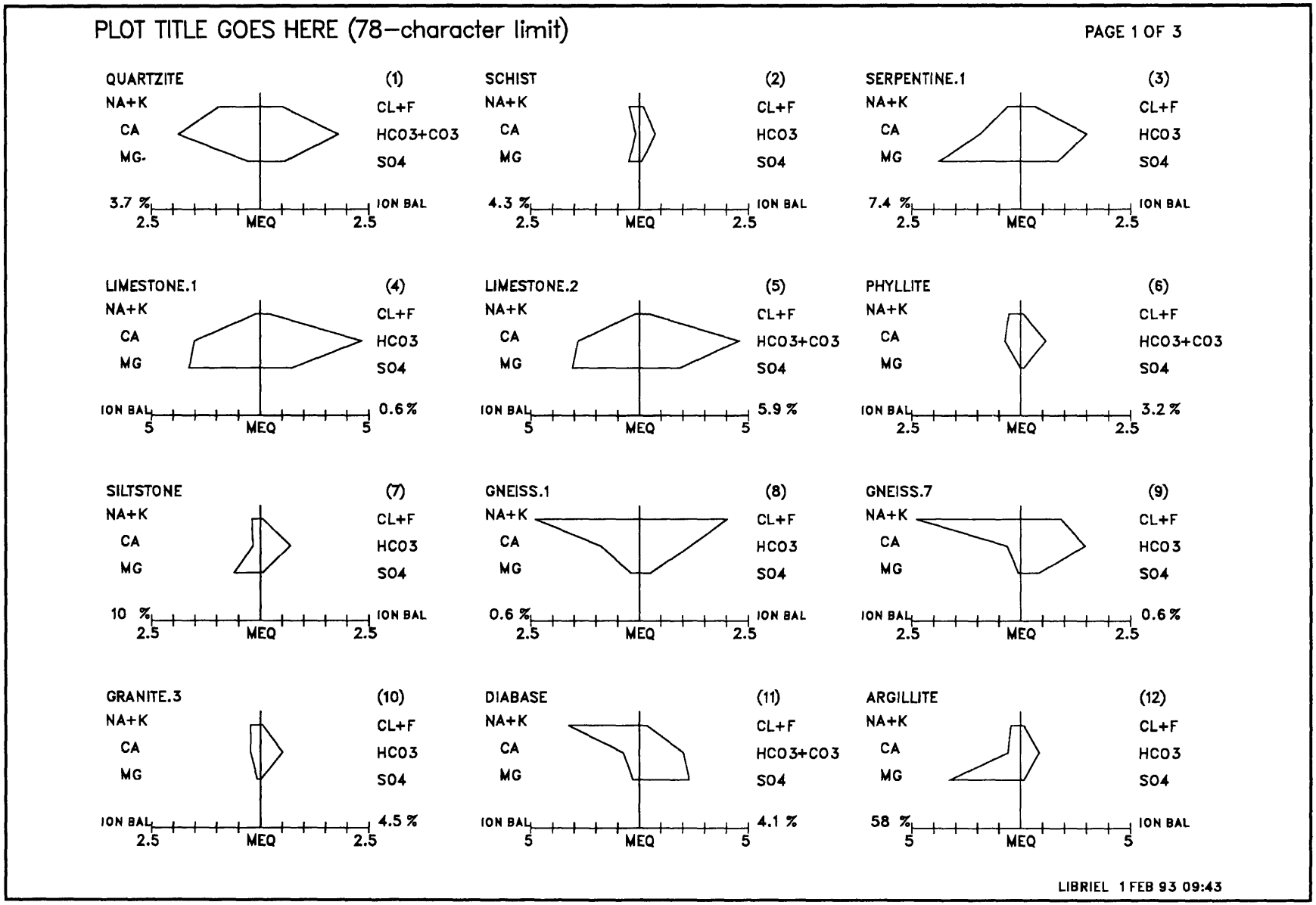

Figure 8. Stiff diagrams generated by the program from test data showing six constituents on three horizontal axes.

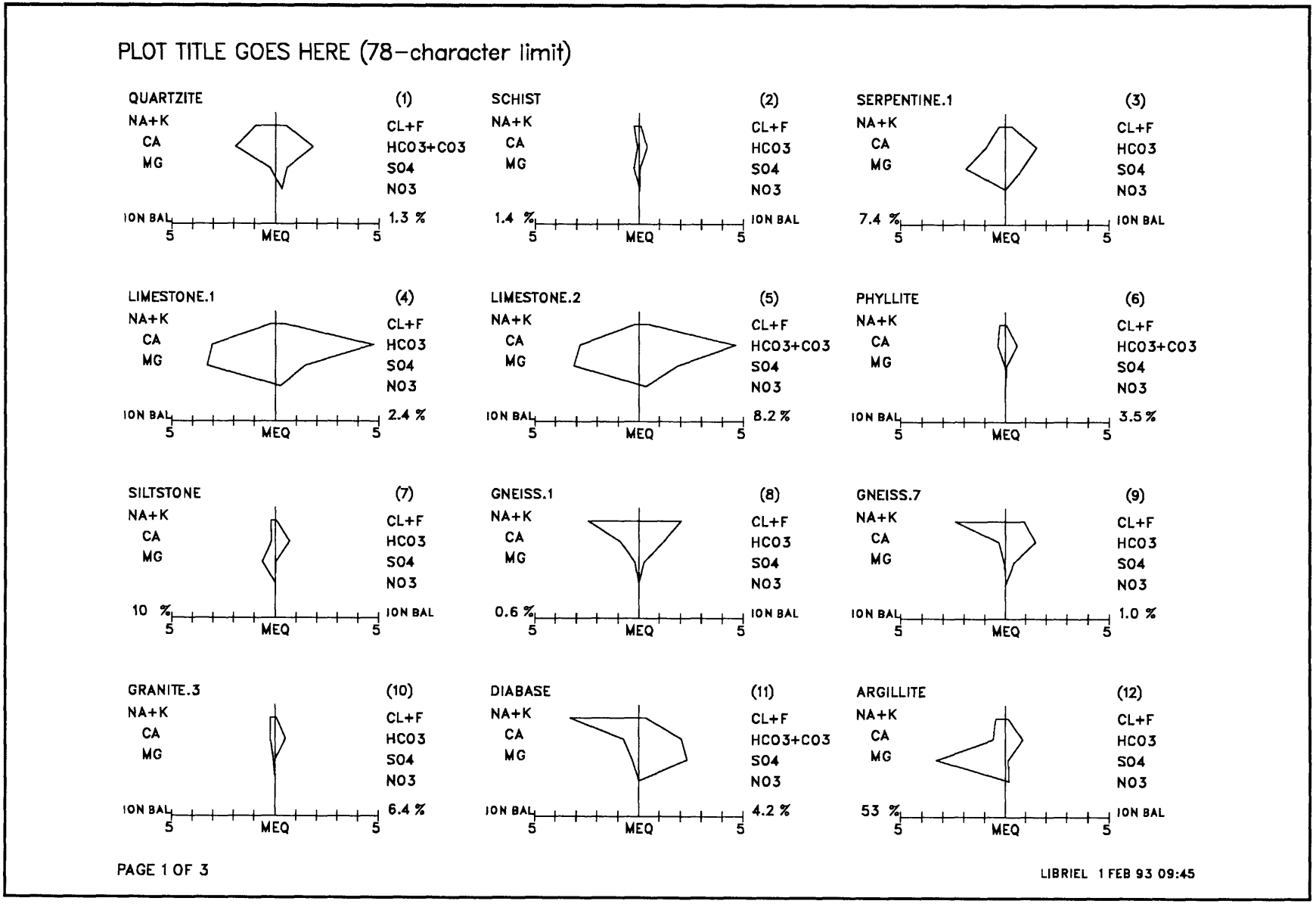

Figure 9. Stiff diagrams generated by the program from test data showing seven constituents on four horizontal axes.

CHAPTER 4.—PROPORTIONATE-AREA DIAGRAMS

Proportionate-area diagrams are commonly used in science and accounting to summarize the distribution of fractional parts of a whole. These diagrams are frequently found in budgets, which must account for all parts of a conservative property, such as mass or worth. At least two different methods for constructing proportionate-area diagrams have been used to show water composition: the bar diagrams of Rogers (1917) and Collins (1923), and the pie diagrams of Hem (1985). The program draws pie diagrams to show relations among major-ion constituents.

Pie-Diagram Technique

On all pie diagrams, the sum of the data is equal to 100 percent. Slices of the pie show the relative proportion of data in each class. On a water-quality pie diagram, the area of the circle represents the total concentration of ions in a sample, in milliequivalents per liter, and the area of each slice represents the percentage of a particular ionic constituent. Slices are commonly grouped so that cations appear in one half of the circle and anions appear in the other half. If the milli-equivalent concentrations of cations and anions are equal, the circle is divided into equal halves.

The diameter of a pie diagram can be drawn to any convenient size. Hem (1985) showed that pie diagrams for a set of samples can be drawn with different-sized diameters, so that the area of each circle is proportional to the total ionic concentration of each sample (fig. 10). Hem's pie diagrams show differences in both the total ionic concentration and the relative proportions of constituents. This technique works best when the range of concentrations does not exceed two orders of magnitude. Over a wider range of concentrations, the resolution of the slice areas becomes a problem for dilute samples (smallest circles), and a choice must be made between a series of diagrams that shows differences in the concentration of the samples and a series of diagrams that shows differences in the proportions of the constituents. The choice made in the program is to show the proportions of constituents and label the concentrations of cations and anions beside each diagram.

A distinct advantage of the pie-diagram technique is the summation principle on which pie diagrams are based: The area of each pie is equal to the sum of the areas of its constituent slices. Relative proportions of all constituents are shown on the diagram in a direct and unified way. The major and minor constituents of each sample and the dominant type of water composition (if any) are obvious at a glance. Pie diagrams commonly do not require as much time to interpret as some other types of water-quality diagrams, and this provides a rapid means to screen the composition of large numbers of samples. Like Stiff polygons, pie diagrams are compact, and both figures provide distinctive ways to show similarities and differences in water composition as symbols on a map.

A disadvantage of the pie-diagram technique is that small differences among samples with similar chemical composition are not as easily perceived on pie diagrams as on Stiff polygons. Recent studies in visual perception indicate that it is easier for the human eye to discern small differences in the length of parallel vectors (Stiff axes) than to discern corresponding differences in the area of pie slices (Helsel and Hirsch, 1992). This does not mean that pie diagrams are a less accurate form of data representation than Stiff polygons—only that small differences in chemical composition are easier to see on the Stiff figures. Although perceptual precision favors the use of Stiff polygons, these diagrams do not show the relative proportions of the constituents in a holistic way. For some applications, a set of pie diagrams can be completely appropriate, whereas for other applications, a higher degree of perceptual precision is needed. This program can draw both Stiff and pie diagrams for the same set of data, which allows the user to determine the diagram of choice.

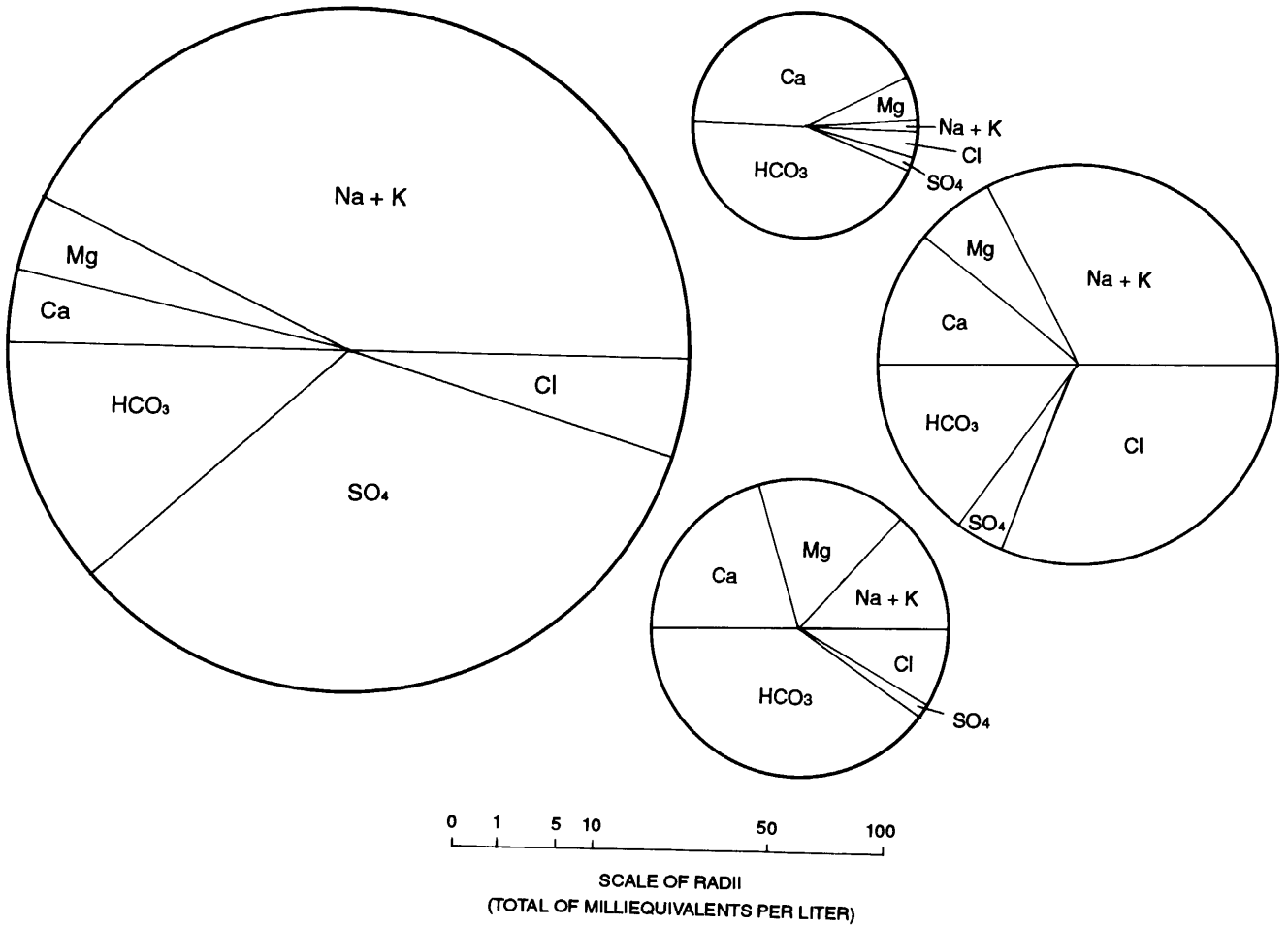

Figure 10. Hem's pie diagrams for representing water-quality analyses showing differences in both the proportions of major ionic constituents and the total ionic concentration (modified from Hem, 1985).

Pie-Diagram Output from the Program

Pie diagrams generated by the program depart from Hem's model in several ways: (1) Pie diagrams are all drawn to the same size, and the total concentrations of cations and anions is written beside each diagram; (2) pie diagrams are drawn with cation slices on the left and anion slices on the right, so that these diagrams have the same orientation as the Stiff polygons. The upper radius between cations and anions is always vertical, and deviation of the lower radius from vertical gives an indication of ionic charge balance. For additional emphasis, (3) the cation and anion halves of the pie diagram are separated by a small gap, which the user can eliminate if needed. (4) Pie slices appear in the same order as the Stiff axes and use the same scheme for grouping constituents.

The arrangement of pie diagrams on a page is also similar to the arrangement of Stiff diagrams: As many as 12 pie diagrams can be displayed, each diagram in a separate field. If more than 12 samples are in a file, a new plot page is generated to accommodate each set of 12 diagrams. All multiple pages have the same plot title and user-date-time tag, and each page has a unique tag in the upper right corner. The page tag is automatically moved to the lower left corner, if the length of the plot title exceeds 67 characters. Examples of pie plots generated by the program are shown in figures 11 and 12.

Figure 11 shows the default output for the pie procedure: A file of samples is identified by a plot title at the top of the page. The composition of each sample is represented by a pie diagram drawn in a separate area of the page. A sample-identification label from the input file is shown at the upper left of each diagram, and a sequential sample number is shown at the upper right.

Sequential sample numbers on the plot pages provide a means of cross-reference between each pie diagram and its data in the data-table file (chap. 9). Each slice is labeled with standard chemical notation to indicate which cations and anions are being represented. Like the Stiff procedure (chap. 3), the pie procedure uses pH to select an appropriate label for the bicarbonate slice: If pH is less than 7.3, the label is shown as HCO_3; otherwise, the label is shown as $HCO_3 + CO_3$. Pie slice labels can be omitted if they are not needed.

In Hem's model (fig. 10), pie diagrams are represented by open circles. Pie diagrams drawn by the program, however, have a distinctive combination of shade pattern and color assigned to each of the ions (fig. 11). These enhancements can increase perception of the area of individual slices, and this facilitates rapid screening of large numbers of samples. Slice patterns and colors can be changed (fig. 12) or omitted if needed. Different colors for pie slices can be specified in the data file; different shade patterns (and colors) can be placed in an auxiliary file (appendix B, fig. B–2). The numeric codes for colors and slice patterns are discussed in appendix A, and details of the format of the patterns file are discussed in appendix B.

Figure 12 shows user-selected modifications to the pie output: The gap has been eliminated, slice labels are not shown, and colors and patterns have been changed by reading an alternative set. Labels and patterns can be omitted independently, but it is generally preferable to show one or the other.

The pie-diagram procedure deals with samples in the data file one at a time; no data are stored, and the procedure does not limit the number of diagrams that can be drawn during a run. Pie plots are the most complex form of output generated by the program; for the same set of data, pie-plot files usually need about three times as much disk space as the least complex form (Stiff plots).

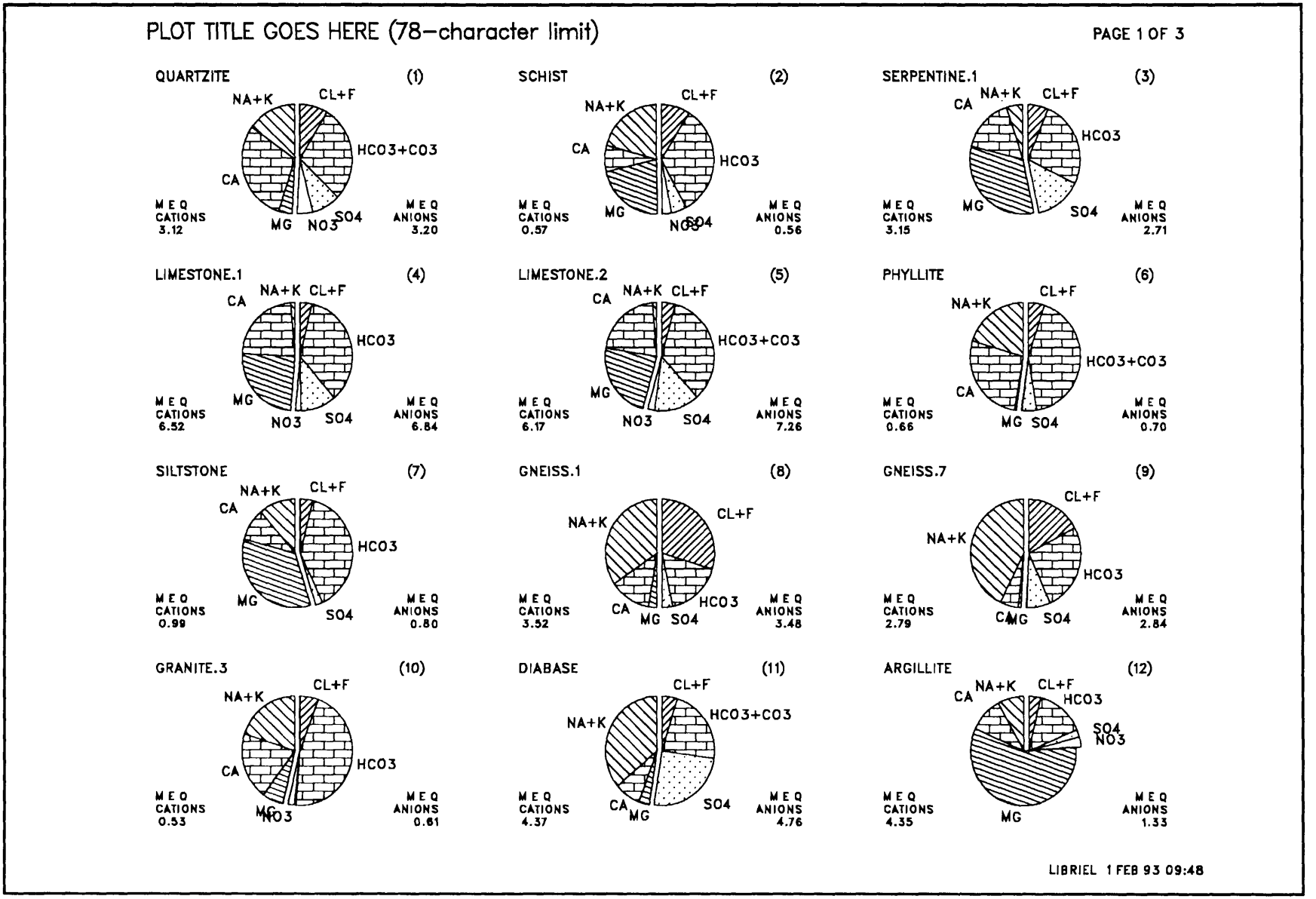

Figure 11. Pie diagrams generated by the program from test data showing standard features of the diagram for a group of 12 water samples.

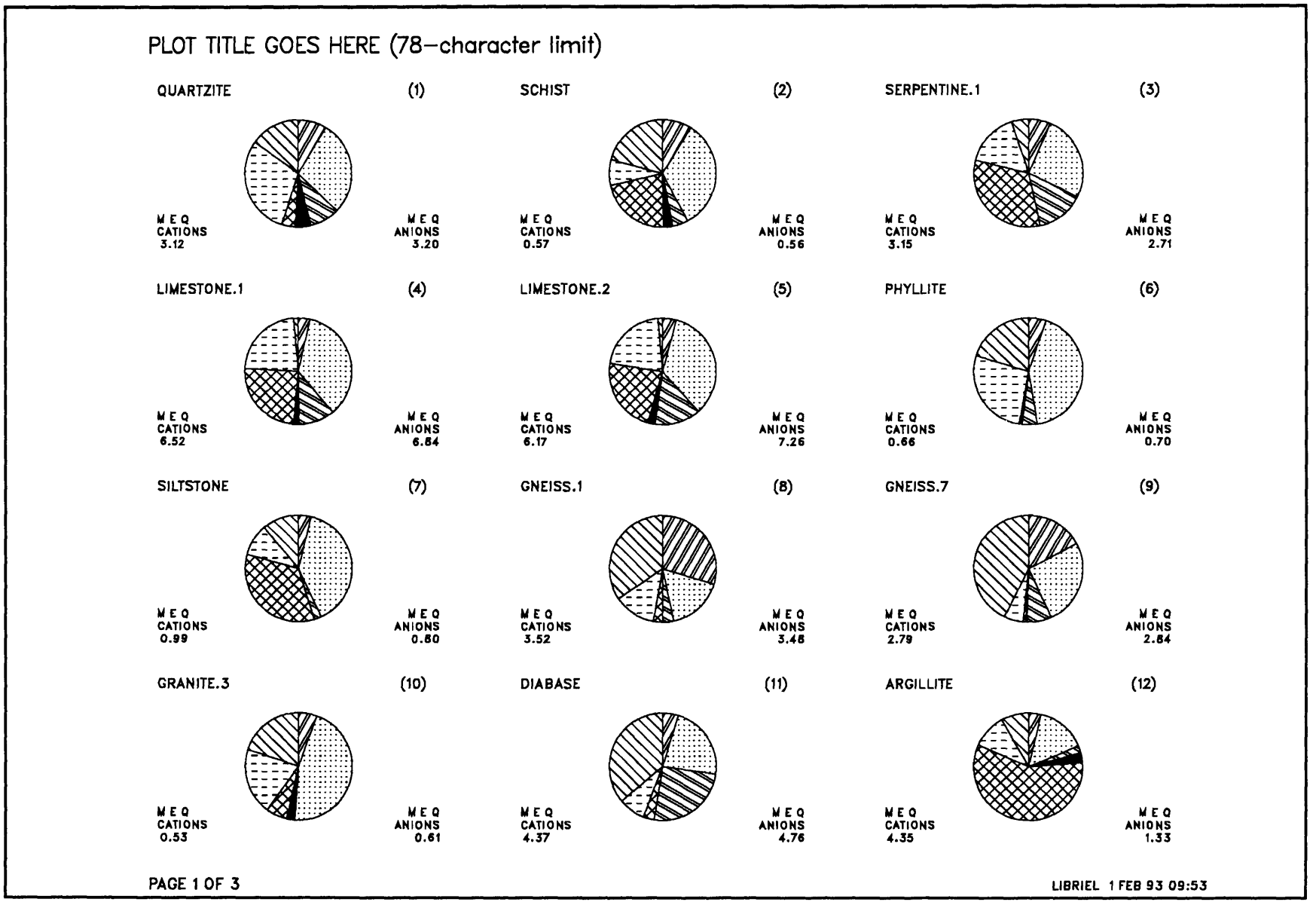

Figure 12. Pie diagrams generated by the program from test data showing user-modified shade patterns and reduced annotation around the diagrams.

CHAPTER 5.—RECTANGULAR-COORDINATE DIAGRAMS

Rectangular-coordinate (X–Y) diagrams are the most familiar method for displaying point and line data on a graph: Paired values for two variables are presented on a set of perpendicular axes, X and Y, and a rectangular-grid coordinate system is used to locate points. It is not necessary to use the same size or type of measurement scale on both axes. An X–Y diagram, or "scatterplot," shows the relation (if any) between the two variables. If points on an X–Y diagram are aligned in a discernible pattern, a relation may exist between the variables, and a mathematical equation can be sought to quantify the relation. A random scattering of points across an X–Y diagram shows that the variables are probably not related and that efforts to find a mathematical equation to relate the variables are not justified. Although not as comprehensive as a trilinear diagram, an X–Y diagram is usually easier to understand.

X–Y Diagram Technique

One type of X–Y diagram that can be constructed from water-quality data is a milliequivalent-concentration diagram, which shows concentration, in milliequivalents per liter, for selected pairs of constituents, or groups of constituents. Milliequivalent-concentration diagrams always show concentration units on both axes, though the scales can be different. If a mineral dissolves without chemical reaction, the solution acquires the ratio of ionic constituents of the mineral. A water that is in chemical equilibrium with a single mineral species shows the ratio of ionic constituents of the mineral on a milliequivalent-concentration diagram. Because most natural waters have more than one mineral in solution, a milliequivalent-concentration diagram commonly shows that more than one ratio exists among the dissolved constituents. A milliequivalent-concentration diagram can indicate which minerals are likely to be present in each sample.

A second type of X–Y diagram that can be constructed from water-quality data is a characteristic-constituent diagram, which shows a characteristic—such as specific conductance, in microsiemens per centimeter—on one axis and a constituent—such as calcium, in milliequivalents per liter—on the other. This type of X–Y diagram shows the variation in relative magnitude of two dissimilar water-quality variables, each expressed in different units. A characteristic-constituent diagram can indicate that a relation exists between the magnitude of a particular characteristic and the concentration of a particular ion.

A third type of X–Y diagram that can be constructed from water-quality data is a characteristic-characteristic diagram, which shows a characteristic—such as specific conductance, in microsiemens per centimeter—on one axis and a second characteristic—such as water temperature, in degrees Celsius—on the other. Like the characteristic-constituent diagram, the two axes are commonly expressed in different units. A characteristic-characteristic diagram can indicate that a relation exists between the magnitudes of two water-quality characteristics.

X–Y Diagram Output from the Program

X–Y diagrams generated by the program have some features in common with diagrams drawn by other procedures: (1) Like the Piper diagram (chap. 2), the X–Y diagram shows data for all samples on the same plot, providing an overall view of the relation between selected pairs of variables; and (2) like the Stiff- (chap. 3) and pie-diagram (chap. 4) output, multiple X–Y diagrams can be constructed on a single page to give a simultaneous view of the relation of different pairs of variables across the entire set of samples. When a page is full, a new page is generated to accommodate additional X–Y diagrams. All multiple-page X–Y diagrams have the same title and user-date-time tag, and each page has a unique

tag in the upper right corner. The page tag can be omitted, but it cannot be moved to the bottom of the page, as it can on Stiff and pie plots.

An important difference between X–Y diagrams and Piper, Stiff, or pie diagrams is that major features of an X–Y diagram, such as variables, axes, scales, and page layout, can be selected by the user, whereas major features of the other three diagrams are determined by the procedure. Any of the required constituents, pH, total cations, total anions, and six optional numeric variables in the data file can be displayed on either axis of an X–Y diagram. The program can also sum the milliequivalent concentrations of as many as five different ions and display the sum on either axis. This feature allows groups of ions, such as sodium plus potassium, or chloride plus fluoride plus nitrate plus phosphate, to be shown as a unit on an X–Y diagram. Total cations and total anions can be displayed without the use of the sum option. Scales for both X and Y axes can be selected either by the user or by the program. The user can also select the number of X–Y diagrams (1, 4, or 12) to be drawn on each page; the program default is 12 diagrams per page. Because X–Y diagrams can be drawn in so many different ways, more information from the user is needed to generate X–Y diagrams than is needed for Piper, Stiff, and pie diagrams.

This additional information can come from the terminal or from external files. Details of these files are discussed at the end of this chapter; examples are shown in appendix B. The X–Y diagram procedure has a limit of 1,000 samples per run.

A user can make many modifications to the output of the X–Y diagram procedure. A series of examples of X–Y diagrams generated by the program is shown in figures 13–16. These figures illustrate some of the special features of the X–Y diagram procedure, which are described in greater detail in the following sections.

Page Layouts for X–Y Diagrams

A special feature of the X–Y diagram procedure is that three different page layouts are available, so that 1, 4, or 12 X–Y diagrams can be constructed on each page. The layout of 12 X–Y diagrams per page is similar to the layouts for Stiff and pie diagrams, and it allows a rapid comparison of 12 different selected pairs of variables (fig. 13). In this layout, all samples are represented on the diagrams by the same symbol shape and color, because there is not sufficient space on the page for an explanation field. Symbol shape and color can be selected by the user.

The full-page layout (one X–Y diagram per page) is similar to the layout for Piper diagrams, and it provides space for the identification of 48 samples (fig. 14). Each sample in the data file is identified by means of a distinctive plotting symbol, which appears on the diagram and in the explanation field at the right. In the explanation field, symbols are paired with sample-identification labels taken from the data file. Unlike the Piper procedure, the X–Y diagram procedure does not recognize groups of consecutive samples in the data file with the same sample-identification label; each sample is plotted independently. Because the graphics library contains only 18 different symbol shapes (appendix A, fig. A–1), if the number of samples exceeds 18, a shape must be used to represent more than one sample. In this situation, the program changes the color of the symbols, and the 18 shapes are used again in the same order. If there are more than 36 samples, the color is changed again.The order of symbol selection can be changed if needed (see appendix B).

To identify a larger number of samples, the program provides an alternative symbol set that contains 60 different symbols (appendix A, fig. A–2). Because the alternative set contains many of the symbols in the library set, the alternative set is the default set for the program. The symbol set can be selected at the beginning of the run. The choice of shape and color for the first symbol to be plotted can also be selected by the user; the program then cycles through the set of shapes in the order shown in figures A–1 and A–2. If the same symbol is used to plot all samples, the user can select that symbol from either symbol set. In the full-page layout, the explanation field can be omitted if it is not needed.

The layout of four X–Y diagrams per page (fig. 15) represents a compromise in size between the other two layouts: A series of four diagrams of intermediate size is drawn on each page. Larger diagrams provide better resolution of adjacent samples, but not as many pairs of variables are shown on the page. The features of the 4-per-page

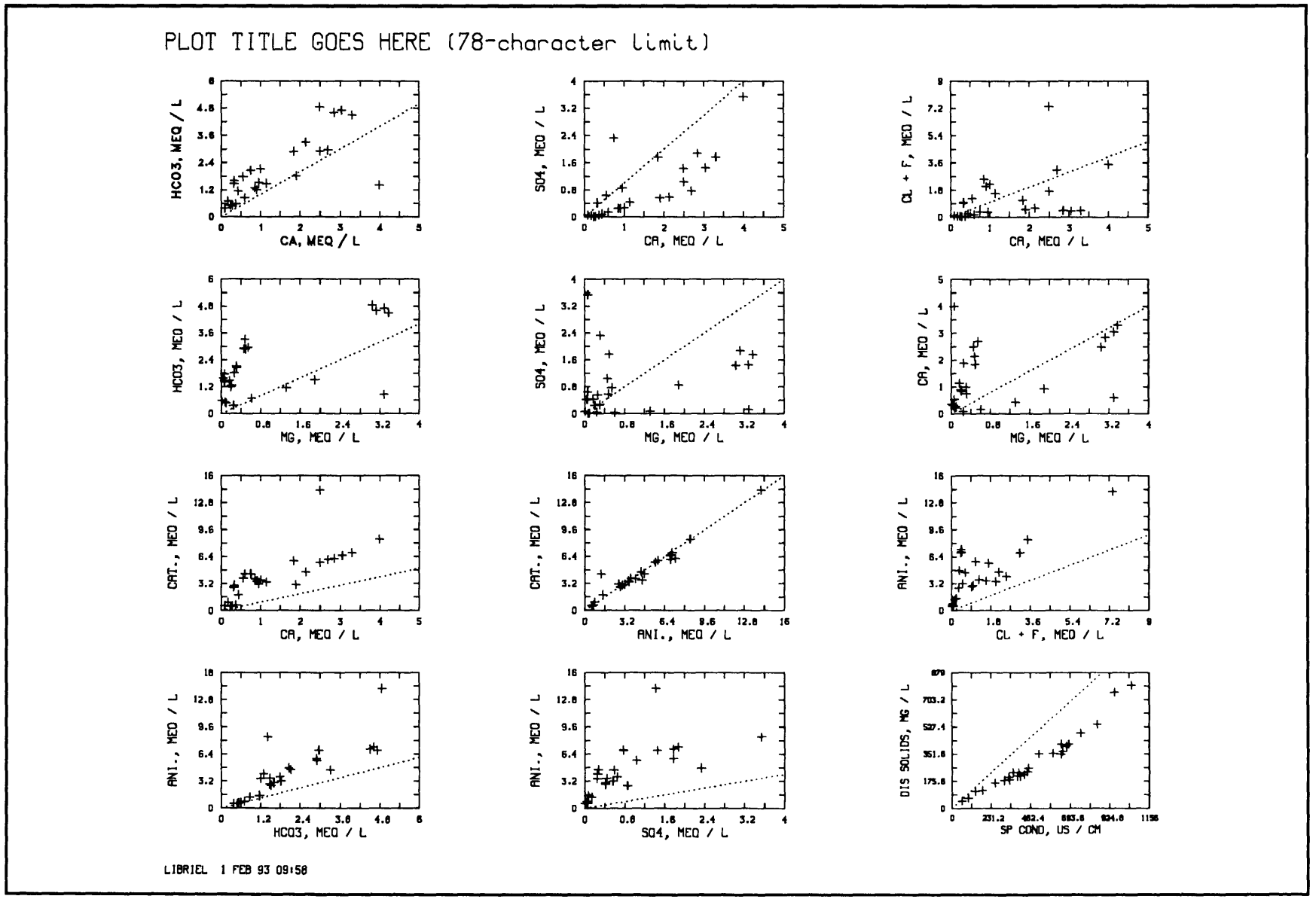

Figure 13. X–Y diagrams generated by the program from test data showing the standard format of 12 diagrams per page.

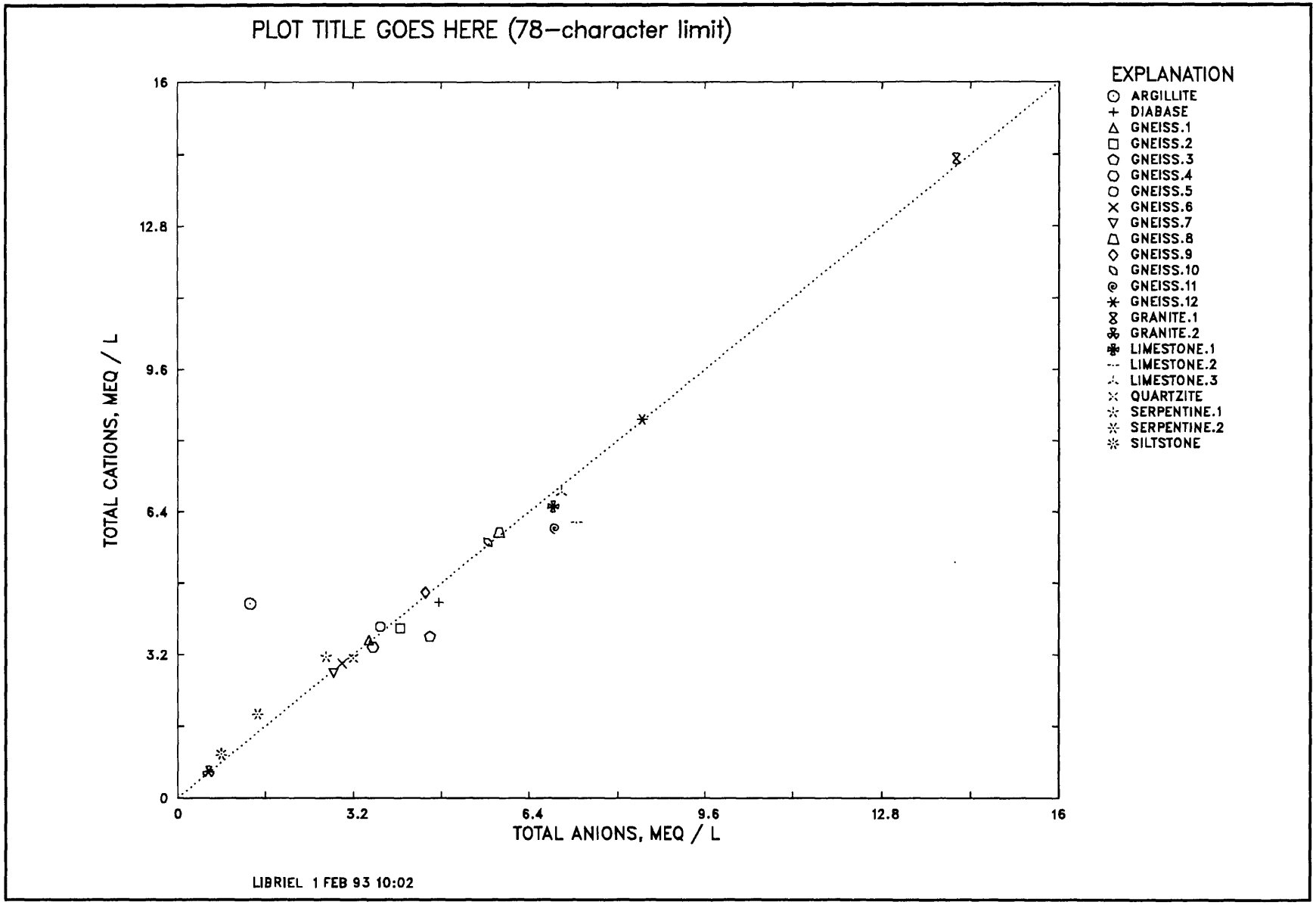

Figure 14. X–Y diagram generated by the program from test data showing the enlarged format of one diagram per page and a symbol-explanation field similar to the Piper diagram.

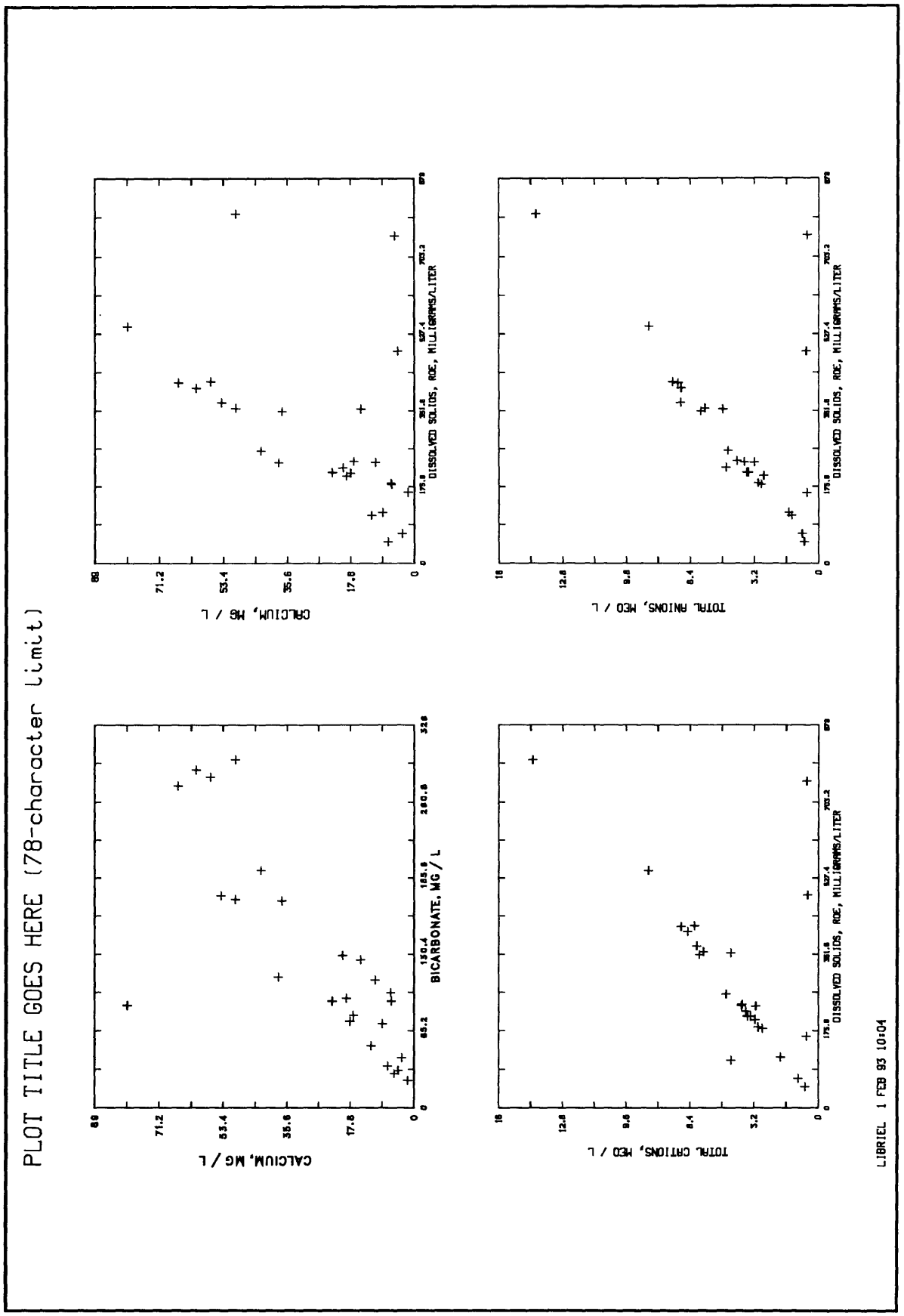

Figure 15. X–Y diagrams generated by the program from test data showing the format of four diagrams per page.

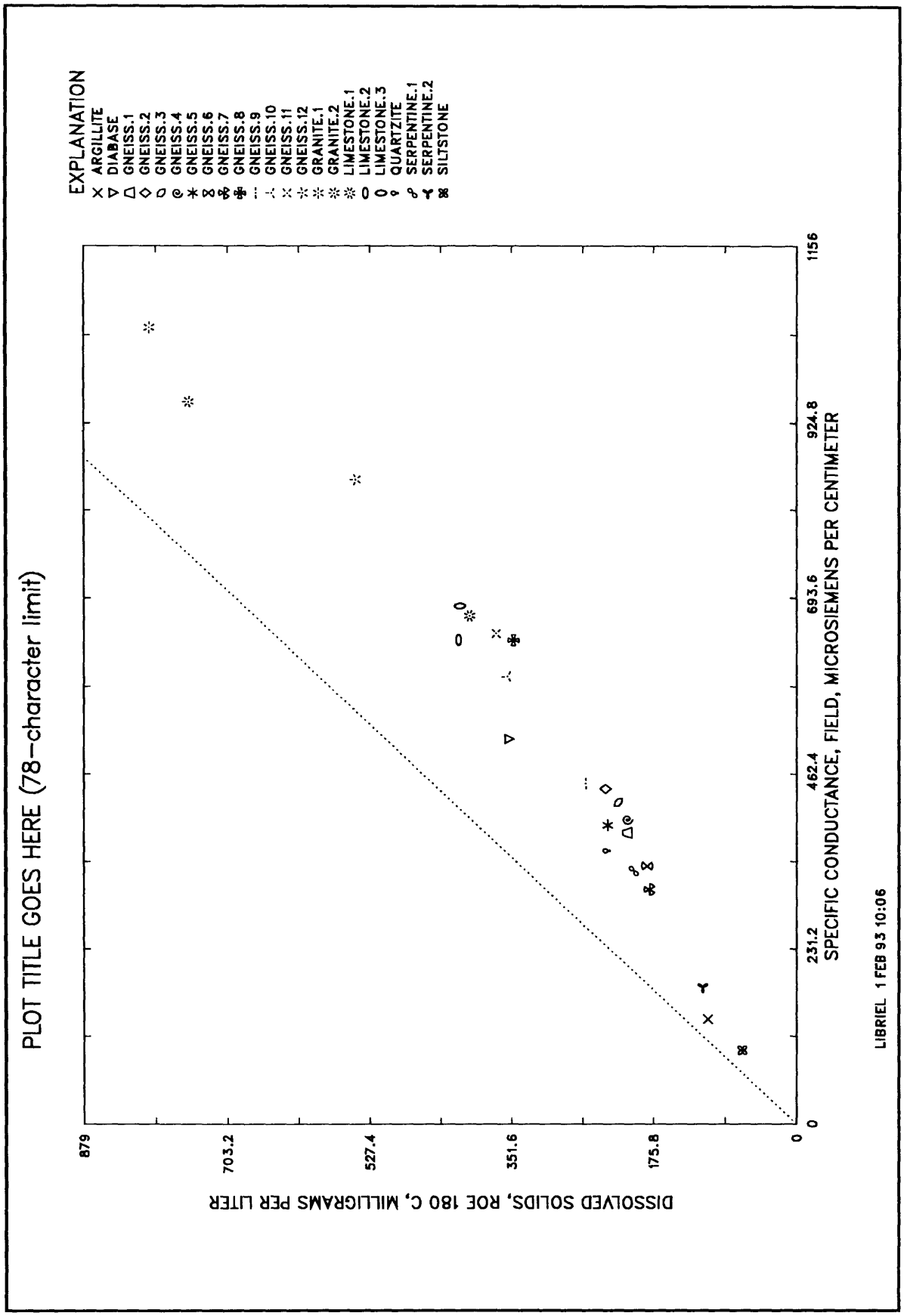

Figure 16. X–Y diagram generated by the program from test data showing user-selected optional variables.

layout are virtually the same as those of the 12-per-page layout: All samples are represented in the diagrams by the same symbol shape and color, because there is no explanation field. Symbol shape and color can be set by the user.

Scales for X–Y Diagrams

Two options are available for scaling X–Y diagrams: (1) X and Y axes are scaled independently by use of the maximum values of the X and Y variables to determine an appropriate scale for each axis, or (2) X and Y axes are drawn to the same physical scale by use of the larger of the two maximums. The minimum value for each axis is always equal to zero. The default option (independent scaling) maximizes the amount of plotting area that is used on a diagram and usually provides better resolution of adjacent samples. The equal-scaling option provides a way to draw both axes to the same scale. Equal scaling can be chosen by the user if needed.

The 1:1 Ratio Line

One disadvantage of independent scaling of X–Y diagrams is that simple ratios between variables are not always obvious. To correct this, a 1:1 ratio line can be drawn on each diagram as a dotted line. The 1:1 ratio line is not a regression line; it is the locus of points where X = Y. The program draws the 1:1 ratio line by default; this line can be omitted if it is not needed.

Optional Variables on X–Y Diagrams

The scope of the X–Y diagram procedure in this program was originally limited to a set of constituents that appear on Piper diagrams. Axis labels for these constituents on X–Y diagrams have been included in the program; the user does not enter axis labels for these constituents. Characterization of water quality, however, commonly involves constructing X–Y diagrams for other familiar constituents and characteristics that do not appear on Piper diagrams. Therefore, the scope of the X–Y diagram procedure was enlarged to include (1) pH, a water-quality characteristic that is required by the program, and (2) as many as six optional numeric variables in the data file. Optional variables can be characteristics or constituents; the selection and number (up to 6) of optional variables is left to the user.

Optional variables can be displayed on either or both axes of an X–Y diagram. If optional variables are displayed, the user must supply a set of axis labels to identify the variables and their units. A set of labels does not need to be complete, because labels are not required for optional variables that are not displayed. The first time an optional variable is displayed, axis labels are requested for that variable. Once labels have been entered for an optional variable, the labels are available for the duration of a run and do not have to be re-entered each time that variable is displayed.

Because X–Y diagrams can be drawn in three different physical sizes (layouts), axis labels for optional variables can be entered in three different lengths: (1) For the full-page layout, labels can contain as many as 80 characters; (2) for the 4-diagrams-per-page layout, labels are limited to 40 characters; (3) for the 12-diagrams-per-page layout, labels are limited to 20 characters. On the variable-selection menu (fig. 17) that appears on the screen, optional variables are represented by the first 11 characters of the 20-character label. If an optional variable has not been identified, the label—**Extra var.**—appears on the menu.

Axis labels for optional variables can be either entered from the terminal or read from an external file. If labels are entered from the terminal, the user is prompted for each of the three different lengths needed. The length entered can be shorter than the limiting length, but all labels must contain at least one non-blank character. If a null response (carriage return) is entered for an axis label, a surrogate label (**Extra var.**) is used for that variable.

If axis labels are read from an external file, the local directory is searched for a file named QWPLOT.LABELS; if this file is not found, the user is asked for the name of a file containing the axis labels. The details of the format of the axis-labels file are discussed in appendix B.

```
Variable    Code     Variable    Code     Variable    Code     Variable    Code

Calcium        1     Fluoride       6     Tot Cations   11     Dis Solids,   15
Magnesium      2     Bicarbonate    7     Tot Anions    12     Extra var.    16
Sodium         3     Sulfate        8     SUM: Ca-PO4   99     Silica, in    17
Potassium      4     Nitrate        9     pH            13     Iron, in ug   18
Chloride       5     Phosphate     10     Cond, in uS   14     Manganese,    19

Enter Code for X-AXIS variable  > 11
Enter Code for Y-AXIS variable  > 12
```

Figure 17. Variable-selection menu for the X–Y diagram procedure showing the numeric code for each variable and menu labels for optional variables. Labels for optional variables can be read from a file, which is shown in appendix B (fig. B–4).

X–Y Variables File

If a user needs to plot the same combinations of X and Y variables on more than one run, the menu code for these variables (fig. 17) can be read from a file. This can reduce significantly the amount of information that has to be entered from the terminal in each run. If a variables file is used, the local directory is searched for a file named QWPLOT.VARS; if this file is not found, the user is asked to enter the name of a file containing these codes. The codes for all diagrams generated during an interactive run can be written to a file for use in a later run. Details of the format of the X–Y variables file are discussed in appendix B.

CHAPTER 6. —VALUE-DISTRIBUTION DIAGRAMS

Sets of water-quality data commonly contain more than one variable and more than one value for each variable. One or two summary statistics for each variable —such as the mean and standard deviation—frequently do not provide an adequate description of the distribution of values, because water-quality data can be distributed in many different ways. Several general types of distributions are possible. It is useful to know if a set of values can be treated as a normal distribution (values distributed symmetrically around a central value), a skewed distribution (values distributed asymmetrically around a central value), a multicenter distribution (values clustered around more than one center), or another type of distribution. Value distributions for water-quality variables commonly have a positive skew, which means that more extreme values are on the higher side of the distribution than on the lower side (Helsel and Hirsch, 1992).

Value-distribution diagrams are graphical summaries of the distribution of values for individual variables. A number of methods have been proposed for constructing diagrams to show value distributions. Extended discussions of this topic can be found in Chambers and others (1983) and in Helsel and Hirsch (1992). The program incorporates the boxplot-diagram technique introduced by Tukey (1977).

Boxplot-Diagram Technique

Tukey's boxplot diagrams show only selected values for a data distribution. The data are ranked (or nonparametric), and values are displayed on a single-axis system. Boxplot diagrams are useful because they provide concise visual summaries of the 25th, 50th, and 75th percentiles and any extreme values in a distribution. Boxplot diagrams are commonly put side by side to compare and contrast different distributions of data. A rectangular figure (or box) on the diagram emphasizes the central range of values between the 25th and 75th percentiles. This central range, called the interquartile range (or IQR), always contains one-half of the data. The IQR is a robust measure of the spread of values, which means that the IQR is insensitive to the presence of extreme values in a distribution. The 50th percentile (or median) divides the box in half. Any difference in area between the two halves of a box (quartile skew) is an indication of asymmetry in the distribution. Several methods have been devised for displaying the confidence interval for the median value on boxplot diagrams (Helsel and Hirsch, 1992), but this feature is commonly omitted.

Data values located outside the box are shown on the diagram in different ways. Values located within 1.5 times the IQR are connected to the box by lines drawn outward from the 25th and 75th percentiles. These lines are called whiskers. Boxplot diagrams do not show the location of individual values along whisker lines. Data values located beyond the ends of the whiskers are called extreme values, and they are plotted individually. Two groups of extreme values are shown: (1) Values located from 1.5 to 3 times the IQR are called outliers (or near outliers), and they are plotted with an X. (2) Values located beyond 3 times the IQR are called far outliers, and they are plotted with a circle.

The occurrence of extreme values on a boxplot diagram can indicate that the data are not normally distributed, and the use of any statistical procedures based on the assumption of normality is not justified. For data from a normal distribution, near outliers occur fewer than once in 100 times and far outliers occur fewer than once in 300,000 times (Helsel and Hirsch, 1992).

Some researchers prefer not to show any outlying values on a boxplot diagram. Instead, a pair of whiskers is drawn outward from the 25th and 75th percentiles to the 10th and 90th percentiles, or to the 5th and 95th percentiles, or even to the minimum and maximum data values, respectively. These boxplot diagrams are called box-and-whisker plots and schematic boxplots. This program follows Tukey's method and shows outliers.

Boxplot-Diagram Output from the Program

Boxplot diagrams generated by the program have some features in common with diagrams drawn by the other procedures. Like Stiff-, pie-, and X–Y diagram output (chaps. 3–5), as many as 12 boxplot diagrams can be placed side by side on a single page to compare and contrast the value distributions for different water-quality variables. A fixed width is used for all box figures drawn by the program; this width accommodates 12 diagrams in the main plotting area. If more than 12 boxplots are needed, the program generates a new page to hold the additional diagrams. All multiple-page boxplots have the same title and user-date-time tag, and each page has a unique tag in the lower right corner. For emphasis, five different parts of the boxplot diagram—IQR box, median line, whisker lines, near outliers, and far outliers—are shown with different colors; this is the program default. All diagrams on a page use the same color scheme. If the user prefers, all parts of the diagram can be drawn with one color. The main features of a boxplot diagram are labeled in an explanation field shown at the right (figs. 18 and 20). The explanation field can be omitted if needed. The boxplot procedure has a limit of 10,000 samples.

Figure 18 shows the default output for the boxplot procedure: A plot title at the top of the page identifies the group of samples. Value distributions for selected constituents and characteristics are compared by a series of box figures with parallel Y-axes. The numerical scale is the same for all Y-axes and is shown along the left edge of the diagram. Because units for different constituents and characteristics can vary from box to box, units are shown with the identification of each variable at the bottom of the diagram. The number of values in each distribution is shown along the top of the diagram. If the number of values in a distribution is less than 10, values are plotted individually and the box figure is not shown. The principal features of boxplot diagrams are labeled in the explanation field at the right. This field can be omitted if it is not needed.

In figure 18, a six-cycle logarithmic scale is used instead of a linear scale to plot the distribution of values, so that the diagram is less sensitive to large values. Figure 18 does not represent a log transformation of the data; instead, the values are plotted on a logarithmic scale. The use of this scale distorts the symmetry of the box, and quartile skew is especially difficult to determine, because the log scale changes the proportions of the figure.

Figure 19 shows a series of boxplots with a linear scale. The proportions of the boxes (quartile skew) are easy to compare on this scale, but the diagram as a whole is highly sensitive to large values. A comparison of figures 18 and 19 shows the differences between the log and linear scales for displaying boxplots.

Displaying Groups of Values for One Parameter

Figure 20 shows a series of boxplots for groups of samples that have a common label variable. The boxplot and Piper 2–D procedures can recognize groups of samples that have the same value for the label variable. A change in the value of the label variable signals the beginning of each group of samples. This feature allows the data for any characteristic or constituent in the file to be divided into as many as 60 groups of values and each group displayed as a separate boxplot. If this option is used, only one parameter can be displayed during a run, and samples having the same label must be arranged consecutively in the file. Multiple plot-pages are created automatically for each set of 12 figures. This procedure has a storage limit of 60 different values for the 15-character label variable. Label variables cannot contain imbedded blanks (see The Label Variable, chap. 8).

Boxplot Variable-Selection Menu

A screen menu (fig. 21) is used to select the variables that appear on the boxplot diagram. Any of the required constituents, pH, total cations, total anions, and six optional variables can be displayed in any order the user chooses. Labels for the first 13 variables have been included in the program. If an optional variable is selected, the user must supply a set of three labels to identify the variable and the unit on the diagram and in the menu. The length of a label on the diagram is limited to 15 characters; the menu label is limited to 11 characters. Once labels have been entered, they are available for the duration of a run and do not have

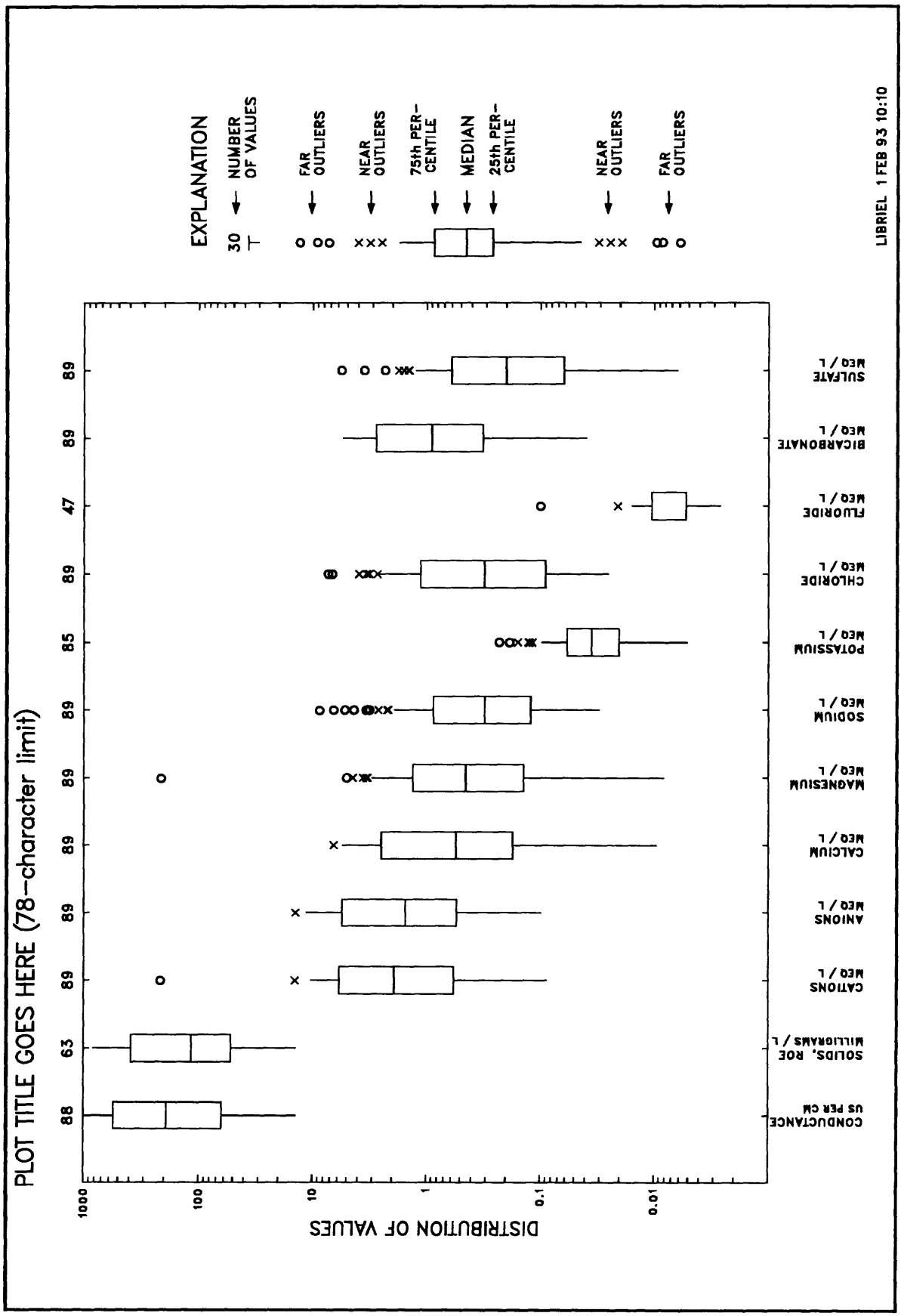

Figure 18. Boxplot diagrams generated by the program from test data showing value distributions for 12 parameters on a log scale.

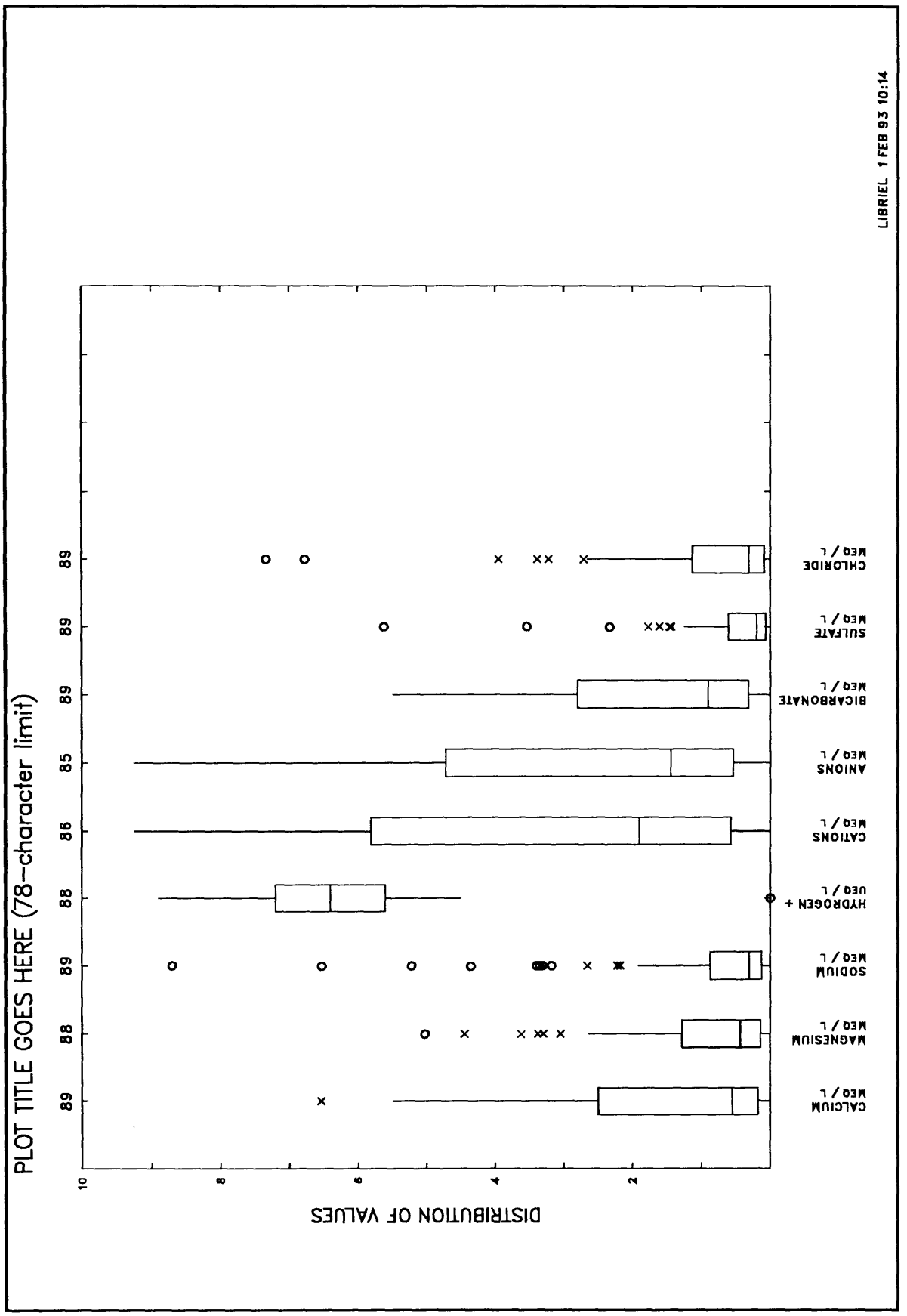

Figure 19. Boxplot diagrams generated by the program from test data showing value distributions for nine parameters on a linear scale and no explanation field.

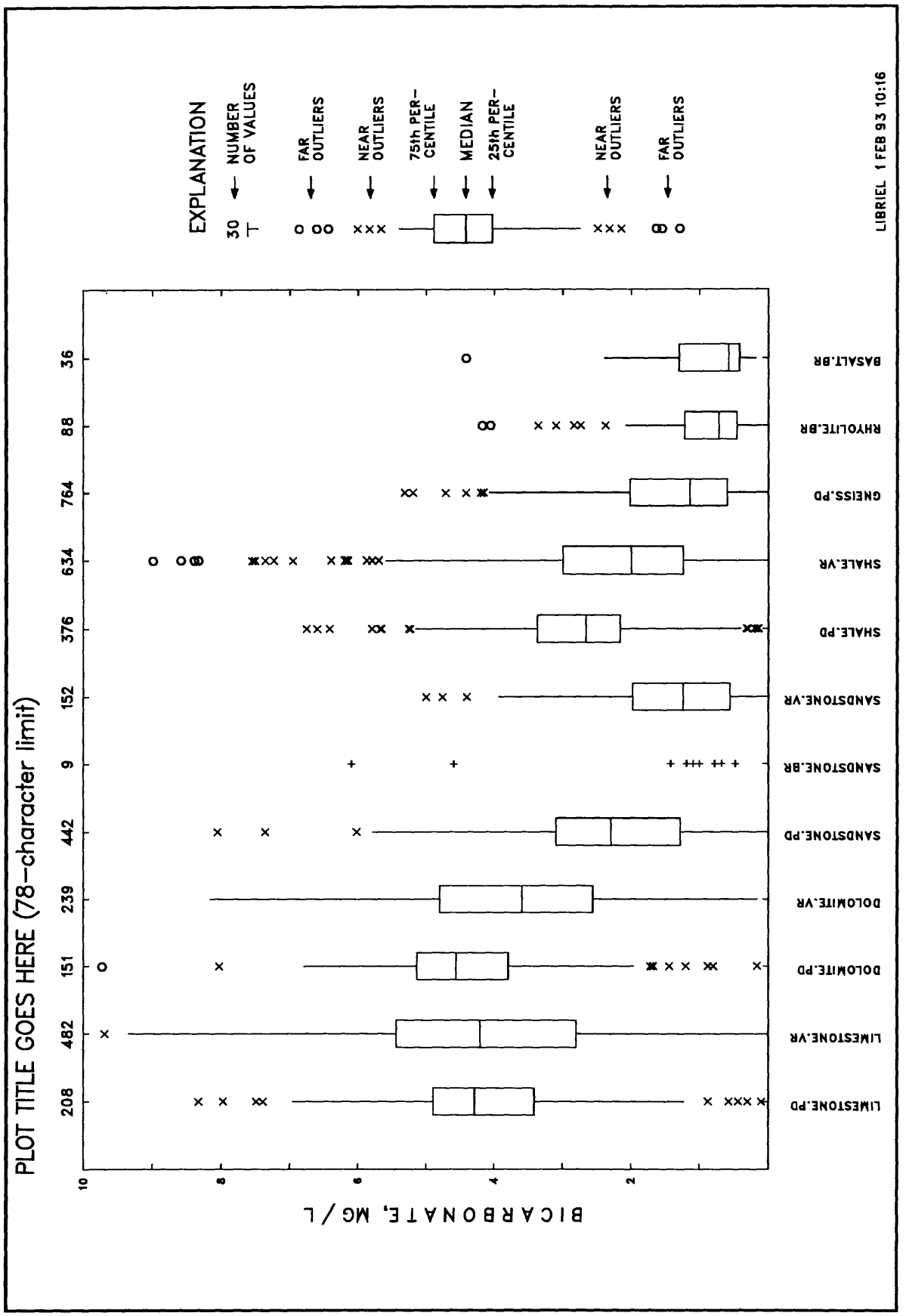

Figure 20. Boxplot diagrams generated by the program from test data showing value distributions for one parameter for groups of samples having a common label variable.

```
Variable    Code     Variable    Code     Variable    Code     Variable    Code

Calcium       1      Fluoride      6      Tot Cations  11      Temperature  16
Magnesium     2      Bicarbonate   7      Tot Anions   12      Dis Silica   17
Sodium        3      Sulfate       8      Ph           13      Iron         18
Potassium     4      Nitrate       9      Sp Conduct   14      Manganese    19
Chloride      5      Phosphate    10      Dis Solids   15

Enter variable code for box # 1  > 14
Enter variable code for box # 2  > 15
Enter variable code for box # 3  > 11
Enter variable code for box # 4  > 12
```

Figure 21. Variable-selection menu for the boxplot-diagram procedure showing the numeric code for each variable and menu labels for optional variables. Labels for optional variables can be read from a file, which is shown in appendix B (fig. B–3).

to be re-entered each time the variable is redisplayed. Labels are not required for optional variables that are not displayed.

Box labels for optional variables can also be read from an external file. If optional variables are displayed, the local directory is searched for a file named BOXPLOT.LABELS; if this file is not found, the user is asked for the name of a file containing the box labels. A set of labels can be written to a file for use in a later run; details of the format of the box-labels file are discussed in appendix B.

Boxplot Variables File

If a user needs to plot the same order of boxplot variables on more than one run, the menu codes (fig. 21) for each variable can be read from a file. This can reduce significantly the amount of information that has to be entered from the terminal in each run. If a variables file is used, the local directory is searched for a file named BOXPLOT.VARS; if this file is not found, the user is asked to enter the name of a file containing the list of codes. Variable codes for all diagrams generated during an interactive run can be written to a file for use in a later run. The format of a boxplot variables file is not the same as the format of an X–Y variables file (chap. 5); details of both formats are discussed in appendix B.

Treatment of pH on Boxplot Diagrams

The pH of a sample is the negative base-10 log of the effective concentration (activity) of the hydrogen ion (H^+); thus, pH values are already in a log form. If pH data are shown on a boxplot diagram with a log scale, the diagram does not show the log of pH values; instead, pH values are converted to H^+ concentration in microequivalents per liter (μeq/L), and the log of this value is shown. H^+ concentration could be shown in the same units as the major dissolved constituents, but H^+ concentrations in milliequivalents per liter are very small for waters that are not strongly acid. Conversion of pH to microequivalents of H^+ per liter allows the distribution of values for H^+ concentration to be displayed in the range used for the major dissolved constituents.

CHAPTER 7. —PROJECTED DIAGRAMS

Projected diagrams have been used for many years in science and engineering to show relations among three (or more) variables on a 2–D surface. The science of metallurgy makes extensive use of projected diagrams for showing complex phase relations among chemical components in metal alloys (Rhines, 1956). Diagram-projection techniques have also been applied to water-quality data to show changes in a pair of variables over time and to show changes in a single variable over a geographic area. An example of the latter are the hydrochemical facies maps of Back (1961).

A new projection technique is proposed here: Sample points on a 2–D Piper plot are projected into the volume of a triangular prism constructed above the diagram to show how variations in chemical composition can be related to changes in an independent (or Z–axis) variable. Piper's original technique used projection to display the chemical composition of samples in the diamond-shaped field; the new technique extends the projection into the space above the plane of the diagram. The name chosen for this new diagram is Piper 3–D.

Piper 3–D Technique

The Piper 3–D technique constructs a 2–D Piper diagram as the lower base of a triangular prism. The full prism is seldom shown, but its dimensions can be inferred from the area of the base and the length of the Z–axis shown along one edge. From each sample point on the Piper diagram (represented by a small cross), a vector is projected upward perpendicular to the basal plane. The length of the vector is proportional to the magnitude of the Z–axis variable. The upper end of the vector (marked by another plotting symbol) represents the location of the sample in the prism. Vectors are drawn on the 3–D diagram as dotted lines that connect the two symbols. A label and a scale for the Z–axis variable is always shown along one of the edges of the prism.

The location of sample points in the prism is a cofunction of chemical composition in the basal plane and the magnitude of the variable displayed on the Z–axis. The chemical composition of each sample is shown on the basal plane by three symbols, one in each of the three fields of the Piper diagram. To simplify the 3–D diagram, Z–axis vectors are usually projected only from sample points in the diamond field, which shows the chemical composition with respect to both cations and anions; vectors can be projected, however, from sample points in any or all three of the fields if needed. Another set of vectors might also be projected downward from the basal plane into the space below the Piper diagram to display a second Z–axis variable, but this option has not been provided in the current version of the program.

An advantage of the Piper 3–D technique is its ability to show on the diagram additional information about the composition of each sample, because complete characterization of water quality commonly depends on many variables. If dissolved solids (or specific conductance) is selected as the Z–axis variable, a Piper 3–D diagram can show both the chemical composition and the ionic concentration of individual samples. On such diagrams, samples having similar chemical composition may be distinguishable by differences in the length of the Z–axis vector. If pH is selected as the Z–axis variable, relations may be apparent between the chemical composition of a sample and its acidity. Piper 3–D diagrams can be used to show variations in chemical composition as a function of any user-selected variable in the data file.

A disadvantage of the projection technique is the distortion introduced by tilting the plane of the Piper diagram: For the same quantity on the Z–axis, vectors at the back of the prism will look taller than those at the front, and only large differences in the length of the vectors can be easily distinguished (Helsel and Hirsch, 1992). If a 3–D figure is projected onto a 2–D surface, a compromise is always made between showing the additional information and showing the data with some distortion. The utility of a projected diagram

is a measure of that compromise: If the diagram clearly provides additional insight into relations between chemical composition and the independent variable, and if these relations were not evident on 2–D diagrams, some degree of distortion may be acceptable. This choice is left to the user.

A major source of distortion in projected diagrams is the viewpoint. Because certain viewing angles can give a highly biased view of a diagram, projection techniques usually have the capability for rotating diagrams freely about all three axes, which allows the data to be seen from many different viewpoints and reduces the bias introduced by any single viewpoint. The Piper 3–D procedure can draw the projected diagram from any viewing angles that the user selects.

Piper 3–D Diagram Output from the Program

Examples of Piper 3–D diagrams generated by the program are shown in figures 22–26. The simplest form of the diagram is shown in figure 22, and various modifications to the diagram are shown in figures 23–26 and discussed in the following sections. Figures 22–24 show samples plotted only above the diamond field, but samples can be plotted above any or all three of the fields if needed (figs. 25–26).

Selection of Z–Axis Variable

The choice of a variable to display on the Z–axis is left to the user; there is no program default for this option. A Z–axis variable can be chosen from any of the required variables, total cations, total anions, or any of the optional variables in the file. The most useful Z–axis variables are probably dissolved solids, specific conductance, and pH, but there are other water-quality characteristics and constituents that a user might need to display on the Piper 3–D diagram. Z–axis variables can be selected from a screen menu or specified in the data file. The format of the variable-selection menu is the same as the one shown in figure 21 for the boxplot-diagram procedure.

Figure 22 shows some of the default features for output from the Piper 3–D procedure with specific conductance chosen by the user as the Z–axis variable. A file of samples is identified by a plot title at the top of the page. The composition of each sample is represented by three small crosses (one in each field) on the Piper diagram. Each cross in the diamond field is connected by a dotted line to a larger symbol in the 3–D space of the prism. A labeled and scaled Z–axis is shown perpendicular to the lower-left corner of the plane of the cations triangle. The projected diagram is displayed from a default viewing perspective of X = 30, Y = -30, Z = 15 degrees; these angles are listed in the view-angles tag at the lower left margin of the page. The user-date-time tag is written at the lower right margin. The default position for the page-identification tag is at the upper right corner, but if the length of the plot title exceeds 67 characters, the page tag is automatically moved to the lower left corner.

Z–Axis Labels File

If optional variables are displayed on the Z–axis, labels for these variables can be read from the same external file that is used by the X–Y diagram procedure: The local directory is searched for a file named QWPLOT.LABELS; if this file is not found, the user is asked for the name of a file containing the Z–axis labels. If a null response is entered, the variable-selection menu is displayed, and Z–axis labels are entered from the terminal. Z–axis labels entered in an interactive run can be saved for use in a later run.

Threshold Values for Z–Axis Variable

One limitation of the Piper 3–D technique is that the diagram becomes cluttered if a number of samples have similar chemical compositions. To limit the number of samples plotted on a diagram, the user can apply a threshold value to the Z–axis variable. If a Z–axis threshold is used, the composition of all (complete) samples in the file is still shown on the basal plane, but only samples whose Z–values are equal to or greater than the threshold value are plotted in the prism (fig. 23). The intersection of a limiting value on the Z–axis with the faces of the prism is shown on the diagram

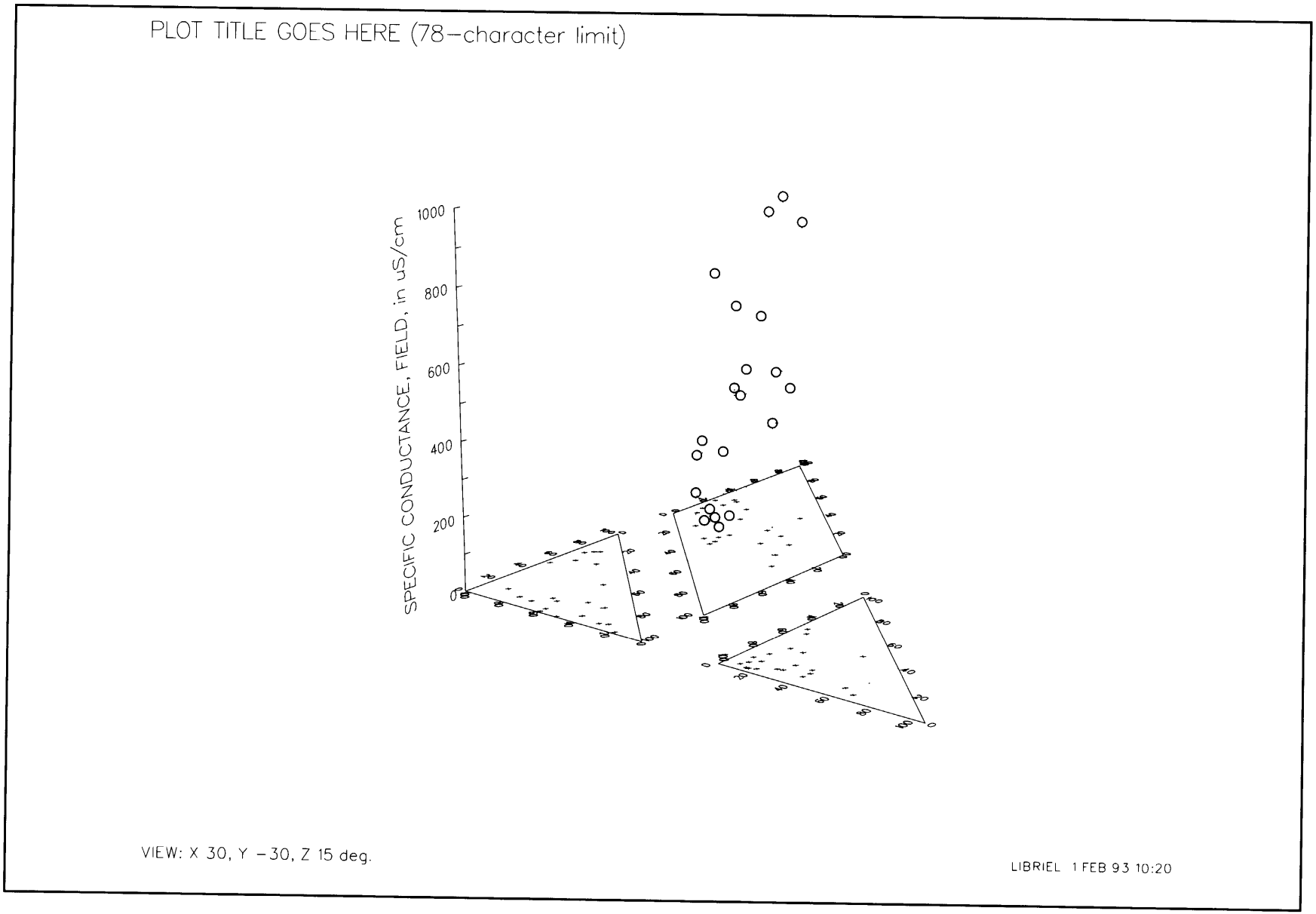

Figure 22. Piper 3–D diagram generated by the program from test data showing the normal viewing perspective and standard features of the 3–D diagram.

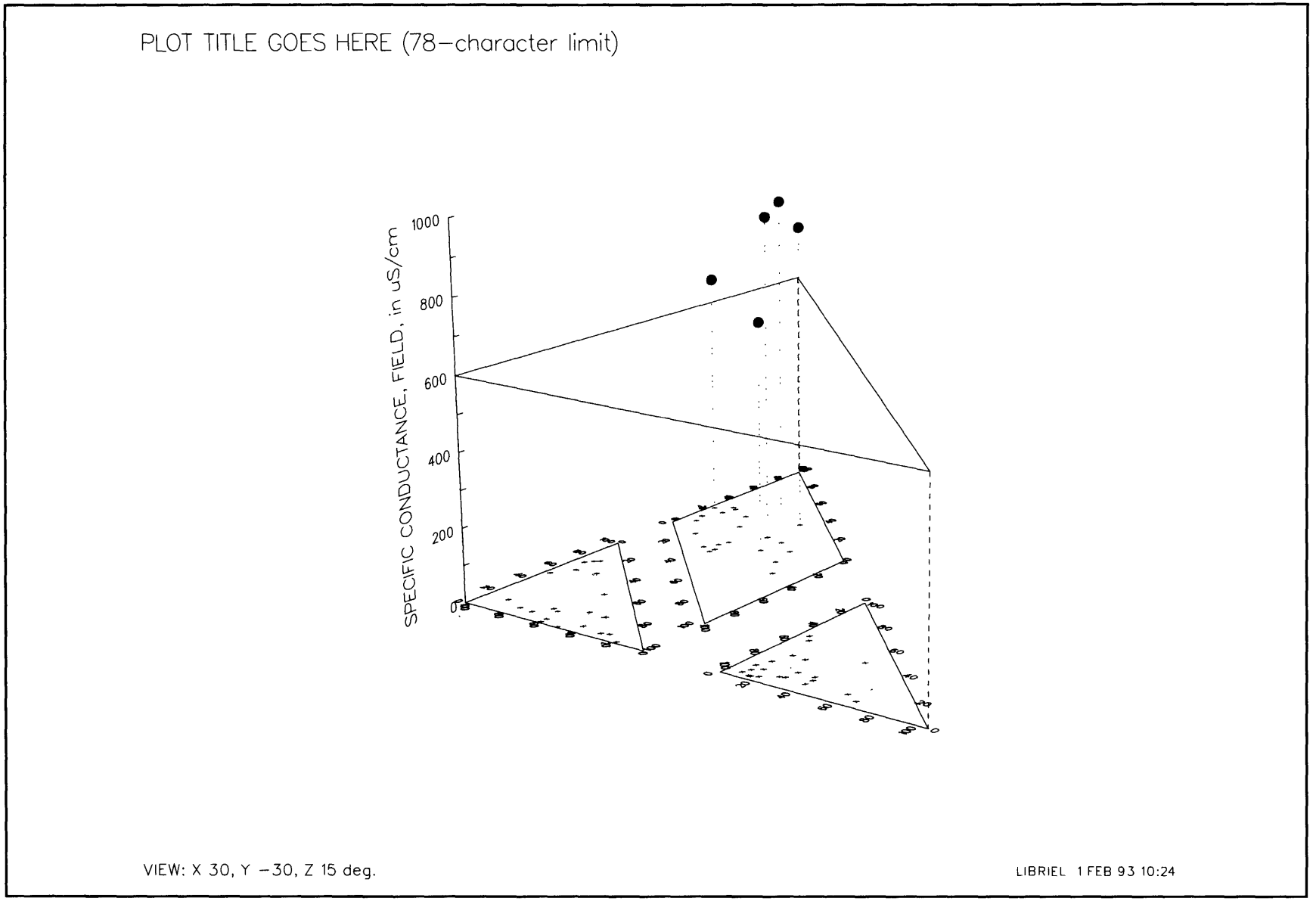

Figure 23. Piper 3-D diagram generated by the program from test data showing the normal viewing perspective and the result of applying a limited value to the variable displayed on the Z-axis.

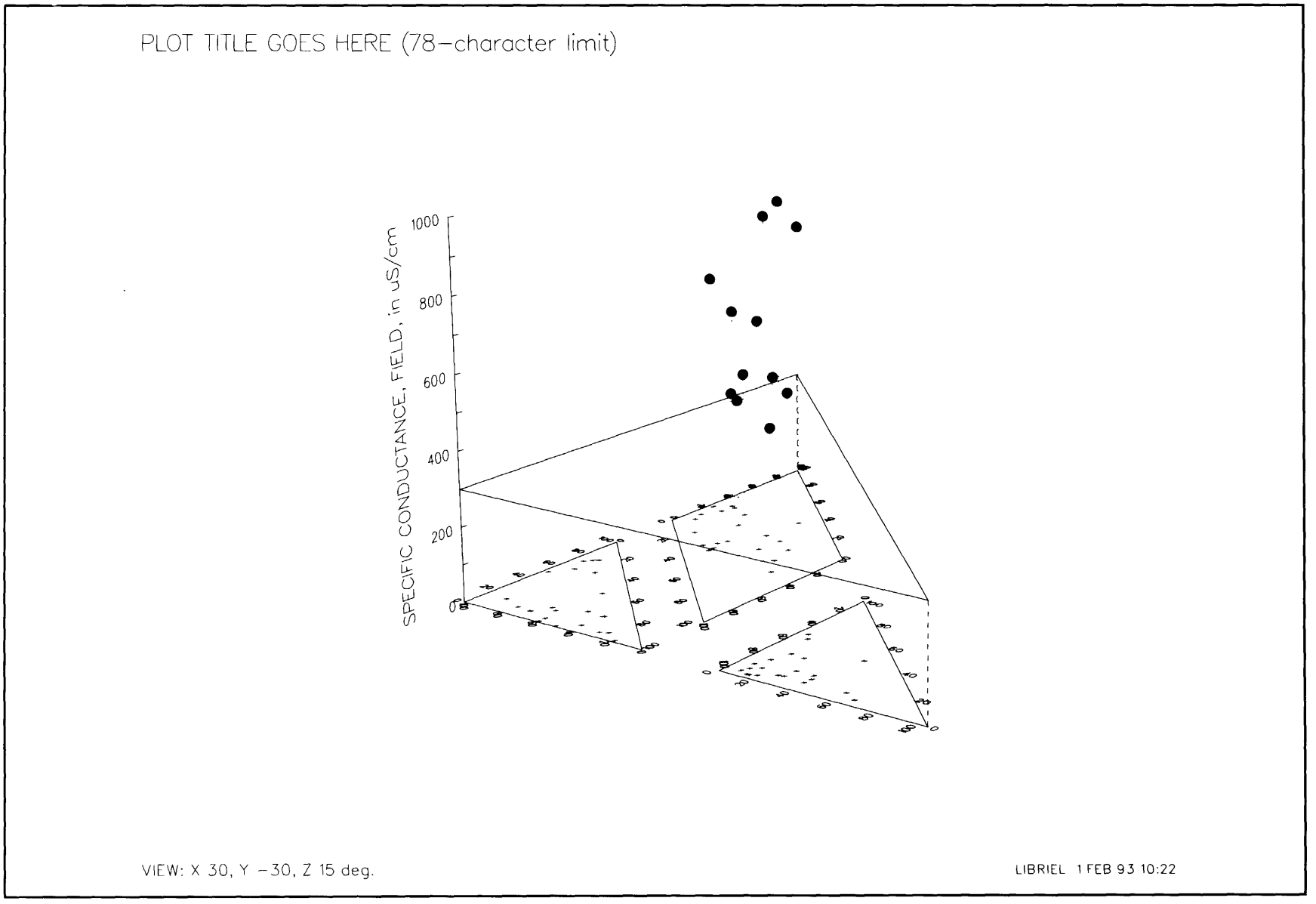

Figure 24. Piper 3–D diagram generated by the program from test data showing the normal viewing perspective and the result of lowering the limiting value on the Z–axis variable.

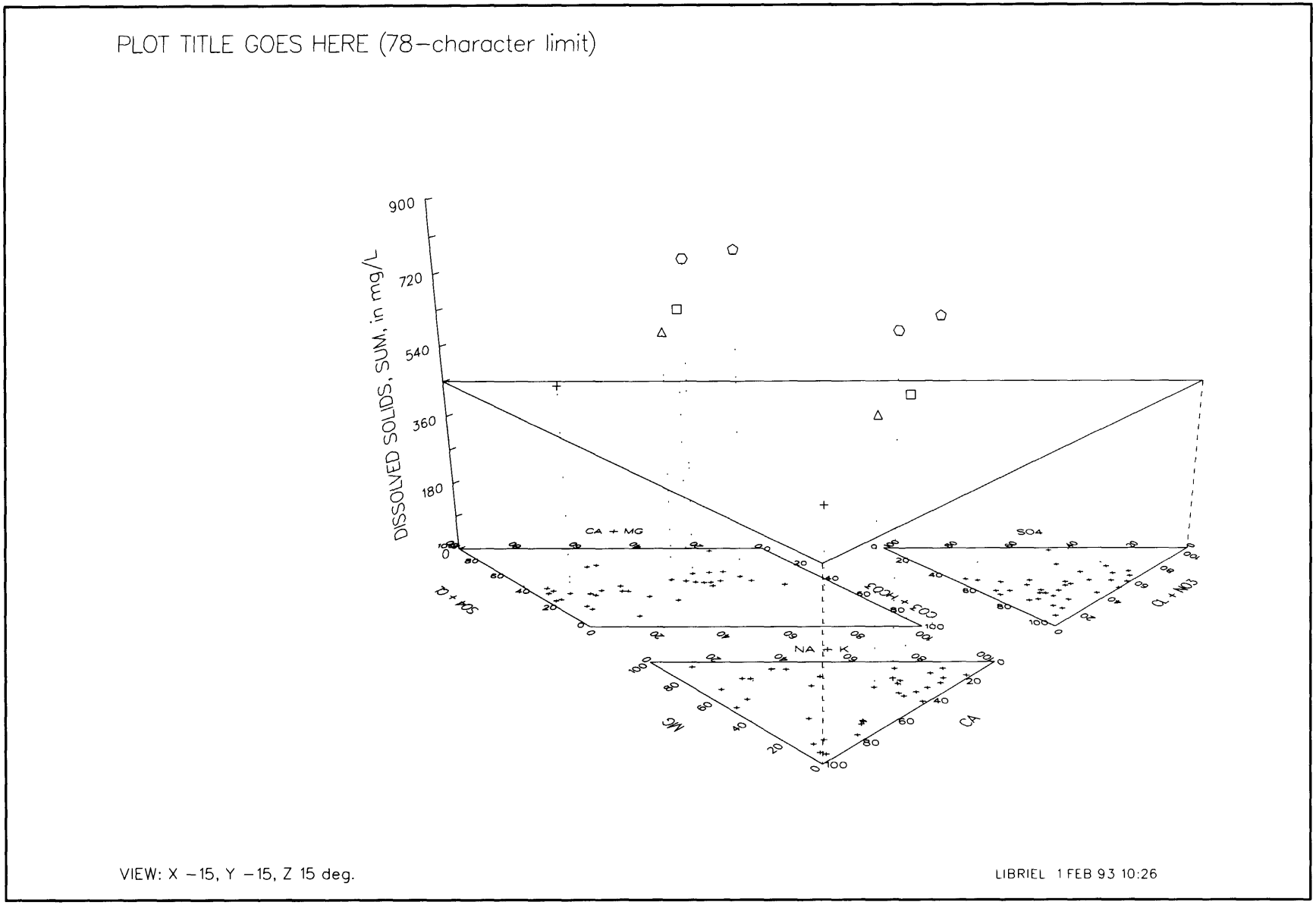

Figure 25. Piper 3–D diagram generated by the program from test data showing a different viewing perspective and with the Z-axis variable displayed over both the diamond and the cations triangle.

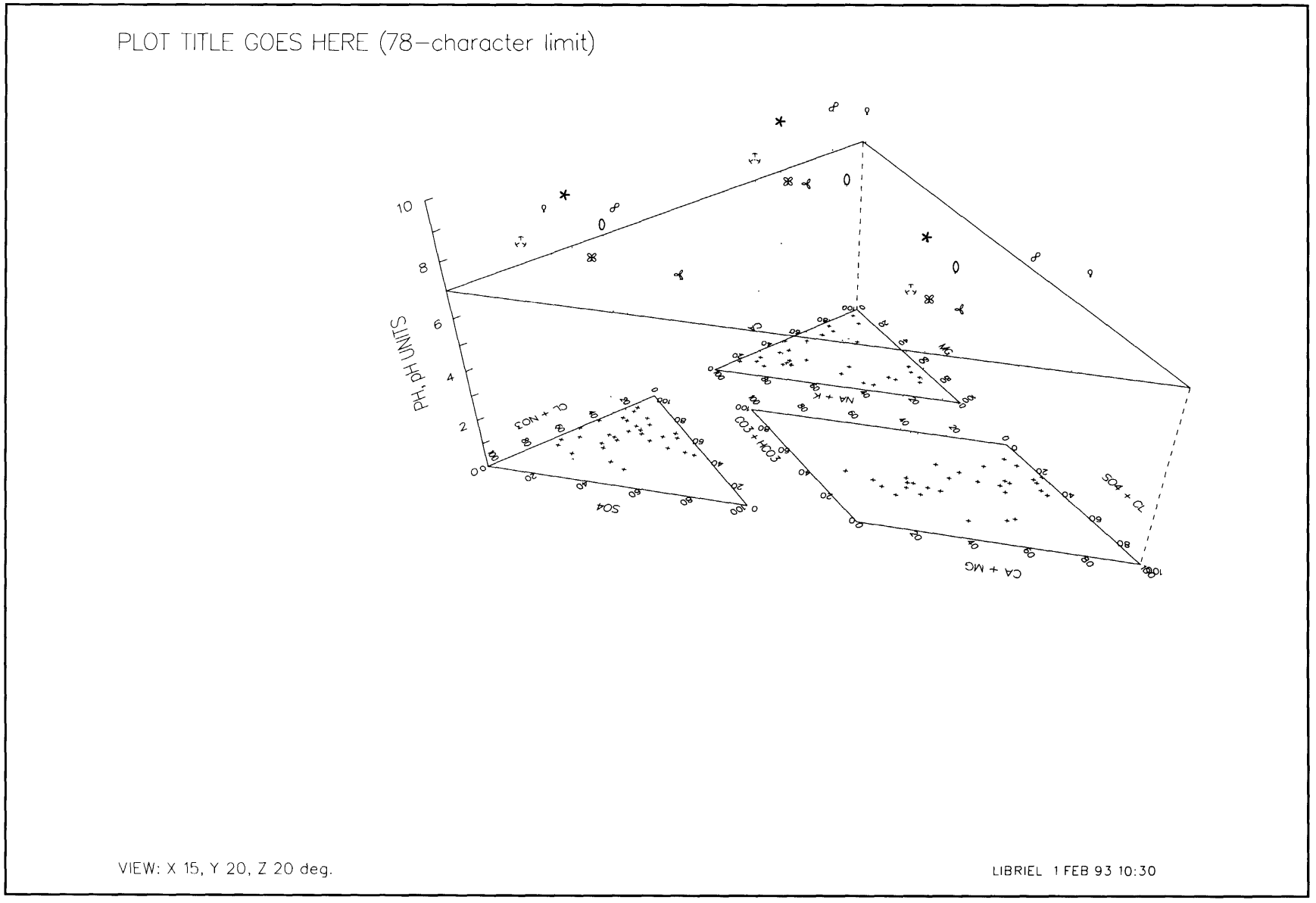

Figure 26. Piper 3–D diagram generated by the program from test data showing another viewing perspective and with the Z-axis variable displayed over all three fields.

by a large open triangle above the basal plane. The plane of the upper triangle is connected to the corners of the Piper diagram by dashed lines called legs. This arrangement shows the volume of the prism that lies between the two planes. The legs can be omitted if needed.

Figures 23 and 24 show the use of a succession of different values for the Z–axis threshold. As the limiting value decreases, more and more samples are plotted in the prism; if the Z–axis threshold is equal to zero, all of the samples are plotted (fig. 22).

Elevation of the Basal Plane

The basal plane of a Piper 3–D diagram is usually drawn at the zero value on the Z–axis. If values for the Z–axis variable are large for all samples, small differences in the lengths of the vectors cannot be easily distinguished. One way to emphasize relative differences in the lengths of these vectors is to displace the basal plane upward along the Z–axis to a point near the minimum value of the Z–axis variable. When the basal plane is elevated, the general appearance of a Piper 3–D diagram remains unchanged, but the lower limit shown on the Z–axis scale is greater than zero. The composition of all (complete) samples in the file is still shown on the basal plane, and the Z–axis vectors are projected as previously described. Elevation of the basal plane of the diagram can also be used to reduce clutter, because a Z–axis vector is shown only for samples lying above the basal plane.

Alternative Perspectives

Another way to resolve the problem of a closely packed diagram is to turn it around and display it from several different viewpoints. Rotation of a diagram also has the advantage of reducing the bias introduced by any single viewpoint. The Piper 3–D procedure can draw the prism from a default viewpoint or from any viewpoint a user selects. The prism can be rotated freely about all three axes by changing the default values for the X–, Y–, and Z–viewing angles. For each axis, viewing angles can range from -360 to +360 degrees. The default angles are X = +30, Y = -30, and Z = +15 degrees; this perspective is shown in figures 22–24. In this view, the prism is seen from 15 degrees above the Piper plane, and the normal baseline of the Piper diagram is rotated clockwise by 30 degrees. Some advantages of this viewpoint are: (1) The normal orientation of a Piper diagram (cation field at the left and anion field at the right) has been maintained; (2) the equilateral structure of a Piper diagram has not been greatly altered, and (3) the prism appears centered on the page. One disadvantage of this viewpoint is that axis annotation at the back of the prism is difficult to read. Because the orientation of the Piper figure is normal, axis labels have been omitted; these labels can be displayed if needed.

Alternative viewpoints are shown in figures 25–26. In both of these figures, axis annotation is easy to read, but the orientation of the Piper diagram is strange and its proportions are distorted. These figures illustrate the fact that some combinations of viewing angles increase the distortion of the Piper 3–D diagram, and practice may be needed to achieve a satisfactory alternative viewpoint.

Chapter 8. —SOURCES OF INPUT

Program input can come from the terminal and from external files. Input from the terminal is usually limited to brief responses: In all procedures, various options are displayed on the screen and the user is asked to select the preferred option. The main menu of options for each plotting procedure is discussed at the end of this section (Interactive Input: Knobs Menus); water-quality data and other information that comes from files are discussed first.

Water-quality data for samples *cannot* be entered from the terminal. Samples data are read from a file that has specific requirements and a definite format. Only one data file is read during each run. The name of this file is supplied by the user at the beginning of the run; there is no default name for the data file. Because a properly constructed data file is essential, the program can produce an example if needed. The contents and structure of the data file are discussed in the next sections. The user should study the following information carefully before the program is run.

The data file is not the only file that can be read by the program; some of the plotting procedures can read information from auxiliary files. This information includes: variables to display on the plot, labels for axes, and preferred colors, patterns, and symbols. The use of auxiliary files can expedite a run by reducing the amount of information that needs to be entered from the terminal. These files have already been mentioned under each of the procedures that use them; the details and structure of auxiliary files are discussed in appendix B.

Contents and Structure of the Data File

Each of the plotting procedures has different data requirements. One of the advantages of this program is that all of the procedures use the same input file. For each procedure, therefore, some of the information in the data file is required and some of it is optional. All of the procedures require water-quality data for 11 variables (see table 1). Optional information can include data for nitrate and phosphate, data for as many as six additional numeric variables, a plot title, a user-identification label, data for subtitles on Piper 2–D diagrams, and a set of 26 flags that are used to control the program. The format of the data file is shown in figure 27. The program can produce this example if needed.

The structure of the data file consists of two sections: (1) a 10-line header section, which contains most of the optional information; and (2) a data section, which contains all of the required information. The header section can be left blank, but it cannot be omitted. The data section begins on line 11 and continues to the end of the file. Each line in the data section represents a different sample, because data cannot be continued from one line to the next. A line of data is incomplete if values are missing for any of six essential ionic constituents (listed below). Incomplete lines are automatically ignored in the Piper, Piper 3–D, Stiff, and pie-diagram procedures.

The number of lines in the data section is not limited in the Piper, Stiff, and pie-diagram procedures. The X–Y and Piper 3–D procedures have a storage limit of 1,000 samples, and the boxplot procedure has a limit of 10,000 samples. Samples in the file beyond these limits are ignored.

Column 1: The Ignore-Data Code

Any line in the data section can be ignored if needed by the use of a semicolon (;) in column 1. This feature allows the user to create a subset of data without actually removing lines from the file. The number of data lines that can be ignored is not limited; if all lines in the data section have a semicolon in column 1, all samples are removed from the plot. The ignore-data code does not apply to lines in the header section.

Data Required for Each Sample

Eleven variables are required for each sample plotted. To be interpreted correctly, data for required variables must appear in the order shown in table 1, and the fields must be separated by one or more

Table 1. Order of water-quality variables in the data file

[mg/L, milligrams per liter; sbu, units for optional variables are supplied by the user]

Position	Identification of variable	Type of variable	Units	Essential for Piper, Stiff, and pie diagrams
		Required		
1	Label 1–15 characters with no blanks	alpha-numeric	unitless	yes
2	Calcium	numeric	mg/L	yes
3	Magnesium	numeric	mg/L	yes
4	Sodium	numeric	mg/L	yes
5	Potassium	numeric	mg/L	no
6	Chloride	numeric	mg/L	yes
7	Fluoride	numeric	mg/L	no
8	Sulfate	numeric	mg/L	yes
9	Bicarbonate	numeric	mg/L	yes
10	Alkalinity	numeric	mg/L	no
11	pH	numeric	standard units	yes
		Optional		
12	Nitrate	numeric	mg/L	no
13	Phosphate	numeric	mg/L	no
14	Extra variable 1	numeric	sbu	no
15	Extra variable 2	numeric	sbu	no
16	Extra variable 3	numeric	sbu	no
17	Extra variable 4	numeric	sbu	no
18	Extra variable 5	numeric	sbu	no
19	Extra variable 6	numeric	sbu	no

blank spaces. The column location of data fields is not important, except that data cannot be placed in column 1; column 1 is reserved for the ignore-data code. Blank fields are not allowed for required variables. Missing or zero values are also not allowed for six essential constituents that are needed to determine the chemical composition of a sample. Required variables can be divided by function into three groups: a sample-identification label, the ionic constituents, and pH.

The Label Variable

The first field required on each line of sample data contains a label that identifies the sample on the plot and in the data table. This label can be either a number or an ASCII character string with *no imbedded blanks*; the label can be the same for all data lines if needed. The length of the label can range from 1 to 15 characters. On Piper and full-page X–Y diagrams, the label identifies each plotting symbol in the explanation field. In the Piper 2–D and boxplot procedures, the label variable can also be used to identify a group of samples: A change in the value of the label variable signals the beginning of each group of samples. On Stiff and pie diagrams, the label variable is used as a subtitle to identify individual samples. The Piper 3–D procedure cannot display the label variable.

Ionic Constituents

The next nine fields required on each line of sample data contain ionic constituents. To plot a water sample on a Piper diagram, concentration data are needed for at least six ionic constituents:

```
v
 PLOT TITLE GOES HERE (78-character limit)                                  00000 00000 00000 00000 00000 0
 USER IDENTIFICATION  (32-character limit)                  knob location => ^^^^^ ^^^^^ ^^^^^ ^^^^^ ^^^^^ ^
                          P50     P50     P50     BAL         knob number => 12345 67890 12345 67890 12345 6
 BEGIN DATE   END DATE    00095   70301   00400   LIM   PASS   FAIL

 13-AUG-1991  15-AUG-1991 500.0   352.0    6.59     5     14      7


 LABEL           Ca  Mg  Na  K   Cl   F   SO4  HCO3   ALK   pH    NO3  PO4  SC P70301 Temp  Si  Fe   Mn    Date    IONBAL

 STREAM.SITE.01  38  19  21  37  73   .9  58  134.1  110   6.55  13.0 -1.  620  468   21   10  270  21  19910813 -9.53
 WELL.NO.01      30  14  22  24  56   .5  30  134.1  110   6.59   5.4 -1.  480  372   20   11  210  23  19910814 -6.58
 WELL.NO.02      21  13  30  24  56  2.4  34   73.1   60   6.80   7.9 -1.  600  327   20  7.9  270  26  19910813 -1.71
 STREAM.SITE.02  36  19  18  29  38   .8  43  121.9  100   6.34  13.0 -1.  570  408   21   11  260  23  19910813  -.52
 WELL.NO.03      34  15  20  22  27   .9  30  158.5  130   6.67   4.2 -1.  490  364   20   12  220  17  19910814   .37
 WELL.NO.04      37  19  22  46  27  1.2  33  219.4  180   6.75   4.3 -1.  610  432   23   12  350 110  19910815  1.17
 WELL.NO.05      34  18  23  34  32   .9  34  195.0  160   6.80  -1.0 -1.  600  399   20   13  360  95  19910813  1.95
 STREAM.SITE.03  32  15  19  32  29   .8  42  134.1  110   6.53   4.8 -1.  530  351   21  9.7  320  27  19910815  2.29
 WELL.NO.06      23  12  16  16  23   .6  29   73.1   60   6.38   4.0 -1.  370  166   20   .2  230  17  19910813  7.85
 WELL.NO.07      34  14  20  28  24   .9  42   24.4   20   6.69  11.0 -1.  470  340   19   10  300  42  19910813 22.87
```

Figure 27. Format of the data file showing the location of data fields and other information that can be placed in this file. Data must not be placed in column 1, because column 1 (marked with a "v") is reserved for data-control codes.

three cations (calcium, magnesium, and sodium) and three anions (bicarbonate, sulfate, and chloride). If data for any of these constituents are either missing or equal to zero, the chemical composition of the sample cannot be determined, and the sample is ignored.

The program also requires data for three additional constituents, potassium, fluoride, and alkalinity. Data for these variables are considered to be supplementary, which means that values for these variables can appear as either missing (see below) or equal to zero. On a Piper diagram, potassium is shown combined with sodium, and fluoride is shown combined with chloride; the Piper diagram can still be constructed if data for either potassium or fluoride are not available.

The program requires alkalinity for another reason: Bicarbonate is now commonly determined from alkalinity. If sample data for HCO_3^- concentration is greater than zero, the program uses that value; otherwise, the program calculates HCO_3^- from alkalinity. If both HCO_3^- and alkalinity are missing or equal to zero, the set of data is incomplete, and the sample is ignored.

Sample pH

The 11th field required on each data line contains pH. The pH is used in the Piper, Stiff, and pie-diagram procedures to determine an appropriate label for bicarbonate: If sample pH is less than 7.3, the label is shown as HCO_3; otherwise, the label is shown $HCO_3 + CO_3$. The maximum pH in a file determines the bicarbonate axis label for the Piper 2–D procedure. The X–Y, boxplot, and Piper 3–D procedures can display sample pH on the diagram.

Units for Required Variables

The 1st data field contains a sample label without units. The next nine fields contain the concentration of ionic constituents, in milligrams per liter. The 11th field contains the sample pH in standard pH units.

Optional Data for Each Sample

All of the plotting procedures can display two additional ionic constituents: nitrate, in milligrams of nitrogen per liter, and phosphate, in milligrams of phosphorus per liter. The 12th and 13th data fields have been reserved for these two constituents, respectively. If phosphorus data are included, both the 12th and the 13th data fields must contain a value; zero or missing values can be used in these fields if needed.

The program treats information written to the right of the 13th data field in one of two ways: Piper, Stiff, and pie diagrams cannot display any additional variables, so these procedures ignore this information; whereas, X–Y, boxplot, and Piper 3–D diagrams can display additional numeric data. The 14th to the 19th fields have been reserved for six optional numeric variables. The user must specify the number of optional variables that are in the data file; otherwise, the program does not read any optional variables. If optional variables are read, the fields for nitrate and phosphate must be occupied; a value of zero, or a missing value (-1), can be used if necessary. Any information written to the right of the last optional variable is ignored, and this area can be used for comments; if non-numeric data are present in any of the numeric fields, however, a fatal error results, and the program stops.

Missing Values for Variables

The label variable cannot be missing; surrogate labels can be used if needed. Because most water-quality variables have non-negative values, negative values can be used to represent missing data. A value of minus one (-1) for any of the six essential ionic constituents causes the sample to be ignored. The program converts negative values for other constituents to zero. Negative values for optional variables also represent missing data. If optional variables are used, any missing values for nitrate and phosphate must be represented in the file by negative numbers, so that the 12th and 13th data fields are occupied.

Other Information in the Data File

The first 10 lines (header section) of the data file can be left blank, or they can contain some optional information that is used in several different ways. In the current version of the program, only specific fields on lines 1, 2, 6, and 9 are read. Line 1 is the most important header line. An example of the format of the header section is shown in figure 27.

Line 1: The Plot Title

The plot title is an optional feature; all of the procedures can write a left-justified single-line title at the top of each page. The length of a title can range from 0 to 78 characters, and blanks *can* be included in the title string. Titles can be entered from the terminal or read from line 1 of the data file. The plot title is placed in columns 2–79, because column 1 has been reserved throughout the data file. Placing a title in the data file has several advantages: (1) It provides more complete documentation of the data in the file; (2) it standardizes the plot title for each run; and (3) it reduces the amount of information entered from the terminal.

The plot title is shown by default. If columns 2–79 of line 1 are blank, the user is asked to enter a plot title. If a null response (carriage return) is entered, the plot title is omitted for the current procedure. A title is stored for the duration of each run; if the plotting procedure is changed during a run, the current title is displayed on the screen and the user is asked if that title is still appropriate.

Line 1: The Preferred-Option Knobs

Each of the six plotting procedures has different options for many features of the plot. A set of 26 single-digit numeric variables (called knobs) is used to specify preferred options. Some of these features include: selecting the plotting procedure and format of the plot file; disabling the data-table file (chap. 9); changing the plot title and diagram annotation; specifying a scale to use for axes; selecting symbols, colors, and shade patterns; indicating the use of optional variables on diagrams; and so on. The function of many knobs is procedure-specific, and some of the plotting procedures do not use all of the knobs.

After a procedure has been selected, the current option for each knob can be displayed on a menu and reset (if needed) from the terminal. Examples of the knobs menu for each procedure are shown in the last section of this chapter; the complete list of options for each knob is shown in appendix C. Screen menus provide an easy means for selecting program options, but an alternative approach provides a faster way to run the program: Preferred options can be specified in the data file.

Values for each of the 26 knobs can be read from specific columns on line 1 of the data file. If the column is left blank, a value of 0 is assigned to that knob and the default option is used. If there is no a default option for a particular feature, the information needed to generate the plot can be entered from the terminal. The location assigned to each knob on line 1 is shown on lines 2 and 3 of figure 27. These locations are the same for all plotting procedures: The value for the first knob is placed in column 81, and values for each of the succeeding knobs are placed in groups of five to knob 26 in column 111. Groups of knobs are separated from adjacent groups by a blank column, to make it easier for the user to locate particular knobs. The knob markers shown on lines 2 and 3 of figure 27 are ignored by the program and can be included in a data file if needed.

In all of the procedures, knobs have been grouped by function; where possible, the same knob (number) has been used for functions common to more than one procedure. Knobs that perform the same functions in all procedures include knobs 1–6 and knobs 25 and 26 (appendix C, table C–1). Knobs 7–24 commonly have different functions in different procedures (appendix C, tables C–2 to C–7), although some overlap does occur. Because different procedures have different numbers of options, some knobs are not used in some procedures.

Specifying preferred options in the data file predetermines various features of the output and allows the program to run with a minimum of terminal input. New users are encouraged to gain some experience with the program by selecting preferred options from the screen menus, before setting knobs from the data file.

Line 2: The User-Identification Label

The user-identification label is a character string that contains the name of the person who generates the plot. The length of this label can range from 0 to 32 characters, and blanks *can* be included in the string. The program can read a user-identification label from columns 2–33 of line 2 of the data file (fig. 27), or generate a user-identification label from the user's login name. Information in the data file supersedes a user's login name. By default, the program combines the user-identification label with the date and current time, and writes this information at the bottom of each plot page. Date and time are obtained from the operating system of the computer and do not need to be supplied by the user. Both the user-identification and date-time labels can be omitted if needed.

Line 6: Data for Piper 2–D Subtitles

An optional feature of the Piper 2–D diagrams generated by the program is a set of five subtitles (figs. 4 and 6), which provides supplementary information about the samples. This information includes: the median dissolved-solids concentration, median specific conductance, median pH, ionic charge balance, and the dates of sample collection. Data for these subtitles must be read from line 6 of the input file (fig. 27); these data cannot be entered in any other way. If line 6 is left blank, the subtitles are not displayed.

The column location of the eight data fields on line 6 is not important, except that data cannot be placed in column 1. Fields must be separated by one or more blank spaces and must appear in the following order: (1) the earliest collection date, (2) the latest collection date, (3) the median specific conductance, (4) the median dissolved-solids concentration, (5) the median pH, (6) the limit for ion balance, expressed in percent, (7) the number of samples passing the ion-balance test, and (8) the number of samples failing the ion-balance test. If line 6 is not blank, it must contain all eight fields; missing data in any of these fields must be shown as -1.

In the Piper procedure, all five subtitles are displayed by default. Subtitles can be omitted individually by the use of knobs 7–11. If a subtitle is omitted, all of the remaining subtitles are automatically moved upward, so that gaps are not left in the annotation. These subtitles can be displayed only on Piper 2–D diagrams; the other plotting procedures ignore line 6.

Line 9: Header for Input Variables

In the example shown in figure 27, line 9 of the data file contains a brief identification of each of the input variables. The program stores line 9 and uses it as a header for each sample in the data-table file (chap. 9). If line 9 is blank, a blank line precedes the data for each sample in the data table.

Interactive Input: Knobs Menus

At the beginning of each run after a plotting procedure has been selected, a menu can be displayed that shows the current value for each of the 26 knobs. This menu also shows a brief description of the function of each of the knobs used by the procedure (active knobs). To emphasize the active knobs in each procedure, the function of inactive knobs is not shown on the menu. From the menu, the value of each active knob can be changed. When an alternative value has been entered, the menu is redisplayed to show the change. A user can make as many changes in the active knobs as needed, including changing the plotting procedure, which redefines the active knobs. If the menu is used to change the plotting procedure, all procedure-specific knobs (7–23) are set to default values, and some may need to be reset. A null response is entered to terminate the menu-selection process and allow the program to generate the plot.

The values for active knobs apply to all diagrams on a page and to all multiple pages of a run. For the Piper, Stiff, and pie-diagram procedures, the only time the knobs menu can be displayed is at the beginning of the run; once the program begins to generate the plot, the knobs cannot be reset. This is not the case, however, for the Piper 3–D, X–Y, and boxplot procedures. When each page of diagrams has been completed, the knobs menu can be redisplayed and *some* of the

active knobs can be changed. The initial values for knobs 1–5 and knobs 24–26 cannot be changed between pages of output.

Knobs menus were designed to display specific information about each of the 26 knobs on an 80–column by 24–line terminal screen. To do this, the information shown for each knob has been condensed, and the screen has been divided in half vertically, with data for knobs 1–15 shown on the left side and data for knobs 16–26 shown on the right (figs. 28–33). The two halves are similar, but they are not entirely identical. For all knobs, the knob number (KNOB) is shown in the first column, and the current value (VAL) is shown in the second column. For knobs 1–15 (left side), the function of each knob (FUNCTION) is shown in the third column, and the option associated with the current value (OPTION) is shown in the fourth column. For knobs 16–26 (right side), the function and the option are shown together in the third column. Many of the knobs on the right side of the menus are defined in such a way that the distinction between function and option is not particularly meaningful. For the few exceptions, a colon (:) is used in the third column to separate the function and the current option.

Knobs menus for all six procedures have the same format; an example of the menu for each procedure is shown in figures 28–33.

```
KNOB VAL  FUNCTION          OPTION          KNOB VAL  FUNCTION (AND OPTION)

  1   0   PROGRAM MODE:     MENU             16   0   1st DIGIT FOR SYM SHAPE
  2   1   PROCEDURE:        PIPER            17   0   2nd DIGIT FOR SYM SHAPE
  3   0   OUTPUT:           METAFILE         18   0   SYM SIZE: ENTER CHOICE
  4   0   PLOT NAME:        GENERATE         19   0   COLORS: ENTER CHOICE
  5   0   DATA TABLE:       ON               20   2   CODE FOR 1st COLOR

  6   0   PLOT TITLE:       ON               21   3   CODE FOR 2nd COLOR
  7   0   SOLIDS TITLE:     ON               22   4   CODE FOR 3rd COLOR
  8   0   CONDUCT TITLE:    ON               23   5   CODE FOR 4th COLOR
  9   0   PH TITLE:         ON               24   6   CODE FOR 5th COLOR
 10   0   BALANCE TITLE:    ON               25   1   NITRATE as N: INCLUDE

 11   0   DATES TITLE:      ON               26   0   PHOSPHATE as P: EXCLUDE
 12   0   USER-DATE TAG:    ON
 13   0   AXIS LABELS:      ON                 + - - - - - - - - - - - - - - +
 14   0   LEGEND FIELD:     ON 35 LABELS       |  0  uses default value      |
 15   0   PLOT SYMBOLS:     ENTER CHOICE       | >0  sets another value      |
                                               + - - - - - - - - - - - - - - +

Enter number of KNOB to reset, <cr> = no changes  >
```

Figure 28. Example of the knobs menu for the Piper-diagram procedure.

```
KNOB VAL  FUNCTION          OPTION          KNOB VAL  FUNCTION (AND OPTION)

  1   2   PROGRAM MODE:     TRACE            16   0   1st DIGIT FOR SYM SHAPE
  2   2   PROCEDURE:        PIPER 3-D        17   0   2nd DIGIT FOR SYM SHAPE
  3   1   OUTPUT:           POSTSCRIPT       18   1   SYM SIZE: REDUCED 1/2
  4   1   PLOT NAME:        ENTER            19   2   COLORS: USE 7 COLORS
  5   1   DATA TABLE:       OFF              20   1   CODE FOR 1st COLOR

  6   0   PLOT TITLE:       ON               21   1   1st DIGIT FOR Z-VAR CODE
  7   1   TEXT FONT:        HARDWARE         22   4   2nd DIGIT FOR Z-VAR CODE
  8   1   PAGE-ID TAG:      OFF              23   0   Z-AXIS CA - PO4: MEQ/L
  9   0   SHOW Z OVER:      DIAMOND          24   6   NUM OF EXTRA VARIABLES
 10   0   FILTER Z-VAR:     NO               25   1   NITRATE as N: INCLUDE
      .
 11   0   VIEW-ANGLES TAG:  ON               26   0   PHOSPHATE as P: EXCLUDE
 12   0   USER-DATE TAG:    ON
 13   0   AXIS LABELS:      OFF                + - - - - - - - - - - - - - - +
 14   0   VIEW ANGLES:      DEFAULT            |  0  uses default value      |
 15   0   PLOT SYMBOLS:     ENTER CHOICE       | >0  sets another value      |
                                               + - - - - - - - - - - - - - - +

Enter number of KNOB to reset, <cr> = no changes  >
```

Figure 29. Example of the knobs menu for the Piper 3-D diagram procedure.

```
KNOB VAL  FUNCTION          OPTION          KNOB VAL  FUNCTION (AND OPTION)

  1   0   PROGRAM MODE:     MENU             16   0   DECIMAL PLACES IN SCALE
  2   3   PROCEDURE:        STIFF            17   0   1st DIGIT FOR SCALE
  3   2   OUTPUT:           HPGL-7475        18   0   2nd DIGIT FOR SCALE
  4   1   PLOT NAME:        GENERATE         19   0   3rd DIGIT FOR SCALE
  5   1   DATA TABLE:       OFF              20   0   4th DIGIT FOR SCALE

  6   0   PLOT TITLE:       ON               21   0
  7   3   TEXT FONT:        SIMPLEX          22   0
  8   0   PAGE-ID TAG:      AT UR            23   0
  9   0                                      24   0
 10   0                                      25   1   NITRATE as N: INCLUDE

 11   0                                      26   0   PHOSPHATE as P: EXCLUDE
 12   0   USER-DATE TAG:    ON
 13   0                                        + - - - - - - - - - - - - - - +
 14   0                                        |  0  uses default value      |
 15   0   DIAGRAM SCALE:    ENTER CHOICE       | >0  sets another value      |
                                               + - - - - - - - - - - - - - - +

Enter number of KNOB to reset, <cr> = no changes  >
```

Figure 30. Example of the knobs menu for the Stiff-diagram procedure. Knobs 9–11, 13, 14, and 21–24 are not used in this procedure.

```
KNOB VAL  FUNCTION          OPTION          KNOB VAL  FUNCTION (AND OPTION)

  1   0   PROGRAM MODE:     MENU             16   2   COLOR CODE FOR NA + K
  2   4   PROCEDURE:        QW PIE           17   3   COLOR CODE FOR CA
  3   3   OUTPUT:           HPGL-7586        18   6   COLOR CODE FOR MG
  4   1   PLOT NAME:        ENTER            19   1   COLOR CODE FOR N + P
  5   1   DATA TABLE:       OFF              20   1   COLOR CODE FOR SO4

  6   2   PLOT TITLE:       VERIFY           21   5   COLOR CODE FOR HCO3
  7   4   TEXT FONT:        DUPLEX           22   7   COLOR CODE FOR CL + F
  8   2   PAGE-ID TAG:      AT LL            23   0
  9   0                                      24   0
 10   0                                      25   1   NITRATE as N: INCLUDE

 11   0   CAT-ANI GAP:      YES              26   0   PHOSPHATE as P: EXCLUDE
 12   0   USER-DATE TAG:    ON
 13   0   SLICE LABELS:     ON                 + - - - - - - - - - - - - - - +
 14   0   PATTERNS:         PROGRAM'S          |  0 uses default value      |
 15   0   COLORS:           PROGRAM'S          | >0 sets another value      |
                                               + - - - - - - - - - - - - - - +

Enter number of KNOB to reset, <cr> = no changes  >
```

Figure 31. Example of the knobs menu for the pie-diagram procedure. Knobs 9, 10, 23, and 24 are not used in this procedure.

```
KNOB VAL  FUNCTION          OPTION          KNOB VAL  FUNCTION (AND OPTION)

  1   0   PROGRAM MODE:     MENU             16   0   1st DIGIT FOR SYM SHAPE
  2   5   PROCEDURE:        X-Y PLOT         17   0   2nd DIGIT FOR SYM SHAPE
  3   4   OUTPUT:           CGMB-META        18   0   SYM SIZE: ENTER CHOICE
  4   0   PLOT NAME:        GENERATE         19   0   COLORS: ENTER CHOICE
  5   0   DATA TABLE:       ON               20   2   CODE FOR 1st COLOR

  6   0   PLOT TITLE:       ON               21   0
  7   0   TEXT FONT:        ENTER CHOICE     22   0
  8   0   PAGE-ID TAG:      AT UR            23   0   UNITS CA - PO4: MEQ/L
  9   0   DIAG / PAGE:      ASK              24   6   NUM OF EXTRA VARIABLES
 10   1   PLOT VARIABLES:   READ             25   1   NITRATE as N: INCLUDE

 11   0   ISOSCALE X=Y:     NO               26   0   PHOSPHATE as P: EXCLUDE
 12   0   USER-DATE TAG:    ON
 13   0   1:1 LINE:         ASK                 + - - - - - - - - - - - - - - - +
 14   0   LEGEND FIELD:     ON                  |  0  uses default value        |
 15   0   PLOT SYMBOLS:     ENTER CHOICE        | >0  sets another value        |
                                                + - - - - - - - - - - - - - - - +

Enter number of KNOB to reset, <cr> = no changes  >
```

Figure 32. Example of the knobs menu for the X-Y diagram procedure. Knobs 21 and 22 are not used in this procedure.

```
KNOB VAL  FUNCTION          OPTION          KNOB VAL  FUNCTION (AND OPTION)

  1   0   PROGRAM MODE:     MENU             16   0   COLORS: ENTER CHOICE
  2   6   PROCEDURE:        BOXPLOT          17   3   COLOR OF BOX
  3   5   OUTPUT:           CGMC-META        18   6   COLOR OF MEDIAN
  4   1   PLOT NAME:        ENTER            19   7   COLOR OF WHISKERS
  5   1   DATA TABLE:       OFF              20   2   COLOR OF NEAR OUTLIERS

  6   2   PLOT TITLE:       VERIFY           21   6   COLOR OF FAR OUTLIERS
  7   5   TEXT FONT:        COMPLEX          22   0
  8   1   PAGE-ID TAG:      OFF              23   1   UNITS CA - PO4: MG/L
  9   2   PLOT BY GROUP:    YES              24   6   NUM OF EXTRA VARIABLES
 10   2   PLOT VARIABLES:   SAVE             25   1   NITRATE as N: INCLUDE

 11   2   BOX SCALE:        LINEAR           26   0   PHOSPHATE as P: EXCLUDE
 12   0   USER-DATE TAG:    ON
 13   0                                        + - - - - - - - - - - - - - - - +
 14   0   LEGEND FIELD:     ON                  |  0  uses default value        |
 15   0   NUM OF VALUES:    ON                  | >0  sets another value        |
                                                + - - - - - - - - - - - - - - - +

Enter number of KNOB to reset, <cr> = no changes  >
```

Figure 33. Example of the knobs menu for the boxplot-diagram procedure. Knobs 13 and 22 are not used in this procedure.

CHAPTER 9.—OUTPUT FILES

The principal output from this program consists of a plot file that contains water-quality diagrams and a data-table file that shows both the input data and the values computed for each sample plotted. Six auxiliary output files can also be produced to store user-supplied information, including preferred symbols, colors, and patterns; axis labels for optional variables on boxplot, X–Y, and Piper 3–D diagrams; and variables to display on X–Y and boxplot diagrams. Auxiliary files are discussed in appendix B; details of the two principal output files are discussed in this chapter.

Plot-File Formats

This program does not display water-quality diagrams; instead, coded information about the diagrams is written to the plot file. Displaying the diagrams requires additional processing of the plot file after a run is completed. The type of processing that is needed depends on the format of the plot file; seven different formats are available from the program. Plot files can be written either as device-independent metafiles—including AGTK compressed-binary and three types of CGM metafiles—that require special software to display the plot, or as device-dependent files, which require specific hardware to display the plot. The default format for the plot is the AGTK binary metafile; six other formats have been included to allow the plot to be read by a larger group of software programs. Three device-dependent formats allow the plot to be displayed on specific devices without the need for additional software; these formats are: the Adobe PostScript graphics format, which uses a laser PostScript printer to display the plot, and two HPGL formats (HPGL 7475 and HPGL 7586), which use specific pen plotters or other devices to display the plot. The seven different plot-file formats allow the user to determine the most appropriate format from the equipment that is available.

Displaying Metafiles: the Post-Processor

Metafiles can be displayed by running a program called the post-processor, which is commonly available at sites supporting the PRIOR AGTK or CA–DISSPLA graphics libraries. Most post-processors are versatile and can display metafiles on many different kinds of graphics devices, including: terminal screens, pen plotters, and film recorders. Some post-processors can also write the plot codes to another file in a different format, such as Adobe PostScript and HPGL. Post-processor programs can be modified by authorized personnel, and the local version of this program usually supports all of the graphics devices that are available on the system. The system-level command that is used to initiate the post-processor program can be obtained from the system administrator.

In a metafile, each plot page is assigned a sequential (internal) number that ranges from 1 to the total number of pages in the file. Post-processors can display plot pages independently, and pages that are not needed can be skipped. Before each page is displayed, the post-processor program allows the user to enter certain instructions (called directives) from the terminal. The post-processor directive for displaying a specific plot page is

DRAW = n $

where n is the number assigned to the plot page in the metafile. An extended discussion of post-processor directives can be found in PRIOR (1991, v. 2, p. MET 31–52).

Displaying PostScript Files

Adobe PostScript graphics files can be displayed on laser printers that can interpret this language; the availability of these printers is increasing rapidly. Laser PostScript printers are single-color devices, and this should be considered when the various color options offered by the program are being selected. PostScript printers can indicate different colors by the use of half-tones

and various shades of grey, but in many cases, it is difficult to distinguish one "color" from another. PostScript plots of water-quality diagrams usually look best when all color options have been disabled.

Displaying HPGL Files

HPGL files can be displayed on graphics devices that can interpret this language, including various plotters and photographic film recorders. There are several different versions of HPGL codes. It is necessary to know the version that is required by a particular device, because some devices can use only one set of these codes. Pen plotters that use one of the two sets of HPGL codes written by this program are widely available. Electrostatic plotters and film recorders that use these codes are available at many locations.

Multiple Plot Files

One advantage of metafiles is that all plot pages produced during a run can be stored in the same file, which reduces clutter in the directory. This feature has not been implemented in the other three formats, because multiple-page plot files do not work correctly. For the device-dependent formats, the program creates a separate output file for each plot page and generates a name for each of the additional files. The method used to generate names for plot files is discussed in the following section. Potential users of PostScript and HPGL formats should study this material carefully, before entering a name for the plot file.

Method Used to Generate Plot-File Names

At the beginning of each run, a name for the plot file can be entered from the terminal or generated by the program. The rules for legal filenames depend on the operating system of the computer being used and are beyond the scope of this report; any legal filename can be entered. If this file already exists, the user is asked if this file can be over-written. If the filename is generated by the program, a 5-character prefix that indicates the format of the plot file—**meta., cgmb., cgmc., cgmt., post., hp74., or hp75.**—is added to the name of the data file. For example, if **datafilename** represents the name of the data file, **meta.datafilename** is the name generated for an AGTK binary metafile, **cgmb.datafilename** is the name generated for a CGM binary metafile, **cgmc.datafilename** is the name generated for a CGM character metafile, **cgmt.datafilename** is the name generated for a CGM text metafile, **post.datafilename** is the name generated for a PostScript plot file, and **hp74.datafilename** and **hp75.datafilename** are the names generated for HPGL–7475 and HPGL–7586 plot files, respectively.

This method for generating filenames is extended to multiple-page plot files by adding an additional digit to each of the prefixes—**post1., hp741., or hp751.**—are generated for the first file in each series. This digit, the fifth character in the name, is increased by one for each succeeding file. If a series contains more than nine files, the fourth character in the name is replaced by the tens digit, and for HPGL files, the distinction between the two versions of codes is lost. In a multiple-page series, the program generates the name for all files beyond the first file. If the user enters a name for the first plot file, these prefixes are not added, but the naming convention still applies: The fifth character in the name of the first file is replaced by "2" in the second filename, by "3" in the third filename, and so on. Therefore, although these prefixes are not required, they should be considered when an alternative name is entered.

The Data-Table File

In addition to the plot file, which contains graphics codes for the water-quality diagrams, this program can produce an ASCII data-table file, which lists the data used to generate the diagrams. For each sample that is plotted, the data table shows the values read from the input file and the computed values displayed on the diagram. Samples that have missing data for any of six essential ionic constituents (chap. 8) cannot be plotted and are not listed in this file. To provide a means of cross-reference between the diagrams and the data table, a sequential number is assigned to each sample listed in the table, and this number

is shown on Stiff and pie diagrams (chaps. 3–4). The data table is the same for all procedures and can be omitted if needed.

Format of the Data-Table File

The format of the data-table file is 132 columns by 64 lines. Figure 34 shows the first 39 lines of a data table generated from the input data shown in figure 27. The first page of a data table shows the name of the data file, user-identification label, date, time, page number, plot title, header section, and output data for the first five samples plotted. Figure 34 does not show the entire first page, but the output-data format is the same for all samples. Each succeeding page of the data table shows output data for seven samples, but does not show the header section. Column 1 is reserved for page-control characters; page breaks are indicated by a "1" (Fortran-forms code).

The entry for each sample in the data table consists of seven lines of information: The first line shows the sequential number assigned to the sample; the second line identifies each of the input variables (this line is copied from line 9 of the data file); the third line shows the input data for each sample (this line is also copied from the data file); the fourth line contains dashes that are used to separate the input data from the computed values; the fifth line is used as a header to identify each of the computed variables; the sixth line shows the computed value for concentration, in milliequivalents per liter, for each of the variables identified above; and the seventh line shows the concentration expressed as a percentage of total milliequivalents per liter of cations or anions (chap. 2). A line of double dashes indicates the end of each entry, and successive entries in the table are separated by a blank line.

Displaying the Data-Table File

Data-table files can be displayed on terminal screens and line printers that support 132-column displays. If the data-table file is printed, the Fortran-forms option should be used so that page breaks occur at the correct places.

Naming the Data-Table File

If the data-table file has not been disabled, the program automatically generates a name for this file by adding a prefix—**table.**—to the name of the data file. If a file with this name already exists, the user is asked if this file can be over-written. If the answer is yes, the current version of the data table replaces the earlier version. If the answer is no, the user is asked to enter another name for the new data table. The program does not make any alterations to the new name.

```
1    DATAFILE:   "testdata"  RUN BY: LIBRIEL  on  1 FEB 93  9:30    PAGE    1.
     ===========  HEADER ================================================================================================

 PLOT TITLE GOES HERE (78-character limit)

                              P50     P50     P50   BAL
 BEGIN DATE   END DATE      00095   70301   00400   LIM   PASS   FAIL

 13-AUG-1991  15-AUG-1991   500.0   352.0    6.59     5     14      7

 ==========  END OF HEADER - DATA BEGINS ============================================================================

 SAMPLE NUMBER   1:
 LABEL          Ca   Mg   Na    K   Cl    F  SO4   HCO3  ALK   pH   NO3  PO4  SC  P70301 Temp  Si  Fe   Mn    Date      IONBAL
 STREAM.SITE.01 38   19   21   37   73   .9   58  134.1  110  6.55  13.0  -1  620   468   21   10  270   21  19910813    -9.53
                ------------------------------------------------------------------------------------------------------------
                     CA       MG       NA        K      CATIONS      ANIONS       HCO3       SO4        CL         F        NO3
    MEQ      >     1.896    1.563    0.913    0.946        5.318        6.440      2.198      1.208      2.059      0.047      0.928
    PERCENT  >    35.65    29.39    17.17    17.79          100.         100.      34.13      18.76      31.97       0.73      14.41
                ============================================================================================================

 SAMPLE NUMBER   2:
 LABEL           Ca   Mg   Na    K   Cl    F  SO4   HCO3  ALK   pH    NO3  PO4  SC  P70301 Temp  Si  Fe   Mn    Date    IONBAL
 WELL.NO.01      30   14   22   24   56   .5   30  134.1  110  6.59   5.4   -1  480   372   20   11  210   23  19910814  -6.58
                ------------------------------------------------------------------------------------------------------------
                     CA       MG       NA        K      CATIONS      ANIONS       HCO3       SO4        CL         F        NO3
    MEQ      >     1.497    1.152    0.957    0.614        4.220        4.815      2.198      0.625      1.580      0.026      0.386
    PERCENT  >    35.47    27.30    22.68    14.55          100.         100.      45.65      12.98      32.81       0.54       8.02
                ============================================================================================================

 SAMPLE NUMBER   3:
 LABEL           Ca   Mg   Na    K   Cl    F  SO4   HCO3  ALK   pH    NO3  PO4  SC  P70301 Temp  Si  Fe   Mn    Date    IONBAL
 WELL.NO.02      21   13   30   24   56  2.4   34   73.1   60  6.80   7.9   -1  600   327   20  7.9  270   26  19910813  -1.71
                ------------------------------------------------------------------------------------------------------------
                     CA       MG       NA        K      CATIONS      ANIONS       HCO3       SO4        CL         F        NO3
    MEQ      >     1.048    1.069    1.305    0.614        4.036        4.176      1.198      0.708      1.580      0.126      0.564
    PERCENT  >    25.97    26.49    32.33    15.21          100.         100.      28.69      16.95      37.83       3.02      13.51
                ============================================================================================================
```

Figure 34. Page 1 of a data table showing header information and samples data from the input file (fig 27) and calculated values for the first three samples. All succeeding pages of this table show six samples per page, but do not show the header information. Column 1 is reserved for Fortran page-control codes.

CHAPTER 10.—SUMMARY

This report is a user's manual for a new computer program that incorporates six different graphical techniques to produce diagrams for displaying water-quality data. Piper, Stiff, pie, X–Y, boxplot, and Piper 3–D diagrams can all be generated from the same file of input data. The Piper 3–D diagram is a new method that projects data from the surface of a 2–D Piper plot into a triangular prism to show how variations in chemical composition can be related to variations in other characteristics and constituents. A multiple-technique approach to water-quality diagrams improves the display of data.

The computer program is written in Fortran '77 and uses graphics subroutines from either the PRIOR AGTK or the CA–DISSPLA graphics library. This program has been implemented on Prime series 50 and Data General Aviion computers within the USGS; portability of the program to other computing systems depends primarily on the availability of the graphics library.

This program requires an ASCII file of input data. Some of the information in the data file is required, and some of it is optional. Most of the optional information is placed in the first 10 lines of the file; these lines can be left blank. Data for samples begins on line 11 and continues to the end of the file. Each line represents a different sample and must contain data for 11 variables in the following order: a sample-identification label, calcium, magnesium, sodium, potassium, chloride, fluoride, sulfate, bicarbonate, alkalinity, and pH. Data fields are separated by one or more blank spaces; column location is not important and can vary from line to line. The sample label is unitless; data for ionic constituents are concentrations, in milligrams per liter; and pH is expressed in standard units.

In addition to the 11 required variables, as many as six optional variables can be included on each line. Optional variables can be displayed by the X–Y, boxplot, and Piper 3–D procedures. Other information in the data file can include: a plot title, a user-identification label, data for subtitles on Piper 2–D diagrams, and a set of 26 knobs that are used to control the program.

This program does not display water-quality diagrams; instead, coded information about the diagrams is written to a plot file. Displaying the diagrams requires additional processing of the plot file after a run is completed. The type of processing that is needed depends on the format of the plot file; seven different formats are available: AGTK compressed-binary metafile, three types of CGM metafiles, PostScript file, HPGL–7475 file, and HPGL–7586 file. The default format is the compressed-binary metafile, but the user can select the most appropriate format from the equipment that is available.

In addition to the plot file, this program can produce a 132–column data-table file, which lists the data used to generate the diagrams. The first line of each page of this table shows the name of the input file, user-identification label, date, time, and page number. The first page also shows the information contained in the header section of the data file. The remainder of the table shows the data for plotted samples. Each line of input data is followed by the computed values, in milliequivalents per liter and in milliequivalent percent, for each of the major ionic constituents.

This program originated from an idea to combine three existing independent programs into a integrated unit for plotting different types of water-quality diagrams. From the beginning, the structure of the new program was modular, allowing each unit to perform a separate task but taking advantage of a common set of subroutines. When the original goal had been reached, it was apparent that the versatile structure of this program would support additional modules to generate as many different kinds of water-quality diagrams as needed, and three additional modules were added to the code. If the program proves to be useful, it can be further expanded to include other plotting techniques.

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APPENDIXES

APPENDIX A.—PROGRAM CODES FOR COLORS, SYMBOL SHAPES, AND SLICE PATTERNS

This program uses integer codes to specify colors, symbol shapes, and slice patterns. On some types of diagrams, these features can be set by the user. The codes for colors, symbol shapes, and slice patterns are discussed in the following sections.

Color Codes

Five of the six types of water-quality diagrams generated by this program can be displayed in color on graphics devices that support color output, such as terminal screens, pen plotters, and photographic film. Default colors have been selected to emphasize various features on these diagrams. A user can choose an alternative set of colors, or disable the color display.

Color is specified by the use of a single-digit integer code that ranges from 1 to 7; where 1 = black, 2 = red, 3 = green, 4 = blue, 5 = magenta, 6 = yellow, and 7 = cyan. These codes work correctly on most color terminals and film recorders, but some pen plotters select pens in a different order. For each plotter, the relation between color information in the plot file and the order of pen selection can be determined by experiment.

Symbol-Shape Codes

The AGTK graphics library contains a total of 18 standard symbol shapes, which are specified by the use of a two-digit interger code that ranges from 1 to 18. The default order of selection and numeric code for each symbol shape are shown in figure A–1. To identify a larger number of samples, the program provides an alternative set of 60 symbol shapes, which are specified by the use of a two-digit interger code that ranges from 1 to 60. The default order of selection and numeric code for each symbol shape are shown in figure A–2. The *alternative* set is the default set for the program; the symbol set to be used can be selected from the terminal or specified by setting the symbols knob for the procedure being run. Both symbol sets can be written to a plot file if needed (KNOB(2) = 7).

The order of selection of plot symbols can be changed if needed (KNOB (15) = 5). The new order for both symbol sets can be entered from the terminal and written to a file for use in a later run. The structure of this file is shown in appendix B.

Slice-Pattern Codes

The shade patterns used by the program for pie slices are specified by either a two-digit integer code that ranges from 0 to 19, or a more complex number that ranges from 0 to 1,080,799. If the value of the pattern code is between 0 and 19, the program uses a set of standard patterns from the PRIOR AGTK library. These patterns are shown in figure A–3, which can be written to a plot file if needed (KNOB (2) = 7).

If a user needs to design a different pattern, its code becomes a complex number of the form: WXYZ, where:

- W is a one-, two-, or three-digit integer indicating the angle of shading, in degrees, from 0 to 360;
- X is a one-digit integer indicating a particular type of line pattern (single, double, triple, and others) and ranging from 0 to 7;
- Y is a one-digit integer indicating pattern density and ranging from 0 (most dense) to 9 (least dense); and
- Z is a one-digit integer indicating whether or not the pattern is cross-hatched (a non-zero value indicates cross-hatching; a value of 0 indicates no cross-hatching).

The WXYZ codes for standard patterns in the AGTK library are shown at the top of figure A–3. The corresponding 2-digit program codes are shown at the bottom.

This program provides for some additional modifications to shade patterns by showing the pattern in one of three different line textures: solid, dotted, or dashed. The default texture is solid; for dotted lines, 360000 is added to the WXYZ code, and for dashed lines, 720000 is added to the WXYZ code. The distinctive brick-wall pattern used by default for the calcium and bicarbonate slices is a special pattern that can be obtained by use of the value 99999.

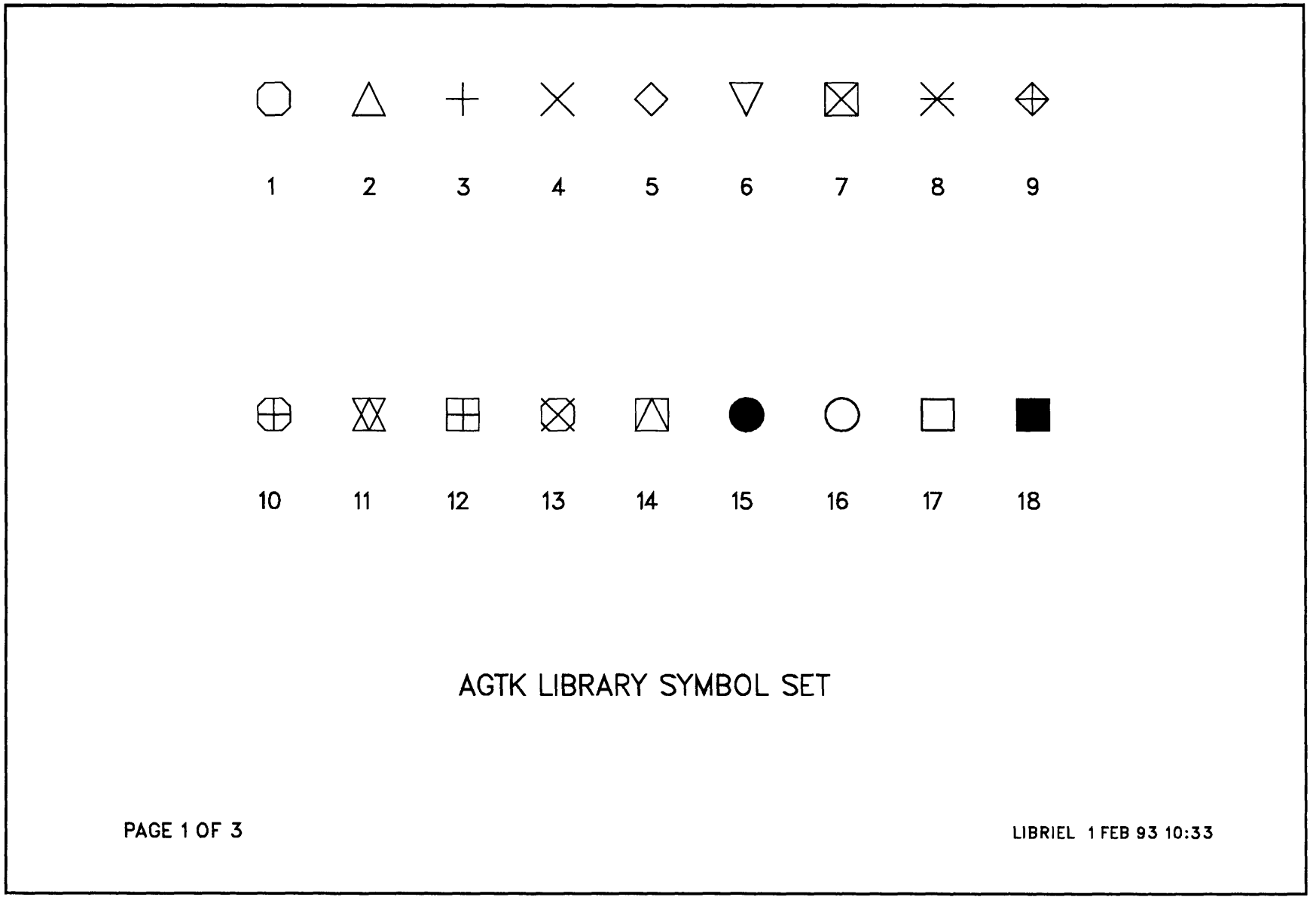

Figure A–1. Program codes for symbols in the AGTK library symbol set. Modified from table 4.2.1, PRIOR Advanced Graphics Toolkit User's Manual, v.1, p. 4–5, PRIOR Data Sciences, Ltd., 1991. Reprinted by permission.

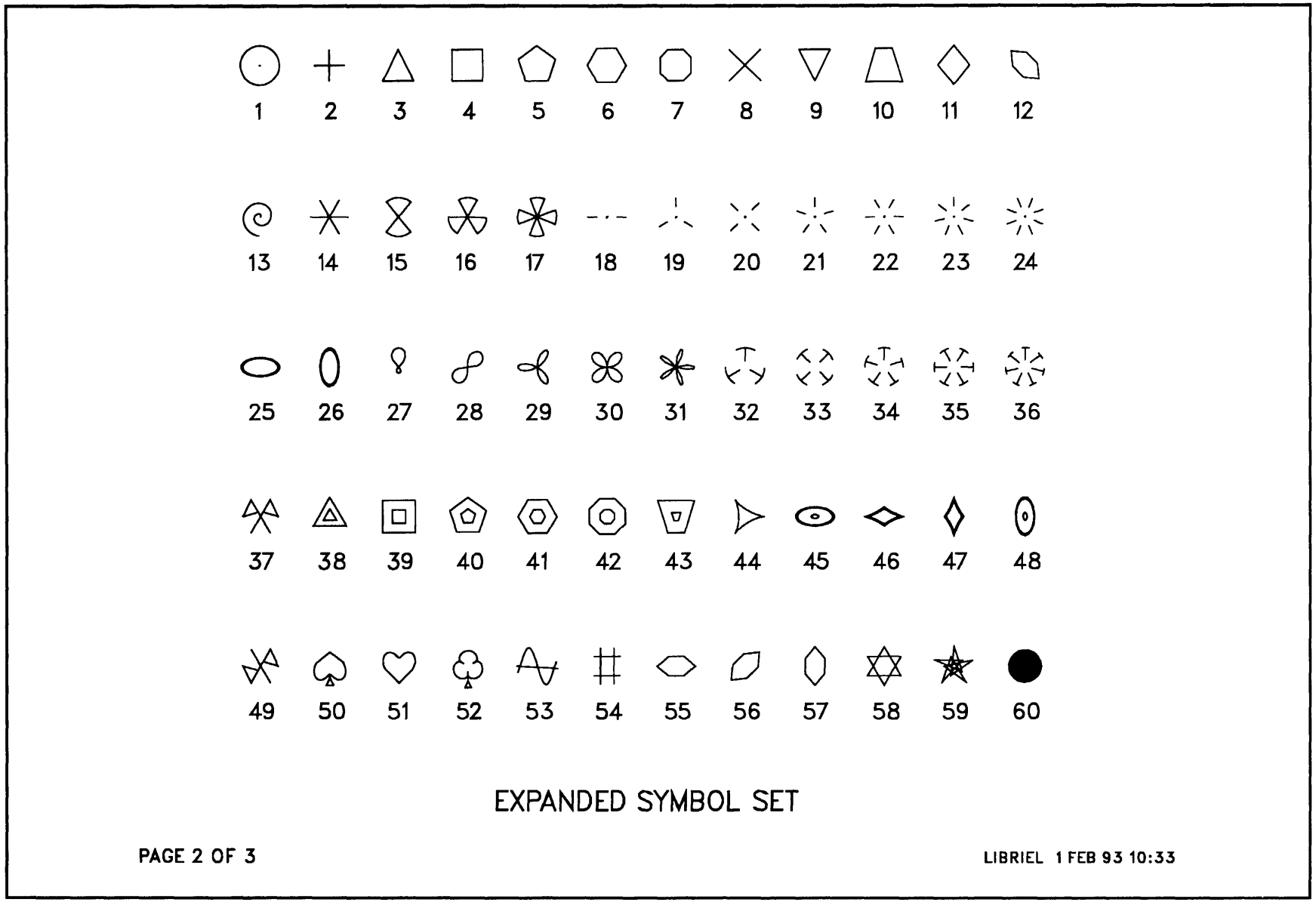

Figure A–2. Program codes for symbols in the expanded symbol set.

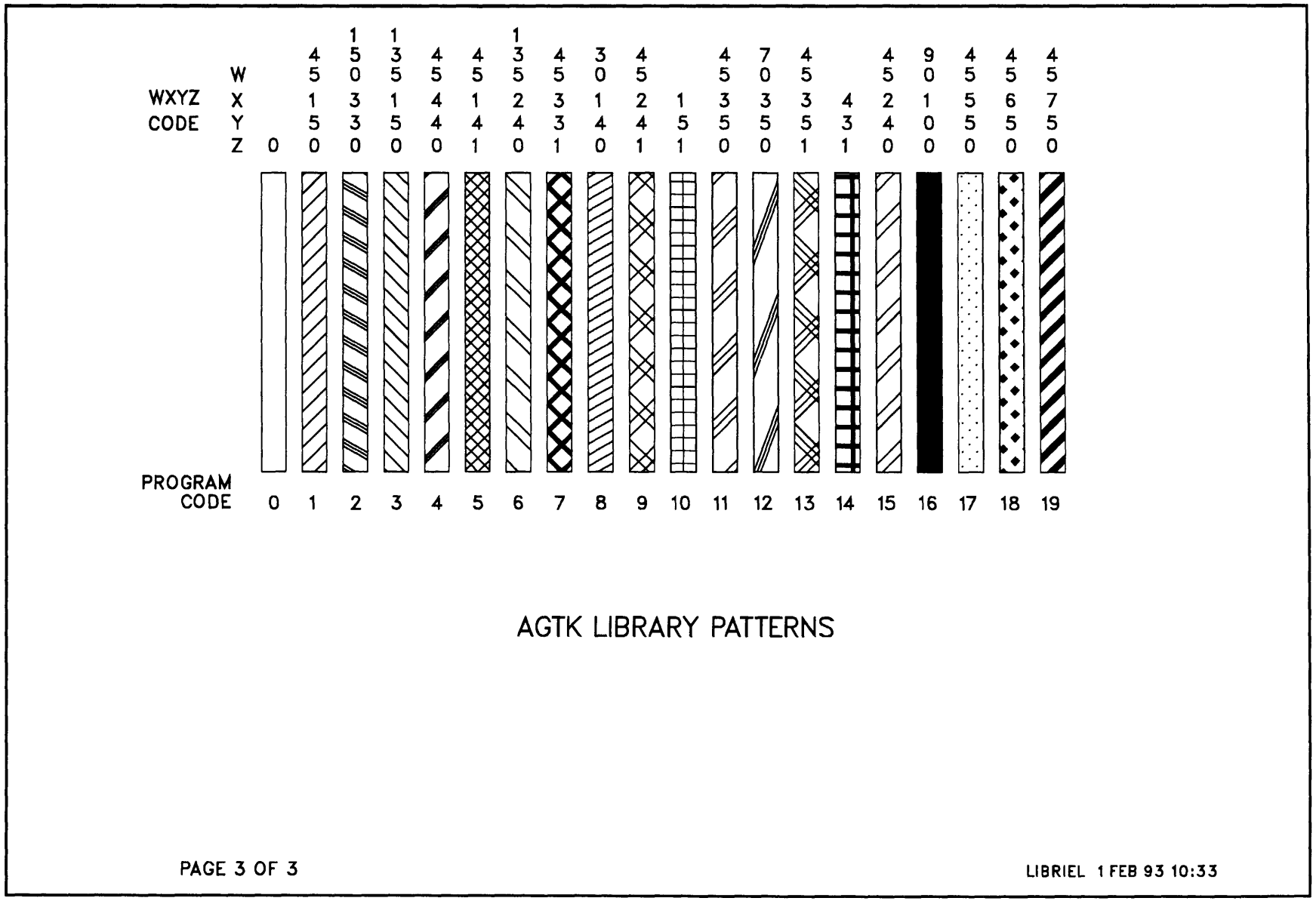

Figure A–3. Program codes for patterns in the AGTK library patterns set. Modified from table 7.2.1, PRIOR Advanced Graphics Toolkit User's Manual, v. 1, p. 7–11, PRIOR Data Sciences, Ltd., 1991, Reprinted by permission.

APPENDIX B.—AUXILIARY INPUT FILES

Some of the plotting procedures can read certain types of information from auxiliary input files. This information includes: (1) alternative choices for plot symbols, slice colors, and shade patterns; (2) axis labels for optional variables on boxplot, X–Y, and Piper 3–D diagrams; and (3) variables to display on X–Y and boxplot diagrams. These files are auxiliary, because this information can also be entered from the terminal. The purpose of auxiliary files is to expedite a run: At the end of an interactive run, user-supplied information can be saved for use in later runs. The information in auxiliary files can also be modified in an ASCII editor if needed.

Structure of Auxiliary Files

The basic structure of all auxiliary input files is similar to the structure of the main data file: The first 10 lines are reserved for header information and data begin on line 11. The header section can be left blank, but it cannot be omitted. Each auxiliary file has a definite format; if the program writes an auxiliary file, the header section contains a brief description of the format. The specific requirements of each type of auxiliary input file are described in the following sections.

Plot-Symbols File

The plot-symbols file contains a list of two-digit integer codes for symbols used on Piper 2–D, Piper 3–D, and X–Y diagrams. This file allows the user to specify a different order of symbol selection for both symbol sets. Each set, however, is independent and symbols cannot be interchanged between sets. The plot-symbols file is not required to list a code for each of the 78 available symbols. When the program is run, symbol positions left blank in the file are filled automatically with unused symbols from each set. Blank positions are filled in ascending numerical order, which is the default symbol order shown in appendix A (figs. A–1 and A–2).

The format of the plot-symbols file is shown in figure B–1. Data begin on line 11, which can contain as many as 18 codes that indicate the preferred order of selection for symbols in the PRIOR AGTK library set. Data for the larger symbol set are found on lines 14–16; each of these lines can contain as many as 20 codes. The column position of each code is specific: codes must begin in columns 2, 5, 8, 11, 14, 17, 20, 23, 26, 29, 32, 35, 38, 41, 44, 47, 50, 53, 56, and 59. Data outside of these locations are ignored and misaligned data are not read correctly. Leading zeros in codes 1–9 can be left blank.

The use of a plot-symbols file is signaled by setting knob (15) = 5. The default filename is QWPLOT.SYMBOLS; if this file exists in the local directory, it is read and the order of symbols is displayed on the screen. The user can then reject this file if needed and enter an alternate name. If QWPLOT.SYMBOLS is not found, the user is asked to enter the name of the plot-symbols file. In an interactive session, codes for symbols can be entered from the terminal and written to a plot-symbols file for use in a later run.

Pie-Slice Patterns File

The pie-slice patterns file contains numeric codes for an alternative set of shade patterns and colors. Codes for the seven slices always occur in the same order (fig. B–2) and must be placed in specific locations on lines 11–17 of the file: Pattern codes are placed in columns 14–20, and color codes in column 29. Data outside of these locations are ignored. The default name of the slice-patterns file is QWPIE.PATTERNS; if this file exists in the local directory, it is used. If QWPIE.PATTERNS is not in the local directory, the user can enter an alternate name for the file containing the slice-pattern codes. If specific codes are missing from the file, the program's default codes are used instead. Labels for the pie slices shown in columns 1–6 are not read by the program; these labels are used to indicate the order of codes in the file.

Axis-Labels Files

Axis-labels files contain a set of three user-supplied labels to identify the optional variables shown on boxplot, X–Y, and Piper 3–D diagrams. These labels are discussed in chapters 5–7. Axis labels begin in column 1, and each label is placed on a separate line of the file. Sets of three labels for each optional variable are separated by a blank line; sets must begin on lines 11, 15, 19, 23, 27, and 31 of the file. One or all of the labels in a set can be left blank. A surrogate label ("Extra var.") is used if an axis label is missing.

On boxplot output, the space for axis labels is limited, and labels cannot exceed 15 characters. Because of this restriction, the program uses a different axis-labels file (BOXPLOT.LABELS) for the boxplot procedure; the X–Y and Piper 3–D procedures use another axis-labels file (QWPLOT.LABELS). The local directory is searched for the default filenames (mentioned above); if these files exist, they are used. If

```
SPECIFYING THE ORDER OF SELECTION OF PLOT SYMBOLS ON PIPER AND X-Y DIAGRAMS
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
INSTRUCTIONS: If KNOB(2) = 7, the default order of selection of plot symbols
is shown on two figures generated by the program.  If needed, this order can
be changed.  Line 11 contains the new order of 18 symbols from the library
set and lines 14-16 contain the order of 60 symbols from the expanded set.
Column position is fixed: 2-digit codes must begin in columns 2, 5, 8, 11,
14, 17, 20, 23, 26, 29, 32, 35, 38, 41, 44, 47, 50, 53, 56, 59.

Order of symbols from the library set:
  18 16 14 12 10  8  6  4  2  1  3  5  7  9 11 13 15 17

Order of symbols from the expanded set:
   2  4  6  8 10 12 14 16 18 20 22 24 26  1  3  5  7  9 11 13
  15 17 19 21 23 25 27 28 29 30 31 32 33 34 35 36 37 38 39 40
  41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60
```

Figure B–1. Format of QWPLOT.SYMBOLS file generated by the program showing an alternate order of symbol selection for both symbol sets.

```
      SUBROUTINE SHDPAT (IPAT)
         where IPAT is the number for a standard pattern (0 - 19),
           or  IPAT is an integer of the form:    wxyz
             w  -  shading angle        (0 - 360)
             x  -  shading type         (0 - 7)
             y  -  shading density      (0 - 9)
             z  -  crosshatching flag   (0 - 9)
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
QWPIE SLICE PATTERNS AND COLORS        Use lines 11-17 for selections
LABEL            IPAT     NPEN         Label not read; use order shown
NA + K         135140        2         Use columns 14-20 for IPAT
CA              99999        3         Use column    29  for NPEN
MG             160130        6         Color codes for NPEN:
N + P               0        1         1 = black     5 = magenta
SO4             45540        4         2 = red       6 = yellow
HCO3            99999        5         3 = green     7 = cyan
CL + F          45140        6         4 = blue
```

Figure B–2. Format of QWPIE.PATTERNS file generated by the program showing the method of indicating slice patterns, order of slices (LABEL), pattern code (IPAT) and color code (NPEN) used for each slice, and the complete list of color codes. The codes shown for IPAT and NPEN are the default codes for each slice.

```
LABELS FOR OPTIONAL VARIABLES ON BOXPLOT DIAGRAMS
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
INSTRUCTIONS:  THREE labels are needed for each optional variable on box-
plot diagrams: (1) a label that identifies the variable, (2) a label that
indicates units for the variable, and (3) a menu label.  Labels can be left
blank.  The length of plot labels (1 and 2) cannot exceed 15 characters;
the menu label cannot exceed 11 characters.  Label groups begin in column
1 on lines 11, 15, 19, 23, 27, and 31.
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

SP CONDUCTANCE                    variable-identification label
MICROSIEMENS/CM                   units-identification label
COND, uS/cm                       menu label

DIS SOLIDS, ROE
MILLIGRAMS / L
SOLIDS mg/L

TEMPERATURE
DEG. CELSIUS
TEMP, deg C

DIS. SILICA
MILLIGRAMS / L
SILICA mg/L

DIS. IRON
MICROGRAMS / L
IRON, ug/L

DIS. MANGANESE
MICROGRAMS / L
MANGANESE
```

Figure B–3. Format of BOXPLOT.LABELS file generated by the program showing the requirements for axis labels on boxplot diagrams, the location of labels in the file, and the labels used for a set of six optional variables.

these files do not exist, the user can enter the name of the axis-labels file. The formats of the two axis-labels files are shown in figures B–3 and B–4.

X–Y Variables File

The X–Y variables file contains sets of menu codes (fig. 17) that indicate the variables to display on all diagrams generated during a run. The use of a variables file eliminates the need to enter these codes from the terminal and allows the X–Y procedure to run in batch mode. Data begin on line 11 and continue unbroken to the end of the file. Each line of a variables file contains all the information needed to produce one X–Y diagram. The numbers on each line are separated by one or more blank spaces; the column position of these numbers is not important and can vary from line to line.

The first number on each line indicates the X–axis variable. This number can range from 1 to 19 (if the data file contains six optional variables); this number can also be equal to 99, which indicates that the variable shown on the X–axis represents the sum of the concentration, in milliequivalents per liter, of several constituents. If the first number is equal to 99, the next number on the line (represented by "n") is the number of variables to include in the X–axis sum, and the n succeeding numbers are menu codes that specify each of the variables. The value of n can range from 1 to 5. Only

```
AXIS LABELS FOR OPTIONAL VARIABLES ON X-Y AND PIPER 3-D DIAGRAMS
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
INSTRUCTIONS: Because X-Y diagrams have 3 different page layouts, labels
can be entered in lengths of 80, 40, and 20 characters.  Piper 3-D diagrams
can show the 80-character label.  Axis labels can be left blank, but groups
must begin on lines 11, 15, 19, 23, 27, & 31.   Length is shown below.

        1         2         3         4         5         6         7
...5....0....5....0....5....0....5....0....5....0....5....0....5....0....5

SPECIFIC CONDUCTANCE, FIELD, MICROSIEMENS PER CENTIMETER
SPECIFIC CONDUCTANCE, FIELD, micro S/CM
SP COND, US / CM

DISSOLVED SOLIDS, SUM, MILLIGRAMS PER LITER
DISSOLVED SOLIDS, SUM, MILLIGRAMS/LITER
DIS SOLIDS, MG / L

WATER TEMPERATURE, DEGREES CELSIUS
WATER TEMPERATURE, DEGREES CELSIUS
TEMP, DEG C

DISSOLVED SILICA, MILLIGRAMS PER LITER
DISSOLVED SILICA, MILLIGRAMS / LITER
SILICA, MG / L

DISSOLVED IRON, MICROGRAMS PER LITER
DISSOLVED IRON, MICROGRAMS / LITER
IRON, UG / L

DISSOLVED MANGANESE, MICROGRAMS PER LITER
DISSOLVED MANGANESE, MICROGRAMS / LITER
MANGANESE, UG / L
```

Figure B–4. Format of QWPLOT.LABELS file generated by the program showing the requirements for axis labels on X–Y and Piper 3–D diagrams, the location and length of the three labels in each group, and the labels used for a set of six optional variables.

codes for the first 10 variables shown in figure 17 (calcium, magnesium, sodium, potassium, chloride, fluoride, bicarbonate, sulfate, nitrate, and phosphate) can be included in a sum.

When the X–axis variable has been specified, the next code on the line indicates the Y–axis variable. In a similar way, as many as five variables can be summed on the Y–axis. When the Y–axis variable has been specified, an optional code can be included at the end of the list to omit the 1:1 ratio line (chap. 5). If this number is equal to 1, the 1:1 ratio line is not shown on the diagram; if this code is equal to 2, this line is shown. An example of an X–Y variables file that generates two diagrams is shown in figure B–5.

The first code on each line indicates the X–axis variable. On the first line, the second number indicates the Y–axis variable. These two codes ("1 7") are all that is needed to construct a diagram that shows the concentration of calcium, in milliequivalents per liter, on the X–axis and the concentration of bicarbonate, in milliequivalents per liter, on the Y–axis. The program will ask if the 1:1 ratio line should appear on the plot, because the code for this feature is missing.

The second line of codes is a more complex example. This diagram shows the sum of two constituents (sodium and potassium, in milliequivalents per liter) on the X–axis and the sum of two constituents (chloride and fluoride, in milliequivalents per liter) on the Y–axis.

```
VARIABLES FOR X-Y DIAGRAMS
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
INSTRUCTIONS: Beginning on line 11, each line contains all codes for one
X-Y diagram.  Column location is not important; codes are separated by
one or more blank spaces. First code on each line is X-AXIS variable; if
first = 99 (sum), next number = number of variables in sum; then 1-5
codes for variables being summed (only codes 1-10).  Next come code(s) for
Y-AXIS variable(s).  Last is an optional flag to control 1:1 ratio line
(0 or blank = ASK, 1 = OFF, 2 - ON).
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

 1 7
99 2 3 4 99 2 5 6 1
```

Figure B–5. Format of an X–Y variables file showing the requirements for the list of codes needed to produce an X–Y diagram and the location of these codes in the file.

The 1:1 ratio line is not shown on this diagram, because the optional code is equal to 1.

Boxplot Variables File

The boxplot variables file contains sets of menu codes (fig. 21) that indicate the variables to display on all diagrams generated during a run. The use of a variables file eliminates the need to enter these codes from the terminal and allows the boxplot procedure to run in batch mode. Data begin on line 11 and continue to the end of the file. Each line of a variables file contains all the information needed to produce one page of boxplot diagrams. The numbers on each line are separated by one or more blank spaces; the column position of these numbers is not important and can vary from line to line.

The first number on each line is the number of boxplot diagrams on the page. This number can range from 1 to 12. The width of each box figure is fixed; box figures are not expanded to fill the plotting area. If fewer than 12 diagrams are drawn on a page, blank space is left on the right side of the plotting area. The remaining numbers on each line are menu codes that specify each of the variables, which can range from 1 to 19 (if the data file contains six optional variables). An example of a boxplot variables file that generates three pages of diagrams is shown in figure B–6.

The first page contains 12 diagrams that show boxplots for each of the 10 constituents listed in order in the previous section. These boxplots are followed by total cations (code 11) and total anions (code 12). The second page contains 8 diagrams that show total cations followed by each of the four required cations, pH (code 13), and two optional variables (codes 18 and 19). The third page contains 7 diagrams that show total anions followed by five anion constituents and one optional variable (code 15).

```
VARIABLES FOR BOXPLOT DIAGRAMS
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
INSTRUCTIONS: Beginning on line 11, each line contains numeric codes for
one page of boxplots.  First number on each line is number of box diagrams
to be constructed on that page.  Column location is not important; codes
are separated by one or more blank spaces.
- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

12 1 2 3 4 5 6 7 8 9 10 11 12
 8   11   1   2   3   4   13   18   19
 7  12  5  6  7  8  9  15
```

Figure B–6. Format of a boxplot variables file showing the requirements for the list of codes needed to produce a page of boxplot diagrams and the location of these codes in the file.

APPENDIX C.–DEFINITION OF KNOBS

Each of the six plotting procedures has different options for many features of the plot. In some procedures, as many as 26 program variables (called knobs) can be used to specify preferred options. The purpose and organization of the knobs is discussed in chapter 8; the range of values for each knob and the option associated with each value are shown in the following sections.

Range of Values

Knobs are single-digit numbers that can range from 0 to 9; this allows each knob to select one of 10 options, and a few knobs use all 10 values. Most knobs, however, have smaller ranges: Some knobs are simply on-off switches for various features of a procedure; these knobs range from 0 to 1, and values outside of this range have no meaning. Some procedures use pairs of adjacent knobs to select values that can range from 0 to 60. In this case, the first knob ranges from 0 to 6, and the second knob ranges from 0 to 9. For most knobs, the range varies with the procedure being run, as shown in tables C–2 to C–7.

Default Values For Knobs

This program is initialized with all knobs equal to 0. Other values can be set from the terminal and from the data file. Blank values for knobs in the data file are read as 0. If a knob is used as an on-off switch, the feature being controlled is usually on by default, and the value of the knob is equal to 0. If the value of the knob is set to 1, the feature is disabled. Some knobs do not have default values; for these knobs, an initial value of 0 must be reset to a higher value in the range for the program to continue. If these knobs are not reset from the data file, this information must be entered from the terminal.

Specific Options For Knobs

On screen menus (chap. 8) and in the following tables, individual knobs are indicated by a number that ranges from 1 to 26. This number represents the position of each knob in the set and is used to identify the knob. The knob number should not be confused with the knob value; the value designates the program option that has been selected by the knob. In the following tables, the first column shows the location of each knob on line 1 of the data file (fig. 27). Because these locations do not change, they are shown only for the first entry of each knob. Knob numbers are shown enclosed in parentheses in the second column and are repeated for emphasis. Each value that has been defined for a knob is shown on a separate line in the third column, and a brief description of the option is given in the last column.

Knobs that have the same function in all procedures include knobs 1–6 and knobs 25 and 26; these knobs are shown in table C–1. Knobs 7-24 commonly have different functions in different procedures; these knobs are shown for each procedure in tables C–2 to C–7. Knob values for figures in this report are shown in table C–8.

Table C–1. Definition of knobs that have the same function in all procedures

Col. no.	Knob no.	Knob value	Description of the options
81	(1)	0	Turns on the knobs menu.
	(1)	1	Turns off the knobs menu; knobs are set from data file.
	(1)	2	Turns on the tracer mode, which lists each item on the screen as it is plotted. This feature can be used to identify items that cause the program to stop before a run is complete.
82	(2)	0	Requests a code for the plotting procedure (1-7).
	(2)	1	Selects the Piper-diagram procedure.
	(2)	2	Selects the Piper 3-D diagram procedure.
	(2)	3	Selects the Stiff-diagram procedure.
	(2)	4	Selects the Pie-diagram procedure.
	(2)	5	Selects the X-Y diagram procedure.
	(2)	6	Selects the Boxplot-diagram procedure.
	(2)	7	Displays both sets of plot symbols.
83	(3)	0	Selects AGTK metafile format for the plot file (default).
	(3)	1	Selects PostScript graphics format for the plot file.
	(3)	2	Selects HPGL-7475 graphics format for the plot file.
	(3)	3	Selects HPGL-7586 graphics format for the plot file.
	(3)	4	Selects CGM-binary metafile format for the plot file.
	(3)	5	Selects CGM-character metafile format for the plot file.
	(3)	6	Selects CGM-text metafile format for the plot file.
84	(4)	0	A name is generated for plot file by adding a prefix ("meta.", "post.", or "hpgl." to name of data file.
	(4)	1	User enters name of plot file from the terminal.
85	(5)	0	A data-table file is produced.
	(5)	1	A data-table file is not produced.
87	(6)	0	A plot-identification title is shown on the plot.
	(6)	1	A plot-identification title is not shown on the plot.
	(6)	2	Requests input on text and location of plot title.
109	(25)	0	The 12th field in the data file is ignored.
	(25)	1	The 12th field is recognized as NO3, in mg/L as N.
111	(26)	0	The 13th field in the data file is ignored.
	(26)	1	The 13th field is recognized as PO4, in mg/L as P.

Table C–2. Definition of knobs for the Piper-diagram procedure

Col. no.	Knob no.	Knob value	Description of the options
82	(2)	1	Selects the Piper-diagram procedure.
88	(7)	0	Median dissolved-solids title is shown on plot.
	(7)	1	Median dissolved-solids title is not shown on plot.
89	(8)	0	Median specific-conductance title is shown on plot.
	(8)	1	Median specific-conductance title is not shown on plot.
90	(9)	0	Median pH title is shown on plot.
	(9)	1	Median pH title is not shown on plot.
91	(10)	0	Ion-balance-limit titles (2 lines) are shown on plot.
	(10)	1	Ion-balance-limit titles are not shown on plot.
93	(11)	0	Period-covered titles (3 lines) are shown on plot.
	(11)	1	Period-covered titles are not shown on plot.
94	(12)	0	Shows user, date, and time at the lower-left margin.
	(12)	1	Does not show user, date, or time on the plot.
	(12)	2	Shows date and time at the lower-left margin.
95	(13)	0	Shows axis labels on the Piper diagram.
	(13)	1	Does not show axis labels on the Piper diagram.
96	(14)	0	Identifies the first 35 samples (or groups) in an explanation field at the right.
	(14)	1	Does not show an explanation field on the plot.
	(14)	2	Identifies the first 48 samples in expanded explanation field at the right. To provide space for an expanded explanation field, the subtitle ("EXPLANATION") is omitted, and main plot title is truncated to 72 characters.
97	(15)	0	Requests the preferred symbol-shape option (1 - 5).
	(15)	1	Uses the same plotting symbol for all samples. User selects the symbol from program's set of 60 shapes.
	(15)	2	Uses a different plotting symbol for each sample. Symbols are used in order from the set of 60 shapes.
	(15)	3	Uses the same plotting symbol for all samples. User selects the symbol from AGTK library set of 18 shapes.
	(15)	4	Uses a different plotting symbol for each sample. Symbols are used in order from the AGTK library set.
	(15)	5	Reads order of symbol selection from an external file.
99	(16)	0-6	First digit of shape code for all samples, if knob (15) = 1.
		0-1	First digit of shape code for all samples, if knob (15) = 3.

Table C–2. Definition of knobs for the Piper-diagram procedure—Continued

Col. no.	Knob no.	Knob value	Description of the options
100	(17)	0-9	Second digit of shape code for all samples, if knob (15) = 1 or 3. If knob (15) = 2 or 4, shapes are selected in the order shown in figures A-1 or A-2, respectively, (appendix A). Knobs (16) and (17) can be used to indicate the code for the starting shape in each set.
101	(18)	0	Requests the preferred symbol-size option (1 or 2).
	(18)	1	Reduces standard symbol size by one-half.
	(18)	2	Uses the standard symbol size.
102	(19)	0	Requests the preferred symbol-color option (1 or 2).
	(19)	1	Uses the same symbol color for all samples. If knob (19) = 1, knobs (20)-(24) can be used to select colors for five groups of samples; colors for additional groups are selected in the same order. Groups are defined by a change in the label variable. If any color knob is equal to 0, default colors are selected in the following order: red, green, blue, magenta, yellow, cyan, and black.
	(19)	2	Uses a different symbol color for each sample (or group).
103	(20)	0-7	Color code for all, or the first group of samples. The default symbol color for this group is red: knob (20) = 2.
105	(21)	0-7	Color code for second group of plot symbols. The default symbol color for this group is green: knob (21) = 3.
106	(22)	0-7	Color code for third group of plot symbols. The default symbol color for this group is blue: knob (22) = 4.
107	(23)	0-7	Color code for fourth group of plot symbols. The default symbol color for this group is magenta: knob (23) = 5.
108	(24)	0-7	Color code for fifth group of plot symbols. The default symbol color for this group is yellow: knob (24) = 6.

Table C–3. Definition of knobs for the Piper 3–D diagram procedure

Col. no.	Knob no.	Knob value	Description of the options
82	(2)	2	Selects the Piper 3-D diagram procedure.
88	(7)	0	Requests the preferred text-font option (1 - 6).
	(7)	1	Shows plot text in AGTK hardware font (default).
	(7)	2	Shows plot text in cartographic font.
	(7)	3	Shows plot text in simplex font.
	(7)	4	Shows plot text in duplex font.
	(7)	5	Shows plot text in complex font.
	(7)	6	Shows plot text in simplex-italic font.
89	(8)	0	Shows a page number on the plot at the upper-right margin.
	(8)	1	Does not number the plot page.
	(8)	2	Shows a page number on the plot at the lower-left margin.
90	(9)	0	Shows the Z-variable over diamond field only.
	(9)	1	Shows the Z-variable over diamond and cations triangle.
	(9)	2	Shows the Z-variable over diamond and anions triangle.
	(9)	3	Shows the Z-variable over cations and anions triangles.
	(9)	4	Shows the Z-variable over cations triangle only.
	(9)	5	Shows the Z-variable over anions triangle only.
	(9)	6	Shows the Z-variable over all three fields.
91	(10)	0	Plots a Z-value for all samples less than axis maximum.
	(10)	1	Plots a Z-value only for samples equal to or greater than a user-selected threshold value.
93	(11)	0	Shows viewing angles for diagram at lower-left margin.
	(11)	1	Does not show viewing angles on the plot.
94	(12)	0	Shows user, date, and time at the lower-left margin.
	(12)	1	Does not show user, date, or time on the plot.
	(12)	2	Shows date and time at the lower-left margin.
95	(13)	0	Does not show the axis labels on the Piper 2-D diagram.
	(13)	1	Shows the axis labels on the Piper 2-D diagram.
96	(14)	0	Requests the preferred view-angles option (1 or 2).
	(14)	1	Uses default view angles X: 30, Y: -30, Z: 15 degrees.
	(14)	2	User enters view angles from the terminal.
97	(15)	0	Requests the preferred symbol-shape option (1 - 5).
	(15)	1	Uses the same plotting symbol for all samples. User selects the symbol from program's set of 60 shapes.
	(15)	2	Uses a different plotting symbol for each sample. Symbols are used in order from the set of 60 shapes.
	(15)	3	Uses the same plotting symbol for all samples. User selects the symbol from AGTK library set of 18 shapes.
	(15)	4	Uses a different plotting symbol for each sample. Symbols are used in order from the AGTK library set.
	(15)	5	Reads order of symbol selection from an external file.

Table C–3. Definition of knobs for the Piper 3–D diagram procedure—Continued

Col. no.	Knob no.	Knob value	Description of the options
99	(16)	0-6	First digit of shape code for all samples, if knob (15) = 1.
		0-1	First digit of shape code for all samples, if knob (15) = 3.
100	(17)	0-9	Second digit of shape code for all samples, if knob (15) = 1 or 3. If knob (15) = 2 or 4, shapes are selected in the order shown in figures A-1 or A-2, respectively, (appendix A). Knobs (16) and (17) can be used to indicate the code for the starting shape in each set.
101	(18)	0	Requests the preferred symbol-size option (1 or 2).
	(18)	1	Reduces standard symbol size by one-half.
	(18)	2	Uses the standard symbol size.
102	(19)	0	Requests the preferred symbol-color option (1 or 2).
	(19)	1	Uses the same symbol color for all samples. If knob (19) = 1, knob (20) can be used to select the symbol color for all samples. If knob (20) = 0, the default color is red.
	(19)	2	Uses a different symbol color for each sample. If knob (19) = 2, default colors are selected in the following order: red, green, blue, magenta, yellow, cyan, and black.
103	(20)	0-7	Color code for all, or the first sample. The default symbol color for this is red: knob (20) = 2.
105	(21)	0-1	First digit of menu code for the Z-axis variable.
106	(22)	0-9	Second digit of menu code for the Z-axis variable.
107	(23)	0	Requests the preferred Z-axis units option (1 or 2).
	(23)	1	Shows concentrations for first 10 constituents--calcium to phosphate--in milliequivalents per liter.
	(23)	2	Shows concentrations for first 10 constituents in milligrams per liter.
108	(24)	0-6	Number of optional numeric variables in the data set.

Table C–4. Definition of knobs for the Stiff-diagram procedure

Col. no.	Knob no.	Knob value	Description of the options
82	(2)	3	Selects the Stiff-diagram procedure.
88	(7)	0	Requests the preferred text-font option (1 - 6).
	(7)	1	Shows plot text in AGTK hardware font (default).
	(7)	2	Shows plot text in cartographic font.
	(7)	3	Shows plot text in simplex font.
	(7)	4	Shows plot text in duplex font.
	(7)	5	Shows plot text in complex font.
	(7)	6	Shows plot text in simplex-italic font.
89	(8)	0	Shows a page number on the plot at the upper-right margin.
	(8)	1	Does not number the plot page.
	(8)	2	Shows a page number on the plot at the lower-left margin.
90	(9)	0	Not used.
91	(10)	0	Not used.
93	(11)	0	Not used.
94	(12)	0	Shows user, date, and time at the lower-right margin.
	(12)	1	Does not show user, date, or time on the plot.
	(12)	2	Shows date and time at the lower-right margin.
95	(13)	0	Not used.
96	(14)	0	Not used.
97	(15)	0	Requests the preferred diagram-scale option (1 or 2).
	(15)	1	Draws each Stiff polygon to a scale that maximizes its size.
	(15)	2	Draws all Stiff polygons to the same fixed scale, in milli-equivalents per liter.
			If knob (15) = 2, knobs (16)-(20) can be used to define a four-digit scale for all Stiff diagrams. The position of the decimal point in this scale is given in knob (16), and the maximum value for the scale in knobs (17)-(20).

Table C–4. Definition of knobs for the Stiff-diagram procedure—Continued

Col. no.	Knob no.	Knob value	Description of the options
99	(16)	0-4	Number of decimal places in fixed scale, if knob (15) = 2.
100	(17)	0-9	First digit of fixed scale, in meq/L, if knob (15) = 2.
101	(18)	0-9	Second digit of fixed scale, in meq/L, if knob (15) = 2.
102	(19)	0-9	Third digit of fixed scale, in meq/L, if knob (15) = 2.
103	(20)	0-9	Fourth digit of fixed scale, in meq/L, if knob (15) = 2.
105	(21)	0	Not used.
106	(22)	0	Not used.
107	(23)	0	Not used
108	(24)	0	Not used.

Table C–5. Definition of knobs for the pie-diagram procedure

Col. no.	Knob no.	Knob value	Description of the options
82	(2)	4	Selects the pie-diagram procedure.
88	(7)	0	Requests the preferred text-font option (1 - 6).
	(7)	1	Shows plot text in AGTK hardware font (default).
	(7)	2	Shows plot text in cartographic font.
	(7)	3	Shows plot text in simplex font.
	(7)	4	Shows plot text in duplex font.
	(7)	5	Shows plot text in complex font.
	(7)	6	Shows plot text in simplex-italic font.
89	(8)	0	Shows a page number on the plot at the upper-right margin.
	(8)	1	Does not number the plot page.
	(8)	2	Shows a page number on the plot at the lower-left margin.
90	(9)	0	Not used.
91	(10)	0	Not used.
93	(11)	0	Shows a gap between the cation and anion halves of the pie.
	(11)	1	Does not show a gap between cation and anion halves.
94	(12)	0	Shows user, date, and time at the lower-right margin.
	(12)	1	Does not show user, date, or time on the plot.
	(12)	2	Shows date and time at the lower-right margin.
95	(13)	0	Shows slice labels on the pie diagrams.
	(13)	1	Does not show slice labels on the pie diagrams.
96	(14)	0	Shows program's patterns on pie slices.
	(14)	1	Does not show patterns on pie slices.
	(14)	2	Shows user-defined patterns on pie slices.
97	(15)	0	Shows a different color on each pie slice.
	(15)	1	Shows the same color on all pie slices.
	(15)	2	Shows two colors: one for cation slices and another for anion slices.
	(15)	3	Shows user-defined colors for pie slices.
			If knob (15) = 1, knob (16) can be used to specify the color for all slices. If knob (15) = 2, knob (16) indicates the color for cation slices and knob (17) the color for anion slices. If knob (15) = 3, knobs (16)-(22) indicate colors for each of the seven slices. If knob (15) is greater than zero and the value of any color knob is equal to zero, the default color is black.
99	(16)	0-7	Color code for pie slice 1 (sodium plus potassium). The default color for this slice is red: knob (16) = 2.

Table C–5. Definition of knobs for the pie-diagram procedure—Continued

Col. no.	Knob no.	Knob value	Description of the options
100	(17)	0-7	Color code for pie slice 2 (calcium). The default color for this slice is green: knob (17) = 3.
101	(18)	0-7	Color code for pie slice 3 (magnesium). Default color for this slice is yellow: knob (18) = 6.
102	(19)	0-7	Color code for pie slice 4 (nitrogen plus phosphorus). The default color for this slice is background (no color).
103	(20)	0-7	Color code for pie slice 5 (sulfate). The default color for this slice is blue: knob (20) = 4.
105	(21)	0-7	Color code for pie slice 6 (bicarbonate plus carbonate). The default color for this slice is magenta: knob (21) = 5.
106	(22)	0-7	Color code for pie slice 7 (chloride plus fluoride). The default color for this slice is cyan: knob (22) = 7.
107	(23)	0	Not used.
108	(24)	0	Not used.

Table C–6. Definition of knobs for the X–Y diagram procedure

Col. no.	Knob no.	Knob value	Description of the options
82	(2)	5	Selects the X-Y diagram procedure.
88	(7)	0	Requests the preferred text-font option (1 - 6).
	(7)	1	Shows plot text in AGTK hardware font (default).
	(7)	2	Shows plot text in cartographic font.
	(7)	3	Shows plot text in simplex font.
	(7)	4	Shows plot text in duplex font.
	(7)	5	Shows plot text in complex font.
	(7)	6	Shows plot text in simplex-italic font.
89	(8)	0	Shows a page number on the plot at the upper-right margin.
	(8)	1	Does not number the plot page.
90	(9)	1	Shows one X-Y diagram per plot page.
	(9)	2	Shows 12 X-Y diagrams per plot page.
	(9)	4	Shows four X-Y diagrams per plot page.
			If knob (9) is equal to any other value, the number of X-Y diagrams per plot page is entered from the terminal. A null answer at this point shows 12 diagrams per page.
91	(10)	0	Requests the preferred variables-file option (1 - 3).
	(10)	1	Codes for X and Y variables are read from a variables file.
	(10)	2	Codes for X and Y variables are saved in a variables file.
	(10)	3	Indicates that a variables file is not used.
93	(11)	0	Scales for X- and Y-axes can be different, which maximizes the amount of area used on the diagram.
	(11)	1	Scales for X- and Y-axes are the same.
			If knob (11) = 1, the maximum value for both axes is entered from the terminal; the minimum value for both axes is always equal to 0.
94	(12)	0	Shows user, date, and time at the lower-right margin.
	(12)	1	Does not show user, date, or time on the plot.
	(12)	2	Shows date and time at the lower-right margin.
95	(13)	0	Requests the preferred ratio-line option (1 or 2).
	(13)	1	Does not show the 1:1 ratio line on the diagram.
	(13)	2	Shows the 1:1 ratio line (dotted) on the X-Y diagram.
96	(14)	0	Identifies first 35 samples in an explanation field, if knob (9) = 1.
	(14)	1	Does not show an explanation field on the plot, if knob (9) = 1.

Table C–6. Definition of knobs for the X–Y diagram procedure—Continued

Col. no.	Knob no.	Knob value	Description of the options
97	(15)	0	Requests the preferred symbol-shape option (1 - 5).
	(15)	1	Uses the same plotting symbol for all samples. User selects the symbol from program's set of 60 shapes.
	(15)	2	Uses a different plotting symbol for each sample. Symbols are used in order from the set of 60 shapes.
	(15)	3	Uses the same plotting symbol for all samples. User selects the symbol from AGTK library set of 18 shapes.
	(15)	4	Uses a different plotting symbol for each sample. Symbols are used in order from the AGTK library set.
	(15)	5	Reads order of symbol selection from an external file.
99	(16)	0-6	First digit of shape code for all samples, if knob (15) = 1.
		0-1	First digit of shape code for all samples, if knob (15) = 3.
100	(17)	0-9	Second digit of shape code for all samples, if knob (15) = 1 or 3. If knob (15) = 2 or 4, shapes are selected in the order shown in figures A-1 or A-2, respectively, (appendix A). Knobs (16) and (17) can be used to indicate the code for the starting shape in each set.
101	(18)	0	Requests the preferred symbol-size option (1 or 2).
	(18)	1	Reduces standard symbol size by one-half.
	(18)	2	Uses the standard symbol size.
102	(19)	0	Requests the preferred symbol-color option (1 or 2).
	(19)	1	Uses the same symbol color for all samples. If knob (19) = 1, knob (20) can be used to select the symbol color for all samples. If knob (20) = 0, the default color is red.
	(19)	2	Uses a different symbol color for each sample. If knob (19) = 2, default colors are selected in the following order: red, green, blue, magenta, yellow, cyan, and black.
103	(20)	0-7	Color code for all, or the first symbol. The default symbol color is red: knob (20) = 2.
105	(21)	0	Not used.
106	(22)	0	Not used.
107	(23)	0	Requests the preferred axis-units option (1 or 2).
	(23)	1	Shows concentrations for first 10 constituents--calcium to phosphate--in milliequivalents per liter.
	(23)	2	Shows concentrations for first 10 constituents in milligrams per liter.
108	(24)	0-6	Number of optional numeric variables in the data set.

Table C–7. Definition of knobs for the boxplot-diagram procedure

Col. no.	Knob no.	Knob value	Description of the options
82	(2)	6	Selects the boxplot-diagram procedure.
88	(7)	0	Requests the preferred text-font option (1 - 6).
	(7)	1	Shows plot text in AGTK hardware font (default).
	(7)	2	Shows plot text in cartographic font.
	(7)	3	Shows plot text in simplex font.
	(7)	4	Shows plot text in duplex font.
	(7)	5	Shows plot text in complex font.
	(7)	6	Shows plot text in simplex-italic font.
89	(8)	0	Shows a page number on the plot at the lower-right margin.
	(8)	1	Does not number the plot page.
90	(9)	0	Requests the preferred group option (1 or 2).
	(9)	1	Includes all values in range for each parameter displayed.
	(9)	2	Changes in the label variable are used to divide the values for one characteristic or constituent into as many as 60 different groups and a separate boxplot is drawn for each group. Note: If this option is used, the data file must be pre-sorted on the label variable.
91	(10)	0	Requests the preferred variables-file option (1 - 3).
	(10)	1	Codes for boxplot variables are read from a file.
	(10)	2	Codes for boxplot variables are saved in a file.
	(10)	3	Indicates that a variables file is not used.
93	(11)	0	Requests the preferred scale for diagrams (1 or 2).
	(11)	1	Logarithmic scale is used for boxplot diagrams.
	(11)	2	Linear scale is used for boxplot diagrams.
94	(12)	0	Shows user, date, and time at the lower-right margin.
	(12)	1	Does not show user, date, or time on the plot.
	(12)	2	Shows date and time at the lower-right margin.
95	(13)	0	Not used.
96	(14)	0	Explanation field shows principal features of diagram
	(14)	1	Explanation field does not appear on the plot.
97	(15)	0	Shows the number of values in each distribution at the top.
	(15)	1	Does not show number of values in each distribution.

Table C–7. Definition of knobs for the boxplot-diagram procedure—Continued

Col. no.	Knob no.	Knob value	Description of the options
99	(16)	0	Requests the preferred color option (1 or 2).
	(16)	1	Uses one color for the entire boxplot diagram. If knob (16) = 1, knob (17) can be used to select a color for the boxplot diagram. If knob (17) = 0, the default color is black.
	(16)	2	Uses five colors for different parts of the boxplot diagram. All diagrams on a page use the same color scheme. If knob (16) = 2, color codes for different parts of the diagram can be indicated by knobs (17)-(21). If any color knob is equal to zero, default colors are used.
100	(17)	0-7	Color code for the IQR box if knob (16) = 2, or for the entire diagram if knob (16) = 1. The default color is green: knob (17) = 3.
101	(18)	0-7	Color code for the median line. The default color for this feature is yellow: knob (18) = 6.
102	(19)	0-7	Color code for the whisker lines. The default color for this feature is cyan: knob (19) = 7.
103	(20)	0-7	Color code for all near-outliers. The default color for this feature is red: knob (20) = 2.
105	(21)	0-7	Color code for all far-outliers. The default color for this feature is yellow: knob (21) = 6.
106	(22)	0	Not used.
107	(23)	0	Requests the preferred Y-axis units option (1 or 2).
	(23)	1	Shows value distributions for first 10 constituents--calcium to phosphate--in milliequivalents per liter.
	(23)	2	Shows value distributions for first 10 constituents in milligrams per liter.
108	(24)	0-6	Number of optional numeric variables in the data set.

Table C–8. Knob values for figures generated by the program

Knob num.	Figure number																			
	4	5	6	8	9	11	12	13	14	15	16	18	19	20	22	23	24	25	26	A1–A3
(1)	0	0	2	0	2	0	2	1	0	2	0	1	0	2	0	0	0	0	2	0
(2)	1	1	1	3	3	4	4	5	5	5	5	6	6	6	2	2	2	2	2	7
(3)	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
(4)	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
(5)	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0
(6)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
(7)	0	1	0	4	4	2	4	1	4	1	4	4	4	4	3	3	3	3	3	4
(8)	0	1	0	2	2	2	2	1	1	1	1	1	1	1	1	1	1	1	1	0
(9)	0	1	0	0	0	0	0	2	1	4	1	1	1	2	0	0	0	1	6	0
(10)	0	1	0	0	0	0	0	1	0	1	0	1	0	0	0	1	1	1	1	0
(11)	0	1	0	0	0	0	1	0	1	0	0	1	2	2	0	0	0	0	0	0
(12)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
(13)	0	1	0	0	0	0	1	0	0	0	0	0	0	1	0	0	0	1	1	0
(14)	0	2	1	0	0	0	2	0	0	0	0	0	1	0	1	1	1	2	2	0
(15)	2	4	1	1	2	1	1	1	2	1	2	0	0	0	3	3	3	2	2	0
(16)	0	0	0	0	0	1	1	0	0	0	0	0	0	0	1	1	1	0	2	0
(17)	1	2	2	0	0	0	0	1	0	2	8	0	0	0	6	5	5	2	6	0
(18)	2	2	1	0	0	0	0	0	0	0	0	1	1	1	0	0	0	0	0	0
(19)	1	2	1	0	0	0	0	1	2	1	1	1	1	1	1	1	1	1	1	0
(20)	0	0	1	0	5	0	0	1	0	1	1	0	0	0	1	1	1	1	1	0
(21)	0	0	1	0	0	0	0	0	0	0	0	0	0	0	2	1	1	1	1	0
(22)	0	0	1	0	0	0	0	0	0	0	0	0	0	0	4	4	4	5	3	0
(23)	0	0	1	0	0	0	0	1	0	2	0	1	1	2	1	1	1	1	1	0
(24)	0	0	1	0	0	0	0	2	0	1	2	2	0	0	1	1	1	2	0	0
(25)	1	0	1	0	1	1	1	1	1	0	0	1	1	1	1	1	1	1	1	0
(26)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0