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ANALYTICAL METHOD FOR DETERMINATION
OF ASBESTOS FIBERS IN WATER

by

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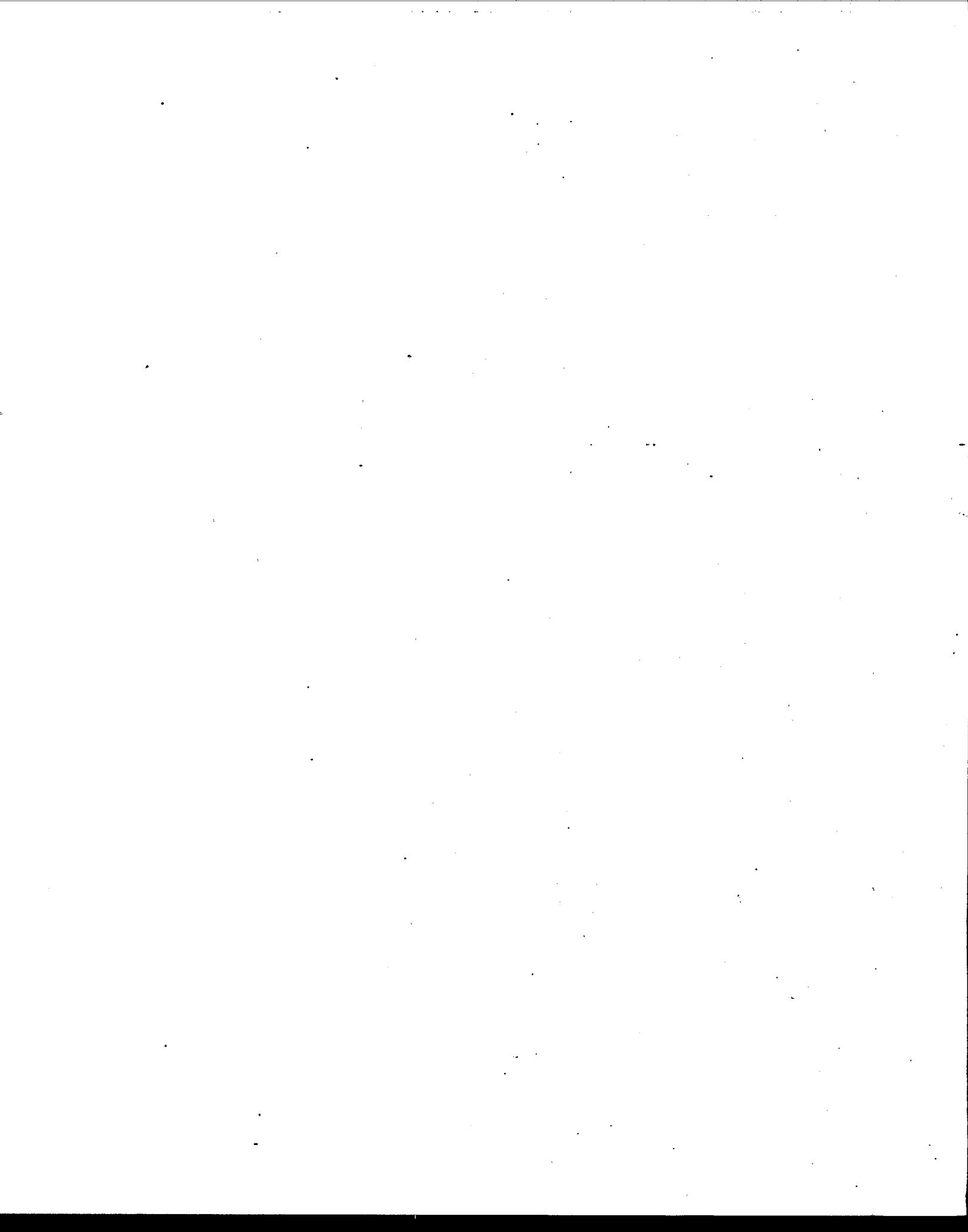
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FOREWORD

Nearly every phase of environmental protection depends on a capability to identify and measure specific pollutants in the environment. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Analytical Chemistry Branch develops and assesses new techniques for identifying and measuring chemical constituents of water and soil.

A 3-year study was conducted to develop improvements in the analytical method for determination of asbestos fiber concentrations in water samples. The research produced an improved sample preparation and analysis methodology, a rapid screening technique to reduce analysis cost, and a new reference analytical method for asbestos in water. The analytical method for determining asbestos fibers in water is perceived as representing the current state-of-the-art.

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PREFACE

The Preliminary Interim Method for Determining Asbestos in Water was issued by the U.S. Environmental Protection Agency's Environmental Research Laboratory in Athens, Georgia. The method was based on filtration of the water sample through a sub-micrometer pore size membrane filter, followed by preparation of the filter for direct examination and counting of the fibers in a transmission electron microscope. Two alternative techniques were specified: one in which a cellulose ester filter was prepared by dissolution in a condensation washer; and another known as the carbon-coated Nuclepore^R technique which used a polycarbonate filter. In January 1980 the method was revised (EPA-600/4-80-005) to eliminate the condensation washer approach, and a suggested statistical treatment of the fiber count data was incorporated.

The analytical method published here is a further refinement of the revised interim method. Major additions include the introduction of ozone-ultraviolet light oxidation prior to filtration, complete specification of techniques to be used for fiber identification and fiber counting rules, and incorporation of reference standard dispersions. A standardized reporting format has also been introduced. The major deletion is the low temperature ashing technique for samples high in organic material content; ashing is not required for the analysis of drinking water and drinking water supplies when samples are treated using the ozone-ultraviolet oxidation technique. The "field-of-view" approach for examination also has been deleted from the method. If a sample is too heavily loaded for examination of entire grid openings, a more reliable result is obtained by preparation of a new filter using a smaller volume of water.

ABSTRACT

An analytical method for measurement of asbestos fiber concentration in water samples is described. Initially, the water sample is treated with ozone gas and ultraviolet light to oxidize suspended organic materials. The water sample is then filtered through a 0.1 μm pore size capillary-pore polycarbonate filter, after which the filter is prepared by carbon extraction replication for examination in a transmission electron microscope (TEM). Fibers are classified using selected area electron diffraction (SAED) and energy dispersive X-ray analysis (EDXA). Measurement of characteristic features on a recorded and calibrated SAED pattern is specified for precise identification of chrysotile. Quantitative determination of the chemical composition, and quantitative interpretation of at least one calibrated zone axis SAED pattern are specified for precise identification of amphibole. Amphibole identification procedures and generation of the standard reporting format specified for the fiber count results are achieved using two computer programs which are integral to the analytical method.

This analytical method is a further development of the interim method issued in 1980, and incorporates results of research performed under Contract 68-03-2717 under sponsorship of the U.S. Environmental Protection Agency. This report covers a period from October 1978 to September 1981 and the work was completed as of September 1981.

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ANALYTICAL METHOD FOR DETERMINATION OF ASBESTOS FIBERS IN WATER

1. SCOPE AND APPLICATION

- 1.1 This method is applicable to drinking water and drinking water supplies, and should be used when the best available analytical procedure is required.
- 1.2 The method determines the numerical concentration of asbestos fibers, the length and width of each fiber, and the estimated mass concentration of asbestos in the water. Fiber size and aspect ratio distributions are also determined.
- 1.3 The method permits, if required, identification of all mineral fibers found in water. In particular, chrysotile can be distinguished from the amphiboles, and fibers of specific amphiboles can be identified.
- 1.4 The analytical sensitivity which can be achieved depends primarily on the amount of other particulate matter which is present in the sample. This limits the proportion of the sample which can be mounted for examination in the electron microscope. In drinking water which meets the AWWA turbidity criterion of 0.1 NTU, an asbestos concentration of 0.01 million fibers per liter (MFL) can be detected. The contamination level in the laboratory environment may degrade the sensitivity. The analytical sensitivity for the determination of mass concentration is a function of the preceding parameters and also depends on the size distribution of the fibers. In low turbidity drinking water the analytical sensitivity is usually of the order of 0.1 nanogram per liter (ng/L).
- 1.5 It is beyond the scope of this document to provide detailed instruction in electron microscopy, electron diffraction, crystallography or X-ray fluorescence techniques. It is assumed that those performing this analysis will be sufficiently knowledgeable in these fields to understand the specialized techniques involved.

2. SUMMARY OF METHOD

Water collected in a polyethylene or glass container is treated with ozone and ultraviolet light to oxidize organic matter. After mild ultrasound treatment to disperse the fibers uniformly, a known volume of the water is filtered through a 0.1 micrometer (μm) pore size Nuclepore^R polycarbonate filter. A carbon coating is then applied in

vacuum to the active surface of the filter. The carbon layer coats and retains in position the material which has been collected on the filter surface. A small portion of the carbon-coated filter is placed on an electron microscope grid and the polycarbonate filter material is removed by dissolution in an organic solvent. The carbon film containing the original particulate, supported on the electron microscope grid, is then examined in a transmission electron microscope (TEM) at a magnification of about 20,000. In the TEM, selected area electron diffraction (SAED) is used to examine the crystal structure of a fiber, and its elemental composition is determined by energy dispersive X-ray analysis (EDXA).

Fibers are classified according to the techniques which have been used to identify them. A simple code is used to record for each fiber the degree to which the identification attempt was successful. The fiber classification procedure is based on successive inspection of the morphology, the selected area electron diffraction pattern, and the qualitative and quantitative energy dispersive X-ray analyses. Confirmation of the identification of chrysotile is only by quantitative SAED, and confirmation of amphibole is only by quantitative EDXA and quantitative zone axis SAED.

Several levels of analysis are specified, three for chrysotile and four for amphibole, defined by the most specific fiber classification to be attempted for all fibers. The procedure permits this target classification to be defined on the basis of previous knowledge, or lack of it, about the particular sample. Attempts are then made to raise the classification of all fibers to this target classification, and to record the degree of success in each case. The lengths and widths of all identified fibers are recorded. The number of fibers found on a known area of the microscope sample, together with the equivalent volume of water filtered through this area, are used to calculate the fiber concentration in MFL. The mass concentration is calculated in a similar manner by summation of the volume of the identified fibers, assuming their density to be that of the bulk material.

3. DEFINITIONS, UNITS AND ABBREVIATIONS

3.1 Definitions

Acicular - The shape shown by an extremely slender crystal with small cross-sectional dimensions.

Amphibole - A group of rock-forming ferromagnesian silicate minerals, closely related in crystal form and composition and having the general formula: $A_{2-3}B_5(Si,Al)_8O_{22}(OH)_2$, where A = Mg, Fe^{+2} , Ca, Na or K, and B = Mg, Fe^{+2}, Fe^{+3} or Al. Some of these elements may also be substituted by Mn, Cr, Li, Pb, Ti or Zn. It is characterized by a cross-linked double chain of Si-O tetrahedra with a silicon:oxygen ratio of 4:11, by columnar or fibrous prismatic crystals and by good prismatic cleavage in

two directions parallel to the crystal faces and intersecting at angles of about 56° and 124° .

Amphibole Asbestos - Amphibole in an asbestosiform habit.

Analytical Sensitivity - The calculated concentration in MFL equivalent to counting of one fiber.

Asbestos - A commercial term applied to a group of silicate minerals that readily separate into thin, strong fibers that are flexible, heat resistant and chemically inert.

Aspect Ratio - The ratio of length to width in a particle.

Camera Length - The equivalent projection length between the sample and its electron diffraction pattern, in the absence of lens action.

Chrysotile - A mineral of the serpentine group: $Mg_3Si_2O_5(OH)_4$. It is a highly fibrous, silky variety of serpentine, and constitutes the most important type of asbestos.

Cleavage - The breaking of a mineral along its crystallographic planes, thus reflecting crystal structure.

Cleavage Fragment - A fragment of a crystal that is bounded by cleavage faces.

d-Spacing - The separation between identical adjacent and parallel planes of atoms in a crystal.

Diatom - A microscopic, single-celled plant of the class Bacillariophyceae, which grows in both marine and fresh water. Diatoms secrete walls of silica, called frustules, in a great variety of forms.

Electron Scattering Power - The extent to which a thin layer of a substance scatters electrons from their original path directions.

Energy Dispersive X-ray Analysis - Measurement of the energies and intensities of X-rays by use of a solid state detector and multichannel analyzer system.

Eucentric - The condition when an object is placed with its center on a rotation or tilting axis.

Fibril - A single fiber, which cannot be separated into smaller components without losing its fibrous properties or appearances.

Fiber - A particle which has parallel or stepped sides, an aspect ratio equal to or greater than 3:1, and is greater than 0.5 μm in length.

Fiber Aggregate - An assembly of randomly oriented fibers.

Fiber Bundle - A fiber composed of parallel, smaller diameter fibers attached along their lengths.

Habit - The characteristic crystal form or combination of forms of a mineral, including characteristic irregularities.

Miller Index - A set of three or four integer numbers used to specify the orientation of a crystallographic plane in relation to the crystal axes.

Replication - A procedure in electron microscopy specimen preparation in which a thin copy, or replica, of a surface is made.

Selected Area Electron Diffraction - A technique in electron microscopy in which the crystal structure of a small area of a sample may be examined.

Serpentine - A group of common rock-forming minerals having the formula: $(\text{Mg}, \text{Fe})_3 \text{Si}_2\text{O}_5(\text{OH})_4$.

Unopened Fiber - Large diameter asbestos fiber which has not been separated into its constituent fibrils.

Zone Axis - That line or crystallographic direction through the center of a crystal which is parallel to the intersection edges of the crystal faces defining the crystal zone.

3.2 Units

eV - electron volt

g/cm^3 - grams per cubic centimeter

kV - kilovolt

$\mu\text{g/L}$ - micrograms per liter (10^{-6} grams per liter)

μm - micrometer (10^{-6} meter)

MFL - Million Fibers per Liter

ng/L - nanograms per liter (10^{-9} grams per liter)

nm - nanometer (10^{-9} meter)

NTU - Nephelometric Turbidity Unit

ppm - parts per million

3.3 Abbreviations

AWWA	- American Water Works Association
EDXA	- Energy Dispersive X-ray Analysis
HEPA	- High Efficiency Particle Absolute
SAED	- Selected Area Electron Diffraction
SEM	- Scanning Electron Microscope
STEM	- Scanning Transmission Electron Microscope
TEM	- Transmission Electron Microscope
UICC	- Union Internationale Contre le Cancer (International Union Against Cancer)
UV	- Ultraviolet

4. EQUIPMENT AND APPARATUS

4.1 Specimen Preparation Laboratory

Asbestos, particularly chrysotile, is present in small quantities in practically all laboratory reagents. Many building materials also contain significant amounts of asbestos or other mineral fibers which may interfere with analysis. It is therefore essential that all specimen preparation steps be performed in an environment where contamination of the sample is minimized. The primary requirement of the sample preparation laboratory is that a blank determination using known fiber-free water must yield a result which will meet the requirements specified in Section 6.8.1. Preparation of samples should be carried out only after acceptable blank values have been demonstrated.

The sample preparation areas should be a separate clean room with no asbestos-containing materials such as flooring, ceiling tiles, insulation and heat-resistant products. The work surfaces should be stainless steel or plastic-laminate. The room should be operated under positive pressure and have absolute (HEPA) filters, electrostatic precipitation, or equivalent, in the air supply. A laminar flow hood is recommended for sample manipulation. It is recommended that a supply of disposable laboratory coats and disposable overshoes be obtained to be worn in the clean room. This will reduce the levels of dust, and particularly asbestos, which might be transferred inadvertently by the operator into the

clean area. Normal electrical and water services are required. An air extract (fume hood) is required to remove surplus ozone from the area near the ozone generator.

4.2 Instrumentation Requirements

4.2.1 Transmission Electron Microscope

A transmission electron microscope having an accelerating potential of a minimum of 80 kV, a resolution better than 1.0 nm, and a magnification range of 300 to 100,000 is required. The ability to obtain a direct screen magnification of at least 20,000 is necessary. An overall magnification of about 100,000 is necessary for inspection of fiber morphology; this magnification may be obtained by supplementary optical enlargement of the screen image by use of a binocular if it cannot be obtained directly. It is also required that the viewing screen be calibrated (as shown in Figure 1) with concentric circles and a millimeter scale such that the lengths and widths of fiber images down to 1 mm width can be measured in increments of 1 mm.

For Bragg angles less than 0.01 radians the instrument must be capable of performing selected area electron diffraction from an area of 0.6 μm^2 or less, selected from an in-focus image at a screen magnification of 20,000. This performance requirement defines the minimum separation between particles at which independent diffraction patterns can be obtained from each. The capability of a particular instrument may normally be calculated using the following relationship:

$$A = \frac{\pi}{4} \left(\frac{D}{M} + 2000 C_s \theta^3 \right)^2$$

where: A = Effective SAED area in μm^2
D = Diameter of SAED aperture in μm
M = Magnification of objective lens
 C_s = Objective lens spherical aberration coefficient in mm
 θ = Maximum Bragg angle in radians

Although almost all instruments of current manufacture meet these requirements, many older instruments which are still in service do not. It is obviously not possible to reduce the area of analysis indefinitely by use of apertures

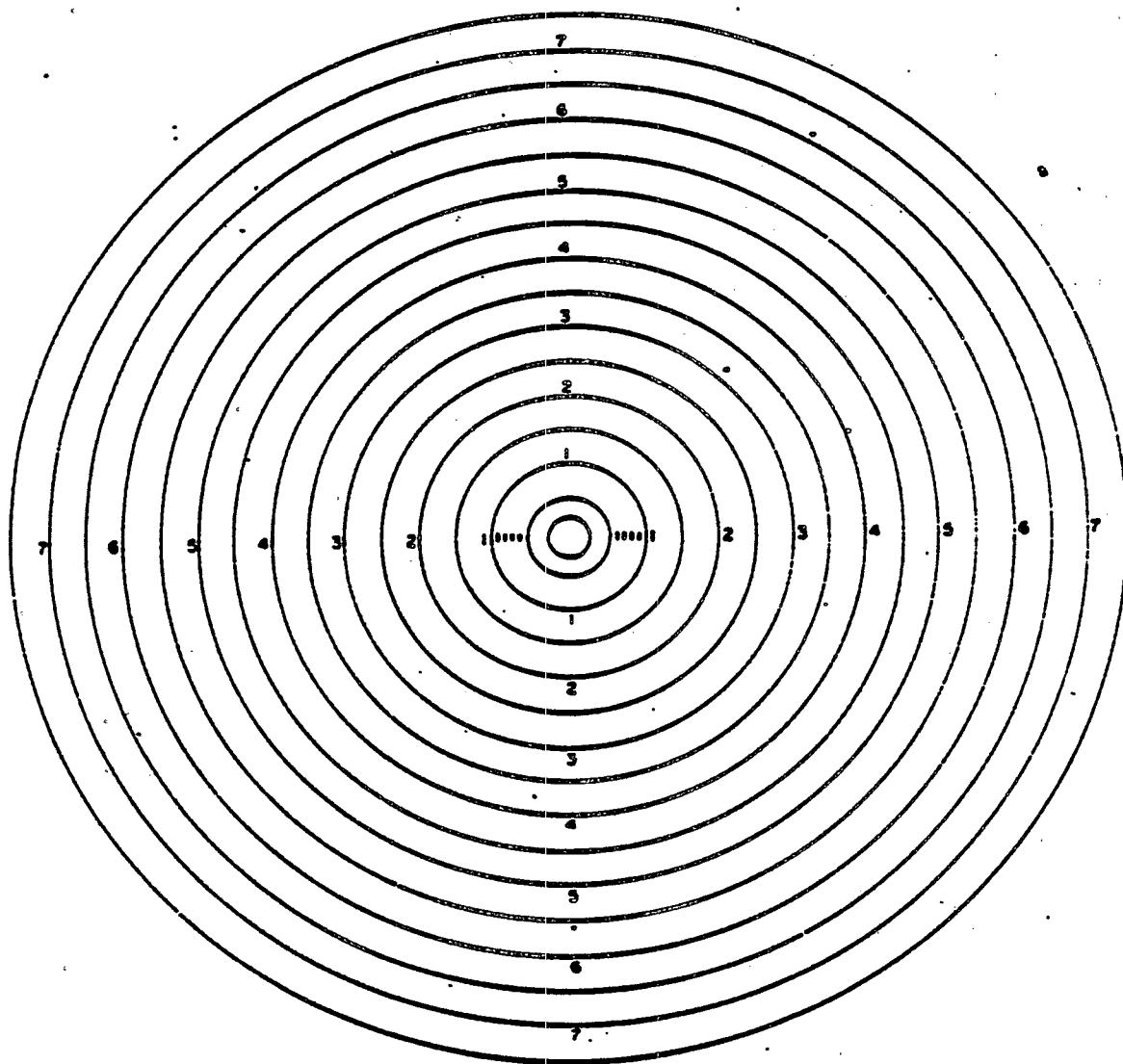


Figure 1. Calibration Markings on TEM Viewing Screen.

smaller in diameter than those specified by the manufacturer, since there is a fundamental limitation imposed by the spherical aberration coefficient of the objective lens.

If zone axis SAED analyses are to be performed, it is required that the electron microscope be fitted with a goniometer stage which permits either a 360° rotation combined with tilting through at least $+30^\circ$ to -30° , or tilting through at least $+30^\circ$ to -30° around two perpendicular axes in the plane of the sample. The work is greatly facilitated if the goniometer permits eucentric tilting.

It is also essential that the electron microscope have an illumination and condenser lens system capable of forming an electron probe smaller than 100 nm in diameter.

Use of an anti-contamination trap around the specimen is recommended if the required instrumental performance is to be obtained.

4.2.2 Energy Dispersive X-ray Analyzer

An energy dispersive X-ray analyzer is required. Since the performance of individual combinations of equipment is critically dependent on a number of geometrical factors, the required performance of the combination of electron microscope and X-ray analyzer is specified in terms of the measured X-ray intensity from a small diameter fiber, using a known electron beam diameter. X-ray detectors are generally least sensitive in the low energy region, and so measurement of sodium in crocidolite is selected as the performance criterion. The combination of electron microscope and X-ray analyzer must yield a background-subtracted NaK α peak integral count rate of more than 1 count per second (cps) from a 50 nm diameter fiber of UICC crocidolite irradiated by a 100 nm diameter electron probe at an accelerating potential of 80 kV. The equivalent peak/background ratio should exceed 1.0.

The EDXA equipment must provide the means for subtraction of the background, identification of elemental peaks, and calculation of net peak areas.

4.2.3 Computer

Many repetitive numerical calculations are necessary, and these can be performed conveniently by relatively simple computer programs. For analyses of zone axis diffraction pattern measurements, a computer facility with minimum available memory of 64K words is required to accommodate

the more complex programs involved. Suggested program listings for standardized data reporting and fiber identification routines are included as part of this analytical procedure. (Appendices A and B).

4.2.4 Vacuum Evaporator

A vacuum evaporator capable of producing a vacuum better than 10^{-4} Torr (0.013 Pa) is required for vacuum deposition of carbon on to the polycarbonate filters. A sample holder is desirable which allows a 51 x 75 mm glass microscope slide to be tilted and rotated during the coating procedure. Use of a liquid nitrogen cold trap above the diffusion pump will minimize the possibility of contamination of the filter surfaces by oil from the pumping system. The vacuum evaporator may also be used for deposition of the thin film of gold, or other reference material, required on electron microscope samples for calibration of electron diffraction patterns. For gold deposition, a sputter coater may allow better control of the process, and is therefore recommended.

4.2.5 Ozone Generator

An ozone generator, in combination with ultraviolet light irradiation, is used for the oxidation of organic material in water samples. This procedure is necessary on all water samples. The generator should be capable of generating at least 400 g of ozone per day at a concentration of at least 1% by weight when supplied with dry oxygen. The ozone generator Model GL-1 (PCI Ozone Corporation, 1 Fairfield Crescent, West Caldwell, New Jersey 07006) or equivalent has been found to meet the requirements of this analytical technique.

4.3 Apparatus, Supplies and Reagents

4.3.1 Gas Supply to Ozone Generator

The ozone generator can be supplied by either compressed air or oxygen. The input gas must be regulated to the pressure specified by the generator manufacturer. It is recommended that oxygen be provided in order to reduce the possibility of acid formation in the sample.

4.3.2 Gas-Line Drying Tube

The ozone generator operates more efficiently when supplied with dry oxygen. An in-line drying tube, filled with a desiccant, followed by a 0.2 μm pore size polytetra-fluoroethylene filter to prevent particulate from the desiccant entering the ozone generator is recommended.

A stainless steel pressure filtration assembly (Millipore Corporation, Bedford MA 01730, Cat. No. XX40 047 00) with a 0.2 μm pore size Fluoropore^R filter (Millipore Corporation, Cat. No. FGLP 047 00) in the normal filter position and silica gel in the reservoir have been found to be satisfactory for this purpose.

4.3.3 In-Line Gas Filtration Assembly

A filter is placed in the ozone line immediately before the gas enters the sample. A 25 mm stainless steel gas line filter holder (Millipore Corporation, Cat. No. XX40 025 00) or equivalent with a 0.2 μm pore size Fluoropore filter (Millipore Corporation, Cat. No. FGLP 025 00) or equivalent is used in each ozone supply line to ensure that the ozone entering the sample is particle-free.

4.3.4 Ultraviolet Lamp

A submersible short wavelength (254 nm) ultraviolet lamp is required for the ozone-UV oxidation treatment of water samples. A 6 inch Pen-Ray^R ultraviolet lamp (Part No. 90-0004-11) and power supply model SCT-4 (Ultra-Violet Products Inc., 5100 Walnut Grove Avenue, San Gabriel, California 91778) or equivalent have been found to meet the requirements of this analytical technique.

4.3.5 Source of Known Fiber-Free Water

For blank determinations, final washing of analytical equipment, and dilution of some samples, a source of water which is free of both particles and fibers is required. Fresh double-distilled water from a glass distillation apparatus (MEGA-PURETM manufactured by Corning and available from all authorized Corning Laboratory Supply Dealers) or equivalent is preferable, and has been found to meet this requirement. De-ionized water, filtered through a 0.1 μm pore size Nuclepore polycarbonate filter has also been found to be satisfactory, but the filtration assembly itself tends to contribute some particles to the filtrate.

4.3.6 Filtration Apparatus

The water sample is filtered through a membrane filter of either 47 mm diameter or 25 mm diameter. The filtration assembly should be chosen to suit the size of filter in use. A glass frit support is required in order to obtain a uniform deposit on the filter. The reservoir must be easily cleaned in order to prevent sample cross-contamination. A 47 mm analytical filter holder (Millipore Corporation, Cat. No. XX10 047 00) or a 25 mm analytical filter holder (Millipore Corporation, Cat. No. XX10 025 00)

or equivalent has been found to be suitable. When using the larger diameter equipment it is necessary to filter proportionately larger volumes of water.

4.3.7 Filtration Manifold

When a number of samples are to be filtered, several filtration units can be operated simultaneously from a single vacuum source by using a multiple port filtration manifold (Millipore Corporation, Cat. No. XX26 047 35) or equivalent. The manifold should include valves to permit each port to be opened or closed independently.

4.3.8 Vacuum Pump

A pump is required to provide a vacuum of 20 kPa for the filtration of water samples. A water jet pump (Edwards High Vacuum Inc., Grand Island, NY 14072, Cat. No. 01-C046-01-000-female connection or 01-C039-01-000-male connection) or equivalent has been found to provide sufficient vacuum for a 3-port filtration manifold and also incorporates a non-return valve to prevent back-streaming.

4.3.9 Membrane Filters

The diameters of the membrane filters should be matched to the diameters of the filtration apparatus in use. For filtration of water samples, two types of filters are required:

- polycarbonate capillary-pore membrane filters, 0.1 μm pore size (Nuclepore Corporation, 7035 Commerce Circle, Pleasanton, California 94566) or equivalent, are used to collect the suspended material from a water sample.
- mixed esters of cellulose membrane filters, 0.45 μm pore size Type HA (Millipore Corporation, Bedford, MA 01730) or equivalent, are used as a support filter placed between the glass frit of the filtration apparatus and the polycarbonate filter.

4.3.10 Jaffe Washer

A Jaffe Washer is used for dissolution of Nuclepore filters. Several designs of Jaffe Washer have been used which are modifications of the original design. Provided that the polycarbonate filter can be completely dissolved, and that the materials used in the different designs of washer are demonstrably free of mineral fiber contamination, the precise design is not considered

important. Because of recent changes in the formulation of Nuclepore polycarbonate filters which have degraded their solubility in chloroform, a more complex dissolution procedure may be required. The additional steps in the preparation are more easily completed if the original washer design is followed. This original design is illustrated in Figure 5A. Figure 5B shows samples being placed on a Jaffe Washer of this design. Alternatively, methylene chloride may be substituted for chloroform, but because this has a higher vapor pressure it is then necessary to ensure that the Jaffe Washer is tightly sealed to avoid excessive evaporation.

4.3.11 Condensation Washer

A condensation washer may be useful if TEM specimens are required more quickly than is possible if the Jaffe Washer is used alone to dissolve some batches of Nuclepore polycarbonate filters. A condensation washer consists of a system with controlled heating, controlled refluxing, and a cold finger for holding the electron microscope sample grids. Figure 6 shows one model of the condensation washer (Cat. No. 15950, Ladd Research Industries, Inc., P.O. Box 901, Burlington, Vermont 05401) which has been found satisfactory.

4.3.12 Electron Microscope Grids

Specimen grids of 200 mesh and 3 mm diameter are required in both copper and gold. The grid openings should be approximately 80 μm square. The fiber count result obtained is proportional to the mean area of the openings examined. Therefore, it is important that an accurate measurement of the dimensions of each grid opening can be obtained. Since there is a wide range of quality in the available copper specimen grids, these should be examined carefully to establish the degree of uniformity of both the grid openings and the grid bars. Copper specimen grids Cat. No. SPI #3020C and 3020T, SPI Supplies Division of Structure Probe, Inc., P.O. Box 342, West Chester, PA 19380, or equivalent, have been found to meet the requirements. In addition, these grids have a mark at the center opening. This reference can be used to indicate the location of openings which have been examined. Alternatively, finder grids may be substituted if re-examination of specific grid openings is to be required. Gold specimen grids Cat. No. 21612, Ernest F. Fullam, Inc., P.O. Box 444, Schenectady, N.Y. 12301, or equivalent, have been found to meet the requirements for gold grids.

4.3.13 Ultrasonic Bath

An ultrasonic bath is required for dispersing particulate in sample containers and for general cleaning of equipment. The size of unit selected is unimportant, and should be related to the volume of work in progress. Bransonic Model B-52 (Branson Cleaning Equipment Company, Parrott Drive, Shelton Connecticut 06484) has a power of 200 watts at a frequency of 50 kHz and has been found to meet the requirements.

4.3.14 Carbon Rod Electrodes

Spectrochemically pure carbon rods are required for use in the vacuum evaporator during carbon coating of filters. Type AGKSP, National Spectroscopic Electrodes, manufactured by Union Carbide, or equivalent, have been found to meet the requirements.

4.3.15 Carbon Rod Sharpener

This device is used to sharpen the carbon rods to a neck of 3.6 mm long and 1.0 mm diameter. The use of necked rods, or equivalent, allows the carbon layer to be applied with a minimum of heating of the polycarbonate membrane. The sharpener, Cat. No. 1204, Ernest F. Fuilam, Inc., Schenectady, N.Y. 12301, or equivalent, meets the requirements.

4.3.16 Standards

- a) Reference Standard Fiber Suspensions. Glass ampoules of stable concentrated chrysotile or amphibole fiber dispersions, (Electron Optical Laboratory, Ontario Research Foundation, Sheridan Park, Mississauga, Ontario, Canada L5K 1B3) can be used to establish quality assurance in analytical programs. The reference suspensions of known mass and numerical fiber concentrations are used to generate control samples for inclusion in analytical programs.
- b) Reference Silicate Mineral Standards on TEM Grids. For calibration of the EDXA system, reference silicate mineral standards are required (Electron Optical Laboratory, Ontario Research Foundation, Sheridan Park, Mississauga, Ontario, Canada L5K 1B3).
- c) Asbestos Bulk Material. Chrysotile (Canadian), Chrysotile (Rhodesian), Crocidolite, Amosite. UICC (Union Internationale Contre le Cancer) Standards. Available from Duke Standards Company, 445 Sherman Avenue, Palo Alto, CA 94306.

4.3.17 Carbon Grating Replica

A carbon grating replica with about 2000 parallel lines per mm (Cat. No. 10020, Ernest F. Fullam, Inc., Schenectady, N.Y. 12301) or equivalent is required for calibration of the magnification of the TEM.

4.3.18 Chloroform

Spectrograde chloroform, distilled in glass (preserved with 1% (v/v) ethanol, Burdick & Jackson Laboratories Inc., Muskegon, Michigan 49442) or equivalent, is required for the dissolution of the polycarbonate filters.

4.3.19 Petri Dishes

Disposable plastic petri dishes (Millipore Corp. Cat. No. PD 10 047 00) or equivalent, are useful for storage of sample filters and specimen grids. If charge build-up on these dishes is experienced, it has been found that rinsing them with a weak detergent solution will reduce the problem.

4.3.20 Quartz Pipets

Quartz pipets are used to bubble ozone through the liquid sample. These pipets are formed by heating quartz tubing and drawing it to a tip of approximately 0.35 mm inside diameter. The pipet should be sufficiently long to reach within 1 inch of the bottom of the sample bottle, to create good mixing of the liquid during oxidation.

4.3.21 Mercuric Chloride Solution

A 0.01 molar solution of mercuric chloride may be required for preservation of water samples. This is prepared by dissolving 2.71 g of reagent grade mercuric chloride in 100 mL of fiber-free water. The solution is then filtered twice through the same 0.1 μm pore size Nuclepore filter, using the filtration apparatus described in Section 4.3.6 and a conventional filtration flask.

4.3.22 Routine Electron Microscopy Preparation Supplies

Electron microscopy preparation supplies such as scalpels, disposable scalpel blades (curved cutting edge), double-sided adhesive tape, sharp point tweezers and specimen scissors are required. These items are available from most EM supply houses.

4.3.23 Routine Laboratory Supplies

Routine laboratory supplies and labware are required. The general supplies include a detergent for cleaning apparatus, marking pens for labelling glass and plastic apparatus, glass microscope slides, lens paper (for preparation of Jaffe Washer and lining of TEM grid storage dishes), lint free tissues. General labware includes such items as graduated cylinders, beakers of several sizes, pipets. Whenever possible, disposable plastic labware is recommended to avoid the problems of contamination from new glassware and cross-contamination between samples.

5. SAMPLE COLLECTION AND PRESERVATION

5.1 Sample Container

The sample container will be an unused, pre-cleaned, screw-capped bottle of glass or low density (conventional) polyethylene and capable of holding at least 1 liter. It is recommended that the use of polypropylene bottles be avoided since problems of particulate being released into water samples have been observed.

Ideally, water samples are best collected in glass bottles. However, glass can have significant levels of asbestos on the surfaces and therefore requires careful cleaning before use. Glass is also difficult to ship because of possible breakage through dropping or freezing. Because of these disadvantages, polyethylene bottles are more convenient to use and therefore are recommended.

The bottles should first be rinsed twice by filling approximately one third full with fiber-free water and shaking vigorously for 30 seconds. After discarding the rinse water, the bottles should then be filled with fiber-free water and treated in an ultrasonic bath for 15 minutes, followed by several rinses with fiber-free water.

It is recommended that blank determinations be made on the bottles before sample collection. The following method has been found satisfactory for these determinations. A pre-washed bottle containing approximately 800 milliliters of fiber-free water is processed as described for preparation of samples, including ozone-UV and ultrasonic treatments. When using polyethylene bottles, 1 bottle in each batch or a minimum of 1 bottle in each 24 is tested for background level. When using glass bottles, the risk of asbestos contamination from the bottle is greater and a minimum of 4 bottles in each 24 are examined for background level. Additional blanks may be desirable when sampling waters suspected of containing very low levels of asbestos, or when additional confidence in the bottle blanks is desired.

5.2 Sample Collection

It is beyond the scope of this procedure to furnish detailed instructions for field sampling; the general principles of obtaining water samples apply. However, some specific considerations apply to asbestos fibers because they are a special type of particulate matter. These fibers are small, and in water range in length from 0.1 μm to 20 μm or more.

Because of the range of sizes there may be a vertical distribution of particle sizes in large bodies of water. This distribution may vary with depth depending upon the vertical distribution of temperature, the water current pattern and the local meteorological conditions. Sampling should take place according to the objective of the analysis. If a representative sample of a water supply is required, a carefully designated set of samples should be taken representing the vertical as well as the horizontal distribution and these samples should be composited for analysis.

When sampling from a faucet, remove all hoses or fittings and allow the water to run to waste for a sufficiently long period to ensure that the sample collected is representative of fresh water. Faucets or valves should not be adjusted until all samples have been collected. If possible, sampling at hydrants and at the ends of distribution systems should be avoided.

As an additional precaution against contamination, before collection of the sample, each bottle may be rinsed several times in the source water being sampled. In the case of depth sampling in bodies of water, this rinsing may compromise the results and should be omitted.

5.3 Quantity of Sample

Two separate samples of approximately 800 milliliters each are required. An air space must be left in the bottle to allow efficient redispersal of settled material before analysis. The second bottle is stored for analysis if confirmation of the results obtained from the analysis of the first bottle is required.

5.4 Sample Preservation and Storage

Samples must be transported to the analytical laboratory as soon as possible after collection. No preservatives should be added during sampling; the addition of acids should be particularly avoided.

If the sample cannot be given ozone-UV treatment and filtered within 48 hours after arrival at the analytical laboratory, amounts (1 milliliter per liter of sample) of a pre-filtered 2.71% solution of mercuric chloride sufficient to give a final concentration of 20 ppm of mercury may be added, to prevent bacterial growth. Appropriate care should be taken when handling mercury compounds.

At all times after collection, it is recommended that the samples should be stored in the dark and refrigerated at about 5°C in order to minimize bacterial and algal growth. The samples should not be allowed to freeze, since the effects on asbestos fiber dispersions are not known.

Before the sample bottles are opened, the exterior surfaces should be thoroughly washed and then rinsed in fiber-free water to avoid inadvertent contamination of the sample by material which may be attached to the bottles.

6. PROCEDURE

6.1 Cleanliness and Contamination Control

It is most important that all glassware and apparatus be cleaned thoroughly in order to minimize the possibility of specimen contamination. All phases of the specimen preparation should be conducted in the clean room facilities or in a laminar flow hood. Glassware should be cleaned in an ultrasonic bath using a detergent solution. After this, it should be rinsed three times using fiber-free water. After drying, equipment should be stored in clean containers and covered using aluminum foil or parafilm. All glassware must be washed by the above procedure before each use.

6.2 Oxidation of Organics

Oxidation of the high molecular weight organic components in water samples prior to filtration has been found necessary if precise results are to be obtained. Asbestos fibers have an affinity for these organic materials. Three separate effects have been identified which result from this affinity and which give rise to serious errors if this oxidation is not carried out:

- a) asbestos fibers associated with organic materials tend to adhere to the container walls;
- b) asbestos fibers tend to aggregate with organic materials;
- c) fibers embedded in organic material are not transferred to the TEM specimen.

All three effects give rise to low results. Before sub-samples are taken from the bottle it is necessary to ensure that all the particulate material is in suspension. The organic material and associated fibers must be released from the container walls. This can be achieved by treating the water sample in the original collection container using the ozone-ultraviolet (ozone-UV) technique to oxidize the organic materials. However, if a sample is known to be free of organic interferences the ozone-UV oxidation may not be required.

The equipment should be assembled as shown in Figures 2 and 3.

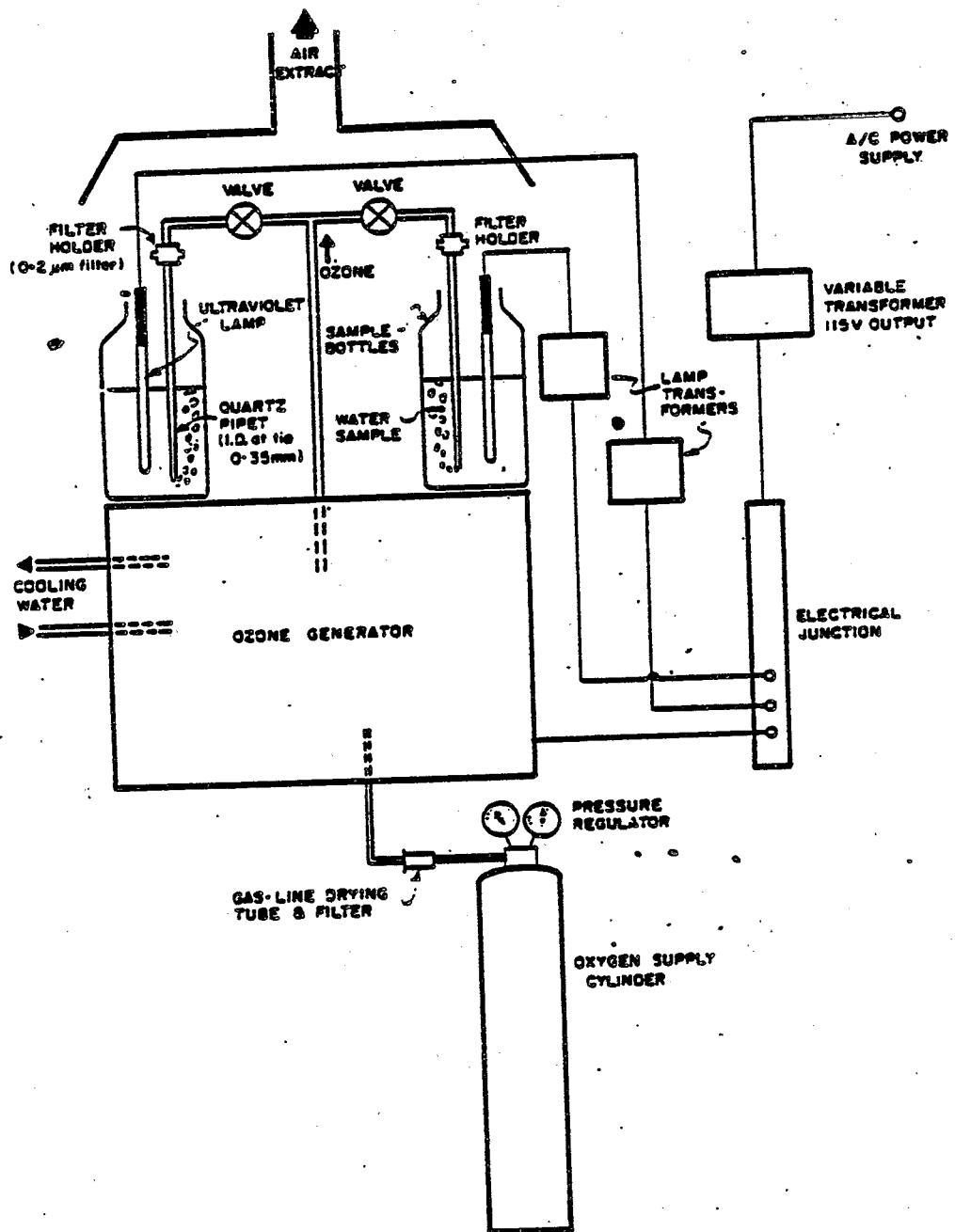


Figure 2. Diagram of Ozone-UV Equipment.

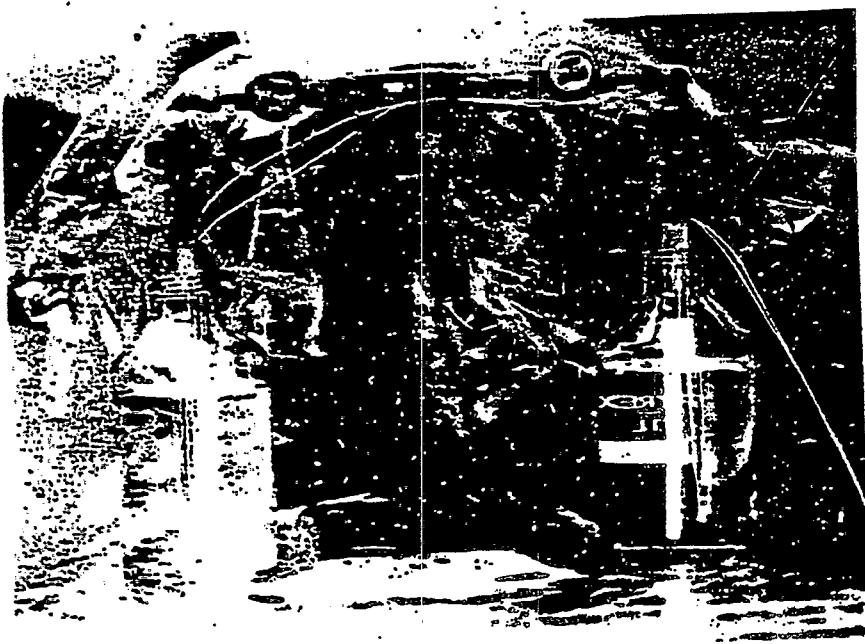


Figure 3. Ozone-UV Oxidation of Water Samples in Glass Bottles. The ozone supply line has been split into two lines to permit simultaneous oxidation of two samples. A valve and a filter holder are incorporated in each of the supply lines to the samples.

An air extract to remove surplus ozone is required. If it is necessary to check that the ozone generator is functioning within the specifications, the output can be verified by normal chemical methods. A suitable technique is to bubble the ozone through a solution of potassium iodide and to titrate the displaced iodine with sodium thiosulfate solution, using starch as an indicator.

Before the ozone-UV treatment, place each polyethylene or glass bottle containing the water sample in the ultrasonic bath for a period of 15 minutes. Mark the level of the liquid in the sample bottle using a waterproof felt marker. The quartz pipets should be thoroughly washed before each use, and installed on the ozone supply as indicated so that the tip is close to the bottom of the sample bottle. The UV lamp is also thoroughly washed and then immersed in the sample and switched on.

At an ozone concentration of 4% in oxygen, treat each sample with about 1 liter/minute of gas for approximately 3 hours. At other ozone concentrations, adjust the oxidation time so that each sample receives about 10 grams of ozone. The gas flow rate should be

sufficient to produce a mixing action in the liquid but should not splash sample out of the container. It is not easy to indicate when oxidation is complete, but this treatment as described has been found to be adequate for all water samples so far handled. When oxidation is complete, remove the UV lamp and quartz pipet, re-cap the bottle and place it in the ultrasonic bath for a period of 15 minutes. This allows particulate released from the oxidized organic materials and the container surfaces to be uniformly dispersed throughout the sample.

The water level in the bottle may have fallen, due to evaporation during the oxidation procedure. The loss of volume should be noted and can be accounted for if it is significant. The sample should be filtered immediately after it is removed from the ultrasonic bath.

6.3 Filtration

6.3.1 General

The separation of suspended particulate by filtration of the sample through a membrane filter is a critical step in the analytical procedure. The objective is to produce a Nuclepore filter on which the suspended solids from the sample are distributed uniformly, with a minimum of overlapping of particles. The volume to be filtered depends on the diameter of the filtration equipment in use, the total suspended solids content of the sample, and in some samples the volume depends on the fiber concentration present.

Table 1 shows the limitation of the analytical sensitivity as a function of the volume of water filtered. In practice, it is usually found that the concentration of suspended solids limits the filtration volume. The maximum particulate loading on the filter which can be tolerated is about $20 \text{ }\mu\text{g/cm}^2$, with an optimum value of about $5 \text{ }\mu\text{g/cm}^2$. Where the concentration of suspended solids is known, the maximum volume which can be used may be estimated. Usually, however, nothing is known about the sample and the best procedure is to prepare several filters using different volumes of the sample. It has been found that suitable filter samples display a faint coloration of the surface, and with experience over-loaded filters usually can be recognized. The determination of a suitable volume to filter is usually a matter of trial and error in the analysis of samples of relatively low total suspended solids but high asbestos concentration.

No attempt should be made to filter sample volumes less than 10 mL for 25 mm diameter equipment, and 50 mL for 47 mm diameter equipment. If smaller volumes are filtered

TABLE 1. LIMITATION OF ANALYTICAL SENSITIVITY BY VOLUME OF WATER SAMPLE
FILTERED

Volume Filtered ¹ (mL)		Analytical Sensitivity ¹ (Fibers/Liter)
Using 25 mm Diameter Filter ²	Using 47 mm Diameter Filter ³	
0.1	0.6	1.5×10^7
0.5	2.8	3.0×10^6
1.0	5.7	1.5×10^6
2.0	11	0.8×10^6
5.0	28	3.0×10^5
10	57	1.5×10^5
25	142	6.0×10^4
50	285	3.0×10^4
100	570	1.5×10^4

¹Concentration corresponding to 1 fiber detected in 20 grid openings of nominal 200 mesh grid (approximately 80 μm square grid openings)

²Assuming Active Filter Area of 1.99 cm^2

³Assuming Active Filter Area of 11.34 cm^2

it is difficult to ensure that a uniform deposit of particulate will be obtained on the filter. Samples of high solids content, or of high fiber content, may require filtration of volumes less than these. Such samples should be diluted with fiber-free water so that the volumes filtered exceed the minima specified. Dilutions should be made by transferring a known volume of the sample to a disposable plastic beaker and making up to a known volume with fiber-free water. The mixture should be stirred vigorously before sub-sampling takes place.

6.3.2 Filtration Procedure

- a) The sample must be filtered immediately after the ozone-UV and ultrasonic bath treatment. If for any reason the sample has been stored for more than a few hours after these treatments, it is recommended that ozone-UV oxidation be repeated for a short period of about 15 minutes, followed by an additional 15 minutes in the ultrasonic bath.
- b) Assemble the filtration base and turn on the vacuum. The upper surface of the filtration base (both the glass frit and the ground mating surface) must be dry before the membrane filters are installed. Place a 0.45 μm pore size type HA Millipore filter on the glass frit. If the filter appears to become wet by capillary action on residual water in the glass frit it must be discarded and replaced by another filter. Place a 0.1 μm pore size Nuclepore filter, shiny side up, on top of the Millipore filter. If the Nuclepore filter becomes folded it must be discarded and replaced. The mating surface of the reservoir component of the filtration apparatus (the funnel) should be dried by shaking off any surplus water and draining on paper towel or tissue. The funnel should be positioned on the filters and firmly clamped, taking care not to disturb the filters. The vacuum should not be released until the filtration has been completed.

It is necessary to comment on the use of filtration equipment which is still wet after washing, since improper procedures at this point can very seriously compromise the results. If the glass frit is wet when the Millipore filter is applied to it, capillary action will result in some areas of the Millipore filter structure being filled by water. When the Nuclepore filter is applied to the surface of the Millipore filter

and the vacuum is applied, the differential pressure across the Millipore filter will be insufficient to overcome the surface tension of the water in the filled areas. Thus no filtration will take place through the corresponding areas of the Nuclepore filter, and a grossly non-uniform deposit of particulate will be obtained.

- c) Add the required volume of sample water to the filtration funnel. Disposable plastic beakers and pipets provide a means of measuring the required sample volume without introducing problems of sample cross-contamination. The reservoir may not be sufficiently large to accommodate the total volume to be filtered. In this case more of the sample may be added during the filtration, but this should be done carefully and only when the reservoir is more than half full. In this way the addition will not disturb or affect the uniformity of particulate already deposited on the Nuclepore filter. Do not rinse the sides of the funnel, and avoid other manipulations which may disturb the particulate deposit on the filter.
- d) Disassemble the filtration unit, and transfer the Nuclepore filter to a labelled, clean petri dish. Since the Nuclepore filters are more easily handled while they are still wet, it is recommended that the strip of filter to be used for TEM sample preparation should be cut as described in Section 6.4.2 before the filter is dried. Place the cover loosely over the dish to limit any deposition of dust onto the filter. Dry the filter under an infra-red heat lamp for a short time before closing the petri dish completely. Discard the Millipore filter.

6.4 Preparation of Electron Microscope Grids

Preparation of the grid for examination in the electron microscope requires a high degree of manual dexterity and is a critical step in the procedure. The objective is to replicate the filter surface by deposition of a carbon film and then to dissolve away the filter itself with a minimum of particle movement and breakage of the carbon film. The filter dissolution procedure is illustrated in Figure 4.

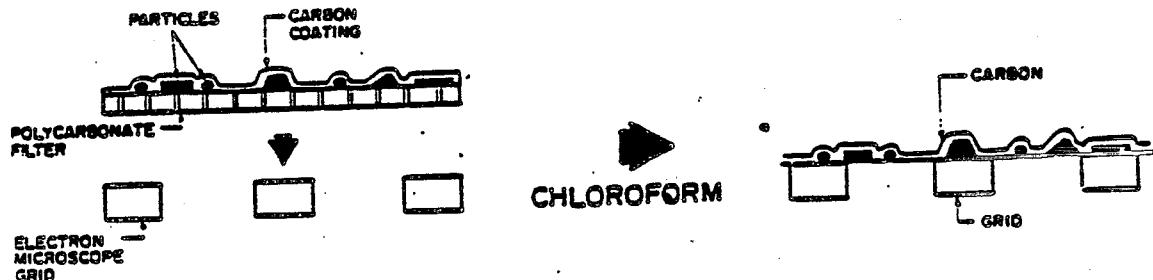


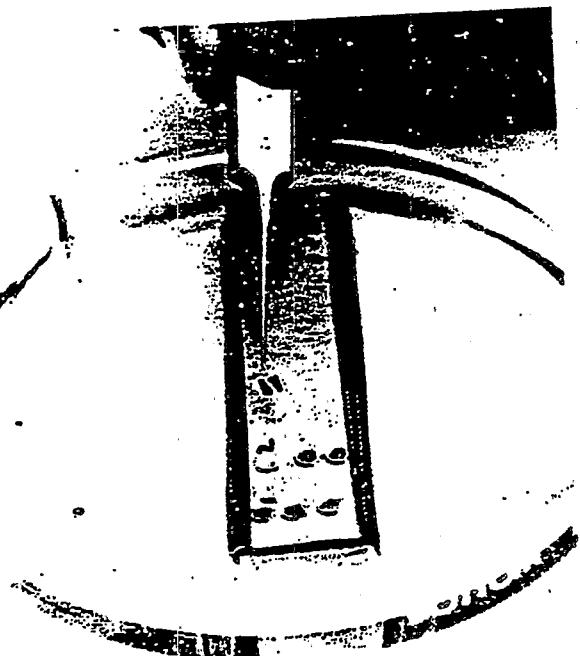
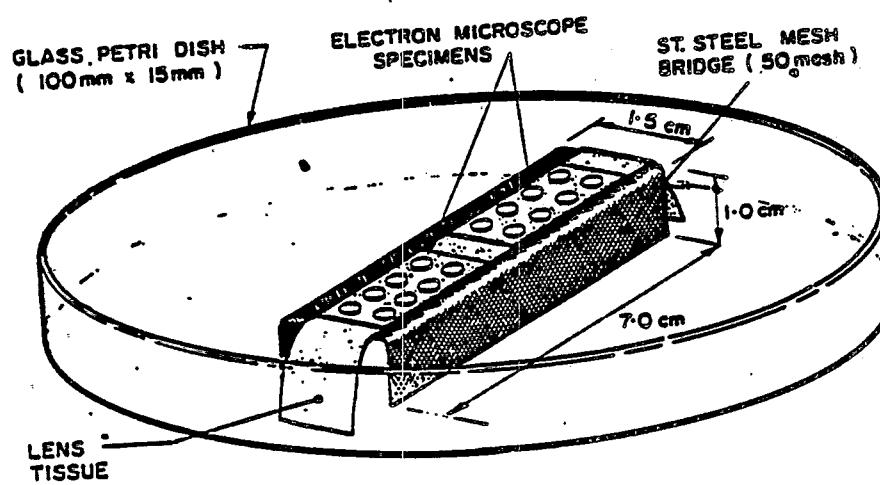
Figure 4. Nuclepore Dissolution Technique

6.4.1 Preparation of Jaffe Washer

Prepare the Jaffe Washer as illustrated in Figure 5A. The stainless steel mesh is formed into a bridge slightly less than 1 cm high, and placed in a 10 cm diameter glass petri dish with a tight fitting lid. A narrow strip of lens cleaning tissue is placed over the bridge with each end of the tissue extending beyond the bridge to the base of the petri dish. The other dimensions of the stainless steel bridge and the length of the lens tissue are not critical, but those specified in Figure 5A have been found to be satisfactory. After the assembly is complete, fill the petri dish with chloroform to a level just below that of the horizontal surface of the stainless steel bridge. It may be found that the chloroform contacts the underside surface of the stainless steel mesh; this is not critical. Cover the petri dish with the lid and the Jaffe Washer is ready for use. Each time the Jaffe Washer is used, the lens tissue and solvent should be discarded and replaced with new lens tissue and fresh solvent. Appropriate precautions should be taken when handling chloroform.

6.4.2 Selection of Filter Area for Carbon Coating

Polycarbonate filters are easily stretched during handling, and cutting of areas for further preparation must be performed with great care. The best method is to use a curved edge scalpel blade to cut the filter while it is in



the plastic petri dish. Press the scalpel point on the filter at the beginning of the desired cut, and rock the blade downwards while maintaining pressure. It will be found that a clean cut is obtained without stressing of the filter. The process should be repeated along all four directions to remove a rectangular portion from the active filtration area of the filter. This filter portion should be selected from along a diameter of the filter, and should be about 3 mm wide by a minimum of 15 mm long. Areas close to the perimeter of the active filtration area should be avoided.

6.4.3 Carbon Coating of the Nuclepore Filter.

The ends of the selected filter strips should be attached to a glass microscope slide using double-sided adhesive tape. This must be performed carefully to ensure that the filter strips lie flat on the slide and are not stretched. The filter strips can be identified by using a wax pencil on the glass slide. After inserting the necked carbon rods into the vacuum evaporator, place the glass slide on the sample rotation and tilting device. The separation between the sample and the tips of the carbon rods should be about 7.5 cm to 10 cm.

If desired, the amount of carbon to be evaporated can be monitored instrumentally so that a thickness of about 30 nm to 50 nm is deposited on the filter strips. Alternatively, a porcelain fragment will serve as a simple carbon deposition monitor. Place a small drop of silicone diffusion pump oil on the surface of a clean fragment of white glazed porcelain. Locate the porcelain in the evaporation chamber with the oil droplet towards the carbon rods and at a distance from the carbon rods equal to that separating the rods from the filter strips. Carbon will not deposit on the oil drop whereas it does on the other areas of the porcelain. With experience, the correct thickness can be monitored visually by observation of the contrast between the darkened areas of the porcelain and the uncoated areas under the oil drop.

Pump down the evaporation chamber to a vacuum better than 10^{-4} Torr (0.013 Pa). Use of a liquid nitrogen cold trap above the diffusion pump will minimize the possibility of contamination of the filter surfaces by oil from the pumping system. Continuously rotate and tilt the glass slide holding the filter strips, while the carbon is evaporated in intermittent bursts, allowing the rods to cool between each evaporation. This procedure is necessary to avoid overheating of the filter strips. Overheating tends to cross-link the polycarbonate which then becomes difficult to dissolve in chloroform.

6.4.4

Transfer of the Filter to Electron Microscope Grids

Remove the glass slide carrying the filter strips from the evaporator, and using the technique described in 6.4.2 cut four pieces slightly less than about 3 mm x 3 mm in size from each filter strip. The square of filter should fit within the circumference of an electron microscope grid. Three of the filter pieces are to be prepared on 200 mesh copper grids, and unless the analysis is to be for chrysotile only, a fourth piece should be prepared on a 200 mesh gold grid. The specimens prepared on copper grids are used for fiber counting and most EDXA examinations. The preparation on the gold grid is intended for EDXA work on fibers containing sodium.

Place a piece of the carbon-coated filter, carbon side up, on to the shiny side of an electron microscope grid. Using fine tweezers, pick up the grid and filter together and place quickly on to the chloroform-saturated lens tissue in the Jaffe Washer, as shown in Figure 5B. It is important that the sample be placed on the lens tissue quickly, since hesitation while the sample is exposed to chloroform vapor will cause it to curl. This is a simplified technique which does not involve dropping of chloroform on to the samples.

Some components of the polycarbonate filters now available dissolve in chloroform only very slowly. Consequently, the grids must be left in the Jaffe Washer for longer than 4 days, and the solvent must be replaced every day. Depending on the particular lot number of the filters, even this period may be insufficient to yield satisfactory grids clear of undissolved plastic. In this event, or if a more rapid sample preparation is desired, after a minimum period of 30 minutes in the Jaffe Washer the lens paper supporting the grids may be transferred to the condensation washer as illustrated in Figure 6. The condensation washer should then be operated for a period of between 30 and 60 minutes, after which the grids will have been cleared of residual plastic. The rate of condensation in the washer is not critical, provided that chloroform drips rapidly from the cold finger for the whole of the washing period and the condensation level is above the samples.

During the dissolution, it is recommended that the grids not be allowed to dry since this has been found to greatly increase the time required for complete dissolution of the polycarbonate.

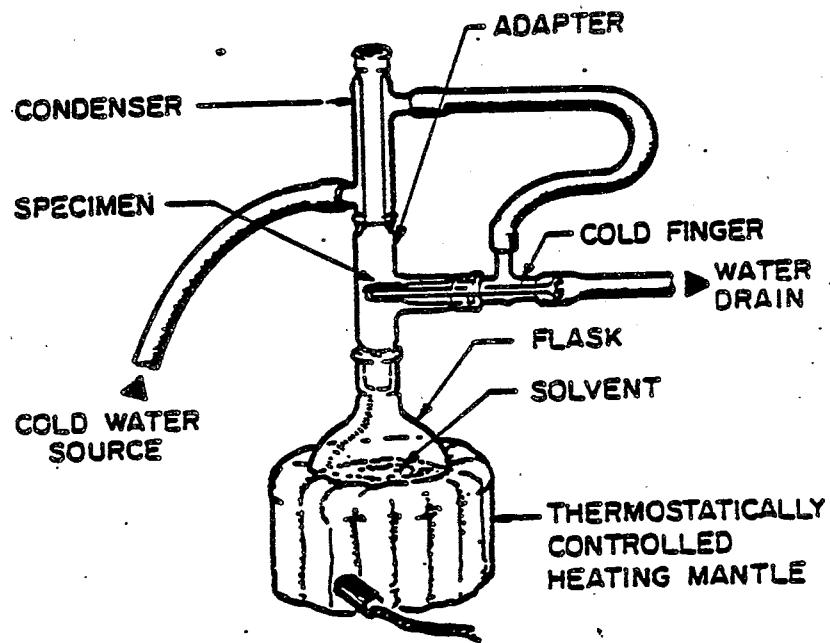


Figure 6. Condensation Washer.

6.5 Examination by Electron Microscopy

6.5.1 Microscope Alignment and Magnification Calibration

Align the electron microscope according to the specifications of the manufacturer. Initially, and at regular intervals, carry out a calibration of the two magnifications used for the analysis (approximately 20,000 and 2,000) using a diffraction grating replica. The calibration should always be repeated after any instrumental maintenance or change of operating conditions. The magnification of the screen image is not the same as that obtained on photographic plates or film. The ratio between these is usually a constant value for the instrument. It is most important that before the magnification calibration is carried out the sample height is adjusted so that the sample is in the eucentric position.

6.5.2 Calibration of EDXA System

The purpose of the calibration is to enable quantitative composition data, at an accuracy of about 10% of the elemental concentration, to be obtained from EDXA spectra of silicate minerals involving the elements sodium, magnesium, aluminum, silicon, potassium, calcium, manganese and iron. If quantitative determinations are required for minerals containing other elements, suitable calibration information may be incorporated in the computer analysis. The well-characterized standards recommended permit calibration of any TEM-EDXA combination which meets the instrumental specifications of Section 4.2, so that data from different instruments can be compared. The standards used for calibration, and the elements which they represent, are shown in Table 2.

TABLE 2. SILICATE MINERAL STANDARDS

Elements	Mineral Standard
Na, Fe, Si	Riebeckite
Mg, Si	Chrysotile
Al, Si	Halloysite
K, Si	Phlogopite
Ca, Si	Wollastonite
Mn, Si	Bustamite

The compositions of these standards have been determined by microprobe analysis, and the TEM grids were prepared from fragments of the same selected mineral specimens. They permit the computer program of Appendix A to be used with any TEM-EDXA system.

Place the first grid into the microscope, form an image at the calibrated higher magnification of about 20,000, and adjust the specimen height to the eucentric point. Tilt the specimen towards the X-ray detector as required by the instrument geometry. Select an isolated fiber or particle less than 0.5 μm in width, and accumulate an EDXA spectrum using an electron probe of suitable diameter. When a well defined spectrum has been obtained, perform an appropriate background subtraction and obtain the net peak areas for each element listed, using energy windows centered on the

peaks and about 130 eV wide. Compute the ratio of the peak area for each specified element relative to the peak area for silicon. Repeat the procedure for about 20 particles of each mineral standard. Analyses of any obvious foreign particles should be rejected, and the data from any one standard should be reasonably self-consistent. Calculate the arithmetic mean peak area ratios for each specified element of each mineral standard. These values are required initially as input for the fiber identification program, and apart from occasional routine checks to ensure that there has been no degradation of the detector resolution, the calibration need not be repeated unless there has been a change of instrumental operating conditions.

6.5.3 Grid Preparation Acceptability

Insert the specimen grid into the electron microscope and adjust the magnification to a value sufficiently low (300 - 1000) so that complete grid openings can be inspected. Examine at least 10 grid openings to evaluate the fiber and total particulate loadings, the uniformity of the particulate deposit, and the extent to which the carbon film is unbroken. The grid must be rejected from further analysis if:

- a) the grid is too heavily loaded with fibers to perform an accurate count. Accurate counts cannot be performed if the grid has more than about 50 fibers per grid opening. A new grid preparation must be made using either a smaller volume of water or a suitable volume of the water diluted with fiber-free water;
- b) the overall distribution of the deposited debris is noticeably non-uniform. A new grid preparation must be made, paying particular attention to proper particulate dispersal and filtration procedures;
- c) the grid is too heavily loaded with debris to allow examination of individual particles by SAED and EDXA. A new grid preparation must be made using either a smaller volume of water or a dilution of the original water sample;
- d) a large proportion of the grid openings have broken carbon film. Since the breakage is usually more frequent in areas of heavy deposit, counting of the intact openings could lead to biased results. Therefore, a new grid preparation must be made from a more completely dispersed sample, a reduced volume of sample, or alternatively, a thicker carbon film may be necessary to support the larger particles.

6.5.4 Procedure for Fiber Counting

The number of fibers to be counted depends on the statistical precision desired. In the absence of fibers, the area of the electron microscope grids which must be examined depends on the analytical sensitivity required. For statistical reasons, discussed in Section 7.2, the fibers on a minimum of 4 grid openings must be counted. The precision of the fiber count depends not only on the total number of fibers counted, but also on their uniformity from one grid opening to the next. In practice, it has been found that termination of the fiber count at a minimum of 100 fibers or 20 grid openings, whichever occurs first, yields results which usually require no further refinement. Additional fiber counting will be necessary if greater precision is required.

At least three grids prepared from the filter must be used in the fiber count. Several grid openings are to be selected from each grid, and the data are all incorporated in the calculation of the results. This permits the measurements to be spread across a diameter of the original filter, so that any gross deviations from a uniform deposition of fibers should be detected.

Figures 7 and 8 show specimen fiber counting raw data sheets which represent the minimum standard of data reporting for this analytical procedure. Figure 7 shows page 1 of the raw data tabulation, which contains all specimen preparation details. Figure 8 is a continuation sheet for the fiber classification and measurement data; several of these sheets may be required for analysis of a sample.

Select a typical grid opening from one of the grids. Set the magnification to the calibrated higher value (about 20,000). Adjust the sample height until the features in the center of the screen are at the eucentric point. Check that the goniometer tilt is set at zero. Reduce the magnification to the lower calibrated value of about 2,000. Measure both dimensions of the grid opening image in millimeters, using the markings on the fluorescent screen. In columns 1 and 2 specify the sequential number of the grid opening, and its dimensions. These two columns are not used again until fiber counting is commenced in the next grid opening to be examined. Adjust the magnification to the upper calibrated value, close to 20,000, and position the grid opening so that one corner is visible on the screen. Move the image by adjustment of only one translation control, carefully examining the sample for fibers, until the opposite side of the opening is encountered. Move the image by one screen width using the

ASBESTOS ANALYSIS - WATER SAMPLE DATA

SEQ:	SAMPLE:										CODE			
JOB:														
PREP:	By _____ Date _____	COUNT:	By _____ Date _____	PROCESS:	By _____ Date _____									
INSTRUMENT:	MAGNIFICATIONS: Grid _____ Count _____													
DILUTIONS: 0														
1 Volume Taken (mL) _____				Final Volume (mL) _____										
2 Volume Taken (mL) _____				Final Volume (mL) _____										
FINAL PREPARATION FILTRATION: Vol. Filtered (mL) _____ Active Area (cm ²) _____														
COMMENTS: (for inclusion in computer print-out; format in 5 lines of 60 characters)														
<hr/> <hr/> <hr/> <hr/> <hr/>														
FIBER CLASSIFICATIONS:														
COUNT: NAM TM CM CD CQ CMQ CDQ UF AD AX ADX AQ ADQ AZQ AZZ														
PROCESS:	FIBER TYPE	CLASSIFICATION	FIBER TYPE	CLASSIFICATION										
NOTES: Preparation:														
<hr/> <hr/> <hr/> <hr/> <hr/>														
Examination:														
<hr/> <hr/> <hr/> <hr/> <hr/>														

Figure 7. Sheet for Recording Water Sample Data.

ASSESSOS MATEVYSSIS - EIBER CLASIFICACION

Figure 8. Sheet for Recording Fiber Classification and Measurement Data.

Continued on Page

other translation control, and then scan the image in the reverse direction. Continue in this manner until the entire grid opening has been inspected. When a fiber is detected, classify it according to the procedures described in Section 6.7, and then insert the appropriate classification on the data sheet. Measure the length and width of the fiber image in millimeters and record these in the appropriate columns of the data sheet. Do not record fibers of obvious biological origin or diatom fragments. Continue the examination until 100 fibers have been recorded in all classification categories of interest, or until 20 grid openings have been inspected. The data should be drawn approximately equally from the three grids. In all samples, fibers on a minimum of 4 grid openings must be counted. Fibers less than 0.5 μm in length will not be incorporated in the fiber concentration calculation.

6.5.5 Estimation of Mass Concentration

If the primary objective of the analysis is to determine the mass concentration, the fiber counting should be approached in a different manner. The number of fibers which must be counted in order to achieve a reliable estimate of the mass concentration depends primarily upon the range of the fiber diameter distribution. The mass concentration measurement is most sensitive to fibers of large diameter, which unfortunately are among those which occur infrequently. When the diameter distribution is narrow, such as that found in the case of chrysotile fibrils, then the mass concentration has approximately the same precision as that of the number concentration. However, the mass concentration may be actually meaningless when calculated from a low number of fibers observed during a routine fiber count, if these fibers have a broad distribution of widths.

If the mass concentration is the primary interest, and the precision required is greater than is possible from the normal fiber count, a different approach to the fiber count must be used. Initially, establish the largest width of fiber which can be detected on the grid by a cursory survey, at a reduced magnification, of a large number of grid openings (about 50). Calculate the volume of this fiber. Adjust the magnification to a value such that a width of 1 mm on the screen corresponds to 10% of the width of the previously selected large fiber. Carry out a routine fiber count for a minimum of 100 fibers, recording only fiber images greater than 1 mm in width. Continue counting until the total volume of fibers is at least 10 times the volume of the originally selected large fiber. The precision and accuracy of this technique has not been

investigated fully, but for samples with broad width distributions it is capable of yielding significantly more precise mass determinations than are obtainable by the conventional fiber count.

The remaining problem concerns the assumption that the widths also represent the thicknesses of the fibers. Measurements of particle thicknesses can be made separately, using the shadow casting technique. Before the filter is carbon coated, apply a vacuum coating of platinum-carbon or gold to the active surface of the Nuclepore filter at an angle of 45°. In the TEM, the fibers will then display shadows on the carbon film which approximate to their thicknesses. Suitable techniques for shadowing are described in the paper by D.E. Bradley included in the Selected Bibliography.

6.6 Fiber Counting Criteria

6.6.1 Fiber Counting Method

Fiber counting with this analytical method will be performed only by the grid opening technique. If a specimen grid is too heavily loaded for examination of entire grid openings, a more reliable result is obtained by preparation of a new filter, using a smaller volume of sample.

6.6.2 Fibers Which Touch Grid Bars

A fiber which intersects a grid bar will be counted only for two sides of the grid opening, as illustrated in Figure 9. The length of the fiber will be recorded as twice the visible length. Fibers intersecting either of the other two sides will not be included in the count.

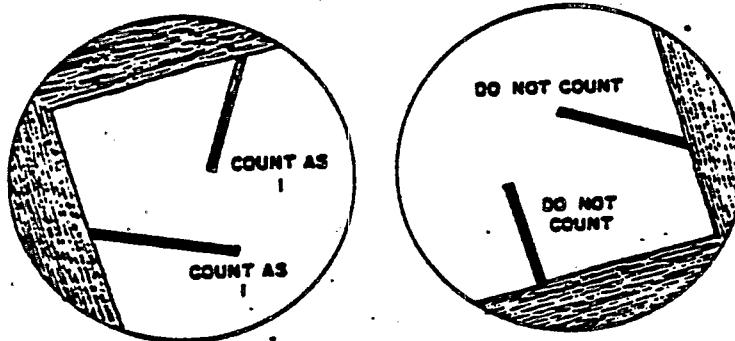


Figure 9. Counting of Fibers Which Overlap Grid Bars.

This procedure ensures that the numerical count will be accurate, and that the best average estimate of length has been made.

6.6.3 Fibers Which Extend Outside the Field of View

During scanning of a grid opening, fibers which extend outside of the field of view must be counted systematically to avoid double-counting. In general, a rule must be established so that fibers extending outside the field of view in only two quadrants are counted. Fibers without terminations in the field of view must not be counted. The procedure is illustrated by Figure 10. The length of each fiber counted is established by moving the sample, and then returning to the original field of view before scanning is continued.

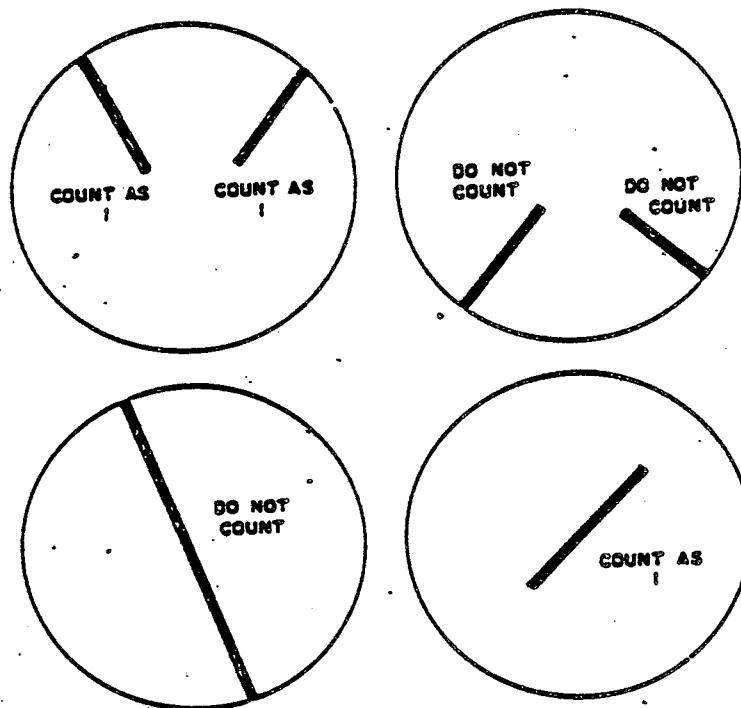


Figure 10. Counting of Fibers Which Extend Outside the Field of View.

6.6.4 Fibers with Stepped Sides

A fiber with stepped sides will be assigned a width mid-way between the minimum and maximum widths.

6.6.5 Fiber Bundles

A fiber bundle composed of many parallel fibers will be counted as a single fiber of a width equal to an estimate of the mean bundle width. Figure 11 shows examples of the procedure.

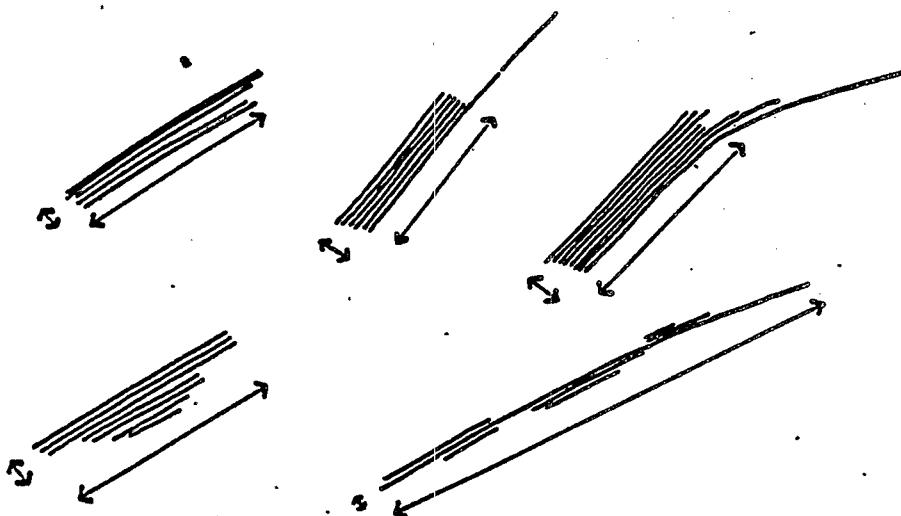


Figure 11. Counting and Measurement of Fiber Bundles. Each bundle to be counted as one fiber with dimensions as indicated by arrows.

6.6.6 Aggregates of Randomly Oriented Fibers

The structure of an aggregate of randomly oriented fibers may be sufficiently visible that the constituent fibers can be counted. This is illustrated in Figure 12. In this



Figure 12. Counting of Fiber Aggregates.

case individual fibers will be recorded. Where the fiber aggregate is too large and complex to count each individual fiber, the identification and aggregate dimensions will be recorded, but it will not be incorporated in the fiber count and mass calculations.

6.6.7 Fibers Attached to Non-Fibrous Debris

A fiber may be attached to, or partially concealed by, a particle of non-fibrous debris. If two ends are visible which appear to be the ends of a single fiber, the fiber will be counted. Where only one end of a fiber is visible, the fiber will be counted as a single fiber having a length equal to twice the visible length, except where this would place the concealed end outside of the particle. In this case the length will be recorded as the visible length plus the extension of it to the opposite side of the particle. Examples of the procedure are shown in Figure 13. There may be more than one fiber attached to a single particle of debris; each one should be counted. If an assembly of fibers and particles is too complex to treat in this way, the overall dimensions should be recorded, but the assembly should not be incorporated in the fiber count and mass calculations.

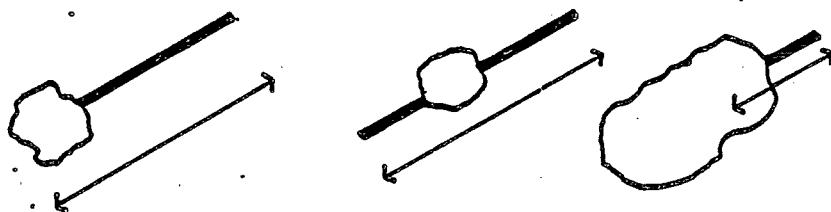


Figure 13. Counting and Measurement of Fibers Attached to Non-Fibrous Debris.

6.7 Fiber Identification Procedures

6.7.1 General

Before it is incorporated into the fiber count, each particle with an aspect ratio of 3 to 1 or greater and not of obviously biological origin must be identified according to defined criteria. It is recognized that economic considerations usually preclude unequivocal identification of every fiber reported. In this analytical method, the

requirement for unequivocal identification is limited to a small proportion of the fibers in order to demonstrate the presence of the particular species. The proportion of fibers examined for unequivocal identification will be stated in the analytical result. The remainder of the fibers are then classified on the basis of crystallographic or chemical similarity, or both, to the identified fibers. If on later examination it is considered necessary to perform a more complete and rigorous identification, additional fibers may be examined in more detail to confirm conclusions based on the fiber classification data.

In general, it will be found that for various instrumental reasons it may be impossible to identify a specific fiber completely, even though the fiber may be of a well-characterized variety. It is, nevertheless, important to record the degree to which the procedures were successful in classification or identification of a particular fiber.

6.7.2 SAED and EDXA Techniques

Fibers are initially classified into two categories on the basis of morphology: those fibers with tubular morphology, and those fibers without tubular morphology. Further analysis of each fiber is conducted using SAED and EDXA methods. Although the precise techniques and classification procedures are specified in Sections 6.7.4 and 6.7.5, some general guidance on the use of SAED and EDXA methods is given here.

The crystal structure of some mineral fibers, such as chrysotile, is easily degraded by the high current densities required for EDXA examination. Therefore, SAED investigation of these sensitive fibers must be completed before attempts are made to obtain EDXA spectra. When examining more stable fibers, such as the amphiboles, the order of work is unimportant.

The SAED technique can be either qualitative or quantitative. Qualitative SAED consists of visual examination of the pattern obtained on the microscope screen from a randomly oriented fiber. SAED patterns obtained from fibers with cylindrical symmetry, such as chrysotile, are an exception since they are not sensitive to axial tilt, and patterns from randomly oriented fibers can be interpreted quantitatively. For non-cylindrical fibers, quantitative (zone axis) SAED requires alignment of the fiber so that a principal crystallographic axis is parallel to the electron beam. The pattern is then recorded and its consistency with known mineral structures is checked by a computer program. The SAED pattern obtained from one zone axis may not be sufficiently

specific to identify the mineral fiber, but it is often possible to tilt the fiber to another angle and to record a different zone axis pattern. The angle between the two axes can also be checked for consistency with the structure of a suspected mineral.

For visual examination of the SAED pattern, the camera length of the TEM should be set to a low value and the SAED pattern then should be viewed through the binoculars. This procedure minimizes the irradiation and possible degradation of the fiber. However, the pattern is distorted by the tilt angle of the viewing screen. For recording purposes, a camera length of at least 2 meters must be used if accurate measurement of the pattern is to be possible. It is of extreme importance that, when obtaining an SAED pattern for either recording or visual evaluation, the sample height be properly adjusted to the eucentric point and the image be focussed in the plane of the selected area aperture. If this is not done there may be some components of the SAED pattern which do not originate from the selected area. It will be found in general that the smallest SAED aperture will be necessary.

For accurate measurements of the SAED pattern, an internal calibration standard is required. A thin coating of gold, or other calibration material, must be applied to the underside of the TEM specimen. This coating can be applied either by vacuum evaporation or, more conveniently, by sputtering. The polycrystalline gold film yields diffraction rings on every SAED pattern and these rings provide the required calibration information.

To form an SAED pattern, move the image of the fiber to the center of the screen and insert a suitable selected area aperture into the electron beam so that the fiber, or a portion of it, is in the illuminated area. The size of the aperture and the portion of the fiber should be such that particles other than the one to be examined are excluded from the selected area. Observe the diffraction pattern with the binocular attachment. If an incomplete diffraction pattern is obtained, move the particle around in the selected area to attempt to get a clearer diffraction pattern or to eliminate possible interferences from neighboring particles.

If a zone axis SAED analysis is to be attempted on the fiber, the sample must be in the appropriate holder. The most convenient holder allows complete rotation of the sample and single axis tilting. Rotate the sample until the fiber image indicates that the fiber is oriented with its length coincident with the tilt axis of the goniometer, and adjust the sample height until the fiber is at the

eucentric position. Tilt the fiber until a pattern appears which is a symmetrical, two dimensional array of spots. The recognition of zone axis alignment conditions requires some experience on the part of the operator. During tilting of the fiber to obtain zone axis conditions, the manner in which the intensities of the spots vary should be observed. If weak reflections occur at some points on a matrix of strong reflections, the possibility of multiple diffraction exists, and some caution should be exercised in selection of diffraction spots for measurement. A full discussion of electron diffraction and multiple diffraction can be found in the references by J.A. Gard, P.B. Hirsch et al, and H.R. Wenk, included in the Selected Bibliography. Not all zone axis patterns which can be obtained are useful or definitive. Only those which have closely-spaced reflections corresponding to low indices in at least one direction should be recorded. Patterns in which all d-spacings are less than about .3 nm are not useful and are usually very wasteful in computer time. A useful guideline is that the lowest angle reflections should be within the radius of the first gold diffraction ring (111), and that patterns with smaller distances between reflections are usually the most definitive.

Five spots, closest to the center spot, along two intersecting lines of the zone axis pattern must be selected for measurement, as illustrated in Figure 14.

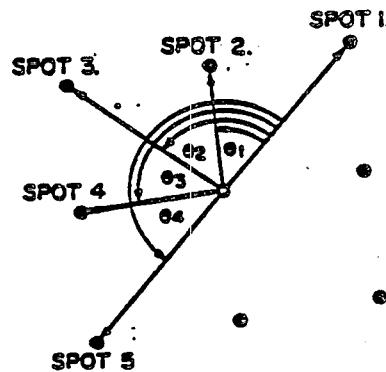


Figure 14. Measurement of Zone Axis SAED Patterns.

The distances of these spots from the center spot and the four angles shown are the input for the computer program. Since the center spot is usually very over-exposed, it does not form a suitable origin for measurement. The required distances must therefore be obtained by measuring between pairs of spots symmetrically disposed about the center spot, preferably separated by several repeat distances. The distances must be measured with a precision of better than 0.3 mm, and the angles better than 2.5°. The diameter of the first or second ring of the calibration pattern (111 and 200) must also be measured with the same precision.

The camera constant (λL) required for the computer program is given by:

$$\lambda L = \frac{aD}{\sqrt{h^2 + k^2 + l^2}}$$

where:

λ = Wavelength of the incident electrons

L = Effective camera length in mm

a = Unit cell dimension in Ångstroms

D = Diameter of the (h , k , l) diffraction rings in millimeters

h , k , l = Miller indices of the scattering plane of the crystal.

Using gold, the camera constant is given by:

$$\lambda L = 2.3548 D \text{ (first ring)}$$

$$\lambda L = 2.0393 D \text{ (second ring)}$$

Analysis of a fiber by EDXA is required in this analytical procedure. Interpretation of the EDXA spectrum may be either qualitative or quantitative. For qualitative interpretation of a spectrum, the elements originating from the fiber are recorded. For quantitative interpretation, the net peak areas, after background subtraction, are obtained for the elements originating from the fiber. As discussed in Section 6.5.2, this method provides for quantitative interpretation for those minerals which contain silicon.

To obtain an EDXA spectrum move the image of the fiber to the center of the screen and remove the objective aperture. Select an appropriate electron beam diameter and deflect the spot to impinge on the fiber. Depending on the instrumentation, it may be necessary to tilt the sample and in some instruments to use Scanning Transmission Electron Microscopy (STEM) mode of operation.

The time for acquisition of a suitable spectrum varies with the fiber diameter, and also with instrumental factors.

For quantitative interpretation, spectra should have a statistically valid number of counts in each peak.

Analyses of small diameter fibers which contain sodium are the most critical, since it is in the low energy range that the X-ray detector is least sensitive. Accordingly, it is necessary to acquire a spectrum for a sufficiently long period that the presence of sodium can be detected in such fibers. It has been found that satisfactory quantitative analyses can be obtained if acquisition is continued until the background-subtracted silicon K_a peak integral exceeds 10000 counts. The spectrum should then be manipulated to subtract the background and to obtain the net areas of the elemental peaks.

After quantitative EDXA classification of some fibers by computer analysis of the net peak areas, it may be possible to classify further fibers in the same sample on the basis of comparison of spectra at the instrument. Frequently, visual comparisons can be made after somewhat shorter acquisition times.

6.7.3 Analysis of Fiber Identification Data

Since the fiber identification procedure can be involved and time-consuming, a Fortran computer program has been provided, the listing of which is given in Appendix A. This program permits the EDXA and zone axis SAED measurements to be compared against a library of compositional and structural data for 226 minerals. The mineral library includes fibrous species which have been listed by several authors, together with other minerals which are known to be similar to amphibole in either their compositions or some aspects of their crystallography. Additional minerals may be added to the library if they are thought to be of concern in particular situations. Rejection of a mineral by the program indicates that either the compositional or crystallographic data for the mineral in the library are inconsistent with the measurements made on the unknown fiber. Demonstration that the measurements are consistent with the data for a particular test mineral does not uniquely identify the unknown, since the possibility exists that data from other minerals may also

be consistent. It is, however, very unlikely that a mineral of another structural class could yield data consistent with that from an amphibole fiber identified uniquely by quantitative EDXA and two zone axis SAED patterns.

The computer program classifies fibers initially on the basis of chemical composition. Either qualitative or quantitative EDXA information may be entered. The procedure using qualitative EDXA consists of entering the list of elements which originate from the particle. For quantitative EDXA (silicon-containing minerals only), the list of elements and the areas under the corresponding X-ray emission peaks, after background correction, form the input data for the computer program. The width of the fiber is also required as input into the program. The program will select from the file a list of minerals which are consistent in composition with that measured for the unknown fiber. To proceed further, it is necessary to obtain the first zone axis SAED pattern, according to the instructions in Section 6.7.2.

It would be attractive to specify a particular zone axis pattern to be obtained for confirmation of amphibole, particularly if such a pattern could be considered characteristic. Unfortunately, for a fiber with random orientation on the grid, no specimen holder and goniometer currently available will permit convenient and rapid location of two pre-selected zone axes. The most practical approach has been adopted, which is to accept those low index patterns which are easily obtained, and then to test their consistency with the structures of the minerals already pre-selected on the basis of the EDXA data. Even the structures of non-amphibole minerals in this pre-selected list must be tested against the zone axis data obtained for the unknown fiber, since non-amphibole minerals may yield similar patterns consistent with amphibole structures in some orientations.

The zone axis SAED interpretation part of the program will consider all minerals previously selected from the file as being chemically compatible with the EDXA data. It will then return a second and usually reduced list of minerals for which solutions have been found. A second set of zone axis data from another pattern obtained on the same fiber can then be processed either as further confirmation or to attempt elimination of an ambiguity. In addition, the angle measured between the orientations of the two zone axes can be entered into the computer to be checked for consistency with the structures of minerals. Caution should be exercised in rationalizing the inter-zone axis angle, since if the fiber contains c-axis twinning the two zone axis SAED patterns may originate from the separate twin crystals.

In practice, the full program will normally be applied to very few fibers, unless precise identification of all fibers is required.

6.7.4 Fiber Classification Categories

It is not always possible to proceed to a definitive identification of a fiber; this may be due to instrumental limitations or to the actual nature of the fiber. In many analyses a definitive identification of each fiber may not actually be necessary if there is other knowledge available about the sample, or if the concentration is below a level of interest. The analytical procedure must therefore take account of both instrumental limitations and varied analytical requirements. Accordingly, a system of fiber classification has been devised to permit accurate recording of data. The classifications are shown in Tables 3 and 4, and are directed towards identification of chrysotile and amphibole respectively: Fibers will be reported in these categories.

The general principle to be followed in this analytical procedure is first to define the most specific fiber classification (target classification) which is to be attempted. Then, for each fiber examined, the classification which is actually achieved is recorded. Depending on the intended use of the results, criteria for acceptance of fibers as "identified" can then be established at any time after completion of the analysis.

In an unknown sample, chrysotile will be regarded as confirmed only if a recorded, calibrated SAED pattern from one fiber in the CD category is obtained. Amphibole will be regarded as confirmed only by obtaining recorded data which yields exclusively amphibole solutions for fibers classified in the AZQ, AZZ or AZZQ categories.

6.7.5 Procedure for Classification of Fibers With Tubular Morphology, Suspected to be Chrysotile

Many fibers are encountered which have tubular morphology similar to that of chrysotile, but which defy further attempts at characterization by either SAED or EDXA. They may be non-crystalline, in which case SAED techniques are not useful, or they may be in a position on the grid which does not permit an EDXA spectrum to be obtained. Alternatively, the fiber may be of organic origin, but not sufficiently definitive that it can be disregarded.

Classification attempts will meet with various degrees of success. Figure 15 shows the classification procedure to be used for fibers which display any tubular morphology.

TABLE 3. CLASSIFICATION OF FIBERS WITH TUBULAR MORPHOLOGY

TM	-	Tubular Morphology not sufficiently characteristic for classification as chrysotile
CM	-	Characteristic Chrysotile Morphology
CD	-	Chrysotile SAED pattern
CQ	-	Chrysotile composition by Quantitative EDXA
CMQ	-	Chrysotile Morphology and composition by Quantitative EDXA
CDQ	-	Chrysotile SAED pattern and composition by Quantitative EDXA
NAM	-	Non-Asbestos Mineral

TABLE 4. CLASSIFICATION OF FIBERS WITHOUT TUBULAR MORPHOLOGY

UF	-	Unidentified Fiber
AD	-	Amphibole by random orientation SAED (shows layer pattern of 0.53 nm spacing)
AX	-	Amphibole by qualitative EDXA. Spectrum has elemental components consistent with amphibole
ADX	-	Amphibole by random orientation SAED and Qualitative EDXA
AQ	-	Amphibole by Quantitative EDXA
AZ	-	Amphibole by one Zone Axis SAED
ADQ	-	Amphibole by random orientation SAED and Quantitative EDXA
AZQ	-	Amphibole by one Zone Axis SAED pattern and Quantitative EDXA
AZZ	-	Amphibole by two Zone-Axis SAED patterns with consistent inter-axial angle
AZZQ	-	Amphibole by two Zone Axis SAED patterns, consistent inter-axial angle and Quantitative EDXA
NAM	-	Non-Asbestos Mineral

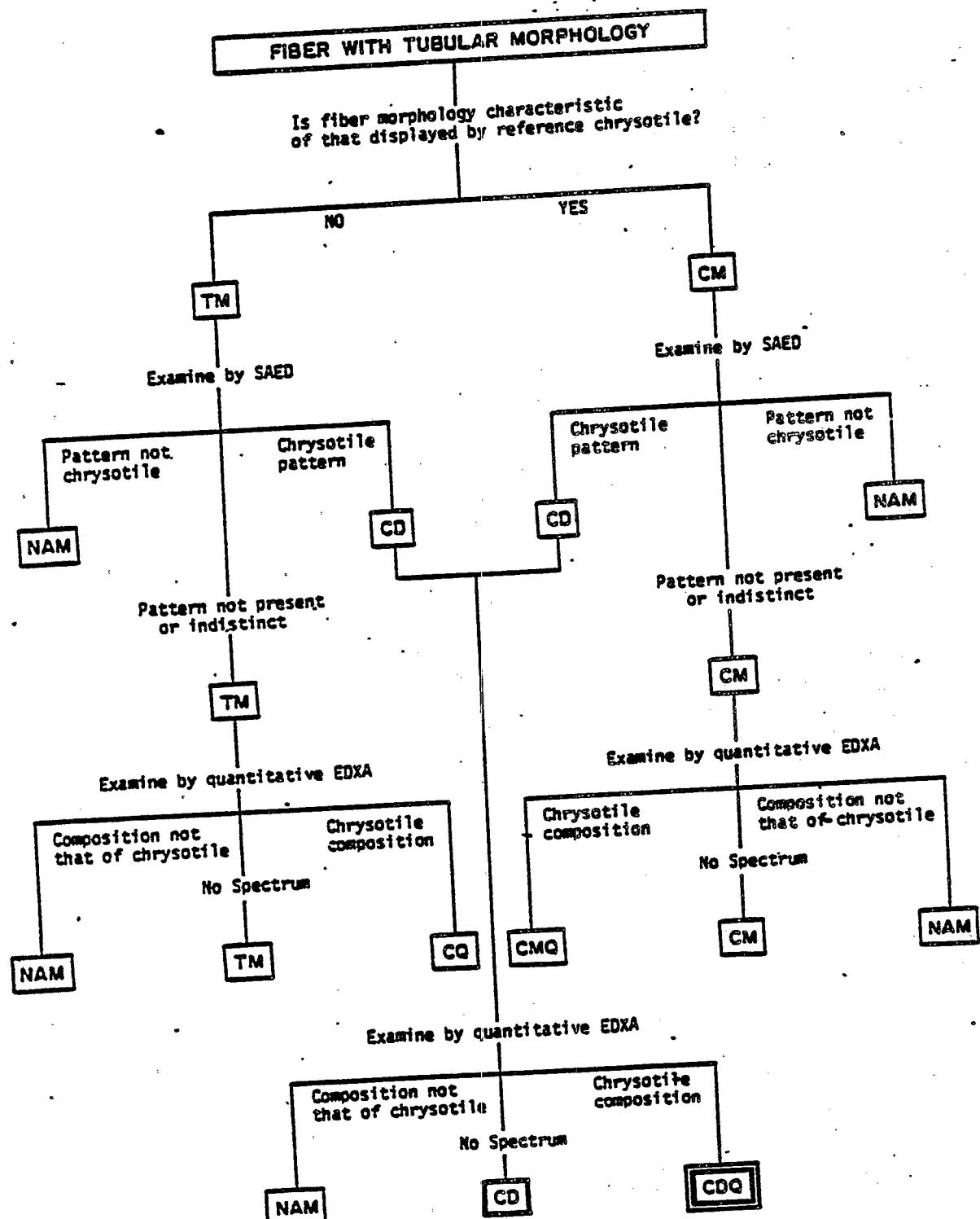


Figure 15. Classification Chart for Fiber With Tubular Morphology.

The chart is self explanatory, and essentially every fiber is either rejected as a non-asbestos mineral (NAM), or classified in some way which could still contribute to the chrysotile fiber count.

Morphology is the first consideration, and if this is not similar to that usually seen in chrysotile standard samples, the initial classification is TM. Regardless of the doubtful morphology, the fiber will still be examined by SAED and EDXA methods according to Figure 15. Where the morphology is more definitive, it may be possible to classify the fiber as having chrysotile morphology (CM).

The morphological characteristics required will be:

- a) the individual fibrils should have high aspect ratios exceeding 10:1 and be about 40 nm in diameter;
- b) the electron scattering power of the fiber at 60 to 100 kV accelerating potential should be sufficiently low for internal structure to be visible; and
- c). there should be some evidence of internal structure suggesting a tubular appearance similar to that shown in Figure 16A, which may degrade in the electron beam to the appearance shown in Figure 16B.

Every fiber having these morphological characteristics will be examined by the SAED technique, and only those which give diffraction patterns with the precise characteristics of Figure 17 will be classified as chrysotile by SAED (CD). The relevant features in this pattern for identification of chrysotile are indicated. The (002) reflections should be examined to determine that they correspond approximately to a spacing of 0.73 nm, and the layer line repeat distance should correspond to 0.53 nm. There should also be "streaking" of the (110) and (130) reflections. Using the millimeter calibrations on the microscope viewing screen, these observations can readily be made at the instrument. A TEM micrograph of at least one representative fiber will be recorded, and its SAED pattern will also be recorded on a separate film or plate. This plate will also carry calibration rings from a known polycrystalline substance such as gold. This calibrated pattern is the only documentary proof that the particular fiber is chrysotile and not some other tubular or scrolled species such as halloysite, palygorskite, talc or vermiculite. The proportion of fibers which can be successfully identified as chrysotile by SAED is variable, and to some extent dependent on both the instrument and the procedures of the operator. The fibers that fail to yield an identifiable SAED pattern will remain in the TM or CM categories unless they are examined by EDXA.

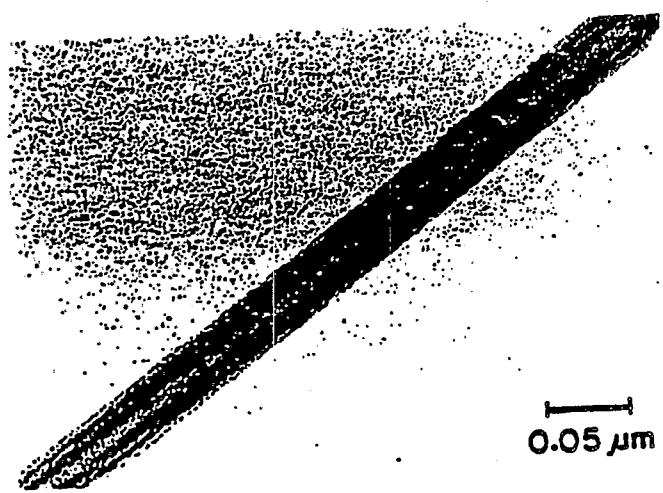


Figure 16A. TEM Micrograph of Chrysotile Fibril, showing Morphology.

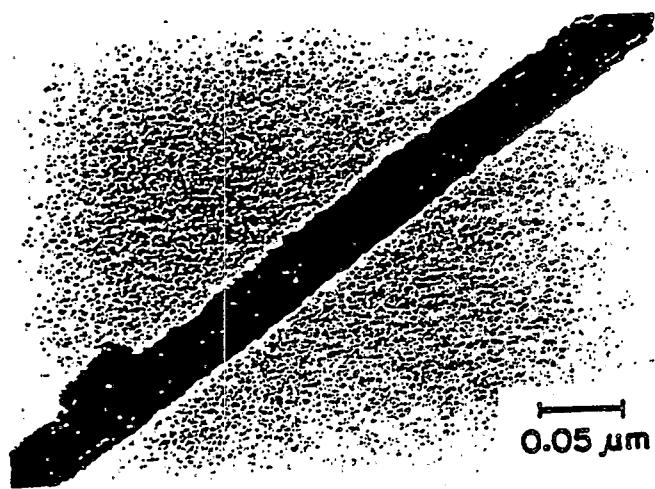


Figure 16B. TEM Micrograph of UICC Canadian Chrysotile Fiber after Thermal Degradation by Electron Beam Irradiation.

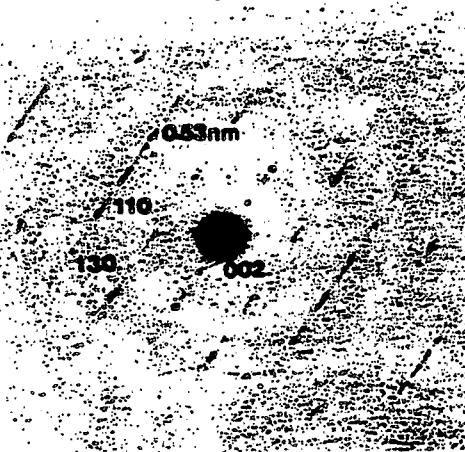


Figure 17. SAED Pattern of Chrysotile Fiber with Diagnostic Features Labelled. Necessary criteria are the presence of 0.73 nm spacing for the 002 reflections, 0.53 nm spacing for the layer line repeat and characteristic streaking of the 110 and 130 reflections.

In the EDXA analysis of chrysotile there are only two elements which are relevant. For fiber classification, the EDXA analysis must be quantitative. If the spectrum displays prominent peaks from magnesium and silicon, with their areas in the appropriate ratio, and with only minor peaks from other elements, the fiber will be classified as chrysotile by quantitative EDXA, in the categories CQ, CMQ or CDQ, as appropriate.

For chrysotile analyses there are essentially three possible levels of analysis:

1. morphological and SAED discrimination only (Target classification CD);
2. in addition, EDXA of only those fibers unclassified by SAED (Target classification CD);
3. EDXA in addition to SAED on all fibers (Target classification CDQ).

6.7.6 Procedure for Classification of Fibers Without Tubular Morphology, Suspected to be Amphibole

Every particle without tubular morphology and which is not obviously of biological origin, with an aspect ratio of 3 to 1 or greater and having parallel or stepped sides, will be considered as a suspected amphibole fiber. Further examination of the fiber by SAED and EDXA techniques will

meet with a variable degree of success, depending on the nature of the fiber and on a number of instrumental limitations. It will not be possible to identify every fiber completely, even if time and cost were of no concern. Moreover, confirmation of the presence of amphibole can be achieved only by quantitative interpretation of zone axis SAED patterns, a very time-consuming procedure. Accordingly, for routine samples from unknown sources, this analytical procedure limits the requirement for zone axis SAED work to a minimum of one fiber representative of each compositional class reported. In some samples, it may be necessary to identify more fibers by the zone axis technique. When analyzing samples from well-characterized sources, the cost of identification by zone axis methods may not be justified.

The 0.53 nm layer spacing of the random orientation SAED pattern is not by itself diagnostic for amphibole. However, the presence of c-axis twinning in many fibers leads to contributions to the layers in the patterns by several individual parallel crystals of different axial orientations. This apparently random positioning of the spots along the layer lines, if also associated with a high fiber aspect ratio, is a characteristic of amphibole asbestos, and thus has some limited diagnostic value. If a pattern of this type is not obtained, the identity of the fiber is still ambiguous, since the absence of a recognizable pattern may be a consequence of an unsuitable orientation relative to the electron beam, or the fiber may be some other mineral species.

Figure 18 shows the fiber classification chart for suspected amphibole fibers. This chart shows all the classification paths possible in analysis of a suspected amphibole fiber, when examined systematically by SAED and EDXA. Initially two routes are possible, depending on whether an attempt to obtain an EDXA spectrum or a random orientation SAED pattern is made first. The normal procedure for analysis of a sample of unknown origin will be to examine the fiber by random orientation SAED, qualitative EDXA, quantitative EDXA, and zone axis SAED, in this sequence. The final fiber classification assigned will be defined either by successful analysis at the target level or by the instrumental limitations. The maximum classification achieved for each fiber will be recorded on the counting sheet in the appropriate column. The various classification categories can then be combined in any desired way for calculation of the fiber concentration, and a complete record of the results from each fiber is maintained for reassessment of the data if necessary.

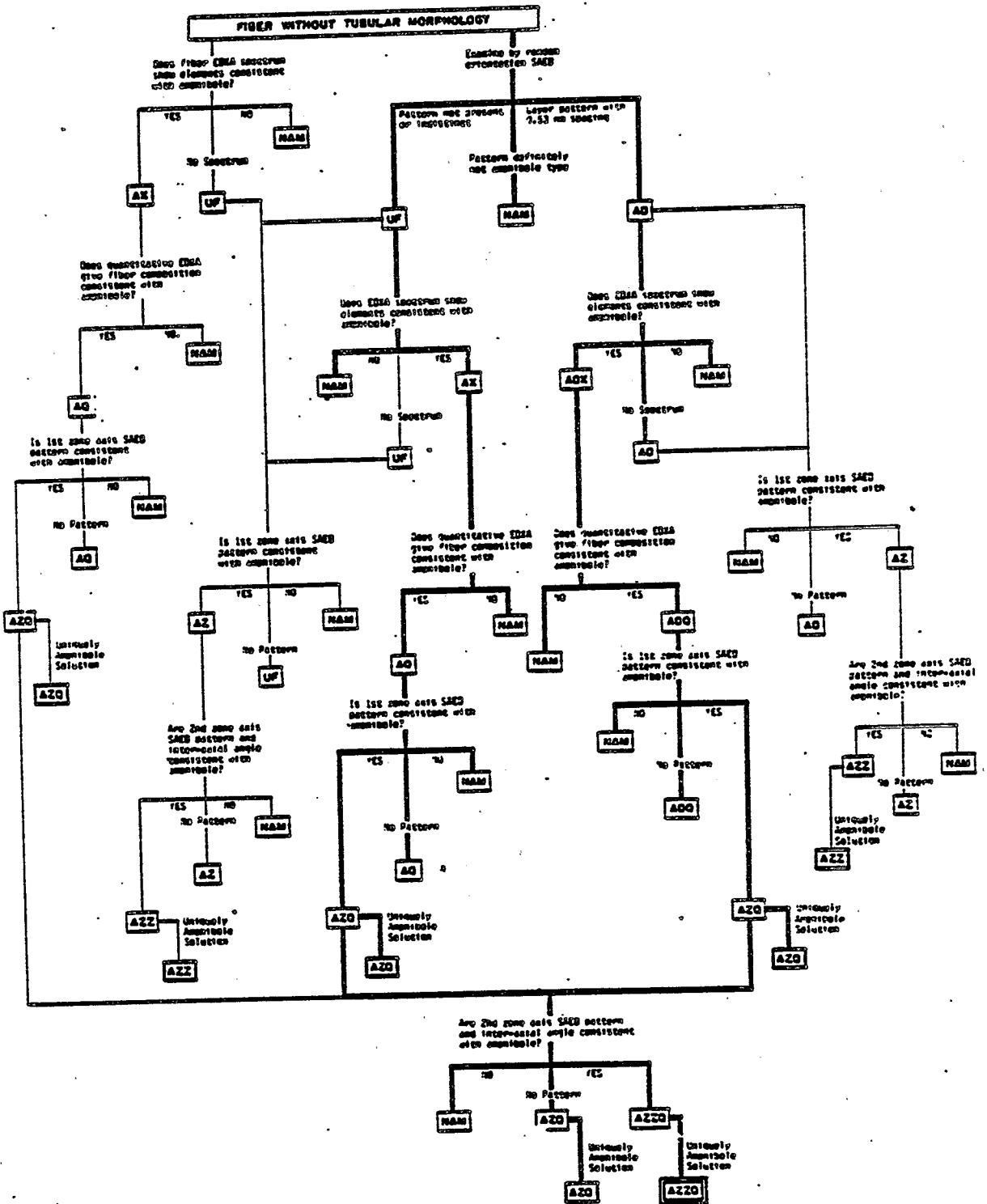
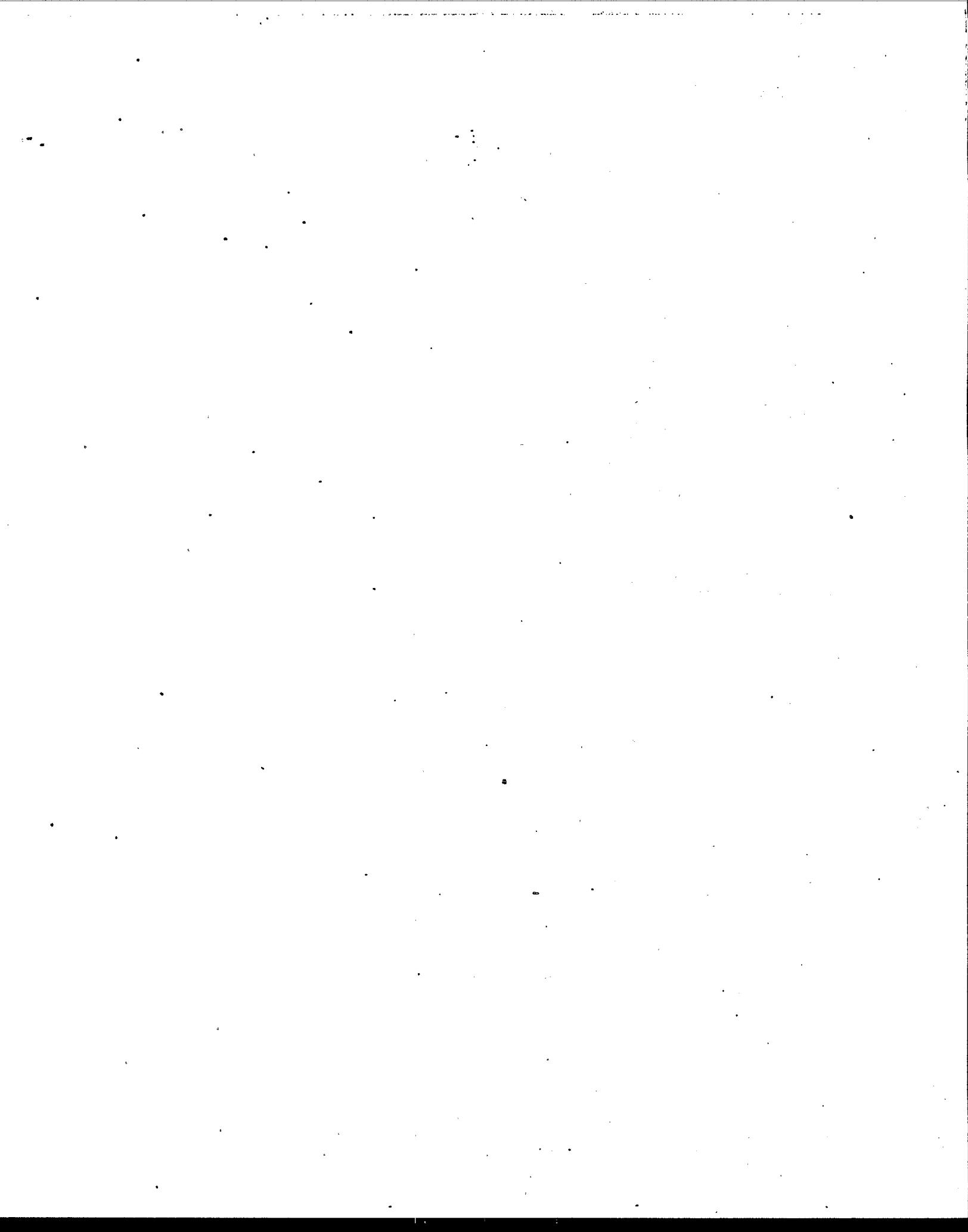


Figure 18. Classification Chart for Fiber Without Tubular Morphology.
Bold Lines indicate the Preferred Paths.



Depending on the particular situation, four levels of analysis can be defined in this analytical procedure, and these are shown in Table 5.

In the routine unknown sample, a level 3 analysis will be required if the presence of amphibole is to be confirmed. For this level of analysis, attempts will be made to raise the classification of every fiber to the ADQ category. In addition, at least one fiber from each type of suspected amphibole found will be examined by zone axis SAED methods to confirm the identification.

TABLE 5. LEVELS OF ANALYSIS FOR AMPHIBOLE

Level of Analysis	Application	Target Classification for all Fibers	Required Classification for Confirmation of Amphibole in a Proportion of the Fibers
1	Routine monitoring of known and well-characterized sources for one mineral fiber type.	ADX	Not Applicable
2	Routine monitoring of known and well-characterized sources where discrimination between two or more amphibole fiber types is required.	ADQ	Not Applicable
3	Routine samples from uncharacterized sources in which presence or absence of amphibole is to be confirmed.	ADQ	AZZ, AZQ or AZZQ - Solutions must include only amphiboles.
4	Samples where precise identification of all amphibole fibers is an important issue.	AZQ	AZZQ - Solutions must include only amphiboles.

6.8 Blank and Control Determinations

To ensure that contamination by extraneous fibers during sample preparation is insignificant compared with the results reported on samples, it is necessary to establish a continuous program of blank measurements. Initially, and at intervals during an analytical program, it is also necessary to ensure that samples of known fiber concentrations can be analyzed satisfactorily.

6.8.1 Blank Determinations

At least one blank determination will be made along with every group of samples prepared at any one time. For the blank determination, a $0.1 \mu\text{m}$ Nuclepore filter will be prepared by filtration of 100 mL of ozone-UV treated fiber-free water if using 25 mm diameter equipment, and 500 mL treated water if using 47 mm diameter equipment. If the samples have been preserved with mercuric chloride, an equivalent amount of the solution should be added to the water used for the preparation of the blank. This blank filter will be carbon coated at the same time as the group of samples, and solvent extracted in the same Jaffe Washer. All aspects of the sample preparation will then be identical to those for the actual samples. All fibers on 20 grid openings of the blank sample will be recorded. The mean fiber concentration for the blank must be less than 0.05 MFL or less than 1% of the lowest individual value reported in the samples concerned, whichever is the greater value. If a value higher than these criteria is encountered, satisfactory blank values must be demonstrated before further analyses are carried out. If it is suspected that samples could have been contaminated during the original preparation, the duplicate bottles should be used for the repreparation of the samples concerned.

6.8.2 Control Samples

Control samples must be incorporated into sample analysis programs in order to demonstrate that the expected results can be produced from samples of known fiber concentration. Such reference suspensions can be prepared using ampoules of stable fiber dispersions listed in Section 4.3.16. It is recommended that the range of fiber concentrations found in the real samples should be simulated using the reference suspensions. The sealed ampoules of fiber dispersions become unstable when they are opened, and the fiber concentration value should not be relied upon for more than 8 hours after opening. Accordingly, it is recommended that, upon opening a dispersion concentrate ampoule, several reference suspensions of different fiber concentrations be prepared in sample bottles. These

bottles can then be stored for preparation and analysis along with water samples of unknown fiber concentrations.

7. CALCULATION OF RESULTS

- The results are conveniently calculated using a computer program, the listing of which is provided in Appendix B. The methods by which the calculations are made are described below.

7.1 Test for Uniformity of Fiber Deposit on Electron Microscope Grids

A check must be made using the chi-square test, to determine whether the fibers found on individual grid openings are randomly and uniformly distributed among the grid openings. If the total number of fibers found in k grid openings is n , and the areas of the k individual grid openings are designated A_1 to A_k , then the total area examined is

$$A = \sum_{i=1}^{i=k} A_i$$

The fraction of the total area examined which is represented by the individual grid opening area, p_i , is given by A_i/A . If the fibers are randomly and uniformly dispersed over the k grid openings counted, the expected number of fibers falling in one grid opening with area A_i is np_i . If the observed number found on that grid opening is n_i , then:

$$\chi^2 = \sum_{i=1}^{i=k} \frac{(n_i - np_i)^2}{np_i}$$

This value is compared with significance points of the χ^2 distribution, having $(k - 1)$ degrees of freedom. Significance levels lower than 0.1% are cause for the sample analysis to be rejected, since this corresponds to a very inhomogeneous deposit. If this occurs, a new filter should be prepared, paying more attention to both uniform dispersal of the suspension and the filtration procedure as described in Section 6.3.2.

7.2 Calculation of the Mean and Confidence Interval of the Fiber Concentration

- In the fiber count, a maximum of 20 grid openings have been sampled from a population of grid openings, and it is required to determine the mean grid opening fiber count for the population on the basis of this sampling. The interval about the sample mean, which, with 95% confidence, contains the population mean, is also required.

The distribution of fibers on the grid openings should theoretically approximate a Poisson distribution. Because of fiber aggregation and size-dependent identification effects, the fiber count data often do not conform to the Poisson distribution, particularly at high fiber counts. Simple assumption of a Poisson distribution may therefore lead to confidence intervals narrower than are justified by the data. Moreover, if a Poisson distribution is assumed, the variance is fixed in relation to the total number of fibers counted. Thus a particular fiber count conducted on one grid opening is considered to have the same confidence interval as that for the same number of fibers found on many grid openings. However, the area of sample actually counted is very small in relation to the total area of the filter, and for this reason fibers must be counted on a minimum of 4 grid openings taken from different areas of the filter in order to ensure representative evaluation of the deposit.

At high fiber counts, where there are adequate numbers of fibers per grid opening to allow a sample estimate of the variance to be made, the distribution can be approximated to Gaussian, with independent values for the mean and variance. Where the sample estimate of variance exceeds that implicit in the Poissonian assumption, use of Gaussian statistics with the variance defined by the actual data is the most conservative approach to calculation of confidence intervals.

At low fiber counts, it is not possible to obtain a reliable sample estimate of the variance, and the distribution also becomes asymmetric, but not necessarily Poissonian. For 30 fibers and below, the distribution becomes sufficiently asymmetric that the Gaussian fit is no longer a reasonable one, and sample variance estimates are unreliable. Accordingly, for fiber counts below 31 fibers, the assumption of a Poisson distribution must be made for calculation of the confidence intervals.

For total fiber counts less than 5, the lower 95% confidence value corresponds to one fiber or less, and in addition, the upper 95% confidence value corresponding to a fiber count of zero is 3.69 fibers. Therefore, it is not meaningful to quote lower confidence interval points for fiber counts of less than 5, and the result should be specified as "less than" the corresponding Poisson upper 95% confidence value.

For fiber counts higher than 30, the sample estimate of variance is also calculated, and the larger of the two confidence intervals is selected. For calculation of Poisson 95% confidence intervals, Table 40 of the reference by E.S. Pearson and H.O. Hartley should be used, with an extension to an expectation of 100. For more than 100 fibers, the Poisson distribution can be accurately approximated by a Gaussian distribution, still using the Poisson variance estimate. For counts of more than 30 fibers, the 95% confidence interval based on a sample estimate of variance is calculated using the Student's "t" distribution. For the two-sided Student's "t" calculation, k values of grid opening fiber count are compared with the expected values for the areas of the grid openings concerned.

In summary, fiber counting data will be reported as follows:

No fibers detected

The value will be reported as less than 369% of the concentration equivalent to one fiber.

1 to 4 fibers

When 1 to 4 fibers are counted, the result will be reported as less than the corresponding upper 95% confidence limit (Poisson).

5 to 30 fibers

Mean and 95% confidence intervals will be reported on the basis of the Poisson assumption.

More than 30 fibers

When more than 30 fibers are counted, both the Gaussian 95% confidence interval and the Poisson 95% confidence interval will be calculated. The larger of these 2 intervals will be selected for data reporting. When the Gaussian 95% confidence interval is selected for data reporting, the Poisson interval will also be noted.

Fiber counts performed on less than 4 grid openings yield very wide 95% confidence intervals when using Gaussian statistics. This is because the value of Student's "t" is very large for 1 and 2 degrees of freedom. Accordingly, fiber counts must not be made on less than 4 grid openings.

The sample estimate of variance s^2 is first calculated:

$$s^2 = \frac{\sum_{i=1}^{i=k} (n_i - np_i)^2}{(k - 1)}$$

where:

- n_i = Number of fibers on the i 'th grid opening
- n = Total number of fibers found in k grid openings
- p_i = Fraction of the total area examined represented by the i 'th grid opening
- k = Number of grid openings

For the 95% confidence interval, the value of $t_{0.975}$ is obtained from tables for $(k - 1)$ degrees of freedom. If the mean value of fiber count is calculated to be \bar{n} , the upper and lower values of the 95% confidence interval are given by:

$$n_U = \bar{n} + \frac{ts}{\sqrt{k}}$$

$$n_L = \bar{n} - \frac{ts}{\sqrt{k}}$$

where:

- n_U = Upper 95% confidence limit
- n_L = Lower 95% confidence limit
- \bar{n} = Mean number of fibers per grid opening
- s = Standard deviation (square root of sample estimate of variance)
- k = Number of grid openings

The fiber concentration in MFL which corresponds to counting of one fiber is given by:

$$C = \frac{A_f \times R_D}{A \times V \times 1000}$$

where:

A_f = Effective filtration area of filter membrane in mm^2 used for filtration of liquid sample

A = Total area examined in mm^2

V = Original volume of sample filtered (mL)

R_D = Dilution ratio of original sample

The mean concentration in MFL is obtained by multiplying the mean number of fibers per grid opening by kC . To obtain the upper and lower 95% confidence limits for the concentration (in MFL) multiply the values n_U and n_L by kC .

7.3 Estimated Mass Concentration

The mass of each amphibole fiber in micrograms is calculated using the relationship:

$$M = L \times W^2 \times D \times 10^{-6}$$

where:

M = Mass in micrograms

L = Length in μm

W = Width in μm

D = Density of fiber in g/cm^3

For chrysotile, the mass may be calculated using the relationship for a cylinder:

$$M = \frac{\pi}{4} \times L \times W^2 \times D \times 10^{-6}$$

The estimated mass concentration is then given by:

$$M_C = C \times \sum_{i=1}^{i=n} M_i \times 10^6$$

where:

M_C = Mass concentration in $\mu\text{g/L}$

C = fiber concentration in MFL, which corresponds to counting of one fiber

M_i = Mass of the i 'th fiber, in micrograms

n = Total number of fibers found in k grid openings

The densities to be assumed are as follows:

Chrysotile	2.55	g/cm^3
Crocidolite	3.37	g/cm^3
Cummingtonite	3.28	g/cm^3
Grunerite	3.52	g/cm^3
Amosite	3.43	g/cm^3
Anthophyllite	3.00	g/cm^3
Tremolite	3.00	g/cm^3
Actinolite	3.10	g/cm^3
Unknown Amphibole	3.20	g/cm^3

7.4 Fiber Length, Width, Mass and Aspect Ratio Distributions

The distributions all approximate to logarithmic-normal, and so the size range intervals for calculation of the distribution must be spaced logarithmically. The other characteristics required for the choice of size intervals are that they should allow for a sufficient number of size classes, while still retaining a statistically-valid number of fibers in each class. Interpretation is also facilitated if each size class repeats at decade intervals. A ratio from one class to the next of 1.468 satisfies all of these requirements. The other constraints are that the length distribution should include 0.5 μm as one interval point, since this is the minimum length to be counted in the method, and the minimum aspect ratio is by definition 3.0. The resulting size classes for the various distributions can be seen in the example shown in Appendix B. The distributions, being approximately logarithmic-normal, must be plotted using a logarithmic ordinate scale and a Gaussian abscissa.

7.4.1 Fiber Length Cumulative Number Distribution

This distribution allows the fraction of the total number of fibers either shorter or longer than a given length to be determined. It is calculated using the relationship:

$$C(N)_k = \frac{\sum_{i=1}^{i=k} n_i}{\sum_{i=1}^{i=N} n_i} \times 100$$

where:

- $C(N)_k$ = Cumulative number percentage of fibers which have lengths less than the upper bound of the $k^{\text{'}}\text{th}$ class
- n_i = Number of fibers in the $i^{\text{'}}\text{th}$ length class
- N = Total number of length classes

7.4.2 Fiber Width Cumulative Number Distribution

This distribution allows the fraction of the total number of fibers either narrower or wider than a given width to be determined. It is calculated in a similar way to that used in 7.4.1 for the length distribution.

7.4.3 Fiber Length Cumulative Mass Distribution

This distribution allows the fraction of the total mass incorporated in fibers either shorter or longer than a given length to be determined. It is computed using the relationship:

$$C_{(M)k} = \frac{\sum_{i=1}^{i=k} \sum_{j=1}^{j=n_i} l_j w_j^2}{\sum_{i=1}^{i=N} \sum_{j=1}^{j=n_i} l_j w_j^2} \times 100$$

where:

- $C_{(M)k}$ = Cumulative mass percentage of fibers which have lengths less than the upper bound of the k 'th class
- n_i = Number of fibers in the i 'th length class
- l_j = Length of the j 'th fiber in the i 'th length class
- w_j = Width of the j 'th fiber in the i 'th length class
- N = Total number of length classes

7.4.4 Fiber Aspect Ratio Cumulative Number Distribution

This distribution allows the fraction of the total number of fibers which have aspect ratios either smaller or larger than a given aspect ratio to be determined. It is

calculated in a similar way to that used in 7.4.1 for the length distribution.

7.4.5 Fiber Mass Cumulative Number Distribution

This distribution allows the fraction of the total number of fibers which have masses either smaller or larger than a given mass to be determined. It is calculated by placing the fibers into logarithmically-spaced mass categories, after which the cumulative frequency distribution is obtained in a similar way to that used in 7.4.1 for the length distribution.

7.5 Index of Fibrosity

It is possible to discriminate between amphibole asbestos fibers and amphibole cleavage fragments on the basis of the distribution of their aspect ratios. The concept of fibrosity in a mineral embodies a high median aspect ratio, together with a large spread of aspect ratios above the median value. A single number can be used to describe the fibrosity of a mineral fiber dispersion, and in many cases the value can be used to state if the material is or is not asbestos. The fibrosity index can be defined thus:

$$F = R^g$$

where R is the median of the aspect ratio distribution and g is the geometric standard deviation of the aspect ratio distribution above the median. The value of g is obtained from that portion of the distribution lying between one and two geometric standard deviations above the median. Meaningful values of the index of fibrosity can be obtained for most waterborne fiber dispersions if more than 50 fibers have been measured.

The fibrosity index as defined above has values exceeding 100 for waterborne dispersions of asbestos. Values below 50 indicate a distribution characteristic of cleavage fragments, or one from which the high aspect ratio fibers have been selectively removed.

8. REPORTING

The computer program provided in Appendix B satisfies all of the reporting requirements for this analytical method, and it is recommended that this format be used. The size classifications used must be the same as those in Appendix B.

8.1 Before the fiber count data can be processed to give concentration values, a decision must be made as to which fiber classifications are to be considered adequate as identification of the fiber species in question. This decision will depend on how much is known about the particular source from which the sample was collected.

For a sample from a completely uncharacterized source, the following procedure will be used to accumulate the classified fibers:

- a) Confirmed Amphibole: AZZQ + AZQ + AZZ
(solutions must include only amphiboles)
- b) Amphibole Best Estimate*: AZZQ + AZQ + AZZ + AZ + ADQ + AQ
- c) Suspected Amphibole: ADX + AX + AD
- d) Confirmed Chrysotile: CDQ + CD
- e) Chrysotile Best Estimate*: CDQ + CD + CMQ + CQ
- f) Suspected Chrysotile: CM

*NOTE: Best estimate can be reported only if some fibers are also reported in the confirmed category, otherwise all fiber classifications must be reported as suspected amphibole or chrysotile.

8.2 The concentration in MFL, together with 95% confidence intervals, will be reported for the groupings in Section 8.1 (a) to (f).

8.3 Two significant figures will normally be used for concentrations greater than 1 MFL, and one significant figure for concentrations less than 1 MFL.

8.4 For confirmation of chrysotile, a micrograph and a calibrated diffraction pattern will be provided from a typical fiber. The identification features in Figure 17 must be visible on the diffraction pattern.

For confirmation of amphibole, either (1) or (2) or (3) below must be provided for a typical fiber of each amphibole variety reported. The data provided must yield solutions which include only amphibole.

- 1) A micrograph, a calibrated zone axis SAED pattern, and an EDXA spectrum together with peak area measurements and EDXA calibration data;

- 2) A micrograph, and two calibrated zone axis SAED patterns with a measurement of the angular rotation between the two patterns;
- 3) A micrograph, two calibrated zone axis SAED patterns with a measurement of the angular rotation between the two patterns, and an EDXA spectrum together with peak area measurements and EDXA calibration data.

- 8.5 Tabulate the length, width and aspect ratio distributions.
- 8.6 Report the estimated mass concentration in $\mu\text{g/L}$ for each of the groupings in Section 8.1 (a) to (f).
- 8.7 One significant figure will normally be used for reporting mass concentration.
- 8.8 Report the concentration in MFL corresponding to one fiber detected.
- 8.9 Report the total number of fibers counted in each of the groupings in Section 8.1 (a) to (f).
- 8.10 Report the χ^2 value for each of the groupings in Section 8.1 (a) to (f).
- 8.11 Report the number of fiber aggregates not included in the fiber count
- 8.12 Report any special circumstances or observations such as aggregation, presence of organic materials, amount of debris, presence of other fibers and their probable identity if known.

9. LIMITATIONS OF ACCURACY

9.1 Errors and Limitations of Identification

Complete identification of every chrysotile fiber is not possible, due to both instrumental limitations and the nature of some of the fibers. The requirement for a calibrated SAED pattern eliminates the possibility of an incorrect identification of the fiber selected. However, there is a possibility of misidentification of other chrysotile fibers for which both morphology and SAED pattern are reported on the basis of visual inspection only. The only significant possibilities of misidentification occur with halloysite, vermiculite scrolls or palygorskite, all of which can be discriminated from chrysotile by the use of EDXA and by observation of the 0.73 nm (002) reflection of chrysotile in the SAED pattern.

As in the case of chrysotile fibers, complete identification of every amphibole fiber is not possible due to instrumental

limitations and the nature of some of the fibers. Moreover, complete identification of every amphibole fiber is usually not practical due to limitations of both time and cost. Particles of a number of other minerals having compositions similar to those of some amphiboles could be erroneously classified as amphibole when the classification criteria do not include zone axis SAED techniques. However, the requirement for quantitative EDXA measurements on all fibers as support for the random orientation SAED technique makes misidentification very unlikely, particularly when other similar fibers in the same sample have been identified as amphibole by zone axis methods. The possibility of misidentification is further reduced with increasing aspect ratio, since many of the minerals with which amphibole may be confused do not display its prominent cleavage parallel to the c-axis.

9.2 Obscuration

If large amounts of other materials are present, some asbestos fibers may not be observed because of physical overlapping. This will result in low values for the reported asbestos content.

9.3 Inadequate Dispersion

If the initial water sample contains organic material which is incompletely oxidized in the ozone-UV treatment, it will not be possible to disperse any fibers associated with the organic material. This may lead to adhesion of some fibers to the container walls and aliquots taken during filtration will then not be representative. It may also lead to a large proportion of fiber aggregates which are either not transferred during the replication and filter dissolution step or which cannot be counted during the sample examination. The result obtained from such an analysis will be low. The sample will also be inadequately dispersed if it is not treated in an ultrasonic bath prior to filtration, and therefore instructions regarding this treatment must be followed closely.

9.4 Contamination

Contamination by introduction of extraneous fibers during the analysis is an important source of erroneous results, particularly for chrysotile. The possibility of contamination, therefore, should always be a consideration.

9.5 Freezing

The effect of freezing on asbestos fibers is not known but there is reason to suspect that fiber breakdown could occur and result in a higher fiber count than was present in the original sample. Therefore, the sample should be transported to the laboratory and stored under conditions that will avoid freezing.

10. PRECISION AND ACCURACY

10.1 General

The precision that can be obtained is dependent upon the number of fibers counted, and on the uniformity of particulate deposit on the original filter. If 100 fibers are counted and the loading is at least 3.5 fibers/grid square, computer modeling of the counting procedure shows that a relative standard deviation of about 10% can be expected. As the number of fibers counted decreases, the precision will also decrease approximately as \sqrt{N} where N is the number of fibers counted. In actual practice, some degradation from this precision will be observed. This degradation is a consequence of sample preparation errors, non-uniformity of the filtered particulate deposit, and fiber identification variability between operators and between instruments. The 95% confidence interval about the mean for a single fiber concentration measurement using this analytical method should be about $\pm 25\%$ when about 100 fibers are counted over 20 grid openings. For these conditions the precision of the computed mass concentration is generally lower than the precision for the fiber number concentration. The precision to be expected for a single determination of mass concentration is critically dependent on the fiber width distribution. For a result based on measurement of a minimum of about 100 fibers, the 95% confidence interval about the mean computed mass concentration may vary between $\pm 25\%$ and $\pm 60\%$. If better precision is required for a mass determination, the alternative counting method described in Section 6.5.5 should be used.

10.2 Precision

10.2.1 Intra-Laboratory Comparison Using Environmental Water Sources

Table 6 shows the results obtained from analysis of 10 replicate samples from each of 8 water sampling locations. Four of these locations were associated with a source of chrysotile and four associated with a source of amphibole. It can be seen that the relative standard deviations of the number concentrations range between 13% and 22%. The corresponding relative standard deviations for the mass concentrations range between 29% and 69%.

10.2.2 Inter-Laboratory Comparison of Filters Prepared Using Standard Dispersions and Environmental Water Sources

Tables 7 and 8 show the fiber counting results obtained when sectors of filters prepared in the ORF Laboratory were distributed to six laboratories considered experienced in asbestos analysis by the identification and counting techniques incorporated in this manual. The samples as

TABLE 6. INTRA-LABORATORY COMPARISON OF ENVIRONMENTAL WATER SAMPLES

Type of Filter in Water Source	Sampling Location	Number Concentration Results				Mass Concentration Results			
		Number of Samples		Fiber Concentration, NFL	Relative Standard Deviation	Mass Concentration, µg/L		Relative Standard Deviation	Mean Number of Fibers Counted per sample
		Mean	95% Confidence Interval			Mean	95% Confidence Interval		
Chrysotile	Domestic Faucet	10	44.3	39.7 - 48.9	15%	0.27	0.19 - 0.35	41%	140
	Domestic Faucet	10	39.7	34.6 - 44.8	18%	0.25	0.19 - 0.32	37%	84
	River	10	15.7	14.0 - 17.3	15%	0.16	0.07 - 0.20	68%	23
	Treatment Plant	10	24.9	22.5 - 27.3	14%	0.17	0.13 - 0.20	25%	93
Ampibole	Domestic Hose	10	16.6	15.1 - 18.1	13%	12.4	9.0 - 15.8	38%	190
	Domestic Hose	10	9.73	8.93 - 10.5	12%	7.0	5.21 - 10.4	46%	110
	Lakeside	10	5.25	4.72 - 5.79	14%	6.55	3.32 - 9.78	69%	38
	Treatment Plant	10	3.42	2.98 - 3.97	22%	2.18	1.45 - 2.92	47%	46

TABLE 7. INTER-LABORATORY COMPARISON: STANDARD DISPERSIONS

Laboratory	Sample 1			Sample 2			Sample 3		
	Concentration, MFL		Concentration, MFL		Concentration, MFL				
	Mean	95% Confidence Interval	Number of Fibers Counted	Mean	95% Confidence Interval	Number of Fibers Counted	Mean	95% Confidence Interval	Number of Fibers Counted
1	9.16	7.02 - 11.3	81	20.2	20.1 - 36.3	300	1.58	1.17 - 1.99	69
2	9.48	4.79 - 14.2	66	32.3	Not Available	75	2.67	1.82 - 3.52	56
3	12.1	9.20 - 16.0	86	27.0	19.6 - 34.4	186	1.68	1.17 - 2.19	55
4	9.26	7.12 - 11.4	96	20.3	11.2 - 29.4	150	1.76	0.97 - 2.55	32
5	9.66	7.37 - 11.9	85	34.0	28.9 - 39.1	284	1.18	0.85 - 1.51	42
6	8.99	1.22 - 16.7	55	16.2	3.27 - 29.1	202	1.90	1.14 - 2.65	63
Mean Concentration		9.78	26.3		1.79				
Standard Deviation		0.92	6.89		0.49				
Relative Standard Deviation		8.4%	26%		27%				
Fiber Species Reported		Chrysotile		Chrysotile		Amphibole			

TABLE 8. INTER-LABORATORY COMPARISON: ENVIRONMENTAL WATER SAMPLES

Laboratory	Sample 4		Sample 5		
	Concentration, AFL Mean	95% Confidence Interval	Number of Fibers Counted	Concentration, AFL Mean	95% Confidence Interval
1	1.71	1.19 - 2.23	48	10.6	9.06 - 12.1
2	1.47	0.61 - 2.33	27	5.87	3.30 - 8.44
3	2.11	1.36 - 2.86	29	6.10	4.92 - 7.28
4	2.50	2.01 - 2.99	35	6.74	5.22 - 8.26
5	1.31	0.63 - 1.99	19	5.17	4.14 - 6.20
6	1.53	0.62 - 2.44	30	6.27	0.72 - 11.8
				78	
				6.79	
				1.94	
				29%	
				Amphibole	
				Chrysotile	

distributed were identified by number only. In Table 7 it can be seen that the relative standard deviations for the six results on each of the standard dispersion filters did not exceed 27%. In Table 8, the environmental water sources used to prepare the filter samples contained similar types of suspended materials as those used to generate the intra-laboratory results in Table 6. The relative standard deviations do not exceed 29%, which appears higher than the values obtained for the intra-laboratory results. However, when the 6 inter-laboratory results are compared with the 10 intra-laboratory values, there is no statistically significant difference to indicate that there has been any degradation of precision.

10.3 Accuracy

10.3.1 Intra- and Inter-Laboratory Comparison of Standard Dispersions of Asbestos Fibers

Tables 9 and 10 show the results obtained between two laboratories when stable aqueous fiber dispersions of known mass concentrations were analyzed. The fiber concentrations reported displayed no significant difference between values from the two laboratories. The relative standard deviation of the mean fiber concentration was 17% for chrysotile and 16% for crocidolite. The corresponding relative standard deviations for the mass concentration were 16% for chrysotile, and 37% for crocidolite. The higher variability for crocidolite is a consequence of the low statistical reliability of the large diameter fiber counts. The computed mean mass concentration for chrysotile was about 46% higher than the known mass concentration. This may be a consequence of the difficulty of diameter measurement for single chrysotile fibrils or the assumption of the bulk value for the density. The computed mean value for mass concentration for the crocidolite sample was 67.4 $\mu\text{g/L}$, which is very close to the known concentration of 50 $\mu\text{g/L}$:

TABLE 9. INTER- AND INTRA-LABORATORY COMPARISON: CHRYSOTILE
ANALYSIS OF REPLICATES OF A 1120 ng/L CHRYSOTILE FIBER DISPERSION

Laboratory	Sample	Fiber Concentration, MFL		Estimated Mass Concentration, ng/L	Number of Fibers Counted
		Mean	95% Confidence Interval		
1	1C	210	165 - 255	1792	147
	2C	199	149 - 248	1435	147
	3C	196	166 - 226	1352	141
2	4C	132	89 - 176	1600	50
	5C	172	146 - 198	1980	79
				1632	
Mean Concentration		182			
Standard Deviation		31		257	
Relative Standard Deviation		17%		16%	

TABLE 10. INTER- AND INTRA-LABORATORY COMPARISON: CROCIDLITE

ANALYSIS OF REPLICATES OF A 50 $\mu\text{g/L}$ CROCIDLITE FIBER DISPERSION

Laboratory	Sample	Fiber Concentration, MFL Mean	Fiber Concentration, MFL 95% Confidence Interval	Estimated Mass Concentration, $\mu\text{g/L}$	Number of Fibers Counted
1	1A	148	112 - 183	94.0	218
	2A	143	123 - 163	89.4	195
	3A	136	98 - 175	66.4	195
2	4A	188	132 - 243	33.0	73
	5A	189	149 - 229	54.1	178
Mean Concentration		161		67.4	
Standard Deviation		26		25.3	
Relative Standard Deviation		16%		37%	

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APPENDIX A

TEST DATA AND COMPUTER LISTINGS FOR FIBER IDENTIFICATION

TEST DATA EXAMPLE 1: AMPHIBOLE IDENTIFICATION

A fiber of riebeckite (FIBER 2) has been used to illustrate the amphibole identification process. Photographs 34 and 41 were taken of two zone axis electron diffraction patterns from this fiber. The measured inter-zone axis angle was 21°.

Electron Diffraction Pattern 34

Electron Diffraction Pattern 41

TWO DIFFRACTION PATTERNS (ACTUAL SIZE) ILLUSTRATING SPOTS AND GOLD RINGS.

DATE: 23-JUN-82

PARTICLE IDENTIFICATION

PARTICLE: UNKNOWN SAMPLE X

WIDTH OF PARTICLE: 0.700 micrometers

X-RAY SPECTRUM:	ELEMENT	PEAK AREA	ELEMENT	PEAK AREA
	SI	5325.00	FE	2157.00
	NA	597.00		

CALCULATED ATOMIC RATIOS:	ELEMENT	RATIO	ELEMENT	RATIO
	SI	1.000	FE	0.425
	NA	0.430		

MINERALS WITH COMPOSITIONS CONSISTENT WITH X-RAY SPECTRUM

AEGIRINE
CROSSITE
FE-RICHTERITE
RIEBECKITE

NA FE SI₂ O₆
NA₂ (Mg,Fe)₃ (Fe,Al)₂ Si₈ O₂₂ (OH)₂
NA CA NA Fe₅ Si₈ O₂₂ (OH)₂
NA₂ Fe₃ Fe₂ Si₈ O₂₂ (OH)₂

DATE: 23-JUN-82

PARTICLE IDENTIFICATION

PARTICLE: UNKNOWN SAMPLE X

ELECTRON DIFFRACTION PATTERN: FIBER 2 PATTERN 34

CAMERA CONSTANT= 83.030 mm*Å

DISTANCES OF DIFFRACTION SPOTS (mm)

4.580 15.520 30.700 15.520 4.580

ANGLES BETWEEN SPOTS (degrees)

80.70 89.80 97.50 180.00

COMPLETE ELECTRON DIFFRACTION ANALYSES MAY BE FOUND IN FILE "XINDEX"

RESULTS OF ZONE AXIS ANALYSIS

MINERAL	A	B	C	ALPHA	BETA	GAMMA
CROSSITE -2 0 -1 2 0 1	9.65	17.91	5.32	90.00	103.60	90.00
FE-RICHTERITE 2 0 1 -2 0 -1	9.82	17.96	5.27	90.00	104.33	90.00
RIEBECKITE 2 0 1 -2 0 -1	9.75	18.00	5.30	90.00	103.00	90.00

DATE: 23-JUN-82

PARTICLE IDENTIFICATION

PARTICLE: UNKNOWN SAMPLE X

ELECTRON DIFFRACTION PATTERN: FIBER 2 PATTERN 41

CAMERA CONSTANT= 81.480 mm⁻¹A

DISTANCES OF DIFFRACTION SPOTS (mm)

12.120 9.070 15.420 10.520 12.110

ANGLES BETWEEN SPOTS (degrees)

57.50 98.50 134.00 179.90

COMPLETE ELECTRON DIFFRACTION ANALYSES MAY BE FOUND IN FILE "XINDEX"

RESULTS OF ZONE AXIS ANALYSIS

MINERAL		A	B	C	ALPHA	BETA	GAMMA
CROSSITE					9.65	17.91	5.32
	5 -1 2	-5 -1 -2	-1 0 1	1 0 -1		90.00	103.60
FE-RICHTERITE					9.82	17.96	5.27
	5 -1 2	-5 -1 -2	-1 0 .1	.1 0 -1		90.00	104.33
RIEBECKITE					9.75	18.00	5.30
	5 -1 2	1 C -1	-1 0 1	-5 -1 -2		90.00	103.00

DATE: 23-JUN-82

PARTICLE IDENTIFICATION

PARTICLE: UNKNOWN SAMPLE X

ELECTRON DIFFRACTION PATTERNS:

- #1: FIBER 2 PATTERN 34
- #2: FIBER 2 PATTERN 41

MEASURED INTER-ZONE AXIS ANGLE= 21.00 +/- 6.00 degrees

COMPLETE INTER-ZONE AXIS ANGLE ANALYSIS MAY BE FOUND IN FILE "PHIDAT"

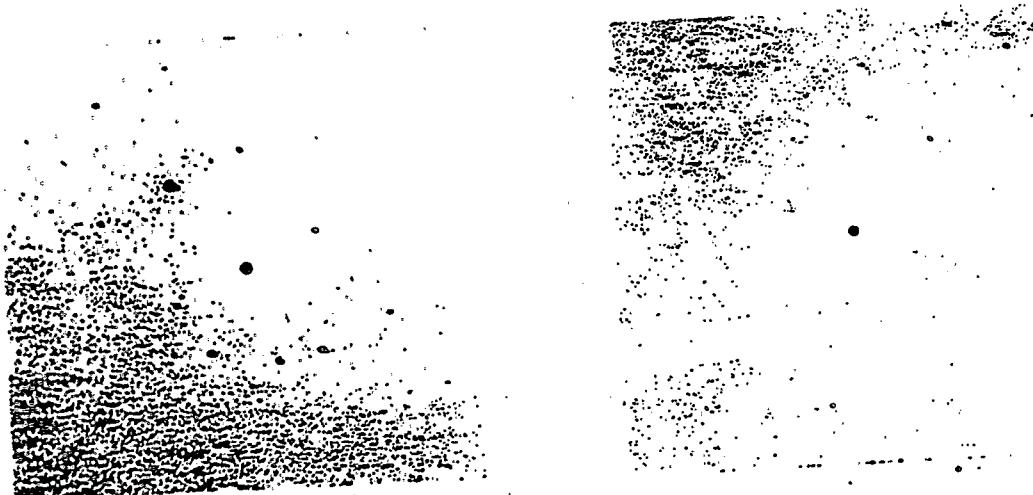
RESULTS OF INTER-ZONE AXIS ANGLE ANALYSIS

MINERAL	ZONE AXIS OF #1	ZONE AXIS OF #2	ANGLE
---------	-----------------	-----------------	-------

CROSSITE	-2 0 -1	-5 -1 -2	21.14
CROSSITE	2 0 1	5 -1 2	21.14
FE-RICHTERITE	2 0 1	5 -1 2	20.90
FE-RICHTERITE	-2 0 -1	-5 -1 -2	20.90
RIEBECKITE	2 0 1	5 -1 2	20.99
RIEBECKITE	-2 0 -1	-5 -1 -2	20.99

TEST DATA EXAMPLE 2: AMPHIBOLE IDENTIFICATION

A fiber of riebeckite (FIBER 3) has been used to illustrate the amphibole identification process. Photographs 30 and 32 were taken of two electron diffraction patterns from this fiber. The measured inter-zone axis angle was 65° .



Electron Diffraction Pattern 30

Electron Diffraction Pattern 32

TWO DIFFRACTION PATTERNS (ACTUAL SIZE) ILLUSTRATING SPOTS AND GOLD RINGS.

DATE: 23-JUN-82

PARTICLE IDENTIFICATION

PARTICLE: UNKNOWN SAMPLE #1

WIDTH OF PARTICLE: 0.500 micrometers

X-RAY SPECTRUM:	ELEMENT	PEAK AREA	ELEMENT	PEAK AREA
	SI	5249.00	FE	2100.00
	NA	614.00		

CALCULATED ATOMIC RATIOS:	ELEMENT	RATIO	ELEMENT	RATIO
	SI	1.000	FE	0.420
	NA	0.449		

MINERALS WITH COMPOSITIONS CONSISTENT WITH X-RAY SPECTRUM

AEGIRINE
CROSSITE
FE-RICHTERITE
RIEBECKITE

NA FE SI₂ O₆
NA₂ (Mg,Fe)₃ (Fe,Al)₂ Si₈ O₂₂ (OH)₂
NA CA NA Fe₅ Si₈ O₂₂ (OH)₂
NA₂ Fe₃ Fe₂ Si₈ O₂₂ (OH)₂

DATE: 23-JUN-82

PARTICLE IDENTIFICATION

PARTICLE: UNKNOWN SAMPLE #1

ELECTRON DIFFRACTION PATTERN: FIBER 3 PATTERN 32

CAMERA CONSTANT= 83.500 mm*A

DISTANCES OF DIFFRACTION SPOTS (mm)

16.170 8.710 19.740 15.790 16.180

ANGLES BETWEEN SPOTS (degrees)

71.80 123.00 148.30 180.00

COMPLETE ELECTRON DIFFRACTION ANALYSES MAY BE FOUND IN FILE "XINDEX"

RESULTS OF ZONE AXIS ANALYSIS

MINERAL	A	B	C	ALPHA	BETA	GAMMA
AEGIRINE 0 1 0	9.65	8.79	5.29	90.00	107.40	90.00
CROSSITE 0 -1 0 -7 1 -6 7 1 6	9.65	17.91	5.32	90.00	103.60	90.00
FE-RICHTERITE 0 -1 0 7 1 6 -7 1 -6	9.82	17.96	5.27	90.00	104.33	90.00
RIEBECKITE 0 -1 0 7 1 6 -7 1 -6	9.75	18.00	5.30	90.00	103.00	90.00

DATE: 23-JUN-82

PARTICLE IDENTIFICATION

PARTICLE: UNKNOWN SAMPLE #1

ELECTRON DIFFRACTION PATTERN: FIBER 3 PATTERN 30

CAMERA CONSTANT= 81.520 mm*Å

DISTANCES OF DIFFRACTION SPOTS (mm)

20.250 15.040 16.420 10.520 20.290

ANGLES BETWEEN SPOTS (degrees)

30.80 69.70 133.30 180.00

COMPLETE ELECTRON DIFFRACTION ANALYSES MAY BE FOUND IN FILE "XINDEX"

RESULTS OF ZONE AXIS ANALYSIS

MINERAL	A	B	C	ALPHA	BETA	GAMMA
---------	---	---	---	-------	------	-------

CROSSITE -4 -1 -1	4 -1 1	3 -1 6	9.65 -3 -1 -6	17.91	5.32	90.00 103.60	90.00
----------------------	--------	--------	---------------	-------	------	--------------	-------

FE-RICHTERITE -4 -1 -1	4 -1 1	3 -1 6	9.82 -3 -1 -6	17.96	5.27	90.00 104.33	90.00
---------------------------	--------	--------	---------------	-------	------	--------------	-------

RIEBECKITE 4 -1 1	3 -1 6	9 -1 6	9.75 -4 -1 -1	18.00	5.30 -3 -1 -6	90.00 103.00	90.00 -9 -1 -6
----------------------	--------	--------	---------------	-------	---------------	--------------	----------------

DATE: 23-JUN-82

PARTICLE IDENTIFICATION

PARTICLE: UNKNOWN SAMPLE #1

ELECTRON DIFFRACTION PATTERNS:

- #1: FIBER 3 PATTERN 32
#2: FIBER 3 PATTERN 30

MEASURED INTER-ZONE AXIS ANGLE = 65.00 +/- 8.00 degrees

COMPLETE INTER-ZONE AXIS ANGLE ANALYSIS MAY BE FOUND IN FILE "PHIDAT"

RESULTS OF INTER-ZONE AXIS ANGLE ANALYSIS

MINERAL ZONE AXIS OF #1 ZONE AXIS OF #2 ANGLE

CROSSITE	0	-1	0	-4	-1	-1	64.59
CROSSITE	0	-1	0	4	-1	1	64.59
CROSSITE	0	-1	0	3	-1	6	64.59
CROSSITE	0	-1	0	-3	-1	-6	64.59
FE-RICHTERITE	0	-1	0	-4	-1	-1	64.89
FE-RICHTERITE	0	-1	0	4	-1	1	64.89
FE-RICHTERITE	0	-1	0	3	-1	6	64.41
FE-RICHTERITE	0	-1	0	-3	-1	-6	64.41
RIEBECKITE	0	-1	0	4	-1	1	64.75
RIEBECKITE	0	-1	0	3	-1	6	64.69
RIEBECKITE	0	-1	0	-4	-1	-1	64.75
RIEBECKITE	0	-1	0	-3	-1	-6	64.69

PROGRAM USER NOTES

AMPHIBOLE IDENTIFICATION FORTRAN PROGRAMS

XMATCH, ITOMNR

- Programs which compare an input X-ray spectrum with mineral compositions stored in the file DIFDAT. Compositions are compared qualitatively if silicon is not present or X-ray peak areas are not specified. If X-ray peak areas are specified, the composition of the unknown fiber is calculated using standards internal to the program, and the names of minerals with the composition are reported

XIDEN, OARRAY, CELL, PHOHIB

- Programs which analyze zone axis SAED patterns

ANGDIF, ACOSI, PHIZON

- Programs which compute inter-zone angles between all zone axis solutions for two patterns

RESULT, SYM

- Programs which print results

FIBID.CMD

- An example of a command file used to chain together all the above procedures

DATGET, DATEDL, DIFDAT

- Programs which list and allow editing and new entries into the mineral data file DIFDAT

NOTES

- The program XIDEN requires a computer with 64K words of memory.
All the other programs require 32K words.

- Some of the input/output statements are specific to the RSX-11M operating system.

The following main programs are run sequentially in order:

XMATCH, XIDEN, ANGdif, RESULT

They are most easily run from a command file (see command file example)

Data Files Used in Identification Procedures

DIFDAT - a permanent file containing compositional and crystallographic information on all of the minerals being checked for consistency with the experimental data

MATMIN - a temporary file to transfer reduced data from XMATCH to XIDEN

MATPAT and MATPAU - temporary files to transfer reduced data from

XIDEN and ANGdif

MATPHI - a temporary file to transfer reduced data from ANGdif to RESULT

XINDEX and PHIDAT - temporary files containing the calculations from the electron diffraction analysis and the inter-zone axis angle analysis respectively

RESULT - the final output file as shown in the examples

XMATCH

Program to match X-ray peaks with elements of materials in the
file "DIFDAT".

PARTICLE IDENTIFIER - a description up to 80 chars. in length

ELEMENT SYMBOL, X-RAY PEAK AREA - enter a 2 char. element symbol followed by
a space, and then the X-ray peak area, an
8 char. free format number
- enter END to finish
- a maximum number of 8 elements is allowed

WIDTH OF PARTICLE - enter a real number with free format

In order to obtain quantitative results, the X-ray peak area ratios
obtained for the seven selected elements from the set of mineral standards
(Table 2 of Manual) are required. These seven numbers are entered into the
data statement PRATIO of the program, replacing the seven numbers that are
already there. The procedure is only done once in order to initially
calibrate the system.

The peak area ratios must be ordered in the data statement, so that
they are in the order Na, Mg, Al, K, Ca, Mn and Fe.

e.g. DATA_PRATIO/0.245,0.498,1.110,0.980,0.251,0.785,0.783/

XIDEN

Program for the indexing of electron diffraction spot patterns.

See Section 6.7.2 of Methodology Manual.

DIFFRACTION PATTERN - enter a description up to 80 chars. in length

CAMERA CONSTANT - $\lambda \cdot L (\text{nm} \cdot \text{\AA})$ - enter a real number with free format

DISTANCES OF 5 SPOTS - enter 5 real numbers, each separated by a comma,
with free format

FOUR ANGLES BETWEEN SPOTS - enter 4 real numbers, each separated by a
comma, with free format

More than one diffraction pattern may be entered for the same
particle

ANGDIF

Program which calculates inter-zone axis angles.

ANGLE BETWEEN PATTERNS - enter a free format number

ANGULAR TOLERANCE - enter a free format number

ANALYSIS OF ZONE AXIS ANGULAR DIFFERENCES

MINERAL CROSSITE

PATTERN 1 FIBER 3 PATTERN 32

PATTERN 2 FIBER 3 PATTERN 30

ANGLE= 65.00 ANGULAR TOLERANCE= 8.00

ZONE AXIS ANGULAR DIFFERENCES

A 9.65	B 17.91	C 5.32	ALPHA 90.00	BETA 103.60	GAMMA 90.00
PATTERN 1					
PATTERN 2					
U,V,W U1,V1,W1					
0.	-1.	0.	-4.	-1.	-1.
0.	-1.	0.	4.	-1.	1.
0.	-1.	0.	3.	-1.	6.
0.	-1.	0.	-3.	-1.	-6.
-7.	1.	-6.	-4.	-1.	-1.
-7.	1.	-6.	4.	-1.	1.
-7.	1.	-6.	3.	-1.	6.
-7.	1.	-6.	-3.	-1.	-6.
7.	1.	6.	-4.	-1.	-1.
7.	1.	6.	4.	-1.	1.
7.	1.	6.	3.	-1.	6.
7.	1.	6.	-3.	-1.	-6.

TEMPORARY COMPUTER FILE "PHIDAT"

FIBER 3 PATTERN 32

CAMERA CONSTANT = 83.5000

POSITION TOLERANCE = 0.300 MILLIMETERS (MINIMUM OVER-RIDING TOLERANCE OF
+/- 5.0 PERCENT OF DIFF. DISTANCE PREVAILS)

DIFFRACTED DISTANCES OF SPOTS ARE
16.17 8.71 19.74 15.79 16.18 (MILLIMETERS)

ANGLE TOLERANCE = 2.50 DEGREES

MEASURED ANGLES BETWEEN SPOTS ARE
71.80 123.00 148.30 180.00

AEGIRINE

REAL CELL CONSTANTS

A	B	C	ALPHA	BETA	GAMMA
9.650	8.790	5.290	90.000	107.400	90.000

MAXIMUM INDICES ARE 5 5 3

MAXIMUM DIMENSIONS OF ARRAYS ARE 16 18 16

PROHIBITED REFLECTIONS FOR THE FACE CENTRED CELL TYPE C HAVE BEEN OMITTED

TEMPORARY COMPUTER FILE "XINDEX"

SET 1 ZONE AXIS [0 1 0] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(0 0 2)	2.524	2.499
2	(2 0 0)	4.604	4.639
3	(4 0 -2)	2.030	2.047
4	(2 0 -2)	2.559	2.559
5	(0 0 -2)	2.524	2.497

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 80.812
 (INPUT CAMERA CONSTANT = 83.500)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.154 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 72.60 (MEASURED 71.80) DEGREES
 ANGLE BETWEEN PLANES 1 & 3 = 122.72 (MEASURED 123.00) DEGREES
 ANGLE BETWEEN PLANES 1 & 4 = 147.97 (MEASURED 148.30) DEGREES
 ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

FIBER 3 · PATTERN 32

CAMERA CONSTANT = 83.5000

POSITION TOLERANCE = 0.300 MILLIMETERS (MINIMUM OVER-RIDING TOLERANCE OF
+/- 5.0 PERCENT OF DIFF. DISTANCE PREVAILS)

DIFFRACTED DISTANCES OF SPOTS ARE
16.17 8.71 19.74 15.79 16.18 (MILLIMETERS)

ANGLE TOLERANCE = 2.50 DEGREES

MEASURED ANGLES BETWEEN SPOTS ARE
71.80 123.00 148.30 180.00

CROSSITE

REAL CELL CONSTANTS

A	B	C	ALPHA	BETA	GAMMA
9.647	17.905	5.316	90.000	103.600	90.000

MAXIMUM INDICES ARE 5 9 3

MAXIMUM DIMENSIONS OF ARRAYS ARE 36 21 36

PROHIBITED REFLECTIONS FOR THE FACE CENTRED CELL TYPE C HAVE BEEN OMITTED

3 SETS OF POSSIBLE ZONE AXES INDEX WITHIN SPECIFIED LIMITS

SET 1 ZONE AXIS [0 -1 0] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(2 0 -2)	2.520	2.526
2	(2 0 0)	4.688	4.689
3	(2 0 2)	2.067	2.069
4	(0 0 2)	2.583	2.586
5	(-2 0 2)	2.528	2.524

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 81.680
(INPUT CAMERA CONSTANT = 83.500)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.024 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 71.99 (MEASURED 71.80) DEGREES
ANGLE BETWEEN PLANES 1 & 3 = 123.03 (MEASURED 123.00) DEGREES
ANGLE BETWEEN PLANES 1 & 4 = 148.39 (MEASURED 148.30) DEGREES
ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SET 2 ZONE AXIS [-7 1 -6] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(1 7 0)	2.468	2.547
2	(1 1 -1)	4.865	4.729
3	(1 -5 -2)	2.133	2.087
4	(0 -6 -1)	2.584	2.609
5	(-1 -7 0)	2.468	2.546

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 82.384
(INPUT CAMERA CONSTANT = 83.500)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.489 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 70.10 (MEASURED 71.80) DEGREES
ANGLE BETWEEN PLANES 1 & 3 = 124.47 (MEASURED 123.00) DEGREES
ANGLE BETWEEN PLANES 1 & 4 = 150.04 (MEASURED 148.30) DEGREES
ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SET 3 ZONE AXIS [7 1 6] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(1 -7 0)	2.468	2.547
2	(1 -1 -1)	4.865	4.729
3	(1 5 -2)	2.133	2.087
4	(0 6 -1)	2.584	2.609
5	(-1 7 0)	2.468	2.546

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 82.384
 (INPUT CAMERA CONSTANT = 83.500)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.489 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 70.10 (MEASURED 71.80) DEGREES.
 ANGLE BETWEEN PLANES 1 & 3 = 124.47 (MEASURED 123.00) DEGREES
 ANGLE BETWEEN PLANES 1 & 4 = 150.04 (MEASURED 148.30) DEGREES
 ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

FIBER 3 PATTERN 32

CAMERA CONSTANT = 83.5000

POSITION TOLERANCE = 0.300 MILLIMETERS (MINIMUM OVER-RIDING TOLERANCE OF
+/- 5.0 PERCENT OF DIFF. DISTANCE PREVAILS)

DIFFRACTED DISTANCES OF SPOTS ARE
16.17 8.71 19.74 15.79 16.18 (MILLIMETERS)

ANGLE TOLERANCE = 2.50 DEGREES

MEASURED ANGLES BETWEEN SPOTS ARE
71.80 123.00 148.30 180.00

FE-RICHTERITE

REAL CELL CONSTANTS

A	B	C	ALPHA	BETA	GAMMA
9.820	17.960	5.270	90.000	104.330	90.000

MAXIMUM INDICES ARE 5 9 3

MAXIMUM DIMENSIONS OF ARRAYS ARE 28 25 28

PROHIBITED REFLECTIONS FOR THE FACE CENTRED CELL TYPE C HAVE BEEN OMITTED

3 SETS OF POSSIBLE ZONE AXES INDEX WITHIN SPECIFIED LIMITS

SET 1 ZONE AXIS [0 -1 0] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(2 0 -2)	2.525	2.528
2	(2 0 0)	4.757	4.694
3	(2 0 2)	2.048	2.071
4	(0 0 2)	2.553	2.589
5	(-2 0 2)	2.525	2.527

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 81.762
(INPUT CAMERA CONSTANT = 83.500)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.226 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 73.38 (MEASURED 71.80) DEGREES
ANGLE BETWEEN PLANES 1 & 3 = 124.40 (MEASURED 123.00) DEGREES
ANGLE BETWEEN PLANES 1 & 4 = 149.05 (MEASURED 148.30) DEGREES
ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SET 2 ZONE AXIS [7 1 6] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(1 -7 0)	2.477	2.548
2	(1 -1 -1)	4.861	4.731
3	(1 .5 -2)	2.124	2.087
4	(0 6 -1)	2.582	2.610
5	(-1 7 0)	2.477	2.547

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 82.409
(INPUT CAMERA CONSTANT = 83.500)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.437 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 70.55 (MEASURED 71.80) DEGREES
ANGLE BETWEEN PLANES 1 & 3 = 124.51 (MEASURED 123.00) DEGREES
ANGLE BETWEEN PLANES 1 & 4 = 149.94 (MEASURED 148.30) DEGREES
ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SET 3 ZONE AXIS [-7 1 -6] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(1 7 0)	2.477	2.548
2	(1 1 -1)	4.861	4.731
3	(1 -5 -2)	2.124	2.087
4	(0 -6 -1)	2.582	2.610
5	(-1 -7 0)	2.477	2.547

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 82.409
(INPUT CAMERA CONSTANT = 83.500)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.437 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 70.55 (MEASURED 71.80) DEGREES
ANGLE BETWEEN PLANES 1 & 3 = 124.51 (MEASURED 123.00) DEGREES
ANGLE BETWEEN PLANES 1 & 4 = 149.94 (MEASURED 148.30) DEGREES
ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

FIBER 3 PATTERN 32

CAMERA CONSTANT= 33.5000

POSITION TOLERANCE = 0.300 MILLIMETERS (MINIMUM OVER-RIDING TOLERANCE OF
+/- 5.0 PERCENT OF DIFF. DISTANCE PREVAILS

DIFFRACTED DISTANCES OF SPOTS ARE

16.17 8.71 19.74 15.79 16.18 (MILLIMETERS)

ANGLE TOLERANCE = 2.50 DEGREES

MEASURED ANGLES BETWEEN SPOTS ARE

71.80 123.00 148.30 180.00

RIEBECKITE

REAL CELL CONSTANTS

A	B	C	ALPHA	BETA	GAMMA
9.750	18.000	5.300	90.000	103.000	90.000

MAXIMUM INDICES ARE 5 9 3

MAXIMUM DIMENSIONS OF ARRAYS ARE 32 25 32

PROHIBITED REFLECTIONS FOR THE FACE CENTRED CELL TYPE C HAVE BEEN OMITTED

2 SETS OF POSSIBLE ZONE AXES INDEX WITHIN SPECIFIED LIMITS.

SET 1 ZONE AXIS [0 -1 0] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(2 0 -2)	2.519	2.536
2	(2 0 0)	4.750	4.707
3	(2 0 2)	2.081	2.077
4	(0 0 2)	2.582	2.597
5	(-2 0 2)	2.519	2.534

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 82.000
 (INPUT CAMERA CONSTANT = 83.500)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.119 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 71.89 (MEASURED 71.80) DEGREES
 ANGLE BETWEEN PLANES 1 & 3 = 123.63 (MEASURED 123.00) DEGREES
 ANGLE BETWEEN PLANES 1 & 4 = 148.89 (MEASURED 148.30) DEGREES
 ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SET 2 ZONE AXIS [7 1 6] (SET 2 HAS 2 SYMM. EQUIV. SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(1 -7 0)	2.482	2.552
2	(1 -1 -1)	4.851	4.737
3	(1 5 -2)	2.133	2.090
4	(0 6 -1)	2.594	2.613
5	(-1 7 0)	2.482	2.550

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 82.519
 (INPUT CAMERA CONSTANT = 83.500)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.425 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 70.22 (MEASURED 71.80) DEGREES
 ANGLE BETWEEN PLANES 1 & 3 = 124.17 (MEASURED 123.00) DEGREES
 ANGLE BETWEEN PLANES 1 & 4 = 149.79 (MEASURED 148.30) DEGREES
 ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SYMMETRICALLY EQUIVALENT SOLUTIONS FOR SET 2

ZONE AXIS	POINT 1	POINT 2	POINT 3	POINT 4	POINT 5
[-7 1 -6]	(1 7 0)	(1 1 -1)	(1 -5 -2)	(0 -6 -1)	(-1 -7 0)

FIBER 3 PATTERN 30

CAMERA CONSTANT = 81.5200

POSITION TOLERANCE = 0.300 MILLIMETERS (MINIMUM OVER-RIDING TOLERANCE OF
+/- 5.0 PERCENT OF DIFF. DISTANCE PREVAILS)

DIFFRACTED DISTANCES OF SPOTS ARE
20.25 15.04 16.42 10.52 20.29 (MILLIMETERS)

ANGLE TOLERANCE = 2.50 DEGREES

MEASURED ANGLES BETWEEN SPOTS ARE
30.80 69.70 133.30 180.00

AEGIRINE

REAL CELL CONSTANTS

A	B	C	ALPHA	BETA	GAMMA
9.650	8.790	5.290	90.000	107.400	90.000

MAXIMUM INDICES ARE 6 5 3

MAXIMUM DIMENSIONS OF ARRAYS ARE 32 9 28

PROHIBITED REFLECTIONS FOR THE FACE CENTRED CELL TYPE C HAVE BEEN OMITTED

NO IDENTIFICATION

FIBER 3 PATTERN 30

CAMERA CONSTANT = 81.5200

POSITION TOLERANCE = 0.300 MILLIMETERS (MINIMUM OVER-RIDING TOLERANCE OF
+/- 5.0 PERCENT OF DIFF. DISTANCE PREVAILS)

DIFFRACTED DISTANCES OF SPOTS ARE
20.25 15.04 16.42 10.52 20.29 (MILLIMETERS)

ANGLE TOLERANCE = 2.50 DEGREES

MEASURED ANGLES BETWEEN SPOTS ARE
30.80 69.70 133.30 180.00

CROSSITE

REAL CELL CONSTANTS

A	B	C	ALPHA	BETA	GAMMA
9.647	17.905	5.316	90.000	103.600	90.000

MAXIMUM INDICES ARE 6 10 3

MAXIMUM DIMENSIONS OF ARRAYS ARE 70 20 70

PROHIBITED REFLECTIONS FOR THE FACE CENTRED CELL TYPE C HAVE BEEN OMITTED

4 SETS OF POSSIBLE ZONE AXES INDEX WITHIN SPECIFIED LIMITS

SET 1 ZONE AXIS [-4 -1 -1] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(-2 8 0)	2.020	2.012
2	(-1 5 -1)	2.706	2.710
3	(0 2 -2)	2.482	2.482
4	(1 -3 -1)	3.858	3.874
5	(2 -8 0)	2.020	2.008

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 81.502
(INPUT CAMERA CONSTANT = 81.520)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.051 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 30.74 (MEASURED 30.80) DEGREES
ANGLE BETWEEN PLANES 1 & 3 = 69.66 (MEASURED 69.70) DEGREES
ANGLE BETWEEN PLANES 1 & 4 = 133.23 (MEASURED 133.30) DEGREES
ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SET 2 ZONE AXIS [4 -1 1] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(2 8 0)	2.020	2.012
2	(-1 5 1)	2.706	2.710
3	(0 2 2)	2.482	2.482
4	(-1 -3 1)	3.858	3.874
5	(-2 -8 0)	2.020	2.008

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 81.502
(INPUT CAMERA CONSTANT = 81.520)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.051 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 30.74 (MEASURED 30.80) DEGREES
ANGLE BETWEEN PLANES 1 & 3 = 69.66 (MEASURED 69.70) DEGREES
ANGLE BETWEEN PLANES 1 & 4 = 133.23 (MEASURED 133.30) DEGREES
ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SET 3 ZONE AXIS [3 -1 6] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(4 0 -2)	1.984	2.003
2	(3 3 -1)	2.684	2.697
3	(2 6 0)	2.517	2.471
4	(-1 3 1)	3.858	3.856
5	(-4 0 2)	1.984	1.999

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 81.134
 (INPUT CAMERA CONSTANT = 81.520)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.229 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 29.86 (MEASURED 30.80) DEGREES
 ANGLE BETWEEN PLANES 1 & 3 = 69.06 (MEASURED 69.70) DEGREES
 ANGLE BETWEEN PLANES 1 & 4 = 134.31 (MEASURED 133.30) DEGREES
 ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SET 4 ZONE AXIS [-3 -1 -6] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(4 0 -2)	1.984	2.003
2	(3 -3 -1)	2.684	2.697
3	(2 -6 0)	2.517	2.471
4	(-1 -3 1)	3.858	3.856
5	(-4 0 2)	1.984	1.999

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 81.134
 (INPUT CAMERA CONSTANT = 81.520)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.229 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 29.86 (MEASURED 30.80) DEGREES
 ANGLE BETWEEN PLANES 1 & 3 = 69.06 (MEASURED 69.70) DEGREES
 ANGLE BETWEEN PLANES 1 & 4 = 134.31 (MEASURED 133.30) DEGREES
 ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

FIBER 3 PATTERN 30

CAMERA CONSTANT= 81.5200

POSITION TOLERANCE = 0.300 MILLIMETERS (MINIMUM OVER-RIDING TOLERANCE OF
+/- 5.0 PERCENT OF DIFF. DISTANCE PREVAILS

DIFFRACTED DISTANCES OF SPOTS ARE
20.25 15.04 16.42 10.52 20.29 (MILLIMETERS)

ANGLE TOLERANCE = 2.50 DEGREES

MEASURED ANGLES BETWEEN SPOTS ARE
30.80 69.70 133.30 180.00

FE-RICHTERITE

REAL CELL CONSTANTS

A	B	C	ALPHA	BETA	GAMMA
9.820	17.960	5.270	90.000	104.330	90.000

MAXIMUM INDICES ARE 6 10 3

MAXIMUM DIMENSIONS OF ARRAYS ARE 74 26 74

PROHIBITED REFLECTIONS FOR THE FACE CENTRED CELL TYPE C HAVE BEEN OMITTED

4 SETS OF POSSIBLE ZONE AXES INDEX WITHIN SPECIFIED LIMITS

SET 1 ZONE AXIS [-4 -1 -1]

(NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(-2 8 0)	2.030	2.011
2	(-1 5 -1)	2.701	2.708
3	(0 2 -2)	2.456	2.480
4	(1 -3 -1)	3.860	3.871
5	(2 -8 0)	2.030	2.007

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 81.448
(INPUT CAMERA CONSTANT = 81.520)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.162 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 31.02 (MEASURED 30.80) DEGREES
ANGLE BETWEEN PLANES 1 & 3 = 69.58 (MEASURED 69.70) DEGREES
ANGLE BETWEEN PLANES 1 & 4 = 132.56 (MEASURED 133.30) DEGREES
ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SET 2 ZONE AXIS [4 -1 1]

(NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(2 8 0)	2.030	2.011
2	(1 5 1)	2.701	2.708
3	(0 2 2)	2.456	2.480
4	(-1 -3 1)	3.860	3.871
5	(-2 -8 0)	2.030	2.007

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 81.448
(INPUT CAMERA CONSTANT = 81.520)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.162 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 31.02 (MEASURED 30.80) DEGREES
ANGLE BETWEEN PLANES 1 & 3 = 69.58 (MEASURED 69.70) DEGREES
ANGLE BETWEEN PLANES 1 & 4 = 132.56 (MEASURED 133.30) DEGREES
ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SET 3 ZONE AXIS [3 -1 6] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(4 0 -2)	2.005	2.018
2	(3 3 -1)	2.721	2.718
3	(2 6 0)	2.534	2.489
4	(-1 3 1)	3.860	3.885
5	(-4 0 2)	2.005	2.014

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 81.746
(INPUT CAMERA CONSTANT = 81.520)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.178 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 30.26 (MEASURED 30.80) DEGREES
ANGLE BETWEEN PLANES 1 & 3 = 69.79 (MEASURED 69.70) DEGREES
ANGLE BETWEEN PLANES 1 & 4 = 134.37 (MEASURED 133.30) DEGREES
ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SET 4 ZONE AXIS [-3 -1 -6] (NO SYMMETRICALLY EQUIVALENT SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(4 0 -2)	2.005	2.018
2	(3 -3 -1)	2.721	2.718
3	(2 -6 0)	2.534	2.489
4	(-1 -3 1)	3.860	3.885
5	(-4 0 2)	2.005	2.014

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 81.746
(INPUT CAMERA CONSTANT = 81.520)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.178 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 30.26 (MEASURED 30.80) DEGREES
ANGLE BETWEEN PLANES 1 & 3 = 69.79 (MEASURED 69.70) DEGREES
ANGLE BETWEEN PLANES 1 & 4 = 134.37 (MEASURED 133.30) DEGREES
ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

FIBER 3 PATTERN 30

CAMERA CONSTANT = 81.5200

POSITION TOLERANCE = 0.300 MILLIMETERS (MINIMUM OVER-RIDING TOLERANCE OF
+/- 5.0 PERCENT OF DIFF. DISTANCE PREVAILS

DIFFRACTED DISTANCES OF SPOTS ARE
20.25 15.04 16.42 10.52 20.29 (MILLIMETERS)

ANGLE-TOLERANCE = 2.50 DEGREES

MEASURED ANGLES BETWEEN SPOTS ARE

30.80 69.70 133.30 180.00

RIEBECKITE

REAL CELL CONSTANTS

A	B	C	ALPHA	BETA	GAMMA
9.750	18.000	5.300	90.000	103.000	90.000

MAXIMUM INDICES ARE 6 10 3

MAXIMUM DIMENSIONS OF ARRAYS ARE 74 24 74

PROHIBITED REFLECTIONS FOR THE FACE CENTRED CELL TYPE C HAVE BEEN OMITTED

3 SETS OF POSSIBLE ZONE AXES INDEX WITHIN SPECIFIED LIMITS

SET 1 ZONE AXIS [4 -1 1] (SET 1 HAS 2 SYMM. EQUIV. SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(2 8 0)	2.033	2.019
2	(1 5 1)	2.723	2.719
3	(0 2 2)	2.482	2.490
4	(-1 -3 1)	3.858	3.887
5	(-2 -8 0)	2.033	2.015

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 81.774
 (INPUT CAMERA CONSTANT = 81.520)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.112 MILLIMETRES
 ANGLE BETWEEN PLANES 1 & 2 = 31.03 (MEASURED 30.80) DEGREES
 ANGLE BETWEEN PLANES 1 & 3 = 70.01 (MEASURED 69.70) DEGREES
 ANGLE BETWEEN PLANES 1 & 4 = 133.08 (MEASURED 133.30) DEGREES
 ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SYMMETRICALLY EQUIVALENT SOLUTIONS FOR SET 1

ZONE AXIS	POINT 1	POINT 2	POINT 3	POINT 4	POINT 5
[-4 -1 -1]	(-2 8 0)	(-1 5 -1)	(0 2 -2)	(1 -3 -1)	(2 -8 0)

SET 2 ZONE AXIS [3 -1 6] (SET 2 HAS 2 SYMM. EQUIV. SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(4 0 -2)	1.985	2.009
2	(3 3 -1)	2.697	2.704
3	(2 6 0)	2.536	2.477
4	(-1 3 1)	3.858	3.866
5	(-4 0 2)	1.985	2.005

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 81.345
 (INPUT CAMERA CONSTANT = 81.520)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.273 MILLIMETRES
 ANGLE BETWEEN PLANES 1 & 2 = 29.82 (MEASURED 30.80) DEGREES
 ANGLE BETWEEN PLANES 1 & 3 = 69.28 (MEASURED 69.70) DEGREES
 ANGLE BETWEEN PLANES 1 & 4 = 134.66 (MEASURED 133.30) DEGREES
 ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SYMMETRICALLY EQUIVALENT SOLUTIONS FOR SET 2

ZONE AXIS	POINT 1	POINT 2	POINT 3	POINT 4	POINT 5
[-3 -1 -6]	(4 0 -2)	(3 -3 -1)	(2 -6 0)	(-1 -3 1)	(-4 0 2)

SET 3 ZONE AXIS [9 -1 6] (SET 3 HAS 2 SYMM. EQUIV. SOL'NS)

POINT	PLANE	DSPACE	ESTIMATED DSPACE FROM DIFF. PATTERN
1	(-1 -9 0)	1.957	1.967
2	(0 -6 -1)	2.594	2.648
3	(1 -3 -2)	2.422	2.425
4	(1 3 -1)	3.858	3.786
5	(1 9 0)	1.957	1.963

BEST FIT CAMERA CONSTANT USED IN ABOVE ESTIMATES OF D SPACINGS = 79.647
(INPUT CAMERA CONSTANT = 81.520)

MEAN DEVIATION OF MEASURED SPOTS FROM TRUE POSITIONS = 0.318 MILLIMETRES

ANGLE BETWEEN PLANES 1 & 2 = 29.61 (MEASURED 30.80) DEGREES
ANGLE BETWEEN PLANES 1 & 3 = 67.30 (MEASURED 69.70) DEGREES
ANGLE BETWEEN PLANES 1 & 4 = 132.71 (MEASURED 133.30) DEGREES
ANGLE BETWEEN PLANES 1 & 5 = 180.00 (MEASURED 180.00) DEGREES

SYMMETRICALLY EQUIVALENT SOLUTIONS FOR SET 3

ZONE AXIS	POINT 1	POINT 2	POINT 3	POINT 4	POINT 5
[-9 -1 -6]	(-1 9 0)	(0 6 -1)	(1 3 -2)	(1 -3 -1)	(1 -9 0)

C PROGRAM XMATCH
 C PROGRAM TO MATCH XRAY PEAKS WITH ELEMENTS OF MATERIALS
 C IN FILE DIFDAT.
 C WRITTEN BY W.R. STOTT, DEPT OF APPLIED PHYSICS
 C ONTARIO RESEARCH FOUNDATION, MISSISSAUGA, ONT., CANADA
 C 1982 MAY 5
 REAL*8 NAME(4),FORMUL(6)
 INTEGER ELEM(8),SYM,ELEMS(8),MANEL(8),IELEM(100)
 REAL LOWER(8),UPPER(8),A,B,C,ALPHA,BETA,GAMMA,AREAS(8)
 & ,FQUAN(4,7),PRATIO(7),CON(8),PARTIC(20),RATIO(8)
 BYTE ANSWER
 DATA IELEM/10*0,1,2,3,5*0,4,5,4*0,6,7,74*0/
 DATA FQUAN/0.384,0.386,0.422,0.447,
 & 1.319,1.343,1.324,1.373,
 & 1.023,1.046,1.113,1.113,
 & 0.236,0.236,0.236,0.234,
 & 1.085,1.086,1.046,0.998,
 & 0.497,0.494,0.468,0.442,
 & 0.470,0.467,0.442,0.388/
 DATA PRATIO/.11,0.756,0.772,0.255,1.148,0.419,0.421/
 C FQUAN ARE QUANTITATIVE CONSTANTS FROM MEASURED STANDARDS.
 C IN ORDER TO OBTAIN QUANTITATIVE RESULTS, THE X-RAY PEAK
 C AREA RATIOS TO SILICON FROM THE STANDARDS (AS LISTED
 C IN THE METHODOLOGY MANUAL, TABLE 2) ARE REQUIRED.
 C THE PEAK AREA RATIOS THAT ARE OBTAINED ON YOUR INSTRUMENT
 C ARE ENTERED INTO THE DATA STATEMENT PRATIO FOR THE SEVEN
 C ELEMENTS IN ORDER.
 NA,MG,AL,K,CA,MN,FE
 OPEN(UNIT=1,NAME='DIFDAT.',TYPE='OLD',READONLY)
 OPEN(UNIT=2,NAME='MATMIN.',TYPE='NEW')
 IPTR=5
 WRITE(IPTR,510)
 510 FORMAT(' ENTER PARTICLE IDENTIFIER (80 CHARACTERS)',//)
 READ(5,520) (PARTIC(I),I=1,20)
 520 FORMAT(20A4)
 530 WRITE(IPTR,540)
 540 FORMAT(' ENTER ELEMENT SYMBOL (2 LETTER),SPACE,X-RAY PEAK AREA',
 & '(IF AVAILABLE)',/, ' ENTER END TO FINISH ',
 & '(8 ELEMENTS MAXIMUM)',//)
 SIPK=0.0
 NUMPK=0
 550 READ(5,560) SYMBOL,ADATA
 560 FORMAT(A2,1X,F8.0)
 IF(SYMBOL.EQ.'EN') GOTO 570
 NUMPK=NUMPK+1
 IFLAG=0
 ELEMS(NUMPK)=ITOMNR(SYMBOL,IFLAG)
 IF(IFLAG.EQ.1) GOTO 530
 AREAS(NUMPK)=ADATA
 IF(ELEMS(NUMPK).EQ.14) SIPK=AREAS(NUMPK)
 GOTO 550
 570 IF(SIPK.EQ.0.0) GOTO 590

```

580 WRITE(IPTR,580)
      FORMAT(' ENTER WIDTH OF PARTICLE (MICROMETERS)')
      READ(IPTR,*) WIDTH
      IWIDTH=1
      IF(WIDTH.GE.0.25) IWIDTH=2
      IF(WIDTH.GE.0.5) IWIDTH=3
      IF(WIDTH.GE.1.0) IWIDTH=4
590 IF(NUMPK.EQ.0) GOTO 730
      DO 595 I=1,NUMPK
      K=IELEM(ELEMS(I))
      IF (K.EQ.0.OR.SIPK.EQ.0.0)GOTO 593
      RATIO(I)=AREAS(I)*FQUAN(IWIDTH,K)/PRATIO(K)/SIPK
      GOTO 595
593 RATIO(I)=0.0
      IF(IELEM(I).EQ.14.AND.SIPK.NE.0.0)RATIO(I)=1.0
595 CONTINUE
      WRITE(2,596) (PARTIC(I),I=1,20),NUMPK,WIDTH,(RATIO(I),I=1,NUMPK)
596 FORMAT(1X,20A4,I4,F8.3,8F5.3)
      WRITE(2,597) (ELEMS(I),AREAS(I),I=1,NUMPK)
597 FORMAT(1X,8(I4,F8.2))
C      READ DATA FROM DIFDAT. FILE
      READ(1,400,END=730) (NAME(I),I=1,4),(FORMUL(I),I=1,6)
      READ(1,410)(ELEM(I),LOWER(I),UPPER(I),I=1,8)
      READ(1,420)A,B,C,ALPHA,BETA,GAMMA,SYM
      DO 620 I=1,NUMPK
620 MANEL(I)=0
      NUMNOT=0
      NUMAN=0
      SIATOM=100.0
      DO 630 I=1,4
      IF(ELEM(I).EQ.14) SIATOM=(LOWER(I)+UPPER(I))/2
630 CONTINUE
C      EXTRACT MANDATORY ELEMENTS
      DO 650 I=1,4
      IF(ELEM(I).LT.11)GOTO 650
      NUMAN=NUMAN+1
      ELEM(NUMAN)=ELEM(I)
650 CONTINUE
C      IF(NUMAN.GT.NUMPK) GOTO 600
      MATCH MANDATORY PEAKS AND ELEMENTS
C      GET NEW MATERIAL IF NOT MATCHED
      DO 660 J=1,NUMAN
      DO 655 I=1,NUMPK
      K=I
      K1=IELEM(ELEMS(I))
      IF(SIPK.EQ.0.0.OR.K1.EQ.0) GOTO 653
      CONC=RATIO(I)*SIATOM
      IF(ELEM(J).EQ.ELEMS(I)) GOTO 658
653 CONTINUE
      IF(LOWER(J).NE.0.0)GOTO 600
      NUMNOT=NUMNOT+1
      IF(NUMNOT.GT.1)GOTO 600

```

```

658      GOTO 660
        IF(SIPK.EQ.0.0.OR.K1.EQ.0) GOTO 659
        CONLIM=0.2
        IF(ELEM(J).EQ.11)CONLIM=0.5
        IF( CONC.LT.(LOWER(J)*(1.-CONLIM)).OR.
            CONC.GT.((1.+CONLIM)*UPPER(J)))GOTO 600
&       MANEL(K)=1
659      CONTINUE
660      MATCH OPTIONAL ELEMENTS AND PEAKS
C         GET NEW MATERIAL IF NOT MATCHED
C
        NUMOP=4
        NUMNOT=0
        NUSED=0
        DO 690 I=5,8
        IF(ELEM(I).LT.11)GOTO 690
        NUMOP=NUMOP+1
        ELEM(NUMOP)=ELEM(I)
690      CONTINUE
        DO 700 I=1,NUMPK
        IF(MANEL(I).EQ.1) GOTO 700
        K1=IELEM(ELEMS(I))
        FAIL=1.0
        CONC=RATIO(I)*SIATOM
        DO 695 J=5,NUMOP
        CONLIM=0.2
        IF(ELEM(J).EQ.11)CONLIM=0.5
        J1=J
        IF(ELEM(J).EQ.ELEMS(I)) NUSED=NUSED+1
        IF(ELEM(J).EQ.ELEMS(I)) GOTO 698
        CONTINUE
        IF(SIPK.EQ.0.0) NUMNOT=NUMNOT+1
        FAIL=0.0
698      IF(SIPK.EQ.0.0.OR.K1.EQ.0) GOTO 699
        IF( CONC.GT.((1.+CONLIM)*FAIL*UPPER(J1))) NUMNOT=NUMNOT+1
        IF( CONC.GT.(FAIL*UPPER(J1)+0.125*SIATOM)) GOTO 600
C         TWO SPECTRAL ELEMENTAL DISCREPANCIES ARE ALLOWED
699      IF(NUMNOT.GT.2)GOTO 600
700      CONTINUE
        NUMNOT=NUMNOT+NUMOP-NUSED-4
C         UP TO A TOTAL OF THREE MATCHING FAILURES OF SPECTRAL
C         ELEMENTS PLUS OPTIONAL ELEMENTS ARE ALLOWED
        IF(NUMNOT.GT.3)GOTO 600
C         STORE MATCHED MATERIAL
720      WRITE(2,400) (NAME(I),I=1,4),(FORMUL(I),I=1,6)
        WRITE(2,410) (ELEM(I),LOWER(I),UPPER(I),I=1,8)
        WRITE(2,420) A,B,C,ALPHA,BETA,GAMMA,SYM
        GOTO 600
730      CLOSE(UNIT=1)
        CLOSE(UNIT=2)
        CALL EXIT
400      FORMAT('?',10A8)
410      FORMAT(1X,8(I2,2F5.2))

```

420

FORMAT(1X,6F7.3,I1)

END

```
FUNCTION ITOMNR(SYMBOL,IFLAG)
INTEGER SYMBOL,CS(100),SS(17)
DIMENSION NUM(17)
```

```
DATA CS/' H ', ' HE ', ' LI ', ' BE ', ' B ', ' C ', ' N ', ' O ', ' F ', ' NE ', ' NA ',
& ' MG ', ' AL ', ' SI ', ' P ', ' S ', ' CL ', ' AR ', ' K ', ' CA ', ' SC ', ' TI ', ' V ', ' CR ',
& ' MN ', ' FE ', ' CO ', ' NI ', ' CU ', ' ZN ', ' GA ', ' GE ', ' AS ', ' SE ', ' BR ', ' KR ', ' RB ',
& ' SR ', ' Y ', ' ZR ', ' NB ', ' MO ', ' TC ', ' RU ', ' RH ', ' PD ', ' AG ', ' CD ', ' IN ', ' SN ',
& ' SB ', ' TE ', ' I ', ' XE ', ' CS ', ' BA ', ' LA ', ' CE ', ' PR ', ' ND ', ' PM ', ' SM ', ' EU ',
& ' GD ', ' TB ', ' DY ', ' HO ', ' ER ', ' TM ', ' YB ', ' LU ', ' HF ', ' TA ', ' W ', ' RE ', ' OS ',
& ' IR ', ' PT ', ' AU ', ' HG ', ' TL ', ' PB ', ' BI ', ' PO ', ' AT ', ' RN ', ' FR ', ' RA ', ' AC ',
& ' TH ', ' PA ', ' U ', ' NP ', ' PU ', ' AM ', ' CM ', ' BK ', ' CF ', ' ES ', ' FM ', ' SS / ' H ' ,
& ' B ', ' C ', ' N ', ' O ', ' F ', ' P ', ' S ', ' A ', ' K ', ' V ', ' Y ', ' I ', ' W ',
& ' U ', ' A ', ' CB '/,NUM/1,5,6,7,8,9,15,16,18,19,23,39,53,74,92,18,41/
```

DO 1 I=1,100

IF(SYMBOL.EQ.CS(I)) GO TO 5

1 CONTINUE

DO 2 I=1,17

IF(SYMBOL.EQ.SS(I)) GO TO 4

2 CONTINUE

TYPE 3, SYMBOL

3 FORMAT (3X,'NO MATCH FOUND FOR ',A2,'. TRY AGAIN.')

IFLAG=1

RETURN

4 SYMBOL=CS(NUM(I))

I=NUM(I)

5 ITOMNR=I

RETURN

END

C * A COMPUTER PROGRAM FOR THE INDEXING OF ELECTRON DIFFRACTION
 C * SPOT PATTERNS BY B.L. RHOADES - DEPARTMENT OF MECHANICAL
 C * ENGINEERING, UNIVERSITY OF CANTERBURY, NEW ZEALAND
 C *
 C MODIFIED BY W.R. STOTT TO CHAIN WITH AMPHIBOLE IDENTIFICATION
 C PROGRAMS XMATCH XIDEN ANGDIF RESULT
 C SYM IS A CONTROL VARIABLE FOR THE REMOVAL OF PROHIBITED
 C REFLECTIONS
 C
 C 0 FOR PRMITIVE CELL TYPE P
 C 1 FOR ALL FACES CENTRED TYPE F
 C 2 FOR BODY CENTRED CELL TYPE I
 C 3 FOR A FACE CENTRED CELL TYPE A
 C 4 FOR B FACE CENTRED CELL TYPE B
 C 5 FOR C FACE CENTRED CELL TYPE C
 C 6 FOR OBVERSE RHOMB (HEX CELL) TYPE R
 C 7 FOR REVERSE RHOMB (HEX CELL) TYPE R
 C
 C PROGRAM XIDEN
 COMMON ANGLES(4),DIST(5),LE,LES,KT,D2,D4,ANGACT(4),CAMCO
 & ,KSETS,I2OS(3,50)
 COMMON/DIFF/NAME(4),PHOTO(20),A,B,C,ALPHA,BETA,GAMMA,IFILE
 INTEGER READR,PRINTR,H,HMAX,PMAX,QMAX,RMAX,SMAX,TMAX,SYM,SYMI,
 & P,Q,R,ELEM(8)
 DOUBLE PRECISION DSQ2,DSQ4,RDR
 DOUBLE PRECISION A,B,C,PI180,V,DMAX,DSQ,ASTAR,BSTAR
 DOUBLE PRECISION CSTAR,SINA,SINB,SING,COSA,COSB,COSG,COSAS
 DOUBLE PRECISION COSBS,COSGS,A11,A12,A13,A22,A23,A33,DMIN
 DIMENSION IH(5),IK(5),IL(5)
 VIRTUAL RADIX(5,50),DISTIX(5,50)
 VIRTUAL RAD(3,801),IND(3,3,801),DISTX(5),DISTN(5)
 REAL LOWER(8),UPPER(8),PARTIC(20)
 REAL*8 NAME,FORMUL(6)
 BYTE ANSWER
 IRAD=3
 JRAD=801
 IRADIX=5
 JRADIX=50
 IFLAG=0
 AMTOL=0.05
 PAMTOL=AMTOL*100.
 ANGTOL=2.5
 BPR=57.295780
 12 PI180=3.1415926535897932/180.
 OPEN(UNIT=2,NAME='XINDEX',TYPE='NEW')
 OPEN(UNIT=3,NAME='MATMIN.',TYPE='OLD',READONLY)
 OPEN(UNIT=4,NAME='MATPAT.',TYPE='NEW')
 OPEN(UNIT=1,NAME='MATPAU.',TYPE='NEW')
 PRINTR=2
 IFILE=4
 IPAT=0
 WRITE(5,640)

```

640      FORMAT(1X, ' POSSIBLE SOLUTIONS ', /,
&      10X, 'MINERAL', 18X, 'CELL CONSTANTS', //)
NUMMAT=0
READ(3,401) (PARTIC(I),I=1,20),NUMPK
401      FORMAT(1X,20A4,I4)
READ(3,401)
599      READ(3,400,END=610)(NAME(I),I=1,4),(FORMUL(I),I=1,6)
READ(3,410,END=610) (ELEM(I),LOWER(I),UPPER(I),I=1,8)
READ(3,420,END=610) A,B,C,ALPHA,BETA,GAMMA,SYM
400      FORMAT(1X,10A8)
410      FORMAT(1X,8(I2,2F5.2))
420      FORMAT(1X,6F7.3,I1)
WRITE(5,430) (NAME(I),I=1,3),A,B,C,ALPHA,BETA,GAMMA
430      FORMAT(1X,3A8,6F7.3)
NUMMAT=NUMMAT+1
GOTO 599
610      IF(NUMMAT.EQ.0)GOTO 9999
REWIND 3
TYPE 620
620      FORMAT(1X,'DO YOU WISH TO ANALYZE ELECTRON DIFFRACTION PATTERN(S)?')
READ(5,108) ANSWER
IF(ANSWER.EQ.'N') GOTO 9999
C*
C*      ****READ DETAILS OF DIFFRACTION PATTERN
C*
2      READR=5
WRITE (5,533)
C*
11      TYPE 402
402      FORMAT(/,' DETAILS OF DIFFRACTION PATTERN (80 CHARACTERS)',//)
READ(3,401) (PARTIC(I),I=1,20),NUMPK
READ(3,401)
IPAT=IPAT+1
NUMPAT=0
READ(5,101)(PHOTO(I),I=1,20)
C*
C      CAMCO= A*D/(H**2+K**2+L**2)**0.5
C      A IS GOLD CELL CONSTANT IN ANGSTROMS 4.0783
C      D IS DIAMETER OF GOLD RING (H,K,L) IN MM
C      AN ACCURATE MEASURE OF CAMCO IS MANDATORY IN ORDER TO
C      OBTAIN GOOD RESULTS
TYPE 404
404      FORMAT(/,' CAMERA CONSTANT( LAMBDA*L (mm*A))?', '$)
READ(READR,*) CAMCO
TOL=0.30
IOUT=1
TYPE 406
406      FORMAT(/,' DISTANCES OF 5 SPOTS? ', '$)
READ(READR,*)(DIST(N),N=1,5 )
IF (DIST(4).EQ.0.0) GO TO 120
110 LE=5
GO TO 130

```

```

120 LE=3
130 LES=LE-1
        TYPE 408
408   FORMAT( /, ' FOUR ANGLES BETWEEN SPOTS? ', $)
      READ(READR,*)(ANGLES(MM),MM=1,4)
      DO 135 MM=1,LES
      IF(ANGLES(MM).LT.0.0) ANGLES(MM)=ANGLES(MM)+360.0
      ANGLES(MM)=AMOD(ANGLES(MM),360.0)
      IF(ANGLES(MM).GT.180.0) ANGLES(MM)=360.0-ANGLES(MM)
135   CONTINUE
      3 DO 5 N=1,5
      IF(TOL-(DIST(N)*AMTOL)) 14,4,4
14    DISTN(N)=DIST(N)-(DIST(N)*AMTOL)
      DISTX(N)=DIST(N)+(DIST(N)*AMTOL)
      GO TO 5
      4 DISTN(N)=DIST(N)-TOL
      DISTX(N)=DIST(N)+TOL
      5 CONTINUE
C*   ****READ DETAILS OF MATERIALS
C*   ****COMPUTE RECIPROCAL CONSTANTS
C*   SINA=DSIN(ALPHA*PI180)
C*   SINB=DSIN(BETA*PI180)
C*   SING=DSIN(GAMMA*PI180)
C*   COSA=DCOS(ALPHA*PI180)
C*   COSB=DCOS(BETA*PI180)
C*   COSTG=DCOS(GAMMA*PI180)
C*   V=1./(A*B*C*DSQRT(1.+2.*COSA*COSB*COSG-COSA*COSA-COSB*COSB
C*   &-COSG*COSG))
C*   ASTAR=B*C*V*SINA
C*   BSTAR=A*C*V*SINB
C*   CSTAR=A*B*V*SING
C*   COSAS=(COSB*COSG-COSA)/(SINB*SING)
C*   COSBS=(COSA*COSG-COSB)/(SINA*SING)
C*   COSGS=(COSA*COSB-COSG)/(SINA*SINB)
C*   A11=ASTAR*ASTAR
C*   A22=BSTAR*BSTAR
C*   A33=CSTAR*CSTAR
C*   A12=2.*ASTAR*BSTAR*COSGS
C*   A13=2.*ASTAR*CSTAR*COSBS
C*   A23=2.*BSTAR*CSTAR*COSAS
C*   ****DETERMINE LIMITS OF INDICES

```

```

6 DISTMX=DISTX(1)
7 DO 9 N=2,5
8 IF(DISTMX.GT.DISTX(N)) GO TO 9
    DISTMX=DISTX(N)
9 CONTINUE
DMIN=CAMCO/(2.*DISTMX)
DMIN=DMIN*DMIN
DMAX=DSQRT(1./DMIN)
HMAX=(DMAX/(ASTAR*DSQRT(1.-COSBS*COSBS)*SING))+1.
KMAX=(DMAX/(BSTAR*DSQRT(1.-COSGS*COSGS)*SINA))+1.
LMAX=(DMAX/(CSTAR*DSQRT(1.-COSAS*COSAS)*SINB))+1.

C*
C* ****GENERATE RECIPROCAL VECTORS
C*
PMAX=0
RMAX=0
TMAX=0
LIST3=0
NHMAX=2*HMAX+1
NKMAX=2*KMAX+1
NLMAX=2*LMAX+1
DO 72 NH=1,NHMAX
H=(HMAX+1)-NH
DO 74 NK=1,NKMAX
K=(KMAX+1)-NK
DO 75 NL=1,NLMAX
L=(LMAX+1)-NL
L=(LMAX+1)-NL
IF(H.EQ.0.AND.K.EQ.0.AND.L.EQ.0) GO TO 15
IF(H.EQ.0.AND.K.EQ.0.AND.L.EQ.0) GO TO 15
CALL PROHIB (SYMI,H,K,L,INC)
    IF(INC-1) 17,73,73
15 LIST3=1
    GO TO 73
17 DSQ=H*H*A11+H*K*A12+H*L*A13+K*K*A22+K*L*A23+L*L*A33
    RDR=DSQRT(DSQ)
    D=SNGL(1.0/RDR)
    RADI=CAMCO/(2.*D)
    DO 70 N=1,5,2
        IF(RADI-DISTN(N)) 70,19,19
19    IF(RADI-DISTX(N)) 20,20,70
20    IF(N-1) 40,21,22
21    PMAX=PMAX+1
    M=PMAX
    GO TO 40
22    IF(N-3) 40,25,26
25    IF(LIST3.EQ.1) GO TO 70
    RMAX=RMAX+1
    M=RMAX
    GO TO 40
26    TMAX=TMAX+1
    M=TMAX
40    NN=(N+1)/2
    IND(NN,1,M)=H

```

```

IND(NN,2,M)=K
IND(NN,3,M)=L
RAD(NN,M)=D
IF(PMAX.GT.800.OR.RMAX.GT.800.OR.TMAX.GT.800) GO TO 2018
70 CONTINUE
73 CONTINUE
75 CONTINUE
74 CONTINUE
72 CONTINUE
GO TO 71
2018 WRITE(5,218)
GO TO 10
C*
C* *****FORMAT STATEMENTS ----INPUT
C*
101 FORMAT(20A4)
C 102 FORMAT(F8.4,F6.3,I1)
C 104 FORMAT(3F10.3,3F10.2)
C 105 FORMAT(I1)
C 106 FORMAT(4F8.2)
107 FORMAT(I1,9A8)
108 FORMAT(A1)
C*
C* *****FORMAT STATEMENTS ----OUTPUT
C*
201 FORMAT('1',2X,20A4)
205 FORMAT(//-/1X,4A8)
533 FORMAT(/,6X,31H PROGRAM CRYSTAL IDENTIFICATION)
218 FORMAT(/,' ARRAY LIMITS EXCEEDED--MATERIAL CHECK CANCELLED')
71 WRITE(PRINTR,201) (PHOTO(N),N=1,20)
    WRITE(PRINTR,221)
    WRITE(PRINTR,221)
    WRITE(PRINTR,221)
    WRITE(PRINTR,202) CAMCO
    WRITE(PRINTR,203) TOL,PAMTOL
    WRITE(PRINTR,204)(DIST(K),K=1,5)
    WRITE(PRINTR,219) ANGTOL
    WRITE(PRINTR,220) (ANGLES(MM),MM=1,4)
    WRITE(PRINTR,205) (NAME(N),N=1,4)
    WRITE(PRINTR,221)
    WRITE(PRINTR,206)
    WRITE(PRINTR,207) A,B,C,ALPHA,BETA,GAMMA
        WRITE(PRINTR,532) HMAX,KMAX,LMAX
    WRITE(PRINTR,208) PMAX,RMAX,TMAX
    GO TO (38,31,32,33,34,35,36,37),SYMI
31 WRITE(PRINTR,534)
    GO TO 38
32 WRITE(PRINTR,535)
    GO TO 38
33 WRITE(PRINTR,536)
    GO TO 38
34 WRITE(PRINTR,537)

```

```

GO TO 38
35 WRITE(PRINTR,538)
GO TO 38
36 WRITE(PRINTR,539)
GO TO 38
37 WRITE(PRINTR,540)
38 IF(DIST(4)) 43,43,44
43 IF(PMAX.EQ.0.OR.RMAX.EQ.0) GOTO 1007
44 IF(PMAX.EQ.0.OR.RMAX.EQ.0.OR.TMAX.EQ.0) GOTO 1007
C*
C*      ****FORMAT STATEMENTS ——OUTPUT
C*
202 FORMAT(/,' CAMERA CONSTANT= ',F8.4)
203 FORMAT(/,' POSITION TOLERANCE = ',F6.3,' MILLIMETERS (MINIMUM',
  &' OVER-RIDING TOLERANCE OF ',/,' +/- ',F3.1,
  &' PERCENT OF DIFF. DISTANCE PREVAILS')
204 FORMAT(/,' DIFFRACTED DISTANCES OF SPOTS ARE ',/,'5F10.2,'
  & '(MILLIMETERS)')
206 FORMAT(//,1X,' REAL CELL CONSTANTS'//7X,'A',8X,'B',8X,'C',
  &6X,'ALPHA',5X,'BETA',4X,'GAMMA')
207 FORMAT(1X,6F9.3)
208 FORMAT(//,1X,' MAXIMUM DIMENSIONS OF ARRAYS ARE ',5I6)
219 FORMAT(/,' ANGLE TOLERANCE = ',F5.2,' DEGREES')
220 FORMAT(/,' MEASURED ANGLES BETWEEN SPOTS ARE ',/,'4F10.2)
221 FORMAT(' *********')
532 FORMAT(//,2X,19HMAXIMUM INDICES ARE,3I4)
534 FORMAT(/,1X,' PROHIBITED REFLECTIONS FOR THE FACE CENTRED',
  &' CELL TYPE F HAVE BEEN OMITTED')
535 FORMAT(/,1X,' PROHIBITED REFLECTIONS FOR THE BODY CENTRED',
  &' CELL TYPE I HAVE BEEN OMITTED')
536 FORMAT(/,1X,' PROHIBITED REFLECTIONS FOR THE FACE CENTRED',
  &' CELL TYPE A HAVE BEEN OMITTED')
537 FORMAT(/,1X,' PROHIBITED REFLECTIONS FOR THE FACE CENTRED',
  &' CELL TYPE B HAVE BEEN OMITTED')
538 FORMAT(/,1X,' PROHIBITED REFLECTIONS FOR THE FACE CENTRED',
  &' CELL TYPE C HAVE BEEN OMITTED')
539 FORMAT(/,1X,' PROHIBITED REFLECTIONS FOR THE OBVERSE RHOMBO'
  &' HEDRON (HEXAGONAL CELL) TYPE R HAVE BEEN OMITTED')
540 FORMAT(/,1X,' PROHIBITED REFLECTIONS FOR THE REVERSE RHOMBO'
  &' HEDRON (HEXAGONAL CELL) TYPE R HAVE BEEN OMITTED')

```

```

C
C      ***** DETERMINE INDICES OF POINT '2'
C

```

```

DO 1002 I=1,PMAX
DO 1003 K=1,RMAX
ZHB=(IND(1,1,I)+IND(2,1,K))/2.
NHB=ZHB
AZHB=NHB
IF(ZHB-AZHB) 1003,96,1003
96 ZKB=(IND(1,2,I)+IND(2,2,K))/2.
NKB=ZKB
AZKB=NKB

```

```

IF(ZKB-AZKB) 1003,97,1003
97 ZLB=(IND(1,3,I)+IND(2,3,K))/2.
NLB=ZLB
AZLB=NLB
IF(ZLB-AZLB) 1003,98,1003
98 IF(NHB.EQ.0.AND.NKB.EQ.0.AND.NLB.EQ.0) GO TO 1003
CALL PROHIB (SYMI,NHB,NKB,NLB,INC)
IF(INC-1) 99,1003,1003

C*
C* ****CHECK POINT '2' IS WITHIN LIMITS OF RADIUS
C*
99 DSQ2=NHB*NHB*A11+NHB*NKB*A12+NHB*NLB*A13+NKB*NKB*A22+NKB*NLB
&*A23+NLB*NLB*A33
D2=SNGL(DSQRT(1./DSQ2))
RADI2=CAMCO/(2.*D2)
IF(RADI2.GE.DISTN(2).AND.RADI2.LE.DISTX(2)) GO TO 151
GO TO 1003

C*
C* ****DETERMINE INDICES OF POINT '4'
C*
151 CONTINUE
DO 1001 M=1,TMAX
IF((M.EQ.1).AND.(DIST(4).EQ.0.0)) GO TO 159
ZHD=(IND(2,1,K)+IND(3,1,M))/2.
NHD=ZHD
AZHD=NHD
IF(ZHD-AZHD) 1001,153,1001
153 ZKD=(IND(2,2,K)+IND(3,2,M))/2.
NKD=ZKD
AZKD=NKD
IF(ZKD-AZKD) 1001,154,1001
154 ZLD=(IND(2,3,K)+IND(3,3,M))/2.
NLD=ZLD
AZLD=NLD
IF(ZLD-AZLD) 1001,155,1001
155 IF(NHD.EQ.0.AND.NKD.EQ.0.AND.NLD.EQ.0) GO TO 1001
CALL PROHIB (SYMI,NHD,NKD,NLD,INC)
IF (INC-1) 156,1001,1001

C*
C* ****CHECK POINT '4' IS WITHIN LIMITS OF RADIUS
C*
156 DSQ4=NHD*NHD*A11+NHD*NKD*A12+NHD*NLD*A13+NKD*NKD*A22+NKD*
&NLD*A23+NLD*NLD*A33
D4=SNGL(DSQRT(1./DSQ4))
RADI4=CAMCO/(2.*D4)
IF(RADI4.GE.DISTN(4).AND.RADI4.LE.DISTX(4)) GO TO 158
GO TO 1001

C*
C* ****SORT PLANES INTO ARRAYS
C*
159 L=1
158 IH(1)=IND(1,1,I)

```

```

IH(2)=NHB
IH(3)=IND(2,1,K)
IH(4)=NHD
IH(5)=IND(3,1,M)
IK(1)=IND(1,2,I)
IK(2)=NKB
IK(3)=IND(2,2,K)
IK(4)=NKD
IK(5)=IND(3,2,M)
IL(1)=IND(1,3,I)
IL(2)=NLB
IL(3)=IND(2,3,K)
IL(4)=NLD
IL(5)=IND(3,3,M)

```

```

C*
C*      ****CALCULATE ANGLES BETWEEN PLANES
C*
MM=0
II=1
160 IF(DIST(4)) 161,161,162
161 NZ=3
    GO TO 163
162 NZ=5
163 DO 170 NN=2,NZ
    S=((IH(II)*IH(NN)*ASTAR*ASTAR)+(IK(II)*IK(NN)*BSTAR*BSTAR)
    &+(IL(II)*IL(NN)*CSTAR*CSTAR)+((IK(II)*IL(NN)+IL(II)*IK(NN))*BSTAR*
    &CSTAR*COSAS)+((IL(II)*IH(NN)+IL(NN)*IH(II))*CSTAR*ASTAR*COSBS)+
    &((IH(II)*IK(NN)+IK(II)*IH(NN))*ASTAR*BSTAR*COSGS))
    T=((IH(II)*IH(II)*ASTAR*ASTAR)+(IK(II)*IK(II)*BSTAR*BSTAR)
    &+(IL(II)*IL(II)*CSTAR*CSTAR)+(2.0*IH(II)*IK(II)*ASTAR*BSTAR*COSGS)
    &+(2.0*IL(II)*IH(II)*CSTAR*ASTAR*COSBS)+(2.0*IK(II)*IL(II)*BSTAR*
    &CSTAR*COSAS))
    U=((IH(NN)*IH(NN)*ASTAR*ASTAR)+(IK(NN)*IK(NN)*BSTAR*BSTAR)
    &+(IL(NN)*IL(NN)*CSTAR*CSTAR)+(2.0*IH(NN)*IK(NN)*ASTAR*BSTAR*COSGS)
    &+(2.0*IL(NN)*IH(NN)*CSTAR*ASTAR*COSBS)+(2.0*IK(NN)*IL(NN)*BSTAR*
    &CSTAR*COSAS))
    W=SQRT(T*U)
    ANGIE=S/W
    IF(ANGIE.LT.-1.0.OR.ANGIE.GT.1.0)GOTO 166
    SANGIE=SQRT(1.0-ANGIE*ANGIE)
    IF(SANGIE.NE.0.0) GOTO 164
166   YY=0.0
    IF(ANGIE.LE.-1.0) YY=PI180*180.0
    GO TO 165
164   YY=PI180*90.-ATAN(ANGIE/SANGIE)
165   YY=YY*DPR
    MM=MM+1
    IF(YY.GT.(ANGLES(MM)+ANGTOL).OR.YY.LT.(ANGLES(MM)-ANGTOL))
    &GO TO 1001
    ANGACT (MM)=YY
170   CONTINUE
    CALL OARRAY(KONST,IH,IK,IL,I,J,K,L,M,PI180,RAD,IRAD,JRAD,

```

```
& RADIX,IRADIX,JRADIX,DISTIX,IOUT,NUMPAT)
1001 CONTINUE
1003 CONTINUE
1002 CONTINUE
1007 KONST=3
      CALL OARAY(KONST,IH,IK,IL,I,J,K,L,M,PI180,RAD,IRAD,JRAD,
& RADIX,IRADIX,JRADIX,DISTIX,IOUT,NUMPAT)
      GOTO 10
999  IF(NUMPAT.EQ.0) TYPE 622
622  FORMAT(1X,' THERE ARE NO SOLUTIONS')
      IF(IPAT.EQ.2)GOTO 9999
      TYPE *, ' ANOTHER DIFFRACTION PATTERN FOR SAME PARTICLE?'
      READ(5,108) ANSWER
      IF(ANSWER.EQ.'Y') REWIND 3
      IF(ANSWER.EQ.'Y') IFILE=1
      IF(ANSWER.EQ.'Y') GOTO 11
9999 CLOSE(UNIT=1)
      CLOSE(UNIT=2)
      CLOSE(UNIT=3)
      CLOSE(UNIT=4)
      CALL EXIT
      END
```

C*
C*
C*
SUBROUTINE OARRAY(KONST,IH,IK,IL,IA,JA,KA,LA,MA,PI180,
&RAD,IRAD,JRAD,RADIX,IRADIX,DISTIX,IOUT,NUMPAT)

SUBROUTINE 'OARRAY' SORTS SOLUTIONS AND PRINTS RESULTS

INTEGER PRINTR
VIRTUAL ANGIX(4,50),IHP(5,50,50),RAD(IRAD,JRAD),
&RADIX(IRADIX,JRADIX),DISTIX(IRADIX,JRADIX)
VIRTUAL IKP(5,50,50),ILP(5,50,50),IZONES(3,50,50),ISONES(100,3))
COMMON ANGLES(4),DIST(5),LE,LES,KT,D2,D4,ANGACT(4),CAMCO
&,KSETS,IZOS(3,50)
COMMON/DIFF/NAME(4),PHOTO(20),A,BCON,C,ALPHA,BETA,GAMMA,IFILE
DIMENSION IH(5),IK(5),IL(5)
VIRTUAL ANG(5),CAMKO(50),ADEVN(50),DEVSQ(50),KP(50),
&IZON(3),IZO(3),DIV(3),ADIV(3),JDIV(3),DEVN(5),DEV(50),HSUM(50)
DOUBLE PRECISION PI180,A,BCON,C
REAL*8 NAME
PRINTR=2
IF(KONST-3) 1030,600,1030

C*
C* CALCULATE LOWEST ORDER ZONE AXES

C*
1030 IZON(1)=IK(1)*IL(2)-IK(2)*IL(1)
1031 IZON(2)=IL(1)*IH(2)-IL(2)*IH(1)
1032 IZON(3)=IH(1)*IK(2)-IH(2)*IK(1)
DO 1033 I=1,3
IZO(I)=IZON(I)
1033 CONTINUE
1040 IF(LABS(IZO(1))-LABS(IZO(2))) 1041,1042,1042
1041 INV=IZO(2)
IZO(2)=IZO(1)
IZO(1)=INV
1042 IF(LABS(IZO(2))-LABS(IZO(3))) 1043,1045,1045
1043 INV=IZO(3)
IZO(3)=IZO(2)
IZO(2)=INV
GO TO 1040
1045 INCMAX=LABS(IZO(1))
1083 DO 1061 INC=1,INCMAX
DO 1060 IZ=1,3
1046 DIV(IZ)=LABS(IZO(IZ))/((INCMAX+1.)-INC)
JDIV(IZ)=DIV(IZ)+0.001
ADIV(IZ)=JDIV(IZ)
1060 CONTINUE
IF(DIV(1).EQ.ADIV(1).AND.DIV(2).EQ.ADIV(2).AND.DIV(3).EQ.
&ADIV(3)) GO TO 1063
1061 CONTINUE
1063 DO 1070 I=1,3
IF(IZON(I)) 64,65,65
64 IZON(I)=IZON(I)/((INCMAX+1)-INC)-0.001
GO TO 1070
65 IZON(I)=IZON(I)/((INCMAX+1)-INC)+0.001

1070 CONTINUE

C* LOAD SOLUTIONS INTO OUTPUT ARRAYS

C* GO TO (100,400,600,400) KONST

100 KONST=2

DO 110 I=1,50

KP(I)=0

110 CONTINUE

KT=0

KSETS=0

200 IF(KT.LT.50) GO TO 208

900 KONST=4

GO TO 350

208 KT=KT+1

KSETS=KSETS+1

RADIX(1,KT)=RAD(1,IA)

RADIX(2,KT)=D2

RADIX(3,KT)=RAD(2,KA)

RADIX(4,KT)=D4

RADIX(5,KT)=RAD(3,MA)

DO 210 I=1,4

210 ANGIX(I,KT)=ANGACT(I)

DO 220 I=1,5

DISTIX(I,KT)=DIST(I)

220 CONTINUE

KS=KT

300 CONTINUE

KP(KS)=KP(KS)+1

C* CALCULATE MEAN DEVIATION OF SPOTS FROM TRUE POSITIONS

C*

C*

DEV(KS)=0.

DEVSQ(KS)=0.

RADTOT=0.

DISTOT=0.

30 DO 50 N=1,LE

RADTOT=RADTOT+RADIX(N,KS)

50 DISTOT=DISTOT+(CAMCO/(2.*DISTIX(N,KS)))

CAMINC=((RADTOT-DISTOT)/DISTOT)+1.

CAMKO(KS)=CAMCO*CAMINC

ANGDEV=0.

DO 55 N=1,LES

55 ANGDEV=ANGDEV+(ANGIX(N,KS)-ANGLES(N))

ANGDE=ANGDEV/LE

ANG(1)=0.-ANGDE

DO 56 N=1,LES

M=N+1

56 ANG(M)=(ANGIX(N,KS)-ANGLES(N))-ANGDE

DO 58 N=1,LE

58 XI=DISTIX(N,KS)-((CAMKO(KS)/(2.*RADIX(N,KS)))*DCOS(ANG(N)*
&PI180))

```

X2=(CAMKO(KS)/(2.*RADIX(N,KS)))*DSIN(ANG(N)*PI180)
58 DEVSQ(KS)=DEVSQ(KS)+SQRT((X1*X1)+(X2*X2))
IF(KP(KS).GT.50) RETURN
K=KP(KS)
DO 310 I=1,3
IZONES(I,K,KS)=IZON(I)
IZOS(I,KS)=JDIV(I)
310 CONTINUE
DO 320 I=1,5
IHP(I,K,KS)=IH(I)
IKP(I,K,KS)=IK(I)
320 ILP(I,K,KS)=IL(I)
RETURN
C*
C* CHECK FOR SYMMETRICAL EQUIVALENT SOLUTIONS
C*
400 DO 410 KS=1,KT
IF(RAD(1,IA).EQ.RADIX(1,KS).AND. D2 .EQ.RADIX(2,KS).
&AND.RAD(2,KA).EQ.RADIX(3,KS).AND. D4 .EQ.RADIX(4,KS).AND.
&RAD(3,MA).EQ.RADIX(5,KS)) GO TO 420
GO TO 410
420 DO 430 L=1,4
IF(ANGIX(L,KS).NE.ANGACT(L)) GO TO 410
430 CONTINUE
DO 440 I=1,3
IF(IZOS(I,KS).NE.JDIV(I)) GO TO 410
440 CONTINUE
GO TO 300
410 CONTINUE
GO TO 200
600 IF(KSETS) 1600,1600,349
C*
C* SORT SETS OF RESULTS INTO ORDER OF ACCURACY
C*
349 WRITE(IFILE,3998)(PHOTO(I),I=1,20)
WRITE(IFILE,3997) (ANGLES(I),I=1,4),(DIST(I),I=1,5),CAMCO
3997 FORMAT(1X,10F8.3)
3998 FORMAT(1X,20A4)
350 N=KT
M=N
1120 M=M/2
IF(M) 1130,1140,1130
1130 K=N-M
J=1
1141 I=J
1149 L=I+M
IF(DEVSQ(I)-DEVSQ(L)) 1160,1160,1150
1150 B=DEVSQ(I)
DEVSQ(I)=DEVSQ(L)
DEVSQ(L)=B
CAM=CAMKO(I)
CAMKO(I)=CAMKO(L)

```

```

CAMKO(L)=CAM
DO 1153 NM=1,5
AR=RADIX(NM,I)
RADIX(NM,I)=RADIX(NM,L)
RADIX(NM,L)=AR
AD=DISTIX(NM,I)
DISTIX(NM,I)=DISTIX(NM,L)
DISTIX(NM,L)=AD
DO 1153 KK=1,50
IP=IHP(NM,KK,I)
IHP(NM,KK,I)=IHP(NM,KK,L)
IHP(NM,KK,L)=IP
IP=IKP(NM,KK,I)
IKP(NM,KK,I)=IKP(NM,KK,L)
IKP(NM,KK,L)=IP
IP=ILP(NM,KK,I)
ILP(NM,KK,I)=ILP(NM,KK,L)
1153 ILP(NM,KK,L)=IP
DO 1154 NN=1,3
IQ=IZOS(NN,I)
IZOS(NN,I)=IZOS(NN,L)
IZOS(NN,L)=IQ
DO 1154 KK=1,50
IP=IZONES(NN,KK,I)
IZONES(NN,KK,I)=IZONES(NN,KK,L)
1154 IZONES(NN,KK,L)=IP
DO 1155 NA=1,4
AA=ANGIX(NA,I)
ANGIX(NA,I)=ANGIX(NA,L)
1155 ANGIX(NA,L)=AA
KZ=KP(I)
KP(I)=KP(L)
KP(L)=KZ
I=(I-M)
IF(I-1) 1160,1149,1149
1160 J=J+1
IF(J-K) 1141,1141,1120
1140 IF (XONST.NE.4) GO TO 1180
KT=30
DO 1165 LS=31,50
1165 KP(LS)=0
GO TO 208
C*
C*   SORT ZONEAXES WITHIN EACH SET INTO ORDER
C*
1180 IF(KT.LE.30) GO TO 1185
KT=30
1185 DO 1300 KS=1,KT
N=KP(KS)
DO 1210 KK=1,N
1210 HSUM(KK)=IZONES(1,KK,KS)+IZONES(2,KK,KS)+IZONES(3,KK,KS)
M=N

```

```

1220 M=M/2
    IF(M) 1230,1240,1230
1230 K=N-M
    J=1
1241 I=J
1249 L=I+M
    IF(HSUM(L)-HSUM(I)) 1260,1260,1250
1250 HB=HSUM(I)
    HSUM(I)=HSUM(L)
    HSUM(L)=HB
    DO 1252 NN=1,3
    IP=IZONES(NN,I,KS)
    IZONES(NN,I,KS)=IZONES(NN,L,KS)
1252 IZONES(NN,L,KS)=IP
    DO 1254 NN=1,5
    IP=IHP(NN,I,KS)
    IHP(NN,I,KS)=IHP(NN,L,KS)
    IHP(NN,L,KS)=IP
    IP=IKP(NN,I,KS)
    IKP(NN,I,KS)=IKP(NN,L,KS)
    IKP(NN,L,KS)=IP
    IP=ILP(NN,I,KS)
    ILP(NN,I,KS)=ILP(NN,L,KS)
1254 ILP(NN,L,KS)=IP
    I=(I-M)
    IF(I-1)1260,1249,1249
1260 J=J+1
    IF(J-K)1241,1241,1220
1240 DO 1293 IPZ=1,N
    IPZN=IPZ-1
    IF(IPZ.EQ.1) GO TO 1242
    IF(HSUM(IPZ).LT.HSUM(IPZN)) GO TO 1300
1242 IF(IZONES(1,IPZ,KS).LE.IZONES(2,IPZ,KS).AND.
    &IZONES(2,IPZ,KS).LE.IZONES(3,IPZ,KS))GO TO 1290
    GO TO 1293
1290 DO 1291 NN=1,3
    IP=IZONES(NN,IPZ,KS)
    IZONES(NN,IPZ,KS)=IZONES(NN,I,KS)
1291 IZONES(NN,I,KS)=IP
    DO 1292 NN=1,5
    IP=IHP(NN,IPZ,KS)
    IHP(NN,IPZ,KS)=IHP(NN,I,KS)
    IHP(NN,I,KS)=IP
    IP=IKP(NN,IPZ,KS)
    IKP(NN,IPZ,KS)=IKP(NN,I,KS)
    IKP(NN,I,KS)=IP
    IP=ILP(NN,IPZ,KS)
    ILP(NN,IPZ,KS)=ILP(NN,I,KS)
1292 ILP(NN,I,KS)=IP
1293 CONTINUE
1300 CONTINUE

```

C*

C* WRITE OUT RESULTS

C*

```
KSETSS=0
IF(KSETS-1) 1295,1295,1294
1294 WRITE(PRINTR,1001) KSETS
1295 DO 1500 KS=1,KT
    IF((-1)**KS.LT.0)WRITE(PRINTR,2000)
    IF((-1)**KS.GT.0)WRITE(PRINTR,2001)
2000  FORMAT(1H1)
2001  FORMAT(////)
    IF(KP(KS)-1)1302,1302,1301
1301 WRITE(PRINTR,1002)KS,(IZONES(NN,1,KS),NN=1,3),KS,KP(KS)
    WRITE(PRINTR,1016)
    GO TO 1305
1302 WRITE(PRINTR,1003)KS,(IZONES(NN,1,KS),NN=1,3)
    WRITE(PRINTR,1016)
1305 WRITE(PRINTR,1004)
    DO 1308 I=1,LE
        DISTIX(I,KS)=CAMKO(KS)/(2.*DISTIX(I,KS))
1308 WRITE(PRINTR,1005)I,IHP(I,1,KS),IKP(I,1,KS),ILP(I,1,KS),RADIX
&(I,KS),DISTIX(I,KS)
    WRITE(PRINTR,1008)CAMKO(KS)
    WRITE(PRINTR,1009)CAMCO
    ADEVN(KS)=DEVSQ(KS)/LE
    WRITE(PRINTR,1010)ADEVN(KS)
    WRITE(PRINTR,1007)
    DO 1390 I=2,LE
        LES=I-1
1390 WRITE(PRINTR,1006)I,ANGIX(LES,KS),ANGLES(LES)
    IF(IOUT-1)1500,1395,1500
1395 IF(KP(KS).LE.1) GO TO 1500
    WRITE(PRINTR,1011)KS
    KKMAX=KP(KS)
    IF(LE-3)1440,1396,1440
1396 WRITE(PRINTR,1013)
    DO 1400 I=2,KKMAX
1400 WRITE(PRINTR,1015)(IZONES(L,I,KS),L=1,3),IHP(1,I,KS),
&IKP(1,I,KS),ILP(1,I,KS),IHP(2,I,KS),IKP(2,I,KS),
&ILP(2,I,KS),IHP(3,I,KS),IKP(3,I,KS),ILP(3,I,KS)
    GO TO 1500
1440 WRITE(PRINTR,1012)
    DO 1460 I=2,KKMAX
        KSETSS=KSETSS+1
        ISONES(KSETSS,1)=IZONES(1,I,KS)
        ISONES(KSETSS,2)=IZONES(2,I,KS)
        ISONES(KSETSS,3)=IZONES(3,I,KS)
1460 WRITE(PRINTR,1014)(IZONES(L,I,KS),L=1,3),IHP(1,I,KS),
&IKP(1,I,KS),ILP(1,I,KS),IHP(2,I,KS),IKP(2,I,KS),
&ILP(2,I,KS),IHP(3,I,KS),IKP(3,I,KS),ILP(3,I,KS),
&IHP(4,I,KS),IKP(4,I,KS),ILP(4,I,KS),IHP(5,I,KS),
&IKP(5,I,KS),ILP(5,I,KS)
1500 CONTINUE
```

```

KSS=KSETS+KSETSS
4000 WRITE(1FILE,4000)(NAME(I),I=1,4),A,BCON,C,ALPHA,BETA,GAMMA,KSS
      FORMAT(1X,4AB,6F8.3,I4)
      WRITE(1FILE,4010)((IZONES(NN,1,KS),NN=1,3),KS=1,KSETS)
      IF(KSETSS.GT.0) WRITE(1FILE,4010) ((ISONES(KN,I),I=1,3),
      & KN=1,KSETSS)
4010 FORMAT(1X,3I3)
      IPTR=5
      WRITE(IPTR,4020) (NAME(I),I=1,4)
      WRITE(IPTR,4030) ((IZONES(NN,1,KS),NN=1,3),KS=1,KSETS)
      IF(KSETSS.GT.0) WRITE(IPTR,4030) ((ISONES(KN,I),I=1,3),
      & KN=1,KSETSS)
4020 FORMAT(1X,4AB)
4030 FORMAT(5(1X,['3I3.']),1X))
      NUMPAT=NUMPAT+1
      KS=0
      KSETS=0
      RETURN
1600 WRITE(PRINTR,1017)
1000 RETURN
C*   FORMAT STATEMENTS——OUTPUT
C*
1001 FORMAT(/,13,' SETS OF POSSIBLE ZONE AXES INDEX WITHIN ',
      &'SPECIFIED LIMITS')
1002 FORMAT(1X,'SET ',I2,' ZONE AXIS [',3I3,'],',
      &5X,'(SET ',I2,' HAS ',I2,' SYMM. EQUIV. SOL'NS)')
1003 FORMAT(1X,'SET ',I2,' ZONE AXIS [',3I3,'],',
      &5X,'( NO SYMMETRICALLY EQUIVALENT SOL'NS)')
1004 FORMAT(/,1X,'POINT',8X,'PLANE',10X,'DSPACE',5X,'ESTIMA
      &TED ','DSPACE FROM DIFF. PATTERN')
1005 FORMAT(1H ,2X,I1,7X,'(',3I3,')',6X,F6.3,15X,F6.3)
1006 FORMAT(1H ,1X,'ANGLE BETWEEN PLANES 1 & ',I1,
      & ' = ',F6.2,' (MEASURED ',F6.2,', DEGREES')
1007 FORMAT(1H )
1008 FORMAT(/,1X,' BEST FIT CAMERA CONSTANT USED ',
      & 'IN ABOVE ESTIMATES OF D SPACINGS = ',F7.3)
1009 FORMAT(1H ,4IX,'(INPUT CAMERA CONSTANT = ',F7.3,')')
1010 FORMAT(/,1X,'MEAN DEVIATION OF MEASURED SPOTS ',
      & 'FROM TRUE POSITIONS = ',F5.3,' MILLIMETRES')
1011 FORMAT(/,1X,'SYMMETRICALLY EQUIVALENT SOLUTIONS ',
      & 'FOR SET ',I2)
1012 FORMAT(/,3X,'ZONE AXIS',5X,'POINT 1',5X,'POINT 2',
      &5X,'POINT 3',5X,'POINT 4',5X,'POINT 5',/)
1013 FORMAT(/,3X,'ZONE AXIS',5X,'POINT 1',5X,'POINT 2',
      &5X,'POINT 3',/)
1014 FORMAT(1H ,1X,'[',3I3,']',2X,'(',3I3,')',1X,'(',3I3,')',
      &1X,'(',3I3,')',1X,'(',3I3,')',1X,'(',3I3,')')
1015 FORMAT(1H ,1X,'(',3I3,')',2X,'(',3I3,')',1X,'(',3I3,')',
      &1X,'(',3I3,')',1X,'(',3I3,')')
1016 FORMAT(1X,'***** *****')
1017 FORMAT(/,1X,'NO IDENTIFICATION',/21X,'*****')
      END

```

```
SUBROUTINE CELL(NAME,A,B,C,ALPHA,BETA,GAMMA,SYM,IGAIN)
REAL*8 NAME(4),A,B,C,FORMUL(6)
INTEGER ELEM(8),SYM
REAL LOWER(8),UPPER(8),ALPHA,BETA,GAMMA
IGAIN=0
READ(3,400,END=20)(NAME(I),I=1,4),(FORMUL(I),I=1,6)
READ(3,410,END=20)(ELEM(I),LOWER(I),UPPER(I),I=1,8)
READ(3,420,END=20)A,B,C,ALPHA,BETA,GAMMA,SYM
RETURN
20  IGAIN=1
RETURN
400  FORMAT(IX,10AB)
410  FORMAT(IX,8(I2,2F5.2))
420  FORMAT(IX,6F7.3,I1)
END
```

C⁸
C⁹
C¹⁰
SUBROUTINE PROHIB (SYMI,H,K,L,INC)

TEST INDICES AND ELIMINATE PROHIBITED REFLECTIONS

• INTEGER H,SYMI
GO TO (68,13,15,61,62,13,63,64),SYMI
13 AKH=(K+H)/2.
KH=AKH
BKH=KH
IF(AKH.NE.BKH) GO TO 70
IF(SYMI.NE.2) GO TO 68
62 ALH=(L+H)/2.
LH=ALH
BLH=LH
IF(ALH.NE.BLH) GO TO 70
IF(SYMI.NE.2) GO TO 68
61 AKL=(K+L)/2.
KL=AKL
BKL=KL
IF(AKL.NE.BKL) GO TO 70
GO TO 68
15 AKHL=(H+K+L)/2.
GO TO 66
63 AKHL=(K+L-H)/3.
GO TO 66
64 AKHL=(H+L-K)/3.
66 KHL=AKHL
BKHL=KHL
IF(AKHL.NE.BKHL) GO TO 70
68 INC=0
69 GO TO 75
70 INC=1
75 RETURN
END

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PROGRAM ANGdif

PROGRAM WRITTEN BY W.R. STOTT, DEPT OF APPLIED PHYSICS
ONTARIO RESEARCH FOUNDATION, MISSISSAUGA, ONT., CANADA

PROGRAM CALCULATES INTER-ZONE AXIS ANGLES

IS CHAINED IN SEQUENCE XMATCH XIDEN ANGdif RESULT

COMMON/VARI/U(20),V(20),W(20),U1(20),V1(20),W1(20),

A,B,C,ALPHA,BETA,GAMMA,PHI,I,J

REAL PHOTO(20),PHOTO2(20),ANGLES(4),ANGLE2(4),DIST(5),

DIST2(5),CAMCO,CAMCO2

REAL*8 NAME(4),NAME2(4)

BYTE ANSWER

OPEN(UNIT=1,NAME='MATTAT',TYPE='OLD',READONLY)

OPEN(UNIT=2,NAME='MATPAU',TYPE='OLD',READONLY)

OPEN(UNIT=3,NAME='MATPHI',TYPE='NEW')

OPEN(UNIT=4,NAME='PHIDAT',TYPE='NEW')

READ(1,200,END=999)(PHOTO(I),I=1,20)

READ(1,201)(ANGLES(I),I=1,4),(DIST(I),I=1,5),CAMCO

FORMAT(1X,20A4)

FORMAT(1X,10F8.3)

READ(2,200,END=999)(PHOTO2(I),I=1,20)

READ(2,201)(ANGLE2(I),I=1,4),(DIST2(I),I=1,5),CAMCO2

WRITE(5,700)

FORMAT(1X,'DO YOU WISH TO ANALYZE INTER-ZONE AXIS ANGLES?')

READ(5,710) ANSWER

FORMAT(A1)

IF(ANSWER.EQ.'N') GOTO 999

WRITE(5,206)(PHOTO(I),I=1,20),(PHOTO2(I),I=1,20)

FORMAT(1X,'ANGLE BETWEEN PATTERNS?',//,1X,20A4,/,4X,'AND',//
,1X,20A4,/)

READ(5,*) ANGLE

IF(ANGLE.LT.0.0) ANGLE=-ANGLE

WRITE(5,210)

FORMAT(1X,'ANGULAR TOLERANCE? ',\$)

READ(5,*) ANGTOL

REWIND 1

READ(1,200,END=999)(PHOTO(I),I=1,4)

READ(1,201)(ANGLES(I),I=1,4),(DIST(I),I=1,5),CAMCO

READ(1,202)(NAME(I),I=1,4),A,B,C,ALPHA,BETA,GAMMA,KSETS

READ(1,204)(U(I),V(I),W(I),I=1,KSETS)

FORMAT(1X,4A8,6F8.3,I4)

FORMAT(1X,3F3.0)

REWIND 2

READ(2,200,END=260)(PHOTO2(I),I=1,20)

READ(2,201)(ANGLE2(I),I=1,4),(DIST2(I),I=1,5),CAMCO2

READ(2,202)(NAME2(I),I=1,4),A,B,C,ALPHA,BETA,GAMMA,KSETT

READ(2,204)(U1(I),V1(I),W1(I),I=1,KSETT)

IF(NAME(1).EQ.NAME2(1).AND.NAME(2).EQ.NAME2(2).AND.NAME(3).EQ.

NAME2(3).AND.NAME4().EQ.NAME2(4))GOTO 300

GOTO 280

300 WRITE(4,110)(NAME(I),I=1,4),(PHOTO(I),I=1,20),(PHOTO2(I),I=1,20)

110 FORMAT(1H1,10X,'ANALYSIS OF ZONE AXIS ANGULAR DIFFERENCES',//,

```

& 1X," MINERAL ",4A8,/,IX," PATTERN 1 ",20A4,/IX,
&   " PATTERN 2 ",20A4,///
112 WRITE(4,112) ANGLE,ANGTOL
FORMAT(3X,'ANGLE= ',F8.2,' ANGULAR TOLERANCE= ',F8.2)
100 WRITE(4,100) A,B,C,ALPHA,BETA,GAMMA
FORMAT(//,' ZONE AXIS ANGULAR DIFFERENCES',//,
      '          A      B      C      ALPHA     BETA     GAMMA',/,6F8.2,/,,
      '          PATTERN 1           PATTERN 2           ANGLE',/,,
      '          U,V,W           U1,V1,W1           PHI',/,)
DO 5 I=1,KSETS
DO 5 J=1,KSETT
CALL PHIZON
IF(PHI.GT.(ANGLE+ANGTOL).OR.PHI.LT.(ANGLE-ANGTOL)) GOTO 5
320 WRITE(3,310) U(I),V(I),W(I),U1(J),V1(J),W1(J),PHI
310 WRITE(3,320)(NAME(II),II=1,4),(PHOTO(II),II=1,20),(PHOTO2(II),II=1,20),
      & ANGLE,ANGTOL
320 FORMAT(1X,4A8,20A4,/,1X,20A4,2F8.2)
310 FORMAT(1X,6F5.0,F8.2)
5 WRITE(4,10) U(I),V(I),W(I),U1(J),V1(J),W1(J),PHI
GOTO 260
10 FORMAT(1X,3F5.0,5X,3F5.0,5X,F8.2)
20 FORMAT(1H1)
999 CLOSE(UNIT=1)
CLOSE(UNIT=2)
CLOSE(UNIT=3)
CLOSE(UNIT=4)
CALL EXIT
END
SUBROUTINE PHIZON
COMMON /VARI/U(20),V(20),W(20),U1(20),V1(20),W1(20),
      & A,B,C,ALPHA,BETA,GAMMA,PHI,I,J
C C C THE INTER-ROW ANGLE FORMULA IS FROM THE BOOK
      & INTERNATIONAL TABLES FOR X-RAY CRYSTALLOGRAPHY
      & (VOL. II ; MATHEMATICAL TABLES) P. 106
      & CON=3.14159/180.
      & ALPHA1=ALPHA*CON
      & BETA1=BETA*CON
      & GAMMA1=GAMMA*CON
      & PHICOS=U(I)*U1(J)*A*A+V(I)*V1(J)*B*B+W(I)*W1(J)*C*C
      & + (V(I)*W1(J)+W(I)*V1(J))*B*C*COS(ALPHA1)
      & +(W(I)*U1(J)+U(I)*W1(J))*C*A*COS(BETA1)
      & +(U(I)*V1(J)+V(I)*U1(J))*A*B*COS(GAMMA1)
      & QUVW=U(I)*U(I)*A*A+V(I)*V(I)*B*B+W(I)*W(I)*C*C
      & + 2*V(I)*W(I)*B*C*COS(ALPHA1)
      & + 2*W(I)*U(I)*C*A*COS(BETA1)
      & + 2*U(I)*V(I)*A*B*COS(GAMMA1)
      & QUVWI= U1(J)*U1(J)*A*A+V1(J)*V1(J)*B*B+W1(J)*W1(J)*C*C
      & + 2*V1(J)*W1(J)*B*C*COS(ALPHA1)
      & + 2*W1(J)*U1(J)*C*A*COS(BETA1)
      & + 2*U1(J)*V1(J)*A*B*COS(GAMMA1)
      & PHICOS=PHICOS/SQRT(QUVW*QUVWI)
      & IF(PHICOS.LT.-1.0) PHICOS=-1.0

```

```
IF(PHICOS.GT.1.0) PHICOS=1.0
PHI=ACOSI(PHICOS)/CON
RETURN
END
FUNCTION ACOSI(X)
DOUBLE PRECISION SX,X,ACOSI
SX=DSQRT(1.0-X*X)
IF(SX.NE.0.0) GOTO 10
ACOSI=0.0
IF(X.LE.-1.0) ACOSI=3.141592653589793
RETURN
10    ACOSI=3.141592653589793/2.0- DATAN(X/SX)
RETURN
END
```

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PROGRAM RESULT

OUTPUT ROUTINE FOR AMPHIBOLE IDENTIFICATION
PROCEDURE, PROGRAMS RUN IN SEQUENCE

XMATCH XIDEN ANGdif RESULT

REAL*8 NAME(4),FORMUL(6)
REAL LOWER(8),UPPER(8),DIST(5),ANGLES(4),DAT(3),PARTIC(20),AREAS(8)
REAL PHOTO(20),PHOTO2(20),RATIO(8)
INTEGER ELEM(*),IZONES(3,1,50),ELEMS(8),SYM
BYTE SYMI

IPTR=2
NOSOL=0
CALL DATE(DAT)
OPEN(UNIT=1,NAME='MATMIN',TYPE='OLD',READONLY)
OPEN(UNIT=2,NAME='RESULT',TYPE='NEW')

READ(1,130) (PARTIC(I),I=1,20),NUMPK,WIDTH,(RATIO(I),I=1,NUMPK)

READ(1,140) (ELEMS(I),AREAS(I),I=1,NUMPK)

WRITE(IPTR,500) (DAT(I),I=1,3)

WRITE(IPTR,510) (PARTIC(I),I=1,17)

IF(WIDTH.NE.0.0)WRITE(IPTR,514) WIDTH

WRITE(IPTR,520)

WRITE(IPTR,525) (SYM(ELEMS(I)),AREAS(I),I=1,NUMPK)

PRAT=0.0

DO 4 I=1,NUMPK

PRAT=RATIO(I)+PRAT

IF(PRAT.EQ.0.0) GOTO 8

K=0

DO 6 I=1,NUMPK

IF(RATIO(I).EQ.0.0) GOTO 6

K=K+1

ELEMS(K)=ELEMS(I)

RATIO(K)=RATIO(I)

CONTINUE

NUMPK=K

WRITE(IPTR,537)

WRITE(IPTR,538) (SYM(ELEMS(I)),RATIO(I),I=1,NUMPK)

WRITE(IPTR,530)

READ(1,100,END=19) (NAME(I),I=1,4),(FORMUL(I),I=1,6)

NOSOL=NOSOL+1

READ(1,110) (ELEM(I),LOWER(I),UPPER(I),I=1,8)

READ(1,120) A,B,C,ALPHA,BETA,GAMMA,SYMI

IF(NOSOL.EQ.31)WRITE(IPTR,505) (DAT(I),I=1,3)

WRITE(IPTR,535)(NAME(I),I=1,4),(FORMUL(I),I=1,5)

GOTO 10

19 IPAGE=0

IF(NOSOL.EQ.0) GOTO 43

CLOSE(UNIT=1)

NOSOL=0

OPEN(UNIT=1,NAME='MATPAT',TYPE='OLD',READONLY)

```

20    READ(1,200,END=29) (PHOTO(I),I=1,20)
      NOSOL=NOSOL+1
      READ(1,201)(ANGLES(I),I=1,4),(DIST(I),I=1,5),CAMCO
      IF(IPAGE.EQ.1) GOTO 21
      WRITE(IPTR,500) (DAT(I),I=1,3)
      WRITE(IPTR,510) (PARTIC(I),I=1,17)
      WRITE(IPTR,540) (PHOTO(I),I=1,10)
      WRITE(IPTR,550) CAMCO,(DIST(I),I=1,5),(ANGLES(I),I=1,4)
      WRITE(IPTR,587)
      WRITE(IPTR,555)
      WRITE(IPTR,560)
      IPAGE=1
21    READ(1,210) (NAME(I),I=1,4),A,B,C,ALPHA,BETA,GAMMA,KSETS
      READ(1,220) ((IZONES(NN,1,KS),NN=1,3),KS=1,KSETS)
      IF(NOSOL.EQ.7)WRITE(IPTR,565) (DAT(I),I=1,3)
      WRITE(IPTR,570)(NAME(I),I=1,4),A,B,C,ALPHA,BETA,GAMMA
      WRITE(IPTR,585)((IZONES(NN,1,KS),NN=1,3),KS=1,KSETS)
      GOTO 20
C
29    IPAGE=0
      CLOSE(UNIT=1)
      NOSOL=0
      OPEN(UNIT=1,NAME='MATPAU',TYPE='OLD',READONLY)
30    READ(1,200,END=39) (PHOTO(I),I=1,20)
      NOSOL=NOSOL+1
      READ(1,201)(ANGLES(I),I=1,4),(DIST(I),I=1,5),CAMCO
      IF(IPAGE.EQ.1) GOTO 31
      WRITE(IPTR,500) (DAT(I),I=1,3)
      WRITE(IPTR,510) (PARTIC(I),I=1,17)
      WRITE(IPTR,540) (PHOTO(I),I=1,10)
      WRITE(IPTR,550) CAMCO,(DIST(I),I=1,5),(ANGLES(I),I=1,4)
      WRITE(IPTR,587)
      WRITE(IPTR,555)
      WRITE(IPTR,560)
      IPAGE=1
31    READ(1,210) (NAME(I),I=1,4),A,B,C,ALPHA,BETA,GAMMA,KSETS
      READ(1,220) ((IZONES(NN,1,KS),NN=1,3),KS=1,KSETS)
      IF(NOSOL.EQ.7)WRITE(IPTR,565) (DAT(I),I=1,3)
      WRITE(IPTR,570)(NAME(I),I=1,4),A,B,C,ALPHA,BETA,GAMMA
      WRITE(IPTR,585)((IZONES(NN,1,KS),NN=1,3),KS=1,KSETS)
      GOTO 30
C
39    IPAGE=0
      CLOSE(UNIT=1)
      NOSOL=0
      OPEN(UNIT=1,NAME='MATPHI',TYPE='OLD',READONLY)
40    READ(1,400,END=49) U,V,W,U1,V1,W1,PHI
      NOSOL=NOSOL+1
      READ(1,410) (NAME(I),I=1,4),(PHOTO(I),I=1,20),
      & (PHOTO2(I),I=1,20),ANGLE,ANGTOL
      IU=U
      IV=V

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```

IW=W
IU1=U1
IV1=V1
IW1=W1
IF(IPAGE.EQ.1)GOTO 41
WRITE(IPTR,500) (DAT(I),I=1,3)
WRITE(IPTR,510) (PARTIC(I),I=1,17)
WRITE(IPTR,590) (PHOTO(I),I=1,16),(PHOTO2(I),I=1,16)
WRITE(IPTR,600) ANGLE,ANGTOL
WRITE(IPTR,605)
WRITE(IPTR,610)
IPAGE=1
41 WRITE(IPTR,620) (NAME(I),I=1,4),IU,IV,IW,IU1,IV1,IW1,PHI
IF(NOSOL.EQ.31)WRITE(IPTR,625) (DAT(I),I=1,3)
GOTO 40
48 WRITE(IPTR,630)
49 CLOSE(UNIT=1)
CLOSE(UNIT=2,DISPOSE='PRINT')
CALL EXIT

```

```

C
100 FORMAT(1X,10A8)
110 FORMAT(1X,8(I2,2F5.2))
120 FORMAT(1X,6F7.3,I1)
130 FORMAT(1X,20A4,I4,F8.3,8F5.3)
140 FORMAT(1X,8(I4,F8.0))
200 FORMAT(1X,20A4)
201 FORMAT(1X,10F8.3)
210 FORMAT(1X,4A8,6F8.3,I4)
220 FORMAT(1X,3I3)
400 FORMAT(1X,6F5.0,F8.2)
410 FORMAT(1X,4A8,20A4,/,1X,20A4,2F8.2)
500 FORMAT(1H1,6OX,'DATE: ',3A4,/,24X,'PARTICLE IDENTIFICATION',//)
505 FORMAT(1H1,6OX,'DATE: ',3A4,/,5X,'MINERALS WITH COMPOSITIONS',
      & ' CONSISTENT WITH X-RAY SPECTRUM (CONTINUED)',//)
510 FORMAT(1X,' PARTICLE:',1X,17A4,/)
515 FORMAT(5X,' WIDTH OF PARTICLE: ',F8.3,2X,'micrometers',//)
520 FORMAT(5X,' X-RAY SPECTRUM: ELEMENT PEAK AREA ELEMENT'
      & ' PEAK AREA',/)
525 FORMAT(27X,A2,5X,F8.2,11X,A2,5X,F8.2)
530 FORMAT(////5X,'MINERALS WITH COMPOSITIONS CONSISTENT ',
      & 'WITH X-RAY SPECTRUM',//)
535 FORMAT(2X,9A8)
537 FORMAT(///,5X,' CALCULATED ELEMENT RATIO ELEMENT'
      & ' RATIO',/,5X,'ATOMIC RATIOS:')
538 FORMAT(27X,A2,7X,F6.3,11X,A2,7X,F6.3)
540 FORMAT(1X,'ELECTRON DIFFRACTION PATTERN: '1X,10A4,/)
550 FORMAT(1X,'CAMERA CONSTANT= ',F8.3,2X,'mm*A',//,
      & 1X,'DISTANCES OF DIFFRACTION SPOTS (mm)',//,5X,5F8.3,/,/
      & 1X,'ANGLES BETWEEN SPOTS (degrees)',//,5X,4F8.2,//)
555 FORMAT(////,22X,'RESULTS OF ZONE AXIS ANALYSIS',//)
560 FORMAT(10X,'MINERAL',15X,' A   B   C',
      & ' ALPHA   BETA   GAMMA',/)

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```

565   FORMAT(1H1,60X,'DATE: ',3A4,/,22X,'RESULTS OF ZONE AXIS',
      &   ' ANALYSIS (CONTINUED)',//)
570   FORMAT(/,1X,4A8,6F7.2)
585   FORMAT(6(3X,3I3))
587   FORMAT(///,' COMPLETE ELECTRON DIFFRACTION ANALYSES MAY BE'
      &   ' FOUND IN FILE "XINDEX"')
590   FORMAT(/,5X,'ELECTRON DIFFRACTION PATTERNS:',//,
      &   ,10X,'#1: ',16A4,/,10X,'#2: ',16A4,//)
600   FORMAT(5X,'MEASURED INTER-ZONE AXIS ANGLE= 'F6.2,',' +/- ',
      &   F6.2,2X,'degrees',////,1X,'COMPLETE INTER-ZONE AXIS ANGLE',
      &   ' ANALYSIS MAY BE FOUND IN FILE "PHIDAT"')
603   FORMAT(////,16X,'RESULTS OF INTER-ZONE AXIS ANGLE ANALYSIS')
610   FORMAT(/,12X,'MINERAL',20X,'ZONE AXIS OF #1',
      &   2X,'ZONE AXIS OF #2',1X,'ANGLE',//)
620   FORMAT(1X,4A8,8X,3I3,8X,3I3,5X,F5.2)
625   FORMAT(1H1,60X,'DATE: ',3A4,/,16X,'RESULTS OF INTER-ZONE',
      &   ' AXIS ANGLE ANALYSIS (CONTINUED)',//)
630   FORMAT(///,1X,' NO MINERAL IN FILE MATCHES SPECTRUM')
END

FUNCTION SYM(IELEM)
INTEGER CS(100),SS(17),NUM(17),SYM
DATA CS/' H', 'HE', 'LI', 'BE', 'B', 'C', 'N', 'O', 'F', 'NE', 'NA',
      & 'MG', 'AL', 'SI', 'P', 'S', 'CL', 'AR', 'K', 'CA', 'SC', 'TI', 'V', 'CR',
      & 'MN', 'FE', 'CO', 'NI', 'CU', 'ZN', 'GA', 'GE', 'AS', 'SE', 'BR', 'KR', 'RB',
      & 'SR', 'Y', 'ZR', 'NB', 'MO', 'TG', 'RU', 'RH', 'PD', 'AG', 'CD', 'IN', 'SN',
      & 'SB', 'TE', 'I', 'XE', 'CS', 'BA', 'LA', 'CE', 'PR', 'ND', 'PM', 'SM', 'EU',
      & 'GD', 'TB', 'DY', 'HO', 'ER', 'TM', 'YB', 'LU', 'HF', 'TA', 'W', 'RE', 'OS',
      & 'IR', 'PT', 'AU', 'HG', 'TL', 'PB', 'BI', 'PO', 'AT', 'RN', 'FR', 'RA', 'AC',
      & 'TH', 'PA', 'U', 'NP', 'PU', 'AM', 'CM', 'BK', 'CP', 'ES', 'FM', 'SS', 'H',
      & 'B', 'C', 'N', 'O', 'F', 'P', 'S', 'A', 'X', 'V', 'Y', 'I', 'W',
      & 'U', 'A', 'CB', NUM/1,5,6,7,8,9,15,16,18,19,23,39,53,74,92,18,41/
SYM=CS(IELEM)
RETURN
END

```

C
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PROGRAM DATGET

PROGRAM WHICH PRINTS THE FILE DIPDAT.

```
REAL*8 NAME(4),NAME1(4),FORMUL(6)
INTEGER ELEM(8),SYM
REAL LOWER(8),UPPER(8),A,B,C,ALPHA,BETA,GAMMA
BYTE ANSWER
OPEN(UNIT=1,NAME='DIPDAT',TYPE='OLD')
OPEN(UNIT=2,NAME='DATA',TYPE='NEW')
IPTR=2
NUMBER=0
9 WRITE(IPTR,99)
IPAGE=0
10 READ(1,400,END=60) (NAME(I),I=1,4),(FORMUL(I),I=1,6) -
NUMBER=NUMBER+1
IPAGE=IPAGE+1
READ(1,410)(ELEM(I),LOWER(I),UPPER(I),I=1,8)
READ(1,420)A,B,C,ALPHA,BETA,GAMMA,SYM
WRITE(IPTR,300) (NAME(I),I=1,4),(FORMUL(I),I=1,6)
WRITE(IPTR,310) (ELEM(I),LOWER(I),UPPER(I),I=1,4)
WRITE(IPTR,320) (ELEM(I),LOWER(I),UPPER(I),I=5,8)
WRITE(IPTR,330) A,B,C,ALPHA,BETA,GAMMA,SYM
IF(IPAGE.EQ.8)GOTO 9
GOTO 10
60 CLOSE(UNIT=1)
TYPE *, ' NUMBER OF MINERALS= ',NUMBER
CLOSE(UNIT=2)
CALL EXIT
99 FORMAT(1H1)
100 FORMAT(//,1X,'MINERAL NAME? (32)',$)
200 FORMAT(4A8)
110 FORMAT(1X,'FORMULA? (48)',$)
210 FORMAT(6A8)
120 FORMAT(1X,'MANDATORY ELEMENTS,LOWER,UPPER LIMITS? (UP TO 4)')
130 FORMAT(1X,'OPTIONAL ELEMENTS,LOWER,UPPER LIMITS? (UP TO 4)')
140 FORMAT(1X,'A,B,C,ALPHA,BETA,GAMMA,SYM?',$)
300 FORMAT(1X,'NAME : ',5X,4A8,/1X,'FORMULA : ',5X,6A8)
310 FORMAT(1X,'MANDATORY : ',5X,4(1X,I2,1X,2F5.2))
320 FORMAT(1X,'OPTIONAL : ',5X,4(1X,I2,1X,2F5.2))
330 FORMAT(1X,'A,B,C,ALPHA,BETA,GAMMA,SYM: ',5X,6F7.3,3X,I1,/)
400 FORMAT('?',10A8)
410 FORMAT(1X,8(I2,2F5.2))
420 FORMAT(1X,6F7.3,I1)
500 FORMAT(A1)
END
```

C
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PROGRAM DATEDI

PROGRAM TO EDIT FILE DIFDAT.NEW
DIFDAT.NEW SHOULD BE A COPY OF DIFDAT.
AFTER EDITING RENAME DIFDAT.BAK AS DIFDAT.

```
REAL*8 NAME(4),NAME1(4),FORMUL(6)
INTEGER ELEM(8),SYM
REAL LOWER(8),UPPER(8),A,B,C,ALPHA,BETA,GAMMA
BYTE ANSWER
OPEN(UNIT=2,NAME='DIFDAT.BAK',TYPE='NEW')
OPEN(UNIT=1,NAME='DIFDAT.NEW',TYPE='OLD')
5 TYPE *, ' ENTER MINERAL NAME?'
READ(5,200,ERR=5) (NAME1(I),I=1,4)
10 READ(1,400,END=60) (NAME(I),I=1,4),(FORMUL(I),I=1,6)
READ(1,410)(ELEM(I),LOWER(I),UPPER(I),I=1,8)
READ(1,420)A,B,C,ALPHA,BETA,GAMMA,SYM
IF(NAME(1).EQ.NAME1(1).AND.NAME(2).EQ.NAME1(2))GOTO 19
WRITE(2,400) (NAME(I),I=1,4),(FORMUL(I),I=1,6)
WRITE(2,410)(ELEM(I),LOWER(I),UPPER(I),I=1,8)
WRITE(2,420)A,B,C,ALPHA,BETA,GAMMA,SYM
GOTO 10
19 WRITE(5,300) (NAME(I),I=1,4),(FORMUL(I),I=1,6)
20 TYPE *, ' O.K.?' 
READ(5,500) ANSWER
IF(ANSWER.EQ.'N') GOTO 25
IF(ANSWER.NE.'N'.AND.ANSWER.NE.'Y') GOTO 20
GOTO 29
25 WRITE(5,100)
READ(5,200,ERR=25) (NAME(I),I=1,4)
26 WRITE(5,110)
READ(5,210,ERR=26) (FORMUL(I),I=1,6)
29 WRITE(2,400) (NAME(I),I=1,4),(FORMUL(I),I=1,6)
WRITE(5,310) (ELEM(I),LOWER(I),UPPER(I),I=1,4)
30 TYPE *, ' O.K.?' 
READ(5,500) ANSWER
IF(ANSWER.EQ.'N') GOTO 35
IF(ANSWER.NE.'N'.AND.ANSWER.NE.'Y') GOTO 30
GOTO 39
35 WRITE(5,120)
READ(5,* ,ERR=35) (ELEM(I),LOWER(I),UPPER(I),I=1,4)
39 WRITE(5,320) (ELEM(I),LOWER(I),UPPER(I),I=5,8)
40 TYPE *, ' O.K.?' 
READ(5,500) ANSWER
IF(ANSWER.EQ.'N') GOTO 45
IF(ANSWER.NE.'N'.AND.ANSWER.NE.'Y') GOTO 40
GOTO 49
45 WRITE(5,130)
READ(5,* ,ERR=45) (ELEM(I),LOWER(I),UPPER(I),I=5,8)
49 WRITE(2,410) (ELEM(I),LOWER(I),UPPER(I),I=1,8)
WRITE(5,330) A,B,C,ALPHA,BETA,GAMMA,SYM
50 TYPE *, ' O.K.?' 
```

```
READ(5,500) ANSWER
IF(ANSWER.EQ.'N') GOTO 55
IF(ANSWER.NE.'N'.AND.ANSWER.NE.'Y') GOTO 50
GOTO 59
55 WRITE(5,140)
56 READ(5,*) A,B,C,ALPHA,BETA,GAMMA,SYM
59 WRITE(2,420,ERR=56) A,B,C,ALPHA,BETA,GAMMA,SYM
GOTO 5
60 CLOSE(UNIT=1)
CLOSE(UNIT=2)
CALL EXIT
100 FORMAT(///,1X,'MINERAL NAME? (32)',$)
200 FORMAT(4A8)
110 FORMAT(1X,'FORMULA? (48)',$)
210 FORMAT(6A8)
120 FORMAT(1X,'MANDATORY ELEMENTS,LOWER,UPPER LIMITS? (UP TO 4)')
130 FORMAT(1X,'OPTIONAL ELEMENTS,LOWER,UPPER LIMITS? (UP TO 4)')
140 FORMAT(1X,'A,B,C,ALPHA,BETA,GAMMA,SYM?',$)
300 FORMAT(///,1X,'NAME :',5X,4A8,/1X,'FORMULA :',5X,6A8)
310 FORMAT(1X,'MANDATORY :',5X,4(1X,I2,1X,2F5.2))
320 FORMAT(1X,'OPTIONAL :',5X,4(1X,I2,1X,2F5.2))
330 FORMAT(1X,'A,B,C,ALPHA,BETA,GAMMA,SYM:',5X,6F7.3,3X,I1)
400 FORMAT('?',10A8)
410 FORMAT(1X,8(I2,2F5.2))
420 FORMAT(1X,6F7.3,I1)
500 FORMAT(A1)
END
```

C PROGRAM DIFDAT
 C PRGRAM TO GENERATE NEW MINERAL ENTRIES FOR FILE
 C DIFDAT.
 C DIFDAT.NEW IS TO BE APPENDED TO DIFDAT.
 C
 REAL*8 NAME(4),FORMUL(6)
 INTEGER ELEM(8),SYM
 REAL LOWER(8),UPPER(8),A,B,C,ALPHA,BETA,GAMMA
 BYTE ANSWER
 OPEN(UNIT=1,NAME='DIFDAT.NEW',TYPE='NEW')
 10 DO 11 I=1,6
 11 FORMUL(I)=' '
 DO 12 I=1,4
 12 NAME(I)=' '
 DO 13 I=1,8
 13 ELEM(I)=0
 LOWER(I)=0.
 UPPER(I)=0.
 SYM=0
 A=0.
 B=0.
 C=0.
 ALPHA=0.
 BETA=0.
 GAMMA=0.
 WRITE(5,100)
 READ(5,200) NAME(1),NAME(2),NAME(3),NAME(4)
 IF(NAME(1).EQ.'END') CLOSE(UNIT=1)
 IF(NAME(1).EQ.'END') CALL EXIT
 WRITE(5,110)
 READ(5,210) (FORMUL(I),I=1,6)
 1001 WRITE(5,120)
 READ(5,*,ERR=1001) (ELEM(I),LOWER(I),UPPER(I),I=1,4)
 1002 WRITE(5,130)
 READ(5,*,ERR=1002) (ELEM(I),LOWER(I),UPPER(I),I=5,8)
 1003 WRITE(5,140)
 READ(5,*,ERR=1003) A,B,C,ALPHA,BETA,GAMMA,SYM
 WRITE(5,300) (NAME(I),I=1,4),(FORMUL(I),I=1,6)
 WRITE(5,310) (ELEM(I),LOWER(I),UPPER(I),I=1,4)
 WRITE(5,320) (ELEM(I),LOWER(I),UPPER(I),I=5,8)
 WRITE(5,330) A,B,C,ALPHA,BETA,GAMMA,SYM
 20 TYPE *, 'O.K.?'
 READ(5,500) ANSWER
 IF(ANSWER.EQ.'N') GOTO 10
 IF(ANSWER.NE.'N'.AND.ANSWER.NE.'Y') GOTO 20
 WRITE(1,400) (NAME(I),I=1,4),(FORMUL(I),I=1,6)
 WRITE(1,410)(ELEM(I),LOWER(I),UPPER(I),I=1,8)
 WRITE(1,420)A,B,C,ALPHA,BETA,GAMMA,SYM
 GOTO 10
 100 FORMAT(//,1X,'MINERAL NAME? (32)',\$)
 200 FORMAT(4A8)
 110 FORMAT(IX,'FORMULA? (48)',\$)

```
210 FORMAT(6A8)
120 FORMAT(1X,'MANDATORY ELEMENTS,LOWER,UPPER LIMITS? (UP TO 4)')
130 FORMAT(1X,'OPTIONAL ELEMENTS,LOWER,UPPER LIMITS? (UP TO 4)')
140 FORMAT(1X,'A,B,C,ALPHA,BETA,GAMMA,SYM?',$:)
300 FORMAT(//,1X,'NAME :',5X,4A8,/1X,'FORMULA :',5X,6A8)
310 FORMAT(1X,'MANDATORY :',5X,4(1X,I2,1X,2F5.2))
320 FORMAT(1X,'OPTIONAL :',5X,4(1X,I2,1X,2F5.2))
330 FORMAT(1X,'A,B,C,ALPHA,BETA,GAMMA,SYM:',5X,6F7.3,3X,I1)
400 FORMAT('?',10A8)
410 FORMAT(1X,8(I2,2F5.2))
420 FORMAT(1X,6F7.3,I1)
500 FORMAT(A1)
END
```

```
.ENABLE QUIET  
SET /SLAVE-TI:  
RUN XMATCH  
RUN XIDEN  
RUN ANGDIF  
RUN RESULT  
PIP MATMIN./PU  
PIP RESULT./PU  
PIP RESULT.;1=RESULT/RE  
PIP MATMIN.;1=MATMIN./RE  
PIP MATPAT./PU  
PIP MATPAT.;1=MATPAT./RE  
PIP MATPAU./PU  
PIP MATPAU.;1=MATPAU./RE  
PIP XINDEX./PU  
PIP XINDEX.;1=XINDEX./RE  
PIP PHIDAT./PU  
PIP PHIDAT.;1=PHIDAT./RE  
PIP MATPHI./PU  
PIP MATPHI.;1=MATPHI./RE  
SET /NOSLAVE-TI:  
.STOP
```

AN EXAMPLE OF A COMMAND FILE FOR THE AMPHIBOLE IDENTIFICATION ROUTINE

"DIFDAT" LIBRARY OF MINERALS

NAME : FE-ACTINOLITE
FORMULA : CA₂ Fe₅ Si₈O₂₂(OH)₂
MANDATORY : 20 0.67 2.00 14 7.50 8.00 26 2.50 5.00 0 0.00 0.00
OPTIONAL : 12 0.00 2.50 11 0.00 1.17 13 0.00 0.50 19 0.00 0.50
A,B,C,ALPHA,BETA,GAMMA,SYM: 9.850 18.100 5.300 90.000104.833 90.000 5

NAME : ACTINOLITE
FORMULA : Ca₂(Mg,Fe)₅Si₈O₂₂(OH)₂
MANDATORY : 20 0.67 2.00 14 7.50 8.00 12 2.50 4.50 26 0.50 2.50
OPTIONAL : 11 0.00 1.17 13 0.00 0.50 19 0.00 0.50 22 0.00 0.50
A,B,C,ALPHA,BETA,GAMMA,SYM: 9.850 18.100 5.300 90.000104.833 90.000 5

NAME : AEGIRINE
FORMULA : Na Fe Si₂O₆
MANDATORY : 11 1.00 1.00 26 1.00 1.00 14 2.00 2.00 0 0.00 0.00
OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 9.650 8.790 5.290 90.000107.400 90.000 5

NAME : ALBITE
FORMULA : Na Al Si₃O₈;Ca Al₂Si₂O₈
MANDATORY : 13 1.00 2.00 14 2.00 3.00 0 0.00 0.00 0 0.00 0.00
OPTIONAL : 11 1.00 1.00 20 1.00 1.00 0 0.00 0.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 8.140 12.790 7.160 94.330116.570 87.650 0

NAME : ALLANITE
FORMULA : (Ca,Fe)₂(Al,Fe)₃Si₃O₁₂OH
MANDATORY : 20 0.00 2.00 26 0.00 5.00 13 0.30 3.00 14 3.00 3.00
OPTIONAL : 25 0.00 3.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 10.220 5.750 8.950 90.000115.000 90.000 0

NAME : ALUM (POTASH)
FORMULA : K Al (SO₄)₂. 12 H₂O
MANDATORY : 19 1.00 1.00 13 1.00 1.00 16 2.00 2.00 0 0.00 0.00
OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 12.158 12.158 12.158 90.000 90.000 90.000 0

NAME : ALUNOGEN
FORMULA : Al₂(SO₄)₃.16H₂O
MANDATORY : 13 2.00 2.00 16 3.00 3.00 0 0.00 0.00 0 0.00 0.00
OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 0.835 1.000 0.675 89.970 97.430 91.870 9

NAME : AMESITE
FORMULA : (Mg,Al,Fe)12 [(Si,Al)8O₂₀] (OH)16
MANDATORY : 12 6.0012.00 14 4.00 8.00 0 0.00 0.00 0 0.00 0.00
OPTIONAL : 13 0.00 8.00 26 0.00 4.00 0 0.00 0.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 5.300 9.200 14.300 90.000 97.000 90.000 0

NAME : ANORTHITE
 FORMULA : CA AL₂ Si₂ O₈; NA AL Si₃ O₈
 MANDATORY : 13 1.00 2.00 14 2.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 20 1.00 1.00 11 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.180 12.880 14.160 93.170 115.850 91.220 0

NAME : ALANCIME
 FORMULA : NA AL Si₂ O₆.H₂O
 MANDATORY : 11 1.00 1.00 13 1.00 1.00 14 2.00 2.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 13.700 13.700 13.700 90.000 90.000 90.000 2

NAME : ANDALUSITE
 FORMULA : AL₂ Si O₅
 MANDATORY : 13 2.00 2.00 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 7.780 7.920 5.570 90.000 90.000 90.000 0

NAME : ANHYDRITE
 FORMULA : CA (SO₄)
 MANDATORY : 20 1.00 1.00 16 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.940 6.970 6.200 90.000 90.000 90.000 3

NAME : ANORTHOCLASE
 FORMULA : (NA,K) AL Si₃ O₈
 MANDATORY : 13 1.00 1.00 14 3.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 11 0.00 1.00 19 0.00 1.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.200 12.800 7.100 90.000 116.000 90.000 0

NAME : FE-ANTHOPHYLLITE
 FORMULA : (FE,MG)₇ Si₈ O₂₂ (OH)₂
 MANDATORY : 14 7.00 8.00 26 3.00 7.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 13 0.00 0.50 12 0.00 4.00 20 0.00 1.34 11 0.00 1.34
 A,B,C,ALPHA,BETA,GAMMA,SYM: 18.550 17.900 5.290 90.000 90.000 90.000 0

NAME : MG-ANTHOPHYLLITE
 FORMULA : (MG,FE)₇ Si₈ O₂₂ (OH)₂
 MANDATORY : 14 7.00 8.00 12 3.00 7.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 13 0.00 0.50 26 0.00 4.00 20 0.00 1.34 11 0.00 1.34
 A,B,C,ALPHA,BETA,GAMMA,SYM: 18.550 17.900 5.290 90.000 90.000 90.000 0

NAME : ANTIGORITE
 FORMULA : Mg₃ Si₂ O₅ (OH)₂
 MANDATORY : 12 2.00 3.00 14 2.00 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 43.530 9.259 7.263 90.000 91.133 90.000 5

NAME : APATITE
 FORMULA : (SR,CA)5 (PO4)3 (OH,F)
 MANDATORY : 15 3.00 3.00 20 0.00 5.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 19 0.00 1.00 17 0.00 1.00 38 0.00 5.00 58 0.00 5.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.070 6.070 6.070105.290105.290105.290 0

NAME : APOPYLLITE
 FORMULA : K CA4 Si8 O20 (F,OH) . 8H2O
 MANDATORY : 19 1.00 1.00 20 4.00 4.00 14 8.00 8.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.000 9.000 15.800 90.000 90.000 90.000 0

NAME : ARAGONITE
 FORMULA : CA CO3
 MANDATORY : 20 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 4.940 7.940 5.720 90.000 90.000 90.000 0

NAME : FE-ARFVEDSONITE
 FORMULA : NA2 (FE,MG,AL)5 Si8 O22
 MANDATORY : 14 8.00 8.00 11 1.34 2.34 19 0.50 1.00 26 2.50 5.00
 OPTIONAL : 25 0.00 2.50 13 0.00 0.50 12 0.00 2.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.000 5.300 90.000104.000 90.000 5

NAME : MG-ARFVEDSONITE
 FORMULA : NA2 (MG,FE,AL)5 Si8 O22
 MANDATORY : 11 1.34 2.34 26 0.50 3.00 12 2.00 4.00 14 8.00 8.00
 OPTIONAL : 19 0.50 1.00 25 0.00 2.50 13 0.00 0.50 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.000 5.300 90.000104.000 90.000 5

NAME : ARSENOPYRITE
 FORMULA : FE AS S
 MANDATORY : 26 1.00 1.00 33 1.00 1.00 16 1.00 1.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.740 5.680 5.790 90.000112.170 90.000 0

NAME : AUGITE
 FORMULA : (CA,NA,) (MG,FE,AL) (Si,AL)2 O6
 MANDATORY : 20 1.00 1.00 14 0.00 2.00 13 0.00 2.00 0 0.00 0.00
 OPTIONAL : 26 0.00 1.00 11 0.00 1.00 12 0.00 1.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.800 9.000 5.250 90.000105.000 90.000 5

NAME : AURICHALCITE
 FORMULA : (ZN,CU)5 (CO3)2 (OH)6
 MANDATORY : 30 0.00 5.00 29 0.00 5.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 27.700 6.400 5.250 90.000 90.000 90.000 4

NAME : AUSTINITE
 FORMULA : CA ZN AS 04 CH
 MANDATORY : 20 1.00 1.00 30 1.00 1.00 33 1.00 1.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 7.450 9.020 5.910 90.000 90.000 90.000 0

NAME : AXINITE
 FORMULA : (CA,MN,FE,MG)3 AL2 B SI4 O15 (OH)
 MANDATORY : 20 2.00 2.00 13 0.00 2.00 14 4.00 4.00 0 0.00 0.00
 OPTIONAL : 12 0.00 3.00 25 0.00 2.00 26 0.00 2.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 7.150 9.160 8.960 88.070 81.600 77.700 0

NAME : BARRINGTONITE
 FORMULA : MG CO3 . 2H2O
 MANDATORY : 12 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.155 6.202 6.092 94.000 95.530 109.000 0

NAME : FE-BARROISITE
 FORMULA : CA NA (MG,FE)3 (AL,FE)2 SI7 AL 022 (OH)2
 MANDATORY : 14 7.00 7.50 13 0.50 1.00 26 0.00 3.00 11 0.67 1.83
 OPTIONAL : 12 0.00 3.00 20 0.67 1.34 19 0.00 0.50 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 0.000 0.000 0.000 0.000 0.000 0.000 9

NAME : MG-BARROISITE
 FORMULA : CA NA (MG,FE)3 (AL,FE)2 SI7 AL 022 (OH)2
 MANDATORY : 14 7.00 7.50 13 0.50 1.00 12 0.00 3.00 11 0.67 1.83
 OPTIONAL : 26 0.00 5.00 20 0.67 1.34 19 0.00 0.50 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 0.000 0.000 0.000 0.000 0.000 0.000 9

NAME : BELOVITE
 FORMULA : (SR,CE,NA,CA) (PO4)3 (O,OH)
 MANDATORY : 15 3.00 3.00 0 0.00 0.00 0 0.00 0.00 0 0.00 6.00
 OPTIONAL : 38 0.00 1.00 58 0.00 1.00 11 0.00 1.00 20 0.00 1.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.040 6.040 6.040 105.570 105.570 105.570 0

NAME : BERYL
 FORMULA : BE3 AL2 SI6 O18
 MANDATORY : 13 2.00 2.00 14 6.00 6.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.130 6.130 6.130 97.320 97.320 97.320 0

NAME : BIOTITE IM
 FORMULA : K (MG,FE)3 (AL,FE)SI3 O10 (OH,F)2
 MANDATORY : 19 0.25 1.00 14 3.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 12 0.00 3.00 13 0.00 1.00 26 0.00 4.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.300 9.200 10.200 90.000 100.000 90.000 5

NAME : BIOTITE 2M
 FORMULA : K (Mg,Fe)3 (Al,Fe)Si3 O10 (OH,F)2
 MANDATORY : 19 0.25 1.00 14 3.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 12 0.00 3.00 13 0.00 1.00 26 0.00 4.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.300 9.200 20.200 90.000 95.000 90.000 5

NAME : BISMUTHINITE
 FORMULA : Bi2 S3
 MANDATORY : 83 2.00 2.00 16 3.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 11.130 11.270 3.970 90.000 90.000 90.000 0

NAME : BREWSTERITE
 FORMULA : (Sr,Ba,Ca) (Al Si3 O8)2 .5H2O
 MANDATORY : 14 5.00 7.00 13 1.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 56 0.00 1.00 20 0.00 1.00 38 0.00 1.00 11 0.00 1.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.770 17.410 7.660 90.000 93.070 90.000 0

NAME : BRITHOLITE
 FORMULA : (Ca,Ce)5 (SiO4, PO4)3 (OH,F)
 MANDATORY : 20 3.00 5.00 16 0.00 3.00 14 0.00 3.00 0 0.00 0.00
 OPTIONAL : 58 0.00 5.00 26 0.00 0.50 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.030 6.030 6.030105.890105.890105.890 0

NAME : BRITHOLITE (Y)
 FORMULA : (Ca,Y)5 (Si O4 PO4)3 (OH,F)
 MANDATORY : 20 3.00 5.00 14 0.00 3.00 16 0.00 3.00 0 0.00 0.00
 OPTIONAL : 39 0.00 5.00 26 0.00 0.50 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.900 5.900 5.900106.130106.130106.130 0

NAME : BROCHANTITE
 FORMULA : Cu4 SO4 (OH)6
 MANDATORY : 29 4.00 4.00 16 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 13.080 9.850 6.020 90.000103.370 90.000 0

NAME : BROCKITE
 FORMULA : (Ca,Ti,CE) PO4 CO3 .2H2O
 MANDATORY : 20 0.00 1.00 15 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 90 0.00 1.00 58 0.00 1.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 4.560 4.560 4.560 99.880 99.880 99.880 0

NAME : BROOKITE
 FORMULA : Ti O2
 MANDATORY : 22 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.436 9.166 5.135 90.000 90.000 90.000 0

NAME : BRUCITE
 FORMULA : MG(OH)2
 MANDATORY : 12 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 2.400 2.400 2.400 81.220 81.220 81.220 0

NAME : BUERGERITE
 FORMULA : NA FE3 AL6 BE3 O30 F
 MANDATORY : 26 3.00 3.00 13 6.00 6.00 14 6.00 6.00 0 0.00 0.00
 OPTIONAL : 11 1.00 1.00 9 1.00 1.00 4 3.00 3.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.427 9.427 9.427 113.830 113.830 113.830 7

NAME : BUSTAMITE
 FORMULA : (CA,MN) SI2 O6
 MANDATORY : 20 0.10 1.00 25 0.10 1.00 14 2.00 2.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 15.460 7.180 13.840 89.570 94.880 102.780 0

NAME : BUTTGENBACHITE
 FORMULA : CU19 CL4 (NO3)2 (OH)32 . 2 H2O
 MANDATORY : 29 19.00 19.00 17 4.00 4.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.630 9.630 9.630 110.490 110.490 110.490 0

NAME : CALCITE
 FORMULA : CA CO3
 MANDATORY : 20 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.360 3.360 3.360 46.000 46.000 46.000 0

NAME : CARBONATE-APATITE
 FORMULA : Ca5 (PO4,CO3)3 (OH,F)
 MANDATORY : 20 5.00 5.00 15 3.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.940 5.940 5.940 105.990 105.990 105.990 0

NAME : CASSITERITE
 FORMULA : SN O2
 MANDATORY : 50 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 4.738 4.738 3.188 90.000 90.000 90.000 0

NAME : CELESTITE
 FORMULA : SR SO4
 MANDATORY : 38 1.00 1.00 16 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.360 5.360 6.840 90.000 90.000 90.000 0

NAME : CHAMOSITE
 FORMULA : $(\text{Mg}, \text{Fe})_3 \text{Fe}_3 (\text{Al}, \text{Si}_3) \text{O}_{10} (\text{OH})_8$
 MANDATORY : 14 2.00 3.00 13 1.00 2.00 26 3.00 6.00 0 0.00 0.00
 OPTIONAL : 12 0.00 3.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.400 9.330 7.040 90.000 104.500 90.000 0

NAME : CHLORAPATITE
 FORMULA : $\text{Ca}_5 (\text{PO}_4)_3 \text{Cl}$
 MANDATORY : 20 5.00 5.00 15 3.00 3.00 17 1.00 1.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 19.210 6.785 9.605 90.000 120.000 90.000 0

NAME : CHLORITE
 FORMULA : $(\text{Mg}, \text{Al}, \text{Fe})_{12} [(\text{Si}, \text{Al})_8 \text{O}_{20}] (\text{OH})_{16}$
 MANDATORY : 12 6.00 12.00 14 4.00 8.00 13 4.00 8.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 26 0.00 4.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.300 9.200 14.300 90.000 97.000 90.000 5

NAME : CHRYSOCOLLA
 FORMULA : $\text{Cu}_2 \text{H}_2 \text{Si}_2 \text{O}_5 (\text{OH})_4$
 MANDATORY : 29 2.00 2.00 14 2.00 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 1.580 1.597 1.617 90.000 90.000 90.000 0

NAME : CHRYSOTILE
 FORMULA : $\text{Mg}_3 \text{Si}_2 \text{O}_5 (\text{OH})_4$
 MANDATORY : 12 2.00 3.00 14 2.00 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 26 0.00 0.20 13 0.00 0.10 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.300 9.200 14.600 90.000 93.000 90.000 5

NAME : CLINO-ENSTATITE
 FORMULA : Mg SiO_3
 MANDATORY : 12 1.00 1.00 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.610 8.810 5.170 90.000 108.335 90.000 0

NAME : CLINO-FERROSILITE
 FORMULA : Fe SiO_3
 MANDATORY : 26 1.00 1.00 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.530 9.210 5.150 90.000 107.630 90.000 0

NAME : CLINO-HEDRITE
 FORMULA : $\text{Ca Zn SiO}_3 (\text{OH})_2$
 MANDATORY : 20 1.00 1.00 30 1.00 1.00 14 1.00 1.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.430 15.940 5.240 90.000 103.930 90.000 3

NAME : CLINOZOISITE
 FORMULA : CA₂ AL₃ SI₃ O₁₂ OH
 MANDATORY : 20 2.00 2.00 13 3.00 3.00 14 3.00 3.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.870 5.600 10.160 90.000 113.450 90.000 0

NAME : CLINTONITE
 FORMULA : CA (Mg,Al)₃ (Al₃ Si) O₁₀ (OH)₂
 MANDATORY : 20 1.00 1.00 13 1.40 7.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 14 0.00 1.00 12 0.00 3.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.204 9.026 9.812 90.000 100.340 90.000 5

NAME : CONNELLITE
 FORMULA : Cu₁₉ Cl₄ SO₄(OH)₃₂ · 3H₂O
 MANDATORY : 29 19.00 19.00 17 4.00 4.00 16 1.00 1.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.400 8.400 8.400 107.800 107.800 107.800 0

NAME : CORDIERITE
 FORMULA : (Mg,Fe)₂ Al₄ Si₅ O₁₈
 MANDATORY : 12 0.00 2.00 13 4.00 4.00 14 5.00 5.00 0 0.00 0.00
 OPTIONAL : 26 0.00 2.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.700 17.100 9.400 90.000 90.000 90.000 5

NAME : CRISTOBALITE
 FORMULA : Si O₂
 MANDATORY : 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 4.970 4.970 6.920 90.000 90.000 90.000 0

NAME : CRONSTEDTITE
 FORMULA : Fe₂ Fe₂ Si₁₀ (OH)₄
 MANDATORY : 14 1.00 2.00 26 2.00 6.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 12 0.00 4.00 13 0.00 3.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.490 9.520 7.300 90.000 104.500 90.000 0

NAME : CROSSITE
 FORMULA : Na₂ (Mg,Fe)₃ (Fe,Al)₂ Si₈ O₂₂ (OH)₂
 MANDATORY : 11 1.34 2.50 26 3.00 5.00 14 8.00 8.00 0 0.00 0.00
 OPTIONAL : 19 0.00 0.50 13 0.00 1.50 12 0.00 2.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.647 17.905 5.316 90.000 103.600 90.000 5

NAME : CUMMINGTONITE
 FORMULA : (Fe,Mg)₇ Si₈ O₂₂ (OH)₂
 MANDATORY : 14 8.00 8.00 12 2.10 4.90 26 2.10 4.90 0 0.00 0.00
 OPTIONAL : 20 0.00 1.34 11 0.00 1.34 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.600 18.300 5.300 90.000 101.833 90.000 5

NAME : MG-CUMMINGTONITE
 FORMULA : (MG,FE)7 Si8 O22 (OH)2
 MANDATORY : 12 4.90 7.00 14 8.00 8.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 11 0.00 1.34 20 0.00 1.34 26 0.00 2.10 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.600 18.300 5.300 90.000101.833 90.000 5

NAME : DACHIARDITE
 FORMULA : (K,NA,CA)5 Al5 Si19 O48 . 18H2O
 MANDATORY : 13 5.00 5.00 14 19.00 19.00 19 0.00 5.00 0 0.00 0.00
 OPTIONAL : 11 0.00 5.00 20 0.00 5.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 18.030 7.520 10.200 90.000104.770 90.000 5

NAME : DANNEMORITE
 FORMULA : (Fe,Mn,Mg)7 Si8 O22 (OH)2
 MANDATORY : 25 0.50 2.00 14 8.00 8.00 12 2.50 5.00 0 0.00 0.00
 OPTIONAL : 20 0.00 1.34 11 0.00 1.34 26 0.00 2.50 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.600 18.300 5.300 90.000101.833 90.000 5

NAME : DATOLITE
 FORMULA : CA B Si O4 OH
 MANDATORY : 20 1.00 1.00 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 4.840 7.600 9.620 90.000 90.150 90.000 0

NAME : DICKITE
 FORMULA : Al2 Si2 O5 (OH)4
 MANDATORY : 13 2.00 2.00 14 2.00 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.150 8.950 14.420 90.000 96.800 90.000 5

NAME : DIOPSIDIE
 FORMULA : Mg Ca Si2 O6
 MANDATORY : 12 1.00 1.00 20 1.00 1.00 14 2.00 2.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.730 8.910 5.250 90.000105.833 90.000 5

NAME : DIPYRE
 FORMULA : Na4 (Al3 Si9 O24) Cl; Ca4 (Al6 Si6 O24) Co3
 MANDATORY : 13 3.00 6.00 14 6.00 9.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 11 0.00 4.00 17 0.00 1.00 20 0.00 4.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 12.150 12.150 7.550 90.000 90.000 90.000 2

NAME : DRAVITE
 FORMULA : Na Mg3 Al6 B3 Si6 O27 (OH,F)4
 MANDATORY : 12 3.00 3.00 13 6.00 6.00 11 1.00 1.00 14 6.00 6.00
 OPTIONAL : 5 3.00 3.00 6 0.00 4.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.514 9.514 9.514113.870113.870113.870 7

NAME : DUMORTIERITE
 FORMULA : AL₇O₃(SiO₄)₃
 MANDATORY : 13 7.00 7.00 14 3.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 11.790 20.209 4.701 90.000 90.000 90.000 0

NAME : FE-ECKERMANNITE
 FORMULA : Na₃(Mg,Li)₄(Al,Fe)Si₈O₂₂(OH,F)₂
 MANDATORY : 11 1.34 3.00 26 0.00 2.50 13 0.50 1.00 14 8.00 8.00
 OPTIONAL : 19 0.00 1.00 12 2.00 4.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.760 17.890 5.280 90.000 103.168 90.000 5

NAME : MG-ECKERMANNITE
 FORMULA : Na₃(Mg,Li)₄(Al,Fe)Si₈O₂₂(OH,F)₂
 MANDATORY : 11 1.34 3.00 12 2.00 4.00 13 0.50 1.00 14 8.00 8.00
 OPTIONAL : 19 0.00 1.00 26 0.00 2.50 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.760 17.890 5.280 90.000 103.168 90.000 5

NAME : EDENITE
 FORMULA : Na Ca₂(Mg,Fe)₅Si₇Al_{0.22}(OH,F)₂
 MANDATORY : 14 6.75 7.25 20 0.00 2.00 12 2.50 5.00 13 0.75 1.25
 OPTIONAL : 19 0.00 1.00 26 0.00 2.50 11 0.00 3.67 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.000 5.300 90.000 105.000 90.000 5

NAME : FE-EDENITE
 FORMULA : Na Ca₂(Fe,Mg)₅Si₇Al_{0.22}(OH,F)₂
 MANDATORY : 14 6.75 7.25 20 0.00 2.00 26 2.50 5.00 13 0.75 1.25
 OPTIONAL : 11 0.00 3.67 19 0.00 1.00 12 0.00 2.50 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.000 5.300 90.000 105.000 90.000 5

NAME : ELBAITE
 FORMULA : Na(Li,Al)₃Al₆B₃Si₆O₂₇(OH,F)₄
 MANDATORY : 11 1.00 1.00 13 6.00 9.00 14 6.00 6.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.448 9.448 9.448 113.940 113.940 113.940 7

NAME : ENSTATITE
 FORMULA : Mg Si O₃
 MANDATORY : 12 1.00 1.00 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 18.228 8.805 5.185 90.000 90.000 90.000 0

NAME : EPHESITE
 FORMULA : Na(Li,Al₂)(Al₂Si₂)O₁₀(OH)₂
 MANDATORY : 11 1.00 1.00 13 0.00 4.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 14 0.00 2.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.120 8.853 19.303 90.000 95.080 90.000 5

NAME : EPIDIDYMITE
 FORMULA : NA BE SI3 OH
 MANDATORY : 11 1.00 1.00 14 3.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 12.660 7.340 13.480 90.000 90.000 90.000 0

NAME : EPIDOTE
 FORMULA : CA2 (FE,AL) AL2 [OH SI 04 Si2 07]
 MANDATORY : 20 2.00 2.00 13 2.00 3.00 14 1.00 3.00 0 0.00 0.00
 OPTIONAL : 14 0.00 2.00 26 0.00 1.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.900 5.630 10.200 90.000 115.400 90.000 0

NAME : EPISTILBITE
 FORMULA : CA AL2 Si6 O16 . 5H2O
 MANDATORY : 20 1.00 1.00 13 2.00 2.00 14 6.00 6.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.920 17.730 10.210 90.000 124.330 90.000 5

NAME : EPSOMITE
 FORMULA : MG (SO4) 7H2O
 MANDATORY : 12 1.00 1.00 16 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 11.960 12.050 6.879 90.000 90.000 90.000 0

NAME : ERIONITE
 FORMULA : (CA,NA2,K2)1.5 AL9 Si27 072 . 27H2O
 MANDATORY : 20 1.50 1.50 13 9.00 9.00 14 27.00 27.00 0 0.00 0.00
 OPTIONAL : 11 0.00 3.00 19 0.00 3.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.130 9.130 9.130 92.620 92.620 92.620. 0

NAME : PASSAITE
 FORMULA : CA (MG,FE,AL)(SI,AL)2 O6
 MANDATORY : 20 1.00 1.00 12 1.00 1.00 14 2.00 2.00 0 0.00 0.00
 OPTIONAL : 26 0.00 1.00 13 0.00 3.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.710 8.860 5.260 90.000 106.000 90.000 5

NAME : FAYALITE
 FORMULA : FE2 SiO4
 MANDATORY : 14 0.75 1.00 26 1.80 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 12 0.00 0.20 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 4.817 10.477 6.105 90.000 90.000 90.000 0

NAME : FERRIERITE
 FORMULA : (NA,K)2 MG AL3 Si15 O36 (OH) . 9H2O
 MANDATORY : 11 2.00 2.00 12 1.00 1.00 13 3.00 3.00 14 15.00 15.00
 OPTIONAL : 19 0.00 2.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 14.140 19.120 7.480 90.000 90.000 90.000 2

NAME : FLUORAPATITE

FORMULA : Ca₅(PO₄)₃F

MANDATORY : 20 5.00 5.00 15 3.00 3.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 5.870 5.870 5.870 105.700 105.700 105.700 0

NAME : FORSTERITE

FORMULA : Mg₂SiO₄

MANDATORY : 14 0.75 1.00 12 1.80 2.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 26 0.00 0.20 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 4.756 10.195 5.981 90.000 90.000 90.000 0

NAME : Fe-GEDRITE

FORMULA : (Fe,Mg,Al)₇(Si,Al)₈O₂₂(OH)₂

MANDATORY : 13 1.00 8.00 26 0.00 5.00 14 0.00 7.00 0 0.00 0.00

OPTIONAL : 20 0.00 1.34 11 0.00 1.34 12 0.00 5.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 18.594 17.890 5.304 90.000 90.000 90.000 0

NAME : Mg-GEDRITE

FORMULA : (Mg,Fe,Al)₇(Si,Al)₈O₂₂(OH)₂

MANDATORY : 13 1.00 8.00 12 0.00 5.00 14 0.00 7.00 0 0.00 0.00

OPTIONAL : 20 0.00 1.34 11 0.00 1.34 26 0.00 5.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 18.594 17.890 5.304 90.000 90.000 90.000 0

NAME : GLAUCONITE

FORMULA : (K,Na)(Al,Fe,Mg)2(Al,Si)4O10(OH)2

MANDATORY : 19 0.10 1.00 14 3.00 4.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 11 0.00 1.00 26 0.00 2.00 12 0.00 2.00 13 0.00 3.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 5.250 9.090 10.030 90.000 100.000 90.000 5

NAME : Fe-GLAUCOPHANE

FORMULA : Na₂(Fe,Mg)3Al₂Si₈O₂₂(OH)₂

MANDATORY : 11 1.34 2.50 26 0.00 3.60 13 1.40 2.00 14 8.00 8.00

OPTIONAL : 19 0.00 0.50 12 0.00 3.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 9.541 17.740 5.295 90.000 103.667 90.000 5

NAME : Mg-GLAUCOPHANE

FORMULA : Na₂(Mg,Fe)3Al₂Si₈O₂₂(OH)₂

MANDATORY : 11 1.34 2.50 12 0.00 3.00 13 1.40 2.00 14 8.00 8.00

OPTIONAL : 19 0.00 0.50 26 0.00 3.60 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 9.541 17.740 5.295 90.000 103.667 90.000 5

NAME : GOETHITE

FORMULA : H Fe O₂

MANDATORY : 26 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 4.596 9.957 3.021 90.000 90.000 90.000 0

NAME : GONNARDITE
 FORMULA : NA₂ CA [(AL,SI)₅ O₁₀]₂ . 6H₂O
 MANDATORY : 11 2.00 2.00 20 1.00 1.00 13 0.00 5.00 0 0.00 0.00
 OPTIONAL : 14 0.00 5.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 13.380 13.380 6.660 90.000 90.000 90.000 0

NAME : GREENALITE
 FORMULA : (FE,FE)₅ Si₄ O₁₀ (OH)₈
 MANDATORY : 26 5.00 6.00 14 4.00 4.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.560 9.600 7.210 90.000 90.000 90.000 0

NAME : GRUNERITE
 FORMULA : (FE,MG)₇ Si₈ O₂₂ (OH)₂
 MANDATORY : 14 8.00 8.00 26 4.90 7.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 20 0.00 1.34 11 0.00 1.34 12 0.00 2.10 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.600 18.300 5.300 90.000 101.833 90.000 5

NAME : GYPSUM
 FORMULA : CA SO₄ . 2H₂O
 MANDATORY : 20 1.00 1.00 16 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.680 15.180 6.290 90.000 113.833 90.000 3

NAME : HALLOYSITE
 FORMULA : AL₂ Si₂ O₅ (OH)₄ . 2H₂O
 MANDATORY : 13 1.80 2.20 14 1.80 2.20 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.160 8.940 7.400 90.000 100.000 90.000 3

NAME : HALOTRICHITE
 FORMULA : FE AL₂ (SO₄)₄ . 22H₂O
 MANDATORY : 26 1.00 1.00 13 2.00 2.00 16 4.00 4.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 20.510 24.290 6.179 90.000 96.800 90.000 0

NAME : FE-HASTINGSITE
 FORMULA : NA CA₂ (MG,FE,AL)₅ (AL₂,Si₆) O₂₂ (OH)₂
 MANDATORY : 20 0.67 2.00 14 6.00 6.25 13 1.75 2.00 26 0.00 5.00
 OPTIONAL : 19 0.00 1.00 11 0.00 1.67 22 0.00 0.50 12 0.00 5.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.912 18.030 5.296 90.000 103.946 90.000 5

NAME : MG-HASTINGSITE
 FORMULA : NA CA₂ (MG,FE,AL)₅ (AL₂,Si₆) O₂₂ (OH)₂
 MANDATORY : 20 0.67 2.00 14 6.00 6.25 13 1.75 2.00 12 0.00 5.00
 OPTIONAL : 19 0.00 1.00 11 0.00 1.67 22 0.00 0.50 26 0.00 5.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.912 18.030 5.296 90.000 103.946 90.000 5

NAME : HEDENBERGITE
 FORMULA : CA FE SI2 O6
 MANDATORY : 20 1.00 1.00 26 1.00 1.00 14 2.00 2.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.850 9.020 5.260 90.000104.330 90.000 5

NAME : HEDYPHANE
 FORMULA : (CA,PB)5 (AS O4)3 CL
 MANDATORY : 20 0.00 5.00 33 0.00 3.00 17 1.00 1.00 0 0.00 0.00
 OPTIONAL : 82 0.00 5.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.370 6.370 6.370106.300106.300 0

NAME : HEMIMORPHITE
 FORMULA : ZN4 SI2 O7 (OH)2 . H2O
 MANDATORY : 30 4.00 4.00 14 2.00 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.380 10.700 5.110 90.000 90.000 90.000 2

NAME : HENDRICKSITE
 FORMULA : K (ZN,MN)3 (SI3 AL) O10 (OH)2
 MANDATORY : 19 1.00 1.00 30 0.00 3.00 14 2.00 3.00 0 0.00 0.00
 OPTIONAL : 25 0.00 3.00 13 0.00 1.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.370 9.320 10.300 90.000 99.000 90.000 5

NAME : FE-HOLMQUISTITE
 FORMULA : (NA,CA)(AL,LI,MG,FE)7 SI8 O22 (OH,F)2
 MANDATORY : 26 1.00 3.00 13 1.00 2.00 14 7.50 8.00 0 0.00 0.00
 OPTIONAL : 20 0.00 1.34 11 0.00 1.34 12 0.00 2.00 25 0.00 3.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 18.300 17.690 5.300 90.000 90.000 90.000 0

NAME : MG-HOLMQUISTITE
 FORMULA : (NA,CA)(AL,LI,MG,FE)7 SI8 O22 (OH,F)2
 MANDATORY : 12 1.00 3.00 13 1.00 2.00 14 7.50 8.00 0 0.00 0.00
 OPTIONAL : 20 0.00 1.34 11 0.00 1.34 26 0.00 2.00 25 0.00 3.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 18.300 17.690 5.300 90.000 90.000 90.000 0

NAME : FE-HORNBLENDE
 FORMULA : (CA,NA,K)2 (FE,MG,AL)5 (SI,AL)8 O22 (OH)2
 MANDATORY : 20 0.67 2.00 14 6.25 7.49 26 0.00 4.00 13 0.50 1.75
 OPTIONAL : 11 0.00 1.17 19 0.00 0.50 12 0.00 4.00 22 0.00 0.50
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.880 18.020 5.330 90.000105.500 90.000 5

NAME : MG-HORNBLENDE
 FORMULA : (CA,NA,K)2 (MG,FE,AL)5 (SI,AL)8 O22 (OH)2
 MANDATORY : 20 0.67 2.00 14 6.25 7.49 12 0.00 4.00 13 0.50 1.75
 OPTIONAL : 11 0.00 1.17 19 0.00 0.50 26 0.00 4.00 22 0.00 0.50
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.880 18.020 5.330 90.000105.500 90.000 5

NAME : HOWIEITE

FORMULA : NA (FE,MN)10 (FE,AL)2 Si12 O31 (OH)13

MANDATORY : 11 0.50 1.50 26 1.00 12.00 14 12.00 12.00 0 0.00 0.00

OPTIONAL : 25 0.00 10.00 13 0.00 2.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 10.170 9.720 9.560 91.300 70.700 109.000 0

NAME : HYALOPHANE

FORMULA : (K,Ba)(Al,Si)2 Si2 O8

MANDATORY : 19 0.00 1.00 13 0.00 2.00 14 2.00 4.00 0 0.00 0.00

OPTIONAL : 56 0.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 8.520 12.950 7.140 90.000 116.000 90.000 5

NAME : HYDROXYLAPATITE

FORMULA : Ca5 (PO4)3 OH

MANDATORY : 20 5.00 5.00 15 3.00 3.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 5.902 5.902 5.902 105.860 105.860 105.860 0

NAME : HYPERSTHENE

FORMULA : (Mg,Fe) Si O3

MANDATORY : 12 0.50 0.70 14 1.00 1.00 26 0.30 0.50 0 0.00 0.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 18.200 8.600 5.200 90.000 90.000 90.000 0

NAME : IDOCRASE

FORMULA : Ca10 Mg2 Al4 (SiO4)5 (Si2 O7)2 (OH)4

MANDATORY : 20 10.00 10.00 12 2.00 2.00 14 9.00 9.00 13 4.00 4.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 15.550 15.550 11.800 90.000 90.000 90.000 0

NAME : JADEITE

FORMULA : Na Al Si2 O6

MANDATORY : 11 1.00 1.00 13 1.00 1.00 14 2.00 2.00 0 0.00 0.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 9.420 8.560 5.220 90.000 107.600 90.000 5

NAME : JAMESONITE

FORMULA : Pb4 Fe Sb6 Si4.

MANDATORY : 82 4.00 4.00 26 1.00 1.00 51 6.00 6.00 14 4.00 4.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 15.650 19.030 4.030 90.000 91.800 90.000 0

NAME : FE-KAERSUTITE

FORMULA : Ca2 (Na,K)(Fe,Mg)4 Ti Si6 Al2 O22 (O,OH,F)2

MANDATORY : 11 1.00 1.67 14 6.00 6.25 13 1.75 2.00 26 0.00 4.00

OPTIONAL : 20 0.67 2.00 22 0.50 1.00 12 0.00 4.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.210 5.400 90.000 106.000 90.000 5

NAME : MG-KAERSUTITE
 FORMULA : CA₂ (NA,K)(MG,FE)₄ TI SI₆ AL₂ O₂₂ (OH,F)₂
 MANDATORY : 11 1.00 1.67 14 6.00 6.25 13 1.75 2.00 12 0.00 4.00
 OPTIONAL : 20 0.67 2.00 22 0.50 1.00 26 0.00 4.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 17.210 5.400 90.000106.000 90.000 5

NAME : KAOLOWITE
 FORMULA : AL₂ SI₂ O₅ (OH)₄
 MANDATORY : 13 2.00 2.00 14 2.00 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.155 8.959 7.407 91.680104.870 89.940 0

NAME : FE-KATOPHORITE
 FORMULA : NA₂ CA (FE,AL)₅ (AL,SI₇) O₂₂ (OH)₂
 MANDATORY : 11 0.67 2.33 14 6.50 7.50 13 0.50 1.50 26 0.00 4.00
 OPTIONAL : 20 0.00 1.17 19 0.00 1.00 12 0.00 4.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.000 5.300 90.000104.000 90.000 5

NAME : MG-KATOPHORITE
 FORMULA : NA₂ CA (FE,AL)₅ (AL,SI₇) O₂₂ (OH)₂
 MANDATORY : 11 0.67 2.33 14 6.50 7.50 13 0.50 1.50 12 0.00 4.00
 OPTIONAL : 20 0.00 1.17 19 0.00 1.00 26 0.00 4.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.000 5.300 90.000104.000 90.000 5

NAME : KOZULITE
 FORMULA : (NA,K,CA)₃ (Mn,Mg,Fe,Al)₅ SI₈ O₂₂ (OH,F)₂
 MANDATORY : 11 1.34 3.00 26 0.50 1.00 25 1.33 4.00 14 8.00 8.00
 OPTIONAL : 13 0.00 0.50 19 0.00 1.00 12 0.00 3.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.910 18.110 5.300 90.000104.600 90.000 5

NAME : KYANITE
 FORMULA : AL₂ SI O₅
 MANDATORY : 13 2.00 2.00 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 7.100 7.740 5.570 90.100101.300105.740 0

NAME : LAUMONTITE
 FORMULA : CA AL₂ SI₄ O₁₂ . 4H₂O
 MANDATORY : 20 1.00 1.00 13 2.00 2.00 14 4.00 4.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 14.900 13.170 7.550 90.000111.500 90.000 5

NAME : LAWSONITE
 FORMULA : CA AL₂ (OH)₂ (SI₂ O₇) . H₂O
 MANDATORY : 20 1.00 1.00 13 2.00 2.00 14 2.00 2.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.830 5.800 13.210 90.000 90.000 90.000 5

NAME : LEPIDOCROCITE

FORMULA : GAMMA — FE O . OH

MANDATORY : 26 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 3.860 12.500 3.060 90.000 90.000 90.000 3

NAME : LEPIDOLITE A)

FORMULA : K (LI,AL)3 (SI,AL)4 O1O (F,OH)2

MANDATORY : 19 1.00 1.00 14 3.00 4.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 13 0.00 7.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 5.300 9.200 10.200 90.000 100.000 90.000 5

NAME : LEPIDOLITE B)

FORMULA : K (LI,AL)3 (SI,AL)4 O1O (F,OH)2

MANDATORY : 19 1.00 1.00 14 3.00 4.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 13 0.00 7.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 9.200 5.300 20.000 90.000 98.000 90.000 5

NAME : LEPIDOLITE C)

FORMULA : K (LI,AL)3 (SI,AL)4 O1O (F,OH)2

MANDATORY : 19 1.00 1.00 14 3.00 4.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 13 0.00 7.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 10.460 10.460 10.460 29.360 29.360 29.360 0

NAME : LIZARDITE

FORMULA : MG3 SI2 O5 (OH)4

MANDATORY : 12 2.00 3.00 14 2.00 2.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 5.310 9.200 7.310 90.000 90.000 90.000 5

NAME : LOELLINGITE

FORMULA : FE AS2

MANDATORY : 26 1.00 1.00 33 2.00 2.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 5.250 5.920 2.850 90.000 90.000 90.000 0

NAME : MAGNESITE

FORMULA : MG CO3

MANDATORY : 12 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 5.610 5.610 5.610 48.170 48.170 48.170 0

NAME : MARGARITE

FORMULA : CA AL4 SI2 O1O (OH)2

MANDATORY : 2Q 1.00 1.00 13 4.00 4.00 14 2.00 2.00 0 0.00 0.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 5.130 8.900 19.500 90.000 95.000 90.000 5

NAME : MARIALITE
 FORMULA : NA4 (AL3 SI9 O24) CL; CA4 (AL6 SI6 O24) CO3
 MANDATORY : 13 3.00 6.00 14 6.00 9.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 11 0.00 4.00 20 0.00 4.00 17 0.00 1.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 12.075 12.075 7.516 90.000 90.000 90.000 0

NAME : MEIONITE
 FORMULA : CA4 (AL6 SI6 O24)CO3; NA4 (AL3 SI9 O24) CL
 MANDATORY : 13 3.00 6.00 14 6.00 9.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 11 0.00 4.00 20 0.00 4.00 17 0.00 1.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 12.130 12.130 7.690 90.000 90.000 90.000 0

NAME : MESOLITE
 FORMULA : NA2 CA2 AL6 SI9 O30 . 8H2O
 MANDATORY : 11 2.00 2.00 20 2.00 2.00 13 6.00 6.00 14 9.00 9.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 56.700 6.550 18.480 90.000 90.000 90.000 5

NAME : MICROCLINE
 FORMULA : K AL SI3 O8
 MANDATORY : 19 1.00 1.00 13 1.00 1.00 14 3.00 3.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.580 12.970 7.220 90.640 115.930 87.680 5

NAME : MILLERITE
 FORMULA : NI S
 MANDATORY : 28 1.00 1.00 16 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.640 5.640 5.640 116.620 116.620 116.620 7

NAME : MIMETITE
 FORMULA : PBS (AS O4)3 CL
 MANDATORY : 82 5.00 5.00 33 3.00 3.00 17 1.00 1.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 10.240 20.480 7.450 90.000 120.000 90.000 0

NAME : MINNESOTAITE
 FORMULA : (FE,MG)3 SI4 O10 (OH)2
 MANDATORY : 26 2.00 3.00 14 4.00 4.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 12 0.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.500 9.380 19.300 90.000 99.500 90.000 0

NAME : MIZZONITE
 FORMULA : CA4 (AL6 SI6 O24) CO3; NA4 (AL3 SI9 O24) CL
 MANDATORY : 13 3.00 6.00 14 6.00 9.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 20 0.00 4.00 11 0.00 4.00 17 0.00 1.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 12.169 12.169 7.569 90.000 90.000 90.000 2

NAME : MORDENITE
 FORMULA : (CA NA2 K2) AL2 SI10 O24 . 7H2O
 MANDATORY : 13 2.00 2.00 14 10.00 10.00 20 0.00 1.00 0 0.00 0.00
 OPTIONAL : 11 0.00 2.00 19 0.00 2.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 18.130 20.490 7.520 90.000 90.000 90.000 5

NAME : MULLITE
 FORMULA : AL6 SI2 O13
 MANDATORY : 13 6.00 6.00 14 2.00 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 7.550 7.690 2.880 90.000 90.000 90.000 0

NAME : MUSCOVITE
 FORMULA : K AL3 SI3 O10 (OH)2
 MANDATORY : 19 1.00 1.00 13 3.00 3.00 14 3.00 3.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.190 9.040 20.080 90.000 95.500 90.000 5

NAME : NACRITE
 FORMULA : AL2 SI2 O5 (OH)4
 MANDATORY : 13 2.00 2.00 14 2.00 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.909 5.146 15.697 90.000 13.700 90.000 5

NAME : NATROLITE
 FORMULA : NA2 AL2 SI3 O10 . 2H2O
 MANDATORY : 11 2.00 2.00 13 2.00 2.00 14 3.00 3.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 18.295 18.615 6.603 90.000 90.000 90.000 1

NAME : NEFFELINE
 FORMULA : (NA,K) AL SI O4
 MANDATORY : 13 1.00 1.00 14 1.00 1.00 11 0.00 1.00 0 0.00 0.00
 OPTIONAL : 19 0.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.420 6.420 6.420 102.380 102.380 102.380 0

NAME : NUFFIELDITE
 FORMULA : PB10 CU4 BI10 S27
 MANDATORY : 82 10.00 10.00 29 4.00 4.00 83 10.00 10.00 16 27.00 27.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 14.610 21.380 4.030 90.000 90.000 90.000 0

NAME : NONTRONILE
 FORMULA : (NA).33 FE2 (AL,SI)4 O10 (OH)2 . H2O
 MANDATORY : 11 0.33 0.33 26 2.00 2.00 13 0.00 4.00 0 0.00 0.00
 OPTIONAL : 14 0.00 4.00 0 0.00 0.00 0 -0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.230 9.110 15.250 90.000 90.000 90.000 5

NAME : OFFRETTITE
 FORMULA : (X,CA)3 (AL,Si)13 036 . 14H2O
 MANDATORY : 19 0.00 3.00 13 0.00 5.00 14 0.0013.00 0 0.00 0.00
 OPTIONAL : 20 0.00 3.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.170 9.170 9.170 92.690 92.690 92.690 0

NAME : OMPHACITE
 FORMULA : (CA,NA)(Mg,Fe,Fe,Al) Si2 06
 MANDATORY : 11 0.50 1.00 14 1.50 2.00 13 0.10 1.00 0 0.00 0.00
 OPTIONAL : 26 0.00 1.00 20 0.00 0.50 12 0.00 0.50 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.596 8.771 5.265 90.000106.930 90.000 5

NAME : ORTHOCLASE
 FORMULA : K AL Si3 08
 MANDATORY : 19 1.00 1.00 13 1.00 1.00 14 3.00 3.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.560 13.000 7.190 90.000116.000 90.000 5

NAME : ORTHOFERRISILITE
 FORMULA : Fe Si 03
 MANDATORY : 26 1.00 1.00 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 18.433 9.060 5.258 90.000 90.000 90.000 6

NAME : PALYGORSKITE
 FORMULA : (Mg,Al)2 Si4 O10 (OH) . 4H2O
 MANDATORY : 12 0.60 1.70 14 4.00 4.00 13 0.60 1.30 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 12.700 17.900 5.200 90.000 95.000 90.000 5

NAME : PARACELSIAN
 FORMULA : Ba Al2 Si2 08
 MANDATORY : 56 1.00 1.00 13 2.00 2.00 14 2.00 2.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.C9
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.580 9.583 9.080 90.000 90.000 90.000 0

NAME : FE-PARGASITE
 FORMULA : Na Ca (Fe,Na)4 Al (Si,Al)8 O22 (OH)2
 MANDATORY : 20 0.67 3.00 26 0.00 4.00 13 2.75 3.00 14 6.00 6.25
 OPTIONAL : 11 0.90 1.67 19 0.00 1.00 12 0.00 4.00 22 0.00 0.50
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.000 5.300 90.000105.500 90.000 5

NAME : MG-PARGASITE
 FORMULA : Na Ca (Mg,Fe)4 Al (Si,Al)8 O22 (OH)2
 MANDATORY : 20 0.67 3.00 12 0.00 4.00 13 2.75 3.00 14 6.00 6.25
 OPTIONAL : 11 0.00 1.67 19 0.00 1.00 26 0.00 4.00 22 0.00 0.50
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.000 5.300 90.000105.500 90.000 5

NAME : PECTOLITE
 FORMULA : NA CA2 SI3 O8 OH
 MANDATORY : 11 0.00 1.00 20 1.50 2.00 14 3.00 3.00 0 0.00 0.00
 OPTIONAL : 25 0.00 2.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 7.990 7.040 7.020 99.383 95.283102.467 0

NAME : PHLOGOPITE 1M
 FORMULA : K MG3 AL SI3 O10 (OH)2
 MANDATORY : 14 2.50 3.00 12 0.50 3.00 19 0.25 1.00 0 0.00 0.00
 OPTIONAL : 20 0.00 0.50 26 0.00 2.50 13 0.00 1.30 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.360 9.290 10.410 90.000100.000 90.000 5

NAME : PHLOGOPITE 3T
 FORMULA : K MG3 AL SI3 O10 (OH)2
 MANDATORY : 14 2.50 3.00 12 0.50 3.00 19 0.25 1.00 0 0.00 0.00
 OPTIONAL : 20 0.00 0.50 26 0.00 2.50 13 0.00 1.30 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 10.480 10.480 10.480 29.300 29.300 29.300 0

NAME : PIGEONITE
 FORMULA : (MG,FE,CA)(MG,FE) SI2 O6
 MANDATORY : 14 2.00 2.00 12 0.70 1.40 26 0.60 1.30 0 0.00 0.00
 OPTIONAL : 20 0.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.730 8.950 5.260 90.000108.550 90.000 0

NAME : PISTACITE
 FORMULA : CA2 (FE,AL) AL2 (OH SI O4 SI2 O7)
 MANDATORY : 20 2.00 2.00 13 2.00 3.00 14 1.00 2.00 0 0.00 0.00
 OPTIONAL : 26 0.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.900 5.630 10.200 90.000115.400 90.000 0

NAME : POLYLITHIONITE
 FORMULA : K LI2 AL (SI4 O10)(F,OH)2
 MANDATORY : 19 1.00 1.00 13 1.00 1.00 14 4.00 4.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 3.186 8.968 10.029 90.000100.400 90.000 5

NAME : POTASSIUM OCTATITANATE
 FORMULA : K3 Ti8 O17
 MANDATORY : 19 2.00 3.00 22 7.00 8.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 15.680 3.809 12.060 90.000 95.000 90.000 5

NAME : POTASSIUM HEXATITANATE
 FORMULA : K2 Ti6 O13
 MANDATORY : 19 1.00 2.00 22 5.00 6.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 15.600 3.800 9.130 90.000 99.600 90.000 5

NAME : PREHNITE
 FORMULA : CA2 AL2 Si3 O10 (OH)2
 MANDATORY : 20 2.00 2.00 13 2.00 2.00 14 3.00 3.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 4.610 5.470 18.480 90.000 90.000 90.000 0

NAME : PROBERTITE
 FORMULA : NA CA BS 09 . 5H2O
 MANDATORY : 11 1.00 1.00 20 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 13.430 12.570 6.589 90.000 100.250 90.000 0

NAME : PSEUDOBROOKITE
 FORMULA : FE2 Ti 05
 MANDATORY : 26 2.00 2.00 22 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.790 9.930 3.725 90.000 90.000 90.000 4

NAME : PSEUDONITILE
 FORMULA : FE2 Ti3 O9
 MANDATORY : 26 2.00 2.00 22 3.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 2.257 2.257 2.257 79.020 79.020 79.020 0

NAME : PUCHERITE
 FORMULA : BI V 04
 MANDATORY : 83 1.00 1.00 23 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.332 5.060 12.000 90.000 90.000 90.000 0

NAME : PUMPELLYITE
 FORMULA : CA2 MG AL2 (Si 04) (Si 07)(OH)2 . H2O
 MANDATORY : 20 2.00 2.00 12 1.00 1.00 13 2.00 2.00 14 2.00 2.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.810 5.940 19.140 90.000 97.600 90.000 3

NAME : PYRITE
 FORMULA : FE S2
 MANDATORY : 26 1.00 1.00 16 2.00 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.405 5.405 5.405 90.000 90.000 90.000 0

NAME : PYROAURITE
 FORMULA : MG6 FE2 CO3 (OH)16 . 4H2O
 MANDATORY : 12 6.00 6.00 26 2.00 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 15.920 15.920 15.920 22.420 22.420 22.420 7

NAME : PYROBELONITE
 FORMULA : PB MN VO4 OH
 MANDATORY : 82 1.00 1.00 25 1.00 1.00 23 1.00 1.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 7.644 9.508 6.182 90.000 90.000 90.000 0

NAME : PYROMORPHITE
 FORMULA : PB5 (PO4)3 CL
 MANDATORY : 82 5.00 5.00 15 3.00 3.00 17 1.00 1.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.270 6.270 6.270 105.790 105.790 105.790 0

NAME : PYROPHYLLITE
 FORMULA : AL2 [(OH)2 Si4 O10]
 MANDATORY : 13 2.00 2.00 14 4.00 4.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.160 8.900 18.644 90.000 99.920 90.000 5

NAME : ALPHA-QUARTZ
 FORMULA : SI O2
 MANDATORY : 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 3.350 3.350 3.350 95.600 95.600 95.600 0

NAME : RHODONITE
 FORMULA : MN SI O3
 MANDATORY : 25 1.00 1.00 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 7.660 12.270 6.630 86.000 93.200 111.100 0

NAME : FE-RICHTERITE
 FORMULA : NA CA NA FES Si8 O22 (OH)2
 MANDATORY : 11 0.67 3.00 14 7.50 8.00 26 2.50 5.00 0 0.00 0.00
 OPTIONAL : 19 0.00 1.00 20 0.00 2.00 12 0.00 2.50 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.820 17.960 5.270 90.000 104.330 90.000 5

NAME : RICHTERITE
 FORMULA : NA CA NA MG5 Si8 O22 (OH)2
 MANDATORY : 11 0.67 3.00 14 7.50 8.00 12 2.50 5.00 0 0.00 0.00
 OPTIONAL : 19 0.00 1.00 20 0.00 2.00 26 0.00 2.50 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.820 17.960 5.270 90.000 104.330 90.000 5

NAME : RIEBECKITE
 FORMULA : NA2 FE3 FE2 Si8 O22 (OH)2
 MANDATORY : 11 1.34 3.00 26 2.00 5.00 14 8.00 8.00 0 0.00 0.00
 OPTIONAL : 12 0.00 3.00 13 0.00 0.60 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.750 18.000 5.300 90.000 103.000 90.000 5

NAME : MG-RIEBECKITE
 FORMULA : NA₂ MG₂ FE₂ SI₈ O₂₂ (OH)₂
 MANDATORY : 11 1.34 3.00 12 2.00 3.00 14 8.00 8.00 26 1.00 2.00
 OPTIONAL : 13 0.00 0.60 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.790 18.120 5.280 90.000102.850 90.000 5

NAME : ROSCHERITE
 FORMULA : (CA,MN,FE)₃ BE₃ (PO₄)₃ (OH)₃ . 2H₂O
 MANDATORY : 20 0.00 3.00 15 3.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 25 0.00 3.00 26 0.00 3.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 15.950 11.950 6.620 90.000 94.830 90.000 5

NAME : ROSCOELITE
 FORMULA : K (V,AL,MG)₃ (AL,SI₃)O₁₀ (OH)₂
 MANDATORY : 19 1.00 1.00 23 0.00 3.00 13 0.00 4.00 0 0.00 0.00
 OPTIONAL : 12 0.00 3.00 14 0.00 3.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.260 9.090 10.250 90.000101.000 90.000 5

NAME : ROSENBUSCHITE
 FORMULA : (CA,NA)₃ (ZR,TI) SI₂ O₈ F
 MANDATORY : 14 2.00 2.00 20 0.00 3.00 40 0.00 1.00 0 0.00 0.00
 OPTIONAL : 22 0.00 1.00 11 0.00 3.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 10.140 11.410 7.280 91.350 99.640111.910 0

NAME : RUTILE
 FORMULA : TI O₂
 MANDATORY : 22 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 4.580 4.580 2.950 90.000 90.000 90.000 0

NAME : SCHORL
 FORMULA : NA (FE,MN)₃ AL₆ BE₃ SI₆ O₂₇ (OH,F)₄
 MANDATORY : 11 1.00 1.00 13 6.00 6.00 14 6.00 6.00 26 0.00 3.00
 OPTIONAL : 25 0.00 3.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.530 9.530 9.530113.960113.960113.960 7

NAME : SCOLOCITE
 FORMULA : CA AL₂ SI₃ O₁₀ . 3H₂O
 MANDATORY : 20 1.00 1.00 13 2.00 2.00 14 3.00 3.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 18.500 18.990 6.550 90.000 90.650 90.000 5

NAME : SEPIOOLITE
 FORMULA : MG₂ SI₃ O₈ . 2H₂O
 MANDATORY : 12 2.00 2.00 14 3.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 13.500 26.970 5.250 90.000 90.000 90.000 0

NAME : SIDERITE
 FORMULA : FE CO₃
 MANDATORY : 26 1.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.796 5.796 5.796 47.717 47.717 47.717 7

NAME : SILLIMANITE
 FORMULA : AL₂ (O SI O₄)
 MANDATORY : 13 2.00 2.00 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 7.440 7.590 5.750 90.000 90.000 90.000 0

NAME : SPHENE
 FORMULA : CA TI SI O₅
 MANDATORY : 20 1.00 1.00 22 1.00 1.00 14 1.00 1.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.560 8.720 7.440 90.000 119.720 90.000 5

NAME : SPODUMENE *
 FORMULA : LI AL Si₂ O₆
 MANDATORY : 13 1.00 1.00 14 2.00 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.520 8.320 5.250 90.000 110.470 90.000 5

NAME : STAUROLITE
 FORMULA : Fe₂ Al₉ Si₄ O₂₂ (OH)₂
 MANDATORY : 26 2.00 2.00 13 9.00 9.00 14 4.00 4.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 7.870 16.620 5.660 90.000 90.000 90.000 5

NAME : STEATITE
 FORMULA : Mg₃ Si₄ O₁₀ (OH)₂
 MANDATORY : 12 3.00 3.00 14 4.00 4.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.280 9.150 18.900 90.000 100.250 90.000 5

NAME : STIBNITE
 FORMULA : Sb₂ S₃
 MANDATORY : 51 2.00 2.00 16 3.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 11.200 11.280 3.830 90.000 90.000 90.000 0

NAME : STILBITE
 FORMULA : Na Ca₂ Al₅ Si₁₃ O₃₆ . 16H₂O
 MANDATORY : 11 1.00 1.00 20 2.00 2.00 13 5.00 5.00 14 13.00 13.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 13.630 18.170 11.310 90.000 129.166 90.000 5

NAME : STILPNOMELANE
 FORMULA : K (FE,MG,AL)3 Si4 O10 (OH)2 . H2O
 MANDATORY : 14 4.00 4.00 26 1.50 3.50 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 19 0.00 1.00 12 0.00 2.00 13 0.00 2.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 21.720 21.720 17.740 90.000 95.860 90.000 0

NAME : SVABITE
 FORMULA : CAS (AS O4)3 (F,CL,OH)
 MANDATORY : 20 5.00 5.00 33 3.00 3.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 19 0.00 1.00 17 0.00 1.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.170 6.170 6.170 107.500 107.500 107.500 0

NAME : TAENIOLITE
 FORMULA : K Li MG2 Si4 O10 F2
 MANDATORY : 19 1.00 1.00 12 2.00 2.00 14 4.00 4.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.270 9.130 10.120 90.000 100.000 90.000 5

NAME : TALC
 FORMULA : MG3 Si4 O10 (OH)2
 MANDATORY : 12 2.00 3.00 14 4.00 4.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 26 0.00 1.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 5.280 9.150 18.900 90.000 100.250 90.000 5

NAME : FE-TARAMITE
 FORMULA : NA2 CA (FE,MG)3 (FE,AL)2 Si6 Al2 O22 (OH)2
 MANDATORY : 14 6.00 6.50 13 1.50 2.00 11 0.67 2.67 26 0.00 5.00
 OPTIONAL : 20 0.67 1.00 19 0.00 1.00 12 0.00 3.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.000 5.300 90.000 104.000 90.000 5

NAME : MG-TARAMITE
 FORMULA : NA2 CA (MG,FE)3 (FE,AL)2 Si6 Al2 O22 (OH)2
 MANDATORY : 14 6.00 6.50 13 1.50 2.00 11 0.67 2.67 12 0.00 3.00
 OPTIONAL : 20 0.67 1.00 19 0.00 1.00 26 0.00 5.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.000 5.300 90.000 104.000 90.000 5

NAME : THOMSONITE
 FORMULA : NA Ca2 [Al2 (Al,SI) · Si3 O10] 2 . 6H2O
 MANDATORY : 11 1.00 1.00 20 2.00 2.00 13 4.00 6.00 14 6.00 8.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 13.070 13.090 6.630 90.000 90.000 90.000 0

NAME : THORITE
 FORMULA : TH Si O4
 MANDATORY : 90 1.00 1.00 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 7.120 7.120 6.320 90.000 90.000 90.000 2

NAME : TIRODITE
 FORMULA : (Mg,Mn,Fe)7 Si8 O22 (OH)2
 MANDATORY : 25 0.50 2.00 26 2.50 5.00 14 8.00 8.00 0 0.00 0.00
 OPTIONAL : 20 0.00 1.34 11 0.00 1.34 12 0.00 2.50 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.799 17.990 5.289 90.000103.890 90.000 5

NAME : TOPAZ
 FORMULA : Al2 Si O4 (F,OH)2
 MANDATORY : 13 2.00 2.00 14 11.00 0.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 8.394 8.800 4.650 90.000 90.000 90.000 0

NAME : TREMOLITE
 FORMULA : Ca2 Mg5 Si8 O22 (OH)2
 MANDATORY : 20 0.67 2.00 12 4.50 5.00 14 8.00 8.00 0 0.00 0.00
 OPTIONAL : 11 0.00 0.67 19 0.00 0.50 26 0.00 0.50 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.840 18.020 5.270 90.000104.950 90.000 5

NAME : FE-TSCHERMAKITE
 FORMULA : Ca2 (Fe,Mg)3 (Fe,Al)2 Si6 Al2 O22 (OH)2
 MANDATORY : 20 0.67 2.00 26 0.00 5.00 14 6.00 6.25 13 1.75 2.00
 OPTIONAL : 11 0.00 1.17 19 0.00 0.50 12 0.00 3.00 22 0.00 0.50
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.000 5.300 90.000105.000 90.000 5

NAME : Mg-TSCHERMAKITE
 FORMULA : Ca2 (Mg,Fe)3 (Fe,Al)2 Si6 Al2 O22 (OH)2
 MANDATORY : 20 0.67 2.00 12 0.00 3.00 14 6.00 6.25 13 1.75 2.00
 OPTIONAL : 11 0.00 1.17 19 0.00 0.50 26 0.00 5.00 22 0.00 0.50
 A,B,C,ALPHA,BETA,GAMMA,SYM: 9.900 18.000 5.300 90.000105.000 90.000 5

NAME : TSCHERMIGITE
 FORMULA : NH4 Al (SO4)2 . 12H2O
 MANDATORY : 13 1.00 1.00 16 2.00 2.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 12.215 12.215 12.215 90.000 90.000 90.000 0

NAME : VALENTINITE
 FORMULA : SB2 O3
 MANDATORY : 51 2.00 2.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 4.920 12.460 5.420 90.000 90.000 90.000 0

NAME : VANADINITE
 FORMULA : Pb5 (VO4)3 Cl
 MANDATORY : 82 5.00 5.00 23 3.00 3.00 17 1.00 1.00 0 0.00 0.00
 OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
 A,B,C,ALPHA,BETA,GAMMA,SYM: 6.443 6.443 6.443106.500106.500106.500 0

NAME : VERMICULITE

FORMULA : (Mg,Ca) (Mg,Fe,Al)6 (Al,Si)8 O20(OH)4 8H2O
MANDATORY : 14 5.50 6.00 13 2.00 5.00 12 3.50 6.00 0 0.00 0.00
OPTIONAL : 26 0.00 2.50 20 0.00 1.00 0 0.00 0.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 5.300 9.200 29.000 90.000 97.000 90.000 0

NAME : VINOGRADOVITE

FORMULA : (Na,Ca,K)4 Ti4 Al Si6 O23 . 2H2O
MANDATORY : 11 0.00 4.00 22 4.00 4.00 13 1.00 1.00 14 6.00 6.00
OPTIONAL : 20 0.00 4.00 19 0.00 4.00 0 0.00 0.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 1.180 1.000 0.760 90.000 91.970 90.000 9

NAME : VIVIANITE

FORMULA : Fe3 (PO4)2 . 8H2O
MANDATORY : 26 3.00 3.00 15 2.00 2.00 0 0.00 0.00 0 0.00 0.00
OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 10.059 13.415 4.696 90.000 104.300 90.000 5

NAME : FE-WINCHITE

FORMULA : Ca Na (Fe,Mg)4 (Fe,Al) Si8 O22 (OH)2
MANDATORY : 14 7.50 8.00 26 3.00 5.00 11 0.67 1.83 20 0.67 1.34
OPTIONAL : 12 2.00 4.00 19 0.00 0.50 13 0.00 1.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 9.820 17.960 5.270 90.000 104.330 90.000 5

NAME : MG-WINCHITE

FORMULA : Ca Na (Mg,Fe)4 (Fe,Al) Si8 O22 (OH)2
MANDATORY : 14 7.50 8.00 12 2.00 4.00 11 0.67 1.83 20 0.67 1.34
OPTIONAL : 26 3.00 5.00 19 0.00 0.50 13 0.00 1.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 9.820 17.960 5.270 90.000 104.330 90.000 5

NAME : WOLLASTONITE

FORMULA : ALPHA- CA Si O3
MANDATORY : 20 1.00 1.00 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00
OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 7.940 7.320 7.070 90.050 95.283 102.467 0

NAME : XONOTLITE

FORMULA : Ca3 Si3 O8 (OH)2
MANDATORY : 20 3.00 3.00 14 3.00 3.00 0 0.00 0.00 0 0.00 0.00
OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 16.950 7.340 7.030 90.000 90.000 90.000 0

NAME : ZINNWALDITE

FORMULA : K (Li,Al,Fe)3 (Al,Si)4 O10 (OH,F)2
MANDATORY : 19 1.00 1.00 13 1.00 4.00 14 3.00 3.50 0 0.00 0.00
OPTIONAL : 26 0.00 3.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00
A,B,C,ALPHA,BETA,GAMMA,SYM: 5.270 9.090 20.144 90.000 100.000 90.000 5

NAME : ZIRCON

FORMULA : ZR SI O4

MANDATORY : 40 1.00 1.00 14 1.00 1.00 0 0.00 0.00 0 0.00 0.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 6.600 6.600 5.980 90.000 90.000 90.000 2

NAME : ZOISITE

FORMULA : CA2 AL3 SI3 O12 OH

MANDATORY : 20 2.00 2.00 13 3.00 3.00 14 3.00 3.00 0 0.00 0.00

OPTIONAL : 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00 0 0.00 0.00

A,B,C,ALPHA,BETA,GAMMA,SYM: 16.250 5.540 10.120 90.000 90.000 90.000 0

APPENDIX B

TEST DATA AND COMPUTER LISTINGS FOR DATA PROCESSING AND REPORTING

EXAMPLE OF ANALYSIS TO DETERMINE CONCENTRATION OF CHRYSOTILE

The following pages show an example of raw data tabulation including specimen preparation details, magnifications, and the classification and measurement data recorded during TEM examination of a water sample. The 15 pages which follow the raw data tabulation show the results generated by computer processing of these raw data.

ASBESTOS ANALYSIS - WATER SAMPLE DATA

SFO: SF-EX JOB: 22055	SAMPLE: River Water I		CODE
PREP: By LD Date 7-1-81		COUNT: By EE Date 12-9-81	PROCESS: By AL Date 19-9-81
INSTRUMENT: Philips 400F	MAGNIFICATIONS: Grid 2160	Count 21000	
DILUTIONS: ①			
1 Volume Taken (mL)	Final Volume (mL)		
2 Volume Taken (mL)	Final Volume (mL)		
FINAL PREPARATION FILTRATION: Vol. Filtered (mL) 10 Active Area (cm ²) 1.99			
COMMENTS: (for inclusion in computer print-out; format in 5 lines of 60 characters)			
<u>Sample also contained many diatoms and irregular shaped tabular particles.</u> <hr/> <hr/> <hr/> <hr/>			
FIBER CLASSIFICATIONS:			
COUNT: NAM TN <input checked="" type="radio"/> CD <input type="radio"/> CT <input type="radio"/> CDO <input type="radio"/> CDA	UE AD AX ADX AQ <input type="radio"/> ADD <input checked="" type="radio"/> AZQ AZZ		
PROCESS:			
FIBER TYPE	CLASSIFICATION	FIBER TYPE	CLASSIFICATION
CHRYSTOTILE - CONFIRMED	CDQ + CD		
CHRYSTOTILE - DIFFERENT	CONFIRMATION		
CHRYSTOTILE - SUSPECTED	CM		
NOTES: Preparation: Sample contained fine sand which settled quickly. Sample was water colored, and cleared to colorless solution after UV treatment.			
Examination: Sample contained many irregular shaped platy particles. No amphibole-like particles detected. Many diatoms present.			

ASBESTOS ANALYSIS - FIBER CLASSIFICATION

SAMPLE: River Water I

Grid Opening No. (mm)	Fiber Classification										EDTA Peak Areas	Fiber Size	Length (mm)	Width (mm)	Comments
	MM	M	CM	CD	CD	CQ	CQ	CF	AD	AD					
1 116 x 191	x	x	x	x	x	x	x	x	x	x	15	1			
	x	x	x	x	x	x	x	x	x	x	2.5	1			
	x	x	x	x	x	x	x	x	x	x	4.5	2			
	x	x	x	x	x	x	x	x	x	x	1.7	1			
	x	x	x	x	x	x	x	x	x	x	2.3	2			
	x	x	x	x	x	x	x	x	x	x	1.0	1			
	x	x	x	x	x	x	x	x	x	x	1.2	1	$\text{mg/g} \pm 0.072$		
	x	x	x	x	x	x	x	x	x	x	5.2	3			
	x	x	x	x	x	x	x	x	x	x	1.5	1			
	x	x	x	x	x	x	x	x	x	x	2.7	1			
	x	x	x	x	x	x	x	x	x	x	1.9	1			
	x	x	x	x	x	x	x	x	x	x	7.2	1	$\text{mg/g} \pm 0.010$		
	x	x	x	x	x	x	x	x	x	x	2.7	1			
	x	x	x	x	x	x	x	x	x	x	3.2	1	$\text{mg/g} \pm 0.083$		
	x	x	x	x	x	x	x	x	x	x	6.5	0			
2 145 x 191	x	x	x	x	x	x	x	x	x	x	9.3	2			
	x	x	x	x	x	x	x	x	x	x	7.2	1			
	x	x	x	x	x	x	x	x	x	x	1.5	1			
	x	x	x	x	x	x	x	x	x	x	2.7	1			
	x	x	x	x	x	x	x	x	x	x	3.8	1			
	x	x	x	x	x	x	x	x	x	x	1.9	1			
3 187 x 193	x	x	x	x	x	x	x	x	x	x	5.1	2			
	x	x	x	x	x	x	x	x	x	x	1.7	1			
	x	x	x	x	x	x	x	x	x	x	1.2	1			
	x	x	x	x	x	x	x	x	x	x	1.0	1			

Continued on Page 2.

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Smart: River Water |

Continued on Page 3

ASBESTOS ANALYSIS - FIBER CLASSIFICATION

SAMPLE: River Water 1

Grid Opening No.	Fiber Classification										EDTA Peak Area			Comments		
	Dimensions (mm)	MM	TM	DN	CD	CQ	CM	CF	AD	AX	AQ	AM	AZ	AZZ	Length	Width
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.9	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.7	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	2.3	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	3.9	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.4	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	2.1	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.3	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.9	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	3.5	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.2	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.7	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.3	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	2.5	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.9	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.1	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.0	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.4	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	2.5	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	2.9	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	7.2	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.2	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	2.4	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.7	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.2	"
"	"	"	"	"	"	"	"	"	"	"	"	"	"	"	3.8	"
															$m_3/s_1 = 0.885$	
															$m_3/s_1 = 0.879$	
															$m_3/s_1 = 0.883$	
															$m_3/s_1 = 0.882$	

ASSESSING SWAMP SOILS - FIBER CLASSIFICATION

River-Water

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Continued on Page

ASBESTOS ANALYSIS - FIBER CLASSIFICATION

SAMPLE: River Water I

Grid Opening No.	Fiber Classification										EDTA Peak Areas	Comments			
	NAH	TM	CH	CD	CQ	CHQ	WF	AD	AI	AQ	AG	AWQ	AZQ	Length (mm)	Width (mm)
"	"	"	"	"	"	"	"	"	"	"	"	"	"	2.9	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.7	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	5.2	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.9	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.1	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	2.1	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	152.	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.9	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	3.2	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.9	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.1	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	2.9	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.7	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.0	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	2.3	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	3.9	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.9	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	2.7	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.8	1
"	"	"	"	"	"	"	"	"	"	"	"	"	"	1.2	1
1010 x 157	"	"	"	"	"	"	"	"	"	"	"	"	"	m ₂ /s ₁ = 0.877	.
	"	"	"	"	"	"	"	"	"	"	"	"	"	m ₂ /s ₁ = 0.891	.
	"	"	"	"	"	"	"	"	"	"	"	"	"	m ₂ /s ₁ = 0.887	.
	"	"	"	"	"	"	"	"	"	"	"	"	"	m ₂ /s ₁ = 0.879	.

Continued on Page —

RESULTS OF FIBER COUNT

SAMPLE: River Water 1.

The results below are for fibers classified as CHRYSOTILE
which have aspect ratios equal to or greater than 3:1
and lengths exceeding 0.5 micrometers.

Mean Fiber Concentration	27.1	MFL
Upper 95% Confidence Limit	33.1	MFL
Lower 95% Confidence Limit	21.1	MFL
Analytical Sensitivity	0.26	MFL
Estimated Mass Concentration	0.26	micrograms/liter

ANALYST'S COMMENTS ON THIS SAMPLE

This sample was treated by bubbling filtered ozone gas through the liquid while irradiating the sample with ultraviolet light. This treatment is used to oxidize organics in the liquid. After oxidation, a known volume of the sample was filtered through a 0.1 micrometer pore size Nuclepore polycarbonate filter. The deposited material on the surface of the filter was transferred to an electron microscope specimen grid by the direct carbon coating extraction replication technique.

The sample also contained many diatoms and irregular tabular particles.

* MFL = million fibers per liter

22058

DATE: 18-JUN-82

SAMPLE: River Water I.

DETAILED ANALYTICAL DATA

Active Area of Filter	1.99	sq. cm.
Final Volume Filtered	10.00	ml
Magnification for Grid Measurement	2160	
Magnification for Fiber Counting	21000	
Mean Dimension of Grid Square	87.43	micrometers
Number of Grid Squares Counted	10	
Number of Specified Fibers Counted	104	
Aspect Ratio Limit (>)	3:1	
Fiber Lengths Exceed	0.50	micrometers
Density of Chrysotile Used in Calculations	2.55	g/cc

Type of Fiber Counted

CHRYSTILE

Sample Preparation Technique

Ozone Treating

FIBER LENGTH DISTRIBUTION

Particle Size Range, um	Number Counted	Cum Number	Cum No Percent	Cum Mass Percent
0.23 - 0.34	0	0	0.00	0.00
0.34 - 0.50	0	0	0.00	0.00
0.50 - 0.73	23	23	22.12	6.64
0.73 - 1.08	26	49	47.12	17.03
1.08 - 1.58	29	78	75.00	37.66
1.58 - 2.32	12	90	86.54	51.18
2.32 - 3.41	6	96	92.31	71.03
3.41 - 5.00	6	102	98.08	87.20
5.00 - 7.34	2	104	100.00	100.00
7.34 - 10.77	0	104	100.00	100.00
10.77 - 15.81	0	104	100.00	100.00
15.81 - 23.21	0	104	100.00	100.00
23.21 - 34.06	0	104	100.00	100.00
34.06 - 50.00	0	104	100.00	100.00
50.00 - 73.40	0	104	100.00	100.00
73.40 - 107.70	0	104	100.00	100.00
107.70 - 158.10	0	104	100.00	100.00
158.10 - 232.10	0	104	100.00	100.00
232.10 - 340.60	0	104	100.00	100.00

22058

DATE: 18-JUN-82

SAMPLE: River Water I.

FIBER WIDTH DISTRIBUTION

Particle Width Range, um	Number Counted	Cum Number	Cum No Percent
0.023 - 0.034	0	0	0.00
0.034 - 0.050	97	97	93.27
0.050 - 0.073	0	97	93.27
0.073 - 0.110	6	103	99.04
0.110 - 0.160	1	104	100.00
0.160 - 0.230	0	104	100.00
0.230 - 0.340	0	104	100.00
0.340 - 0.500	0	104	100.00
0.500 - 0.730	0	104	100.00
0.730 - 1.080	0	104	100.00
1.080 - 1.580	0	104	100.00
1.580 - 2.320	0	104	100.00
2.320 - 3.410	0	104	100.00
3.410 - 5.000	0	104	100.00
5.000 - 7.340	0	104	100.00
7.340 - 10.770	0	104	100.00
10.770 - 15.810	0	104	100.00
15.810 - 23.210	0	104	100.00
23.210 - 34.060	0	104	100.00

22058

DATE: 18-JUN-82

SAMPLE: River Water 1.

FIBER ASPECT RATIO DISTRIBUTION

Aspect Ratio Range	Number Counted	Cum Number	Cum No Percent
3.00 - 6.40	0	0	0.00
6.40 - 9.46	0	0	0.00
9.46 - 13.92	0	0	0.00
13.92 - 20.44	14	14	13.46
20.44 - 30.00	37	51	49.04
30.00 - 44.00	26	77	74.04
44.00 - 64.60	14	91	87.50
64.60 - 94.90	6	97	93.27
94.90 - 139.20	0	103	99.04
139.20 - 204.40	1	103	99.04
204.40 - 300.00	0	104	100.00
300.00 - 440.00	0	104	100.00
440.00 - 646.00	0	104	100.00
646.00 - 949.00	0	104	100.00
949.00 - 1392.00	0	104	100.00
1392.00 - 2044.00	0	104	100.00
2044.00 - 3000.00	0	104	100.00
3000.00 - 4403.00	0	104	100.00

Median of Aspect Ratio Distribution 20.81

Slope Parameter of Distribution 2.17

Index of Fibrosity of Distribution 732.20

22058

DATE: 18-JUN-82

SAMPLE: River Water I.

FIBER MASS DISTRIBUTION

Particle Mass Range, pg	Number Counted	Cum Number	Cum No Percent
0.0005 - 0.0010	0	0	0.00
0.0010 - 0.0022	0	0	0.00
0.0022 - 0.0046	49	49	47.12
0.0046 - 0.0100	38	87	83.65
0.0100 - 0.0215	10	97	93.27
0.0215 - 0.0464	4	101	97.12
0.0464 - 0.1000	2	103	99.04
0.1000 - 0.2150	1	104	100.00
0.2150 - 0.4640	0	104	100.00
0.4640 - 1.0000	0	104	100.00
1.0000 - 2.1500	0	104	100.00
2.1500 - 4.6400	0	104	100.00
4.6400 - 10.0000	0	104	100.00
10.0000 - 21.5400	0	104	100.00
21.5400 - 46.4100	0	104	100.00
46.4100 - 100.0000	0	104	100.00
100.0000 - 215.4300	0	104	100.00
215.4300 - 464.1400	0	104	100.00
464.1400 - 1000.0000	0	104	100.00

22058

DATE: 24-JUN-82

SAMPLE: River Water I.

INDIVIDUAL GRID SQUARE FIBER COUNTS: CHRYSOTILE
Aspect Ratio Limit $\geq 3:1$ Minimum Length Limit is 0.5 μm

Grid Square Size			Number of Fibers/Grid Square	
Length μm	Width μm	Area	Actual	Normalized
86.1	88.4	7614.	10	10.04
90.3	88.4	7983.	8	7.66
86.6	89.4	7736.	8	7.90
89.4	85.2	7611.	13	13.05
86.6	88.9	7695.	9	8.94
88.4	86.1	7614.	10	10.04
87.0	88.9	7737.	8	7.90
90.3	86.6	7816.	16	15.65
85.2	87.0	7414.	9	9.28
83.3	86.6	7215.	13	13.77

Mean Count per Average Grid Square 10.40

Standard Deviation 2.80

Total Chi-Square 6.73

Significance Level of Uniformity 50 %

Upper and lower 95% confidence levels have been
determined on the basis of Poisson statistics.

22058

DATE: 18-JUN-82

SAMPLE: River Water 1.

ASBESTOS FIBER COUNT ANALYSIS

SELECTED RAW DATA

Fibers Classified as: CHRYSOTILE
Aspect Ratio Limit \geq 3:1 Minimum Length Limit is 0.5 um

Length um	Width um	Aspect Ratio	Length um	Width um	Aspect Ratio	Length um	Width um	Aspect Ratio
0.71	0.048	15.0	1.19	0.048	25.0	2.05	0.095	21.5
0.81	0.048	17.0	1.10	0.095	11.5	2.48	0.143	17.3
0.71	0.048	15.0	1.29	0.048	27.0	0.90	0.048	19.0
3.43	0.048	72.0	1.29	0.048	27.0	1.52	0.048	32.0
3.10	0.048	65.0	4.43	0.095	46.5	3.43	0.048	72.0
0.71	0.048	15.0	1.29	0.048	27.0	1.81	0.048	38.0
0.90	0.048	19.0	2.43	0.095	25.5	0.81	0.048	17.0
0.57	0.048	12.0	0.81	0.048	17.0	1.10	0.048	23.0
1.52	0.048	32.0	0.71	0.048	15.0	0.90	0.048	19.0
1.52	0.048	32.0	1.14	0.048	24.0	2.48	0.048	52.0
0.81	0.048	17.0	1.14	0.048	24.0	0.62	0.048	13.0
1.14	0.048	24.0	2.81	0.048	59.0	3.48	0.048	73.0
2.00	0.048	42.0	0.57	0.048	12.0	0.81	0.048	17.0
1.29	0.048	27.0	0.90	0.048	19.0	2.14	0.048	45.0
0.90	0.048	19.0	1.86	0.048	39.0	0.67	0.048	14.0
1.14	0.048	24.0	0.62	0.048	13.0	0.90	0.048	19.0
1.67	0.048	35.0	2.00	0.048	42.0	0.81	0.048	17.0
0.62	0.048	13.0	1.19	0.048	25.0	0.90	0.048	19.0
0.52	0.048	11.0	0.67	0.048	14.0	1.19	0.048	25.0
1.38	0.048	29.0	3.43	0.048	72.0	1.14	0.048	24.0
0.81	0.048	17.0	0.57	0.048	12.0	1.81	0.048	38.0
0.90	0.048	19.0	0.81	0.048	17.0	1.86	0.048	39.0
1.10	0.048	23.0	2.00	0.048	42.0	0.90	0.048	19.0
0.81	0.048	17.0	5.10	0.095	53.5	1.10	0.048	23.0
1.38	0.048	29.0	0.62	0.048	13.0	3.43	0.048	72.0
0.81	0.048	17.0	0.67	0.048	14.0	2.00	0.048	42.0
0.90	0.048	19.0	0.52	0.048	11.0	0.71	0.048	15.0
1.29	0.048	27.0	0.57	0.048	12.0	1.52	0.095	16.0
1.29	0.048	27.0	0.52	0.048	11.0	1.14	0.048	24.0
0.81	0.048	17.0	2.48	0.048	52.0	0.90	0.048	19.0
0.52	0.048	11.0	1.00	0.048	21.0	7.24	0.048	152.0
0.67	0.048	14.0	1.52	0.048	32.0	0.90	0.048	19.0
1.38	0.048	29.0	0.81	0.048	17.0	1.10	0.048	23.0

22058

DATE: 18-JUN-82

SAMPLE: River Water I.

ASBESTOS FIBER COUNT ANALYSIS

SELECTED RAW DATA

(CONT'D....)

Fibers Classified as: CHRYSOTILE
Aspect Ratio Limit \geq 3:1 Minimum Length Limit is 0.5 um

Length um	Width um	Aspect Ratio	Length um	Width um	Aspect Ratio	Length um	Width um	Aspect Ratio
1.86	0.048	39.0	0.67	0.048	14.0	1.29	0.048	27.0
0.86	0.048	18.0	0.57	0.048	12.0			

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DATE: 18-JUN-82

SAMPLE: River Water 1.

ASBESTOS FIBER COUNT ANALYSIS

SAMPLE RAW DATA

GRID		FIBER											
Length um	Width um	Class	Length um	Width um	Class	Length um	Width um	Class	Length um	Width um			
86.11	88.43	CD	0.71	0.048	CD	1.19	0.048	CD	2.05	0.095			
		CD	0.81	0.048	CD	1.10	0.095	CH	0.48	0.048			
		CM	0.57	0.048	CDQ	2.48	0.143	CD	0.71	0.048			
		CD	1.29	0.048	CD	0.90	0.048	CQ	3.43	0.048			
90.28	88.43	CD	1.29	0.048	CO	1.52	0.048	CD	3.10	0.048			
		CHQ	4.43	0.095	CD	3.43	0.048	CD	0.71	0.048			
		CD	1.29	0.048	CD	1.81	0.048						
86.57	89.35	CD	0.90	0.048	CD	2.43	0.095	CD	0.81	0.048			
		CM	0.57	0.048	CM	0.48	0.048	CD	0.57	0.048			
		CD	0.81	0.048	CHQ	1.10	0.048	CD	1.52	0.048			
		CD	0.48	0.048	CH	1.29	0.048	CD	0.71	0.048			
89.35	85.19	CD	0.90	0.048	CD	1.52	0.048	CD	1.14	0.048			
		CDQ	2.48	0.048	CD	0.81	0.048	CD	1.14	0.048			
		CD	0.62	0.048	CD	1.14	0.048	CH	0.90	0.048			
		CD	2.81	0.048	CD	3.48	0.048	CD	2.00	0.048			
		CQ	0.57	0.048	CD	0.81	0.048						
86.57	88.89	CD	1.29	0.048	CD	0.90	0.048	CH	1.10	0.048			
		CD	2.14	0.048	CD	0.90	0.048	CH	0.81	0.048			
		CH	1.10	0.048	CQ	1.86	0.048	CD	0.67	0.048			
		CD	1.14	0.048	CD	0.62	0.048	CQ	0.90	0.048			
88.43	86.11	CO	1.67	0.048	CD	2.00	0.048	CD	0.81	0.048			
		CD	0.62	0.048	CDQ	1.19	0.048	CD	0.90	0.048			
		CD	0.52	0.048	CH	0.48	0.048	CD	0.67	0.048			
		CD	1.19	0.048	CQ	1.38	0.048						
87.04	88.89	CD	3.43	0.048	CH	2.00	0.048	CD	1.14	0.048			
		CD	0.81	0.048	CD	0.57	0.048	CD	1.81	0.048			
		CH	0.38	0.048	CD	0.90	0.048	CD	0.81	0.048			
		CQ	1.86	0.048									
90.28	86.57	CD	1.10	0.048	CD	2.00	0.048	CD	0.90	0.048			

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DATE: 18-JUN-82

SAMPLE: River Water 1.

ASBESTOS FIBER COUNT ANALYSIS

SAMPLE RAW DATA

(CONT'D....)

		GRID			FIBER					
Length um	Width um	Class	Length um	Width um	Class	Length um	Width um	Class	Length um	Width um
		CQ	0.81	0.048	CDQ	5.10	0.095	CD	1.10	0.048
		CQ	1.38	0.048	CD	0.62	0.048	CM	1.86	0.048
		CQ	3.43	0.048	CD	0.81	0.048	CD	0.67	0.048
		CQ	2.00	0.048	CQ	0.90	0.048	CD	0.52	0.048
		CQ	0.71	0.048	CD	1.29	0.048			
85.19	87.04	CB	0.57	0.048	CH	0.86	0.048	CD	1.52	0.095
		CB	1.29	0.048	CD	0.52	0.048	CD	1.14	0.048
		CB	0.81	0.048	CD	2.48	0.048	CD	0.90	0.046
		CB	0.52	0.048						
83.33	86.57	CQ	1.00	0.048	CD	7.24	0.048	CD	0.67	0.048
		CQ	1.52	0.048	CQ	0.90	0.048	CM	0.52	0.048
		CQ	1.38	0.048	CQ	0.81	0.048	CM	0.48	0.048
		CHQ	1.10	0.048	CD	1.86	0.048	CD	0.67	0.048
		CHQ	1.29	0.048	CD	0.86	0.048	CQ	0.57	0.048

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DATE: 18-JUN-82

SAMPLE: River Water 1.

ASBESTOS FIBER LENGTH DISTRIBUTION
Aspect Ratio Limit \geq 3:1 Minimum Length Limit is 0.5 μm

Fiber Length
Micrometers
200+

Fibers Classified as: CHRYSOTILE
Number of Fibers Sized = 104

100+

80+

60+

40+

20+

10+

8+

6+

4+

2+

1+

0.8+

0.6+

0.4+

0.2+

0.1+

0.5 + 1 + 2 + 5 + 10 + 20 + 30 + 40 + 50 + 60 + 70 + 80 + 90 + 95 + 98 + 99

Percentage Number of Fibers Shorter Than Stated Length

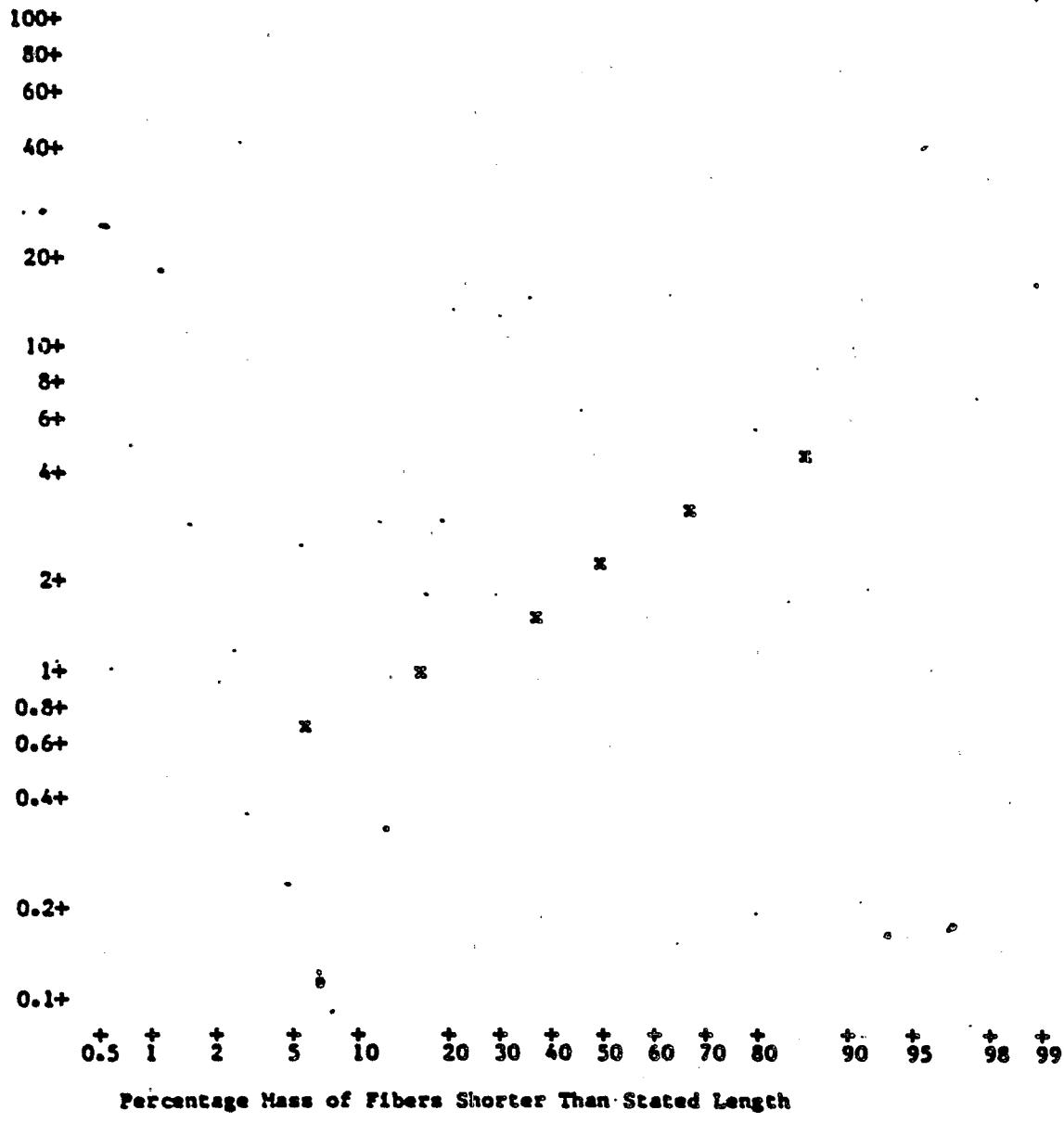
22058

DATE: 18-JUN-82

SAMPLE: River Water I.

ASBESTOS FIBER LENGTH DISTRIBUTION LOG. PROBABILITY PLOT
Aspect Ratio Limit \geq 3:1 Minimum Length Limit is 0.5 um

Fiber Length Fibers Classified as: CHRYSOTILE
Micrometers Number of Fibers Sized = 104
200+



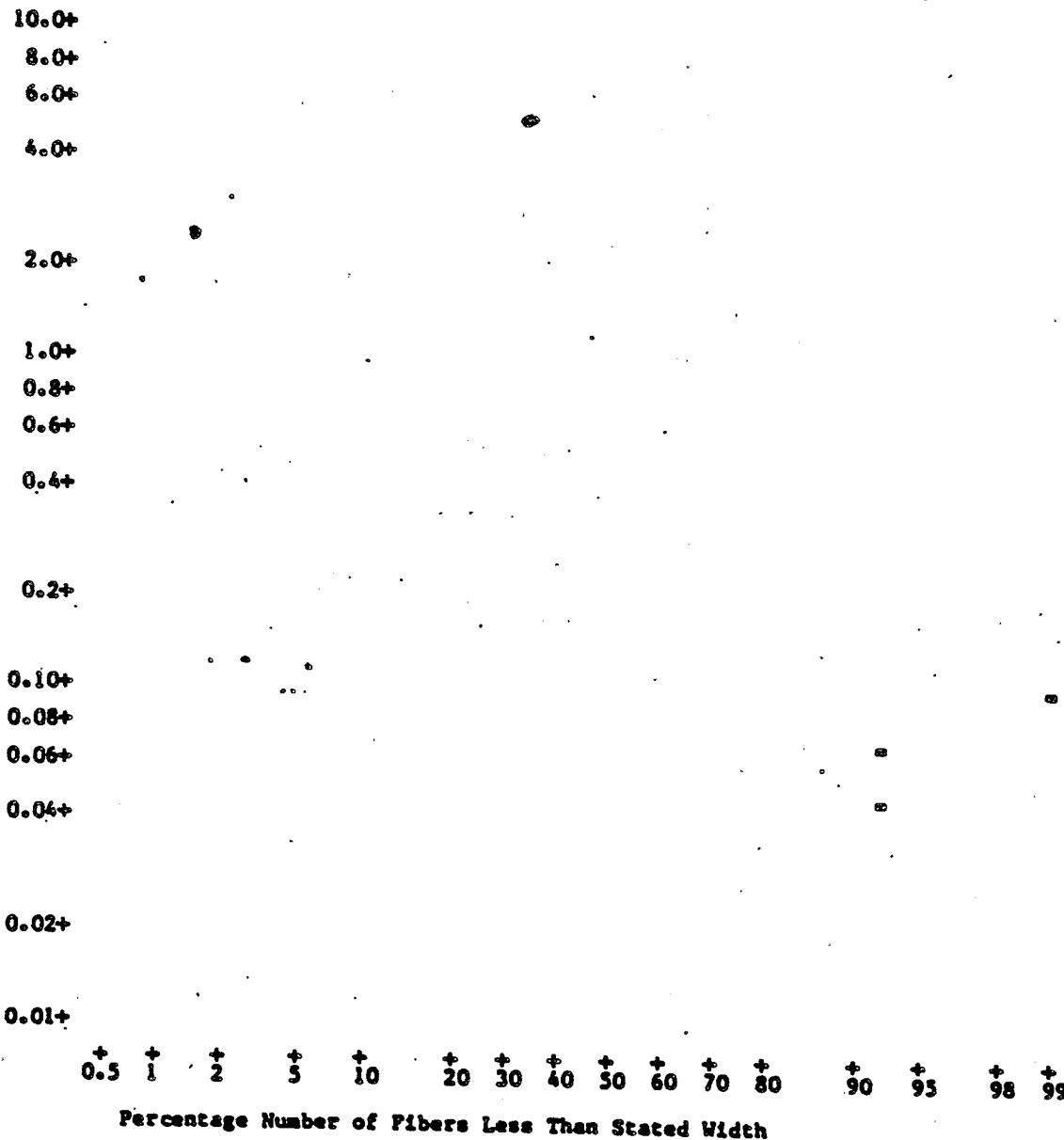
22058

DATE: 18-JUN-82

SAMPLE: River Water 1.

ASBESTOS FIBER WIDTH DISTRIBUTION LOG. PROBABILITY PLOT
Aspect Ratio Limit > 3:1 Minimum Length Limit is 0.5 μ m

Fibers Classified as: CHRYSOTILE
Number of Fibers Sized = 104

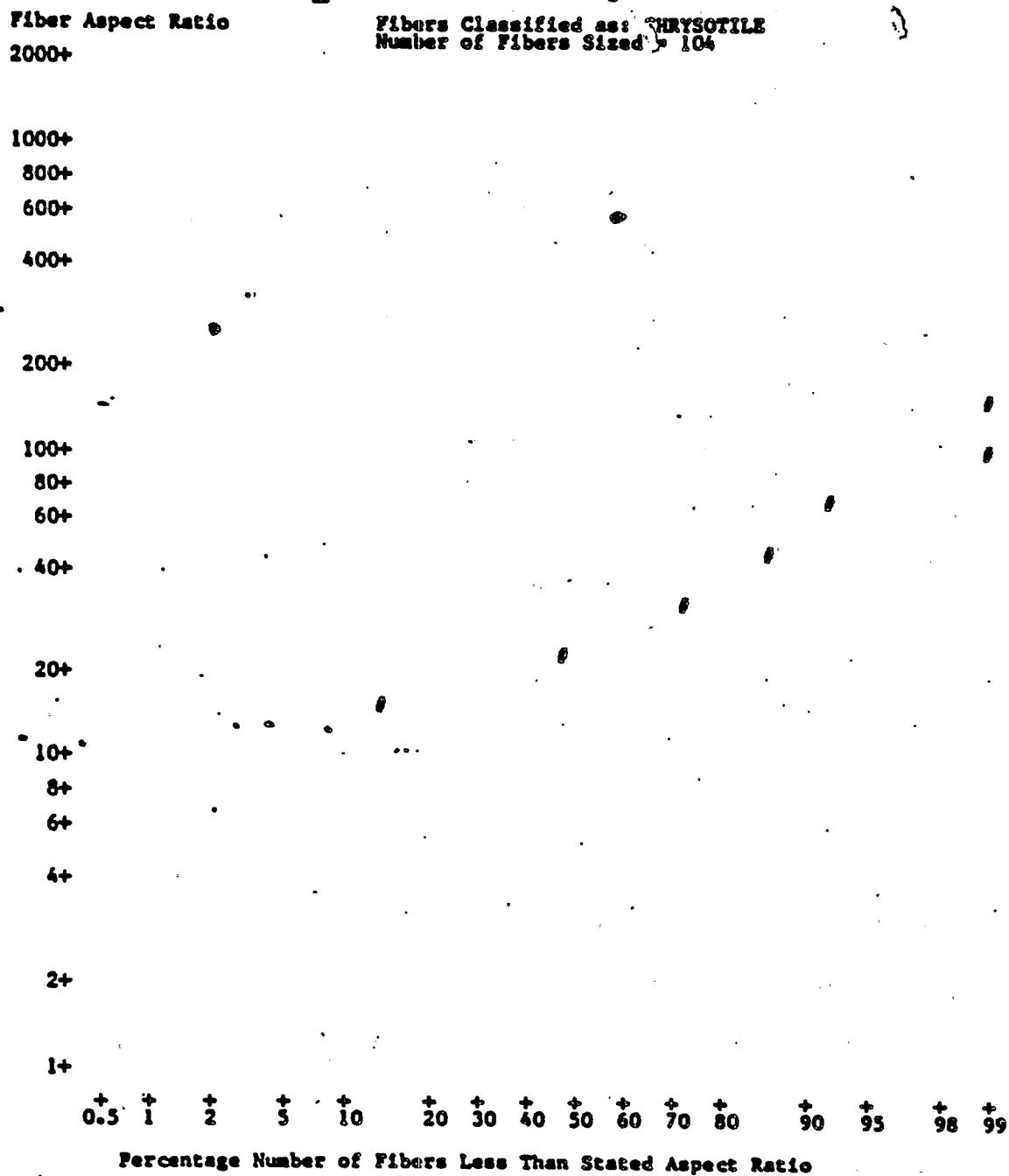


22058

DATE: 18-JUN-82

SAMPLE: River Water 1.

ASBESTOS FIBER ASPECT RATIO DISTRIBUTION LOG. PROBABILITY PLOT
Aspect Ratio Limit \geq 3:1 Minimum Length Limit is 0.5 μm



22058

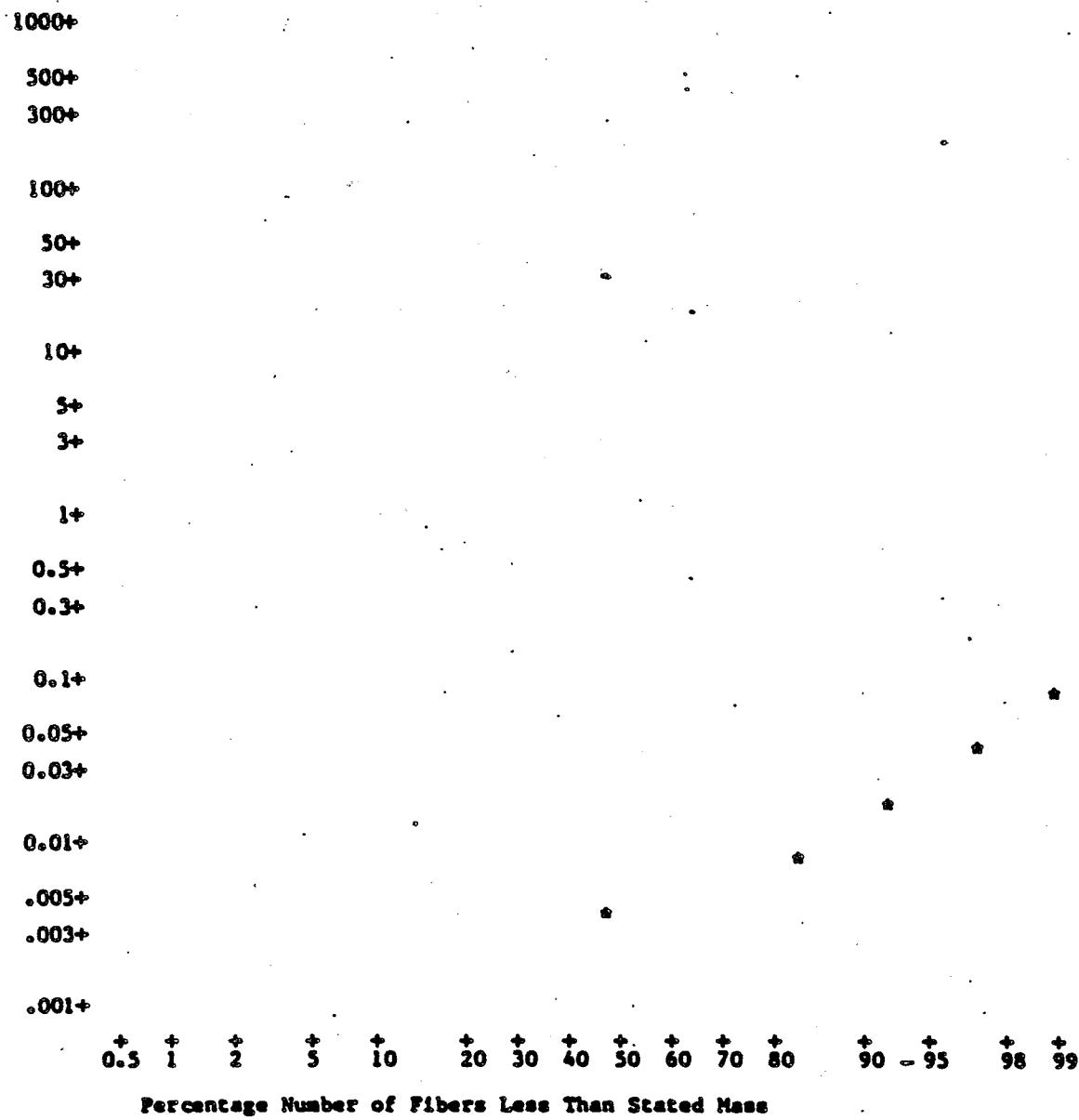
DATE: 18-JUN-82

SAMPLE: River Water 1.

ASBESTOS FIBER MASS DISTRIBUTION LOG. PROBABILITY PLOT
Aspect Ratio Limit \geq 3:1 Minimum Length Limit is 0.5 um

Fiber Mass
Picograms

Fibers Classified as: CHRYSOTILE
Number of Fibers Sized = 104



PROGRAM USER NOTES

FIBER DATA PROGRAMS

The two main programs are run sequentially for each set of data. EPAPFB accepts the data interactively and stores it in a file called FIBANL on the main computer disk which may be transferred onto a long-term storage medium (e.g. floppy diskettes). The second program EPACAL retrieves the data from either the main or long-term storage media and processes the data.

EPAFB

- program which accepts the data and stores it in a computer file

EPACAL and 31 subroutines

- programs which reduce the data and then print results
- the programs can be run on a computer with 32K words of memory
- some of the input-output statements are specific to the RSX-11M operating system
- the program is built with an overlayed structure according to Page 1 of the EPACAL listing.

EPAFIB

Data entry program for classifying fibers. Information is taken from the counting data sheets.

SEQUENCE NO. - any alphanumeric character up to 8 chars. in length
- a designation that is unique to these counting data

JOB NO. - any alphanumeric char. up to 8 chars. in length
- this may be used for accounting purposes

SAMPLE DESCRIPTION - up to 60 chars. in length

PREPARATION - up to 12 chars. in length

COUNT - up to 12 chars. in length

YOUR INITIALS - up to 4 chars. in length

INSTRUMENT USED - up to 12 chars. in length

MAGNIFICATION - Enter two integer numbers, separated by a comma, up to 5 chars. in length. The first number entered is the magnification for counting. The grid magnification range is between 1000 - 3500. The count magnification range is between 18000 - 27000.

NO. OF DILUTIONS - if 1 or 2 is entered the following prompt will appear.

1ST DILUTION: WHAT IS THE VOLUME TAKEN AND FINAL VOLUME (ML)
- enter 2 real numbers, separated by a comma

FINAL VOLUME FILTERED AND ACTIVE FILTER AREA (SQ.CM).

- enter 2 real numbers, separated by a comma
- Comments may be entered if desired, that will print on the bottom of the first page of the report. Up to 5 lines may be entered. Each line has a maximum length of up to 60 chars.
- There are 15 classifications that the program automatically recognizes. These are: TM, CM, CD, CQ, CMQ, CDQ, UF, AD, AX, ADX, AQ, ADQ, AZQ, AZZ, AZZQ. Any other classifications that are needed must be entered by the user. Enter the number of extra classifications when the question is asked, otherwise enter 0 if there are none.

DIMENSIONS OF GRID - enter 2 integer numbers up to 3 chars. in length

FIBER CLASSIFICATION - enter any of the 15 classifications, or any extra classifications

- if there are no more fibers in the grid square, enter END
- if no fibers were found in the grid square, enter END

LENGTH, WIDTH - enter 2 integer numbers up to 4 chars. in length

- the length must be greater than the width
- the width must be greater than 0

ANY MORE DATA SETS? - more than one set of data can be entered at a time

- if there are no more data sets to be entered, type NO

- the data is stored in a file named "FIBANL" on the main disk. For long-term storage, the data may be stored on media such as floppy disk, magnetic tape, etc. by simply appending the "FIBANL" files together.
- "EPACAL" is now ready to be run

EPACAL

Program which processes the data and produces reports for the classifying of fibers.

- Files may either be retrieved from the main disk or the floppy. If "EPAFIB" has just previously been run, it is much faster to retrieve the files from the main disk.
- Records may be processed by sequence no. (SEQ), job no. (JOB), or all (ALL) the records on the file may be processed.

TYPE OF FIBER - up to 32 characters in length

CLASSIFICATION INCLUDED - enter only those classifications that are to be processed for the report, followed by END. If all classifications are desired, enter ALL.

- More than one report may be processed for any data set.


```

99      RECORD=1
399      WRITE (1,399) RECORD
          FORMAT ('START ',I2)
          Q=1
1      TYPE 100
100     FORMAT (/, ' WHAT IS THE SEQUENCE NUMBER? ',$)
200     READ (5,200,ERR=1,END=9999) SEQNUM
          FORMAT(2A4)
C
2      TYPE 101
101     FORMAT (/, ' WHAT IS THE JOB NUMBER? ',$)
          READ (5,200,ERR=2,END=9999) JOBNUM
C
102     TYPE 102
          FORMAT (/, ' ENTEk SAMPLE DESCRIPTION (UPPER AND LOWER CASE): ',$)
C      ENABLES LOWER CASE
          CALL GETADR(PS,BUF(1))
          PS(2)=2
          BUF(1)="25
          BUF(2)=1
          CALL QIO("2440,5,,,PS)
          DO 91 L=1,60
          DESC(L)='
91      READ(5,201,END=9999) I,(DESC(L),L=1,I)
          BUF(2)=0
C
C      DISABLES LOWER CASE
C
          CALL QIO("2440,5,,,PS)
201     FORMAT (Q,60AI)
C
300     WRITE (1,300) SEQNUM,JOBNUM,(DESC(L),L=1,I)
          FORMAT (4A4,60AI)
          Q=2
C
103     TYPE 103
          FORMAT (/, ' PREPARATION: INITIALS AND DATE ',$)
          READ(5,203,END=9999) PREP
          FORMAT (3A4)
203     TYPE 105
          FORMAT (/, ' COUNT: INITIALS AND DATE ',$)
          READ(5,203,END=9999) COUNT
C
107     TYPE 107
          FORMAT (/, ' WHAT ARE YOUR INITIALS? ',$)
          READ(5,207,END=9999) ENTRY
          FORMAT (A4)
207     WRITE (1,305) PREP,COUNT,ENTRY
          FORMAT (7A4)
C
305

```

```

8      PREPTC='020'
109    TYPE 109
FORMAT ('WHAT INSTRUMENT WAS USED? ',$)
READ(5,203,END=9999) INSTR
C
10     TYPE 110
110    FORMAT ('WHAT WAS THE MAGNIFICATION FOR GRIDS & COUNTING? ',$)
READ(5,210,ERR=10,END=9999) GMAG,CMAG
210    FORMAT (2I5)
IF ((GMAG.LT.1000.).OR.(GMAG.GT.3500))
&      TYPE *, 'WARNING GRID MAGNIFICATION NOT IN NORMAL RANGE'
411    IF ((CMAG.LT.18000.).OR.(CMAG.GT.27000.))
&      TYPE *, 'WARNING COUNT MAGNIFICATION NOT IN NORMAL RANGE'
C
C
412    TYPE 112,SEQNUM,DESC,JOBNUM,PREP,PREPTC,COUNT,INSTR,
&      ENTRY,GMAG,CMAG
112    FORMAT ('ONo: ',2A4,/,I3X,'Sample: ',60A1,/, 'Job: ',2A4,/,,
&      'Prep by: ',3A4,17X,'Preparation Technique: ',A4,/,,
&      'Count by: ',3A4,16X,'Instrument: ',3A4,/, 'Entry by: ',,
&      A4,24X,'Magnification, Grid: ',I4,' Count: ',I5,/)
12     TYPE 113
113    FORMAT (' IS THIS INFORMATION CORRECT? ',$)
READ(5,223,END=9999) CORECT
IF (CORECT.EQ.'Y') GOTO 13
IF (CORECT.NE.'N') GOTO 12
BACKSPACE 1
BACKSPACE 1
TYPE *, 'RE-ENTER THE DATA'
GOTO 1
C
13     WRITE (1,310) PREPTC,INSTR(1),GMAG,CMAG
310    FORMAT (2A4,I4,I5)
C
15     RECNUM=2
SMPTYP='LIQU'
WRITE(1,207) SMPTYP
21     UNITS=' ML '
UNITSF=UNITS
97     TYPE 197
197    FORMAT ('HOW MANY DILUTIONS WERE THERE (0,1 OR 2)? ',$)
READ(5,*,ERR=97,END=9999) DIL
IF(DIL.GT.2) GOTO 97
WRITE (1,397)DIL
397    FORMAT(I1)
RECNUM=RECNUM+DIL+1
IF(DIL.EQ.0)GOTO25
23     TYPE 123,'1ST'
123    FORMAT ('0',A3,' DILUTION: WHAT WAS THE VOLUME',
&      ' TAKEN & FINAL VOLUME (ML)? ',$)
READ(5,*,ERR=23,END=9999) DILIVT,DILIFV
WRITE (1,323)DILIVT,DILIFV

```

```

323  FORMAT(F6.1,F6.1)
      IF(DIL.EQ.1) GOTO 25
24   TYPE 123,'2ND'
      READ(5,*,ERR=24,END=9999) DIL2VT,DIL2PV
      WRITE(1,323) DIL2VT,DIL2PV
C
C
223  FORMAT(A1)
C
25   CONTINUE
32   TYPE 132,UNITSF
132   FORMAT ('WHAT IS THE FINAL VOLUME FILTERED (',A4,
           ') & ACTIVE FILTER AREA (SQ.CM)?',\$)
           READ (5,*,ERR=32,END=9999) VOLFIL,FILA
           WRITE (1,335) VOLFIL,FILA
335  FORMAT (F7.2,F5.2)
C
C
SAMPLE SUMMARY
C
TYPE 142
142  FORMAT ('OLIQUID')
      IF(DIL.GT.0)TYPE 144,'1st',DIL1VT,DIL1PV
      IF(DIL.GT.1)TYPE 144,'2nd',DIL2VT,DIL2PV
144  FORMAT ('0',A3,' Dilution: Volume Taken (mL) : ',F6.1,8X,
           'Final Volume (mL) : ',F6.1)
      IF(PREPTC.EQ.'ASH') TYPE 145,UNITS,ASHVF,ASHFA,ASHAT,ASHDIS
145  FORMAT (/,13X,'Volume Filtered (',A4,',') : ',F7.2,
           ' Active Filter Area (sq.cm) : ',F5.2,/, 'ASHING ONLY',/,13X,
           'Area Taken (sq.cm) : ',F4.2,8X,
           'Dispersal Volume (mL) : ',F6.1)
      TYPE 146,UNITSF,VOLFIL,FILA
      FORMAT ('Volume Filtered (',A4,',') : ',F7.2,
           8X,'Active Filter Area (sq.cm) : ',F5.2)
46   TYPE 148
148  FORMAT ('IS THIS INFORMATION CORRECT? ',\$)
      READ(5,223,END=9999) DONE
      GRID=1
      IF (DONE.EQ.'Y') GOTO 73
      IF (DONE.NE.'N') GOTO 46
      DO 48 I=1,RECNUM
      BACKSPACE 1
48   CONTINUE
      TYPE *
      TYPE *, 'RE-ENTER THE INFORMATION'
      GOTO 15
C
C
C
MESSAGE SECTION
73   TYPE 173
      FORMAT('ARE THERE ANY GENERAL COMMENTS ABOUT THE SAMPLE? ',\$)
      READ(5,223,END=9999) DONE
      IF ((DONE.NE.'Y').AND.(DONE.NE.'N')) GOTO 73

```

```

DO 74 L=1,5
LEN(L)=0
DO 74 K=1,60
SMPCOM(L,K)=' '
74 IF(DONE.EQ.'N')GOTO 177
TYPE *, 'COMMENT LINES CAN HAVE A MAXIMUM OF 60 LETTERS'
TYPE *, 'THE SHIFT KEY MUST BE USED TO GET UPPER CASE'

C
C   ENABLE LOWER CASE
C
BUF(2)=1
CALL QIO("2440,5,,,PS)
DO 75 L=1,5
TYPE 175
175 FORMAT (IX,T63,'160'/'+',$,)
READ(5,201,END=9999) I,(SMPCOM(L,K),K=1,I)
LEN(L)=I
75 CONTINUE
BUF(2)=0

C
C   DISABLE LOWER CASE
C
CALL QIO("2440,5,,,PS)
C
76 TYPE 176,((SMPCOM(L,K),K=1,60),L=1,5)
176 FORMAT(//,'THE COMMENTS ARE: ',/,5(/,' ',60A1),//,'IS THIS CORRECT?',$)
READ(5,223,END=9999) DONE
IF(DONE.EQ.'N')GOTO73
IF(DONE.NE.'Y') GOTO 76
177 DO 77 L=1,5
I=LEN(L)
77 WRITE(1,377) (SMPCOM(L,K),K=1,I)
377 FORMAT (6GA1)

C
C   END OF THE INFORMATION ON THE SAMPLE
C
C   INFORMATION ON THE FIBERS PRESENT IN THE SAMPLE
C
C
78 TYPE 178
178 FORMAT('HOW MANY EXTRA CLASSIFICATIONS (0-12) ? ',$,)
READ (5,*,ERR=78,END=9999) EXTRA
IF ((EXTRA.LT.0).OR.(EXTRA.GT.12)) GOTO 78
IF (EXTRA.EQ.0) GOTO 54
DO 79 L=1,EXTRA
TYPE 179
179 FORMAT('ENTER ONE OF THE 3 OR 4 LETTER CLASSES ',$,)
READ(5,256,END=9999) CLS(15+L)
C
C
TYPE *, ' '
TYPE *, ' IF THERE ARE NO MORE FIBERS IN THE GRID SQUARE'

```

```

TYPE *, ' ENTER "END" WHEN IT ASKS FOR CLASSIFICATION'
TYPE *, '
54 RECNUM=1
154 TYPE 154,GRID
FORMAT (/, ' WHAT ARE THE DIMENSIONS OF GRID ',I2,' ? (MM) ',$,)
READ (5,* ,ERR=54,END=9999) GLEN,GWIDTH
IF((GLEN.LE.0).OR.(GLEN.GT.999))GOTO 54
IF((GWIDTH.LE.0).OR.(GWIDTH.GT.999)) GOTO 54
WRITE (1,354) GLEN,GWIDTH,'*'
354 FORMAT (2I3,A1)

C
56 RECNUM=RECNUM+2
57 TYPE 156
156 FORMAT (37HWHAT IS THE FIBER'S CLASSIFICATION? ,$)
READ(5,256,END=9999) CLASS
256 FORMAT(A4)
IF (CLASS.EQ.'END ') GOTO 50
DO 59 L=1,15+EXTRA
IF(CLS(L).EQ.CLASS) L=98
IF(L.EQ.99)GOTO58
TYPE *, 'INCORRECT CLASSIFICATION'
GOTO57

C
58 TYPE 158
158 FORMAT($2HOENTER THE FIBER'S LENGTH, WIDTH (MM), AND COMMENTS ,$)
READ (5,356,ERR=58,END=9999) LENGTH,WIDTH,I,(COM(L),L=1,I)
356 FORMAT (2I4,Q,12A1)
IF (WIDTH.EQ.0) TYPE*, 'ISN''T THIS FIBER A BIT TOO NARROW?'
IF (WIDTH.EQ.0) GOTO58
IF (LENGTH.GT.WIDTH) GOTO458
TYPE 157
157 FORMAT ('OLENGTH MUST BE GREATER THAN WIDTH')
GOTO 58

C
458 WRITE (1,256) CLASS
358 WRITE (1,358) LENGTH,WIDTH,(COM(L),L=1,I)
FORMAT (2I4,12A1)
GOTO 56

C
C
C
C REVIEW DATA FOR LAST GRID
C
50 DO 82 L=3,RECNUM
82 BACKSPACE 1
READ (1,354) GLEN,GWIDTH
C
180 TYPE 180,GRID,GLEN,GWIDTH
FORMAT ('OGRID',I3,I9,' x ',I3)
I=1
81 IF (I.EQ.RECNUM-2) GOTO84
READ (1,256) CLASS

```

```

READ (1,356) LENGTH,WIDTH,K,(COM(L),L=1,K)
182   TYPE 182,CLASS,LENGTH,WIDTH,(COM(L),L=1,K)
FORMAT ('0',8X,A4,8X,I4,' x ',I4,8X,12A1)
I=I+2
GOTO 81
84   IF (RECNUM .EQ.3) TYPE *,'           NO FIBERS'
86   TYPE 186
186   FORMAT ('0IS THIS INFORMATION CORRECT? ',$)
READ(5,223,END=9999) DONE
IF (DONE.EQ.'Y') GOTO 53
IF (DONE.NE.'N') GOTO 86
DO 88 I=1,RECNUM-2
BACKSPACE 1
88   CONTINUE
TYPE 188,GRID
188   FORMAT ('RE-ENTER DATA FOR GRID',I3)
GOTO 52
C
C
53   WRITE (1,256) '///'
GRID=GRID+1
52   IF (GRID.EQ.1) GOTO 54
TYPE 152
152   FORMAT (/,' ARE THERE ANY MORE GRIDS? ',$)
READ(5,223,END=9999) DONE
IF (DONE.EQ.'Y') GOTO 54
IF (DONE.NE.'N') GOTO 52
C
C
70   BACKSPACE 1
WRITE (1,256) 'END'
Q=0
RECORD=RECORD+1
72   TYPE 172
172   FORMAT (/,' ANY MORE DATA SETS? ',$)
READ(5,223,END=9999) DONE
IF (DONE.EQ.'Y') GOTO 99
IF (DONE.NE.'N') GOTO 72
WRITE (1,372)
372   FORMAT ('FINISHED')
CLOSE (UNIT=1)
CALL EXIT
END

```

```

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBRI(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNAM(50), RAWFIB,
LP95, UP95, IPFL, SPAC, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNAM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

```

OVERLAY STRUCTURE: THE MAIN ROOT IS 'EPACAL' WITH THREE OVERLAY REGIONS. EACH REGION CONTAINS THE FOLLOWING SUBROUTINES.

A: INIT, GET, BACK, ENTER1, GETSMP, SMPDIS, CLSGET, CLSCAL
B: GRDCAL, ENTER2, FILTER, STATS, LENDIS, SMPCAL, PAGE1
C: PAGE2, PAGE2A, PAGE2B, PAGE3, PAGE4, PAGES, GRAPH, GRAF, GRAF2,
PAGE2C, GRAF3

**INTEGER ERRA,ERRC,ERRL,ERR
BYTE REPEAT,FLAG**

CHANGE COMMAND CHAR

ICOM I

CALL. INIT

```

CALL INIT          ! GET START UP INFORMATION
IF (REPEAT.NE.'Y') CALL GET(I) ! FIND A FILE SPECIFIED DURING INIT
IF (REPEAT.EQ.'Y') CALL BACK   ! GO BACK TO START OF LAST FILE
IF(I.EQ.1) GOTO 20           ! STOP IF NO FILES ARE LEFT
CALL ENTER1
CALL GETSMP
CALL SMPDIS
CALL CLSGET
CALL CLSCAL
CALL GRDCAL
CALL ENTREE

```

! GET INFO CONCERNING PRINTOUT OF THIS DATA
! READ SAMPLE PREP INFORMATION FROM FILE
! DISPLAY SAMPLE INFO
! READ CLASSIFICATION INFO FROM FILE
! DO CLASSIFICATION AND FIBER CALCULATIONS
! DO GRID CALCULATIONS

CALL ENTER2(REPEAT,ERR)

IF (ERR.EQ.1) GOTO 10

IF (ERR.EQ.2) GOTO 20

OPEN(UNIT=2)

CALL FILTER

CALL STATS

CALL LENDIS

卷之三

! DO LENGTH DISTRIBUTION CALCULATIONS

```
CALL SMPCAL           ! DO SAMPLE PREPARATION CALCULATIONS
CALL PAGE1            ! TYPE PAGE 1
CALL PAGE2            ! TYPE PAGE 2
IF(FIBNO.LT.10) GOTO 15
CALL PAGE2A
CALL PAGE2B
CALL PAGE2C
15      CALL PAGE3          ! TYPE PAGE 3
IF (RAW.EQ.'Y') CALL PAGE4    ! TYPE PAGE 4
IF (RAW.EQ.'Y') CALL PAGES
IF(GRAPHs.NE.'Y')GOTO 18
CALL GRAPH(10)          ! TYPE GRAPHS IF INCLUDED
IF(FIBNO.LT.10) GO TO 18
CALL GRAF2(10)
CALL GRAF(10)
CALL GRAF3(10)
18      CLOSE(UNIT=2,DISP='PRINT')
C       CHANGE COMMAND CHAR BACK
C       !COM !
GOTO 10
20      CLOSE (UNIT=1)
CALL EXIT
END
```

SUBROUTINE INIT

```

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBRI(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, SEQNUM, JOBNUM, CLSLIM, MODE
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, FRACT, WEIGHT, KUMMAS
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

```

FIBANL FILES HAVE BEEN APPENDED TO A FLOPPY DISC FILE CALLED "FIBANL" FOR LONG TERM STORAGE. RETRIEVAL IS BASED ON EITHER THE SEQUENCE NUMBER OR JOB NUMBER.

BYTE TEMP

```

CALL IDATE (I,J,K)
CALL ERRSET(64,,.FALSE.,,.FALSE.,)
IF (K.EQ.74) STOP 'ENTER DATE'
TYPE *, 'WHICH DISC (MAIN OR FLOPPY)?'
ACCEPT 100,TEMP
FORMAT(A1)
IF ((TEMP.NE.'F').AND.(TEMP.NE.'M')) GOTO 10
IF(TEMP.EQ.'M')OPEN(UNIT=1,NAME='FIBANL',TYPE='OLD',READONLY)
IF(TEMP.EQ.'F')OPEN(UNIT=1,NAME='DX:FIBANL',TYPE='OLD',READONLY)

TYPE *, 'WHAT RECORDS DO YOU WANT (JOB SEQ ALL)'
TEMP=
ACCEPT110,MODE
FORMAT(A4)
IF(MODE.EQ.'ALL ') RETURN
IF((MODE.NE.'SEQ ').AND.(MODE.NE.'JOB ')) GOTO20

TYPE120,MODE
FORMAT(' ENTER THE ',A4,'NUMBER(2)',/,,' (ONE PER LINE ',
      ' TYPE END TO STOP)')

```

30 NUMBRO=0
130 ACCEPT130,NUMBR1(NUMBRO+1),NUMBER2(NUMBRO+1)
 FORMAT(2A4)
 IF(NUMBR1(NUMBRO+1).EQ.'END')RETURN
 NUMBRO=NUMBRO+1
 IF(NUMBRO.NE.11)GOTO30
 TYPE140,MODE
140 FORMAT(' LIMIT OF 10 ',A4,'NUMBERS REACHED')
 NUMBRO=10
 RETURN
 END

C
C SUBROUTINE GET(ERR)

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, ASHV, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBRI(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

C
C INTEGER ERR

10 READ (1,310,END=30) STAR
310 FORMAT(A4)

IF(STAR.NE.'STAR') GOTO10

C
320 READ (1,320)SEQNUM,JOBNUM
FORMAT (4A4)

IF (MODE.EQ.'ALL') GOTO 20

DO 15 L=1,NUMBRO

IF ((MODE.EQ.'SEQ').AND.(SEQNUM(1).EQ.NUMBRI(L)).AND.
(SEQNUM(2).EQ.NUMBR2(L))) L=98

IF ((MODE.EQ.'JOB').AND.(JOBNUM(1).EQ.NUMBRI(L)).AND.
(JOBNUM(2).EQ.NUMBR2(L))) L=98

15 CONTINUE

IF (L.NE.99) GOTO 10

20 BACKSPACE 1

ERR=0

RETURN

C
30 ERR=1

RETURN

END

C SUBROUTINE BACK

```
COMMON DESC(60), SMPGOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
      INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
      DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHV, ASHFA,
      ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
      MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
      GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
      FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
      NUMBRI(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
      FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
      RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
      LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
      ASHV, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
      CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPGOM, COM, FIBTYP
```

C BACKSPACE 1

```
C
10  READ (1,20) STAR
20  FORMAT (A4)
IF (STAR.EQ.'STAR') GOTO 30
BACKSPACE 1
BACKSPACE 1
GOTO 10
```

```
C
30  READ (1,40) SEQNUM,JOBNUM
40  FORMAT (4A4)
BACKSPACE 1
RETURN
END
```

C C
SUBROUTINE ENTERI

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBRI(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE
REAL GTAKEN, DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNC, BLANK, NUMFIB, CLSNUM,
CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

C C
REAL JOBNUM, SEQNUM, CLSLIM

C C
TYPE 10, SEQNUM, JOBNUM

10 FORMAT(' FOR SEQUENCE NUMBER: ', 2A4, ' JOB NUMBER: ', 2A4,
& /, ' ENTER TYPE OF FIBER: ', \$)

15 ACCEPT15, FIBTYP

FORMAT(32A1)

LENLIM=5

ASPLIM=3

FORMAT(A1)

GRAPHS='Y'

48 TYPE *, 'DO YOU WANT RAW DATA INCLUDED?'

ACCEPT45, RAW

IF ((RAW.NE.'N').AND.(RAW.NE.'Y')) GOTO 48

RETURN

END

C
C SUBROUTINE GETSMP
C
C

USED TO GET THE SAMPLE INFORMATION
ALL INFORMATION PASSED THROUGH COMMON

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBER1(10), NUMBER2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBER1, NUMBER2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

C
C
10 READ (1,10) SEQNUM, JOBNUM, (DESC(L), L=1, 60)
FORMAT (4A4, 60A1)

20 READ (1,20) PREP, COUNT, ENTRY
FORMAT (7A4)

30 READ (1,30) PREPTC, INST, CMAG, CMAG
FORMAT (2A4, I4, 15)

40 READ (1,40) SMPTYP
FORMAT (A4)

DIL=0

DIL2VT=1

DIL2FV=1

READ(1,80) DIL

FORMAT (I1)

IF (DIL.GT.0) READ (1,90) DILIVT, DILIFV

IF (DIL.GT.1) READ (1,90) DIL2VT, DIL2FV

90 FORMAT (F6.1, F6.1)
110 READ (1,110) VOLFIL, FILA
FORMAT (F7.2, E5.2)

C
DO 160 L=1,5

DO 170 K=1,60

SMPCOM(L,K)=' '

CONTINUE

CONTINUE

130 DO 130 L=1,5
140 READ (1,140) (SMPCOM(L,K),K=1,60)
C FORMAT (60A1)
RETURN
END

SUBROUTINE SMPDIS

C
C
C

ALL INFORMATION RECEIVED THROUGH COMMON

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
& INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
& DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
& ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
& MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
& GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
& FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
& NUMBRI(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
& FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
& RAWLEN(500), RAWWID(500), RAWCLS(500), RAVNUM(50), RAWFIB,
& LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
& ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
& CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

C
C

UNITS='cu.M'
UNITSF=UNITS

C

TYPE 112, SEQNUM, DESC, JOBNUM, PREP, PREPTC, COUNT, INST,
& ENTRY, CMAG, CMAG
112 FORMAT ('ONo: ',2A4,'.',13X,'Sample: ',60A1,'.', Job: ',2A4,'/,
& ' Prep by: ',3A4,17X,'Preparation Technique: ',A4,'/,
& ' Count by: ',3A4,16X,'Instrument: ',A4,'/, ' Entry by: ',
& A4,24X,'Magnification, Grid: ',I4,' Count: ',I5,'/)

C

TYPE 142
142 FORMAT ('OLIQUID')
IF(DIL.GT.0)TYPE 144,'1st',DILIVT,DIL1FV
IF(DIL.GT.1)TYPE 144,'2nd',DIL2VT,DIL2FV
144 FORMAT ('0',A3,' Dilution: Volume Taken (mL) : ',F6.1,8X,
& 'Final Volume (mL) : ',F6.1)
TYPE 146, UNITSF, VOLFIL, FILA
146 FORMAT ('0Volume Filtered (',A4,') : ',F7.2,
& 8X,'Filter Diameter (mm) : ',F5.2)
TYPE 150
150 FORMAT (/, 'OComments: ')
DO 55,L=1,5
IF (SMPCOM(L,1).EQ.' ')TYPE 155,(SMPCOM(L,K),K=1,60)
IF (SMPCOM(L,1).NE.' ')TYPE 155,(SMPCOM(L,K),K=1,60)
55 FORMAT (1X,60A1)

55

CONTINUE
RETURN
END

SUBROUTINE CLSGET

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, GMAG, CMAG, DIL, PREP(3),
INST, SMPPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GIAKEN, KUMMAS(20),
DISVOL, DIL1VT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBR1(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAVNUM(50), RAWFIB,
LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAVNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBR1, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GIAKEN, DISVOL, DIL1VT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, GMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

DO 10 L=1,50
RAVNUM(L)=0
10 NUMFIB(L)=0
C
GRIDNO=1
FIBNO=0
20 READ (1,310) ILEN, IWID
GRIDL(GRIDNO)=ILEN
GRIDW(GRIDNO)=IWID
25 READ (1,320) CLASSI
IF (CLASSI.EQ.' END'.OR.CLASSI.EQ.'END ') GOTO 40
IF (CLASSI.NE.' ///'.AND.CLASSI.NE.'/// ') GOTO 30
GRIDNO=GRIDNO+1
GOTO 20
C
30 NUMFIB(GRIDNO)=NUMFIB(GRIDNO)+1
RAVNUM(GRIDNO)=NUMFIB(GRIDNO)
FIBNO=FIBNO+1
CLASS(FIBNO)=CLASSI
READ (1,330) ILEN, IWID
FIBLEN(FIBNO)=ILEN
FIBWID(FIBNO)=IWID
GOTO 25
C
40 CONTINUE

D
D
TYPE *, 'LEAVING CLSGET - FIBNO-', FIBNO
TYPE *,
RETURN

C
310 FORMAT (2I3)
320 FORMAT (A4)
330 FORMAT (2I4)
END

SUBROUTINE CLSCAL

C
C
C

```

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, GMAG, CMAG, DIL, PREP(3),
& INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
& DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
& ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
& MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
& GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
& FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
& NUMBR1(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
& FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
& RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNAM(50), RAWFIB,
& LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNAM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBR1, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
& ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, GMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
& CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCom, COM, FIBTYP, TYPFIB(32)

```

C
C

```

REAL KCOUNT, DENSIT(15), STAND(15), SHAPE(15), SPECGR(8)
DATA DENSIT/6*2.55, 9*3.2/
DATA STAND/'TM ', 'CM ', 'CD ', 'CQ ', 'CMQ ', 'CDQ ', 'UF ', 'AD ',
& 'AX ', 'ADX ', 'AQ ', 'ADQ ', 'AZQ ', 'AZZ ', 'AZZQ'/
DATA SHAPE/6*0.7854, 9*1.0/
DATA TYPFIB/'C', 'H', 'R', 'Y', 'C', 'R', 'O', 'C', 'C', 'U', 'M', 'M',
& 'G', 'R', 'U', 'N', 'A', 'M', 'O', 'S', 'A', 'N', 'T', 'H', 'T', 'R',
& 'E', 'M', 'A', 'C', 'T', 'I'/
DATA SPECGR/2.55, 3.37, 3.28, 3.52, 3.43, 3.00, 3.00, 3.10/

```

C

KCOUNT=1.E3/CMAG

C
C

IF (FIBNO.EQ.0) GOTO 50
CLSNAM=0

C
20

DO 50 L=1, FIBNO
FIBLEN(L)=FIBLEN(L)*KCOUNT
FIBWID(L)=FIBWID(L)*KCOUNT
ASP(L)=FIBLEN(L)/FIBWID(L)

K=0

IF(L.EQ.1) GOTO 40

DO 40 K=1, CLSNAM

IF (CLASS(L).NE.CLS(K)) GOTO 40
FIBCLS(K)=FIBCLS(K)+1

40 K=98
CONTINUE
IF (K.EQ.99) GOTO 50
CLSNUM=CLSNUM+1
WEIGHT(CLSNUM)=0
DO 35 K=1,15
35 IF(CLASS(L).EQ.STAND(K)) WEIGHT(CLSNUM)=DENSIT(K)
IF(CLASS(L).EQ.STAND(K)) MORF(CLSNUM)=SHAPE(K)
CLS(CLSNUM)=CLASS(L)
FIBCLS(CLSNUM)=1
DO 60 I=1,32,4
IFIB=(I+3)/4
IF(FIBTYP(1).EQ.TYPPFIB(I).AND.FIBTYP(2).EQ.TYPPFIB(I+1)
.AND.FIBTYP(3).EQ.TYPPFIB(I+2).AND.FIBTYP(4).EQ.TYPPFIB(I+3)) GOTO 62
60 CONTINUE
GOTO 50
62 WEIGHT(CLSNUM)=SPECGR(IFIB)
50 CONTINUE
D TYPE778,(CLS(K),WEIGHT(K),MORF(K),K=1,CLSNUM)
D778 FORMAT('0',99(' ',A4,' ',F5.2,' ',F6.3,/))
RETURN
END

C C SUBROUTINE GRDCAL

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, GMAG, CMAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DIL1VT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBER1(10), NUMBER2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNAM(50), RAWFIB,
LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNAM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBER1, NUMBER2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DIL1VT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, GMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP
C
C
REAL KGRID
KGRID=1.E3/GMAG
AREA=0
BLANK=0
DO 60 L=1,GRIDNO
GRIDL(L)=GRIDL(L)*KGRID
GRIDW(L)=GRIDW(L)*KGRID
AREA=AREA+GRIDW(L)*GRIDL(L)
IF (NUMFIB(L).EQ.0) BLANK=BLANK+1
CONTINUE
RETURN
END

60

SUBROUTINE ENTER2(REPEAT,ERR)

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CHAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBRI(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
LP95, UP95, IPFL, CONST

REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS

INTEGER RAWNUM, RAWFIB

REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF

REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM

REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS

INTEGER DIL, CMAG, CHAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, ASPLIM, LENLIM, CLASNO

BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

INTEGER ERR

REAL CLS, TEMP

BYTE REPEAT

TYPE *, 'CLASSIFICATIONS USED IN THIS SET ARE:'

TYPE10, (CLS(I), I=1, CLSNUM)

FORMAT(1X, 24A4)

TYPE *, 'WHAT CLASSIFICATIONS DO YOU WANT INCLUDED'

TYPE *, '(ONE PER LINE TYPE END TO STOP)'

CLASNO=0

ACCEPT15, CLSLIM(CLASNO+1)

FORMAT(A4)

IF(CLSLIM(CLASNO+1).NE.'ALL') GOTO 30

DO 20 K=1, CLSNUM

20 CLSLIM(K)=CLS(K)

CLASNO=CLSNUM

GOTO 60

30 IF (CLSLIM(CLASNO+1).EQ.'END') GOTO 60

CLASNO=CLASNO+1

GOTO 50

60 DO 100 I=1, CLASNO

J=-1

DO 65 K=1, CLSNUM

IF (CLSLIM(I).EQ.CLS(K)) J=K

IF(J.NE.-1) GOTO 75

TYPE 85, CLSLIM(I)

85 FORMAT(' WARNING, NO ', A4, ' FOUND IN SAMPLE')

```
CLSLIM(I)='$$$$'
GOTO 100
75 IF(WEIGHT(J).NE.0) GOTO 100
80 TYPE 70,CLS(J)
70 FORMAT(' WHAT IS THE DENSITY FOR ',A4,' IN G/CC?',S)
READ(S,*,ERR=80) WEIGHT(J)
IF(WEIGHT(J).LE.0) GOTO 80
90 TYPE *, 'WHAT IF THE SHAPE OF THE FIBER CROSS-SECTION? (R/S)'
ACCEPT95,ICHR
95 FORMAT(A1)
IF((ICHR.NE.'R').AND.(ICHR.NE.'S'))GOTO 90
IF(ICHR.EQ.'R') MORF(J)=0.7854
IF(ICHR.EQ.'S') MORF(J)=1
100 CONTINUE
110 TYPE*,'
TYPE*, 'IS THERE GOING TO BE ANOTHER REPORT FROM THIS DATA SET?'
ACCEPT105,REPEAT
105 FORMAT(A1)
IF((REPEAT.NE.'N').AND.(REPEAT.NE.'Y')) GOTO 110
TYPE *, 'IS THE ABOVE INFORMATION CORRECT?'
ACCEPT105,TEMP
ERR=0
IF(TEMP.EQ.'Y') RETURN
ERR=1
IF(TEMP.EQ.'ABOR') ERR=2
REPEAT='Y'
RETURN
END
```

C SUBROUTINE FILTER(ERRA,ERRL,ERRC)

COMMON DESC(60), SMPCom(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
& INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
& DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, ASHVF, ASHFA,
& ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
& MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
& GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
& FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
& NUMBRI(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
& FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
& RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNAM(50), RAWFIB,
& LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNAM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, SD, U95, L95,
& ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
& INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
& CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCom, COM, FIBTYP

C
C INTEGER CNT, GTOTAL, GRID, ERA, ERC, ERL, ERRA, ERRL, ERC

C
CNT=1
GTOTAL=NUMFIB(1)
GRID=1
ERRA=0
ERRL=0
ERC=0
RAWFIB=FIBNO
IF (.NOT.FIBNO) RETURN

C
10 DO 50 L=1,FIBNO
IF (GTOTAL.GE.CNT) GOTO 20
GRID=GRID+1
GTOTAL=GTOTAL+NUMFIB(GRID)
GOTO 10

C
20 IF (ASP(L).LT.ASPLIM-.005) ERA=1

C LOWER LIMIT LENGTH RESTRICTION IS SET TO 0.5 MICROMETERS

C
IF (FIBLEN(L).LT.0.5) ERL=1
IF (CLASNO.EQ.0) GOTO 35
DO 30 K=1,CLASNO
IF (CLASS(L).EQ.CLSLIM(K)) K=98
IF (K.NE.99) ERC=1
RAWLEN(L)=FIBLEN(L)

RAWWID(L)=FIBWID(L)
RAWCLS(L)=CLASS(L)
IF (((ERA.OR.ERL).OK.ERC).EQ.1) GOTO 40

C
FIBLEN(CNT)=FIBLEN(L)
FIBWID(CNT)=FIBWID(L)
ASP(CNT)=ASP(L)
CLASS(CNT)=CLASS(L)
CNT=_CNT+1
GOTO 50

C
40 ERA=ERRA+ERA
ERRL=ERRL+ERL
ERRC=ERRC+ERC
GTOTAL=GTOTAL-1
NUMFIB(GRID)=NUMFIB(GRID)-1
ERA=0
ERL=0
ERC=0
50 CONTINUE
FIBNO=CNT-1
RETURN
END

SUBROUTINE STATS

```

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBRI(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

```

```

REAL CHI(14,26), STUTEE(50), SIGTAB(14), POIS(2,100)
BYTE FREDOM(51)
DATA FREDOM/0,1,2,3,4,5,6,7,8,9,10,11,12,13,14,
      15,16,17,18,19,20,5*21,5*22,5*23,5*24,5*25,5*26/
DATA STUTEE/0.,12.706,4.303,3.182,2.776,2.571,2.447,2.365,2.306,
      2.262,2.228,2.201,2.179,2.160,2.145,2.131,2.120,2.110,2.101,
      2.093,2.086,2.080,2.074,2.069,2.064,2.060,2.056,2.052,2.048,
      2.045,2.042,9*2.03,10*2.01/
DATA SIGTAB/'99.5','99 ','97.5','95 ','90 ','75 ','50 ',
      '25 ','10 ','5 ','2.5','1 ','0.5','0.1'/
DATA CHI/3.93E-5,1.57E-4,9.82E-4,.00393,.016,.101,.46,1.32,2.71,3.84,
      5.02,6.63,7.88,10.83,
      .01,.02,.0506,.103,.21,.57,1.38,2.77,4.61,5.99,7.38,9.21,10.6,13.81,
      .0717,.115,.216,.352,.58,1.2,2.36,4.1,6.25,7.8,9.35,11.34,12.84,16.27,
      .2,.297,.484,.71,1.06,1.92,3.35,5.38,7.78,9.49,11.14,13.28,14.86,18.47,
      .41,.554,.83,1.15,1.61,2.67,4.35,6.62,9.24,11.,12.83,15.09,16.75,20.52,
      .676,.872,1.24,1.64,2.2,3.45,5.35,7.8,10.6,12.59,14.45,16.8,18.55,22.46,
      .989,1.24,1.69,2.17,2.83,4.25,6.34,7.84,12.,14.07,16.,18.48,20.28,24.32,
      1.34,1.65,2.18,2.73,3.49,5.,7.34,10.2,13.36,15.51,17.53,20.,21.95,26.12,
      1.73,2.09,2.7,3.33,4.17,5.9,8.34,11.4,14.68,16.92,19.,21.67,23.59,27.88,
      2.16,2.56,3.25,3.94,4.86,6.73,9.34,12.5,16.,18.3,20.49,23.2,25.19,29.59,
      2.6,3.,3.82,4.57,5.57,7.58,10.3,13.7,17.28,19.68,21.9,24.73,26.76,31.26,
      3.07,3.57,4.4,5.23,6.3,8.44,11.3,14.8,18.55,21.,23.34,26.22,28.3,32.91,
      3.57,4.11,5.01,5.89,7.,9.3,12.3,16.,19.81,22.36,24.74,27.69,29.82,34.53,
      4.,4.66,5.63,6.57,7.79,10.1,13.3,17.1,1.,23.68,26.12,29.14,31.32,36.12,
      4.6,5.23,6.26,7.26,8.54,11.,14.3,18.2,22.31,25.,27.49,30.58,32.8,37.7,
```

& 5.14,5.81,6.9,7.96,9.31,11.9,15.3,19.3,23.54,26.3,28.85,32.,34.27,39.25,
 & 5.7,6.4,7.56,8.67,10.,12.8,16.3,20.5,24.77,27.59,30.19,33.4,35.72,40.79,
 & 6.26,7.,8.23,9.39,10.9,13.6,17.3,21.6,26.,28.87,31.53,34.81,37.16,42.31,
 & 6.84,7.63,8.9,10.,11.6,14.5,18.3,22.7,27.2,30.14,32.85,36.19,38.58,43.8,
 & 7.43,8.26,9.59,10.85,12.4,15.4,19.3,23.8,28.4,31.4,34.17,37.57,40.,45.3,
 & 10.5,11.5,13.1,14.6,16.4,19.9,24.3,29.3,34.38,37.6,40.65,44.3,46.9,5.62,
 & 13.7,14.9,16.8,18.4,20.6,24.4,29.3,34.8,40.26,43.77,47.,50.9,53.67,59.7,
 & 17.2,18.5,20.6,22.5,24.8,29.,34.3,40.2,46.,49.7,53.16,57.29,60.22,66.55,
 & 20.7,22.16,24.4,26.5,29.,33.6,39.3,45.6,51.8,55.7,59.3,63.69,66.77,73.4,
 & 24.3,25.9,28.4,30.6,33.3,38.3,44.3,50.9,57.4,61.6,65.38,69.9,73.13,80.,
 & 28.,29.7,32.3,34.76,37.7,42.9,49.3,56.3,63.17,67.5,71.4,76.1,79.49,86.66/
 DATA POIS/0.025,5.570,0.242,7.220,0.618,8.760,1.088,10.240,1.620,11.650,
 & 2.202,13.080,2.807,14.420,3.456,15.760,4.122,17.082,4.800,18.390,
 & 5.489,19.679,6.204,20.964,6.916,22.230,7.644,23.492,8.400,24.735,
 & 9.152,25.984,9.928,27.217,10.674,28.458,11.438,29.678,12.220,30.880,
 & 12.999,32.109,13.794,33.303,14.582,34.500,15.384,35.616,16.175,36.900,
 & 16.978,38.090,17.793,39.285,18.620,40.460,19.430,41.644,20.250,42.840,
 & 21.049,43.989,21.888,45.184,22.704,46.332,23.528,47.498,24.395,48.685,
 & 25.200,49.824,26.048,5.1.986,26.904,52.174,27.729,53.313,28.600,54.480,
 & 29.438,55.637,30.282,56.784,31.132,57.921,31.988,59.048,32.850,60.210,
 & 33.672,61.364,34.545,62.510,35.376,63.648,36.260,64.778,37.100,65.900,
 & 37.995,67.065,38.844,68.172,39.697,69.324,40.554,70.470,41.415,71.610,
 & 42.280,72.744,43.149,73.872,44.022,74.994,44.899,76.110,45.780,77.220,
 & 46.665,78.385,47.554,79.484,48.384,80.577,49.280,81.728,50.180,82.875,
 & 51.018,83.952,51.925,85.090,52.836,86.224,53.682,87.354,54.600,88.410,
 & 55.451,89.531,56.304,90.648,57.232,91.761,58.090,92.870,59.025,93.975,
 & 59.888,95.152,60.753,96.250,61.620,97.344,62.568,98.434,63.440,99.600,
 & 64.314,100.683,65.190,101.762,66.151,102.920,67.032,103.992,67.915,
 & 105.060,68.800,106.210,69.687,107.358,70.576,108.416,71.467,109.559,
 & 72.360,110.610,73.255,111.748,74.152,112.792,75.051,113.925,75.952,
 & 115.056,76.855,116.090,77.760,117.216,78.667,118.340,79.576,119.462,
 & 80.487,120.483,81.400,121.600/

C
C

```

IF (FIBNO.EQ.0) RETURN
SUM=0
CHISQ=0
AVE=FIBNO/GRIDNO
DO 10 L=1,GRIDNO
TEMP=FIBNO*GRIDL(L)*GRIDW(L)/AREA
CHISQ=CHISQ+(TEMP-NUMFIB(L))**2/TEMP
SUM=SUM+(TEMP-NUMFIB(L))**2

10
C
SIG='<0.1'
IF (GRIDNO.GE.2) SD=(SUM/(GRIDNO-1))**.5
DO 20 L=1,-1
20
IF (CHISQ.LE.CHI(L,FREDOM(GRIDNO))) SIG=SIGTAB(L)
U95=FIBNO+SD*STUTEE(GRIDNO)*(FLOAT(GRIDNO))**.5
IF (U95.LT.0) U95=0
L95=FIBNO-SD*STUTEE(GRIDNO)*FLOAT(GRIDNO)**.5
IF (L95.LT.0) L95=0
IF(FIBNO.GT.100) GOTO 30

```

30

```
LP95=POIS(1,FIBNO)
UP95=POIS(2,FIBNO)
RETURN
X=FIBNO
LP95=FIBNO - STUTEE(GRIDNO)*SQRT(X)
UP95=FIBNO + STUTEE(GRIDNO)*SQRT(X)
RETURN
END
```

C C

SUBROUTINE LENDIS

```

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
INST, SMPTY?, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBR1(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBR1, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM, KUMMAS
REAL GTAKEN, DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP
C C

REAL LOGSIZ(20), ASPSIZ(20), WIDSIZ(20), MASSIZ(20)
DATA LOGSIZ/.23,.34,.5,.73,1.08,1.58,2.32,3.41,5.,7.34,10.77,
& 15.81,23.21,34.06,50.,73.4,107.7,158.1,232.1,340.6/
DATA ASPSIZ/3.,4.4,6.46,9.49,13.92,20.44,30.,44.,64.6,94.9,139.2,
& 204.4,300.,440.,646.,949.,1392.,2044.,3000.,4403./
DATA WIDSIZ/.023,.034,.05,.073,.11,.16,.23,.34,.5,.73,1.08,1.58,
& 2.32,3.41,5.,7.34,10.77,15.81,23.21,34.06/
DATA MASSIZ/.00046,.001,.00215,.00464,.01,.0215,.0464,.1,.215,
& .464,1.,2.15,4.64,10.,21.54,46.41,100.,215.43,464.14,1000./
DO 5 L=1,20
CUMWID(L)=0
CUMNUM(L)=0
CUMASP(L)=0
KUMMAS(L)=0
CUMMAS(L)=0
TYPE *, 'FIBNO=' , FIBNO
IF (FIBNO.EQ.0) GOTO 20
DO 20 L=2,20
DO 10 K=1,FIBNO
IF ((FIBLEN(K).LT.LOGSIZ(L-1)).OR.(FIBLEN(K).GE.LOGSIZ(L)))GOTO10
CUMNUM(L)=CUMNUM(L)+1
I=0
DO 7 J=1,CLSNUM
IF(CLASS(K).EQ.CLS(J)) I=J
CUMMAS(L)=CUMMAS(L)+FIBLEN(K)*FIBWID(K)**2*MORF(I)*WEIGHT(I)
CONTINUE

```

```

DO 40 K=1,FIBNO
IF((ASP(K).LT.ASPSIZ(L-1)).OR.(ASP(K).GE.ASPSIZ(L)))GOTO 40
CUMASP(L)=CUMASP(L)+1
40 CONTINUE
DO 50 K=1,FIBNO
IF((FIBWID(K).LT.WIDSIZ(L-1)).OR.(FIBWID(K).GE.WIDSIZ(L)))GOTO 50
CUMWID(L)=CUMWID(L)+1
50 CONTINUE
DO 60 X=1,FIBNO
DO 61 J=1,CLSNUM
IF(CLASS(K).EQ.CLS(J)) I=J
FMASS=FIBLEN(K)*FIBWID(K)**2*MORF(I)*WEIGHT(I)
IF((FMASS.LT.MASSIZ(L-1)).OR.(FMASS.GE.MASSIZ(L))) GOTO 60
KUMMAS(L)=KUMMAS(L)+1
60 CONTINUE
CUMMAS(L)=CUMMAS(L)+CUMMAS(L-1)
CUMMAS(L-1)=CUMMAS(L)
CUMNUM(L)=CUMNUM(I.)+CUMNUM(L-1)
CUMNUM(L-1)=CUMNUM(L)
CUMASP(L)=CUMASP(L)+CUMASP(L-1)
CUMASP(L-1)=CUMASP(L)
CUMWID(L)=CUMWID(L)+CUMWID(L-1)
CUMWID(L-1)=CUMWID(L)
KUMMAS(L)=KUMMAS(L)+KUMMAS(L-1)
KUMMAS(L-1)=KUMMAS(L)
20 CONTINUE
CUMNUM(20)=FIBNO
IF (CUMNUM(19).EQ.FIBNO) RETURN
CUMMAS(20)=0
DO 30 L=1,FIBNO
DO 25 J=1,CLSNUM
IF(CLASS(L).EQ.CLS(J)) I=J
25 CUMMAS(20)=CUMMAS(20)+FIBLEN(L)*FIBWID(L)**2*MORF(I)*WEIGHT(I)
30 RETURN
END

```

SUBROUTINE SMPCAL
COMMON DESC(60),SMPCOM(5,60),RAW,GRAPHS,CMAG,CMAG,DIL,PREP(3),
& INST,SMPTYP,CLS(24),SEQNUM(2),JOBNUM(2),GTAKEN,KUMMAS(20),
& DISVOL,DILIVT,DIL1FV,DIL2VT,DIL2FV,ASHVF,ASHFA,
& ASHAT,ASHDIS,VOLFIL,FILA,VOLAIR,VOLWAT,PREPTC,CUMWID(20),
& MODE,BLANK,GRIDNO,FIBNO,CHISQ,SIG,NUMFIB(50),SD,U95,L95,
& GRIDL(50),GRIDW(50),FIBCLS(24),MORF(24),AREA,FIBLEN(500),
& FIBWID(500),CLASS(500),ASP(500),COUNT(3),ENTRY,CUMASP(20),
& NUMBR1(10),NUMBR2(10),NUMBRO,CLSNUM,CUMNUM(20),CUMMAS(20),
& FIBTYP(32),WEIGHT(24),FRACT,ASPLIM,LENLIM,CLSLIM(24),CLASNO,
& RAWLEN(500),RAWWID(500),RAWCLS(500),RAWNUM(50),RAWFIB,
& LP95,UP95,IPFL,SPAC,CONST

REAL LP95,UP95,CONST

REAL RAWLEN,RAWWID,RAWCLS

INTEGER RAWNUM,RAWFIB

REAL FIBLEN,FIBWID,CLASS,ASP,INST,NUMBR1,NUMBR2,CUMMAS,MORF

REAL GRIDL,GRIDW,CHISQ,SIG,FIBCLS,MODE,SEQNUM,JOBNUM,CLSLIM

REAL GTAKEN,DISVOL,DILIVT,DIL1FV,DIL2VT,DIL2FV,SD,U95,L95,

& ASHVF,ASHFA,ASHAT,ASHDIS,VOLFIL,FILA,FRACT,WEIGHT,KUMMAS,

& INTEGER DIL,CMAG,CMAG,NUMBRO,FIBNO,GRIDNO,BLANK,NUMFIB,CLSNUM,

& CUMNUM,ASPLIM,LENLIM,CLASNO

BYTE RAW,GRAPHS,DESC,SMPCOM,COM,FIBTYP

C
C

IF (SMPTYP.EQ.'LIQU') FRACT=1E-3

IF (DIL.GT.0) FRACT=FRACT*DILIVT/DIL1FV

IF (DIL.GT.1) FRACT=FRACT*DIL2VT/DIL2FV

FRACT=FRACT*VOLFIL*AREA*1E-8/FILA

RETURN

END

SUBROUTINE PAGE1

C
C
C
C

```

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
& INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
& DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHV, ASHFA,
& ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
& MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMPIB(50), SD, U95, L95,
& GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
& FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
& NUMBR1(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
& FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
& RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNAM(50), RAWFIB,
& LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNAM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBR1, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
& ASHV, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
& INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
& CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

REAL TEMP1, TEMP2, TEMP3, LOW, UPP
REAL DAT(3)

CALL DATE(DAT)
105 WRITE(2,105) JOBNUM, SEQNUM, DAT, DESC, FIBTYP
      & FORMAT (6X,2A4,2X,2A4,37X,'DATE: ',3A4,///,25X,
      & 'RESULTS OF FIBER COUNT',///,12X,'SAMPLE: ',60AI,
      & //,9X,'The results below are for fibers classified as ',32A)
110 WRITE(2,110) ASPLIM
111 FORMAT (/9X,'which have aspect ratios equal to or greater than',I3,:1')
112 WRITE(2,112)
113 FORMAT (/,9X,'and lengths exceeding 0.5 micrometers.')
114 WRITE(2,114)
115 FORMAT (//, ' ')
C

LOW=LP95
UPP=UP95
IPFL=0
CONST=1E-6
IF (FIBNO.NE.0) GOTO 117
CALL SCI((1/FRACT)*CONST*3.69,53,VAL,STR)
GOTO 315
117 IF (FIBNO.LE.4) GOTO 310
CALL SCI((FIBNO/FRACT)*CONST,53,VAL,STR)

```

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IF(VAL.LT.10.0.OR.VAL.GE.10000.0) WRITE(2,120)VAL,STR
IF(VAL.GE.10.0.AND.VAL.LT.100.0) WRITE(2,121)VAL,STR
IF(VAL.GE.100.0.AND.VAL.LT.10000.0) WRITE(2,122)VAL,STR
120 FORMAT(1IX,'Mean Fiber Concentration      ',F11.2,1X,A4,2X,'MFL')
121 FORMAT(1IX,'Mean Fiber Concentration      ',F11.1,1X,A4,2X,'MFL')
122 FORMAT(1IX,'Mean Fiber Concentration      ',F11.0,1X,A4,2X,'MFL')
IF (FIBNO.GT.30) GOTO 145
C
125 CALL SCI((UPP/FRACT)*CONST,53,VAL,STR)
IF(VAL.LT.10.0.OR.VAL.GE.10000.0) WRITE(2,130)VAL,STR
IF(VAL.GE.10.0.AND.VAL.LT.100.0) WRITE(2,131)VAL,STR
IF(VAL.GE.100.0.AND.VAL.LT.10000.0) WRITE(2,132)VAL,STR
130 FORMAT(1IX,'Upper 95% Confidence Limit    ',F9.2,1X,A4,2X,'MFL')
131 FORMAT(1IX,'Upper 95% Confidence Limit    ',F9.1,1X,A4,2X,'MFL')
132 FORMAT(1IX,'Upper 95% Confidence Limit    ',F9.0,1X,A4,2X,'MFL')
CALL SCI((LOW/FRACT)*CONST,53,VAL,STR)
IF(VAL.LT.10.0.OR.VAL.GE.10000.0) WRITE(2,140)VAL,STR
IF(VAL.GE.10.0.AND.VAL.LT.100.0) WRITE(2,141)VAL,STR
IF(VAL.GE.100.0.AND.VAL.LT.10000.0) WRITE(2,142)VAL,STR
140 FORMAT(1IX,'Lower 95% Confidence Limit    ',F9.2,1X,A4,2X,'MFL')
141 FORMAT(1IX,'Lower 95% Confidence Limit    ',F9.1,1X,A4,2X,'MFL')
142 FORMAT(1IX,'Lower 95% Confidence Limit    ',F9.0,1X,A4,2X,'MFL')
GOTO 300
C
310 CALL SCI((UPP/FRACT)*CONST,53,VAL,STR)
315 IF(VAL.LT.10.0.OR.VAL.GE.10000.0) WRITE(2,320)VAL,STR
IF(VAL.GE.10.0.AND.VAL.LT.100.0) WRITE(2,330)VAL,STR
IF(VAL.GE.100.0.AND.VAL.LT.10000.0) WRITE(2,340)VAL,STR
320 FORMAT(1IX,'Fiber Concentration is less than',F8.2,1X,A4,2X,'MFL')
330 FORMAT(1IX,'Fiber Concentration is less than',F8.1,1X,A4,2X,'MFL')
340 FORMAT(1IX,'Fiber Concentration is less than',F8.0,1X,A4,2X,'MFL')
GOTO 300
145 TEMP1=UP95-LP95
TEMP2=U95-L95
IF(TEMP2.LT.TEMP1) GOTO 125
LOW=L95
UPP=U95
IPFL=1
GOTO 125
C
300 CALL SCI((1/FRACT)*CONST,53,VAL,STR)
IF(VAL.LT.10.0.OR.VAL.GE.10000.0) WRITE(2,150)VAL,STR
IF(VAL.GE.10.0.AND.VAL.LT.100.0) WRITE(2,151)VAL,STR
IF(VAL.GE.100.0.AND.VAL.LT.10000.0) WRITE(2,152)VAL,STR
150 FORMAT(1IX,'Analytical Sensitivity      ',F11.2,1X,A4,2X,'MFL')
151 FORMAT(1IX,'Analytical Sensitivity      ',F11.1,1X,A4,2X,'MFL')
152 FORMAT(1IX,'Analytical Sensitivity      ',F11.0,1X,A4,2X,'MFL')
C
IF (FIBNO.EQ.0) GOTO 80
CALL SCI(CUMMAS(20)*1E-6/FRACT,53,VAL,STR)
160 FORMAT(1IX,'Estimated Mass Concentration   ',F7.2,1X,A4,
& ' micrograms/liter')

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C WRITE(2,160) VAL,STR
80 WRITE(2,200)
200 FORMAT(///,21X,33HANALYST'S COMMENTS ON THIS SAMPLE,/)
C
210 IF (DIL.GT.0) WRITE(2,210)
IF (PREPTC.EQ.'OZO') WRITE(2,250)
FORMAT(/,9X,'Because of a high concentration of solids, it',
& ' was necessary to',/,9X,'dilute this sample',
& ' prior to filtration.')
250 FORMAT(/,9X,'This sample was treated by bubbling filtered ozone',
& ' gas through',/,9X,'the liquid while irradiating the sample',
& ' with ultraviolet light.',/,9X,'This treatment is used to oxidize',
& ' organics in the liquid.',/,9X,'After oxidation, a known',
& ' volume of the sample was filtered',/,9X,'through a 0.1',
& ' micrometer pore size Nuclepore polycarbonate',/,9X,'filter.  ',
& 'The deposited material on the surface of the filter was',
& ',/9X,'transferred to an electron microscope specimen',
& ' grid by the direct',/,9X,'carbon coating extraction',
& ' replication technique.',/)
C
C
400 IF (FIBNO.LT.5) WRITE(2,400)
FORMAT (/,9X,'Under the conditions of this measurement,',
& 'fewer than 5 fibers',/,9X,'were found in this sample.',
& ' A mean concentration value',/,9X,'is not calculated; ',
& 'however, the fiber concentration',/,9X,'is reported as',
& 'less than the upper 95% confidence',/,9X,'limit of the',
& 'concentration.')
DO 280 L=1,5
DO 270 I=60,1,-1
IF (SMPCOM(L,I).EQ.' ')GOTO 270
WRITE(2,290) (SMPCOM(L,K),K=1,I)
I=1
270 CONTINUE
290 FORMAT (9X,60A1)
280 CONTINUE
410 WRITE(2,410)
FORMAT(//,6X,'* NFL = million fibers per liter')
RETURN
END
C
C SUBROUTINE SCI(A,ISPACE,VAL,STR)
C
10 BYTE EXP(3)
IF (A.LE.0) GOTO 60
X=ALOG10(ABS(A))
I=INT(X+SIGN(0.499,X)-.499)
IF (I.LT.4.AND.I.GT.-2) GOTO 60
VAL=A*10.**(-I)
ENCODE(3,15,EXP) I

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```
15 FORMAT(I3)
ITAB=ISPACE
IF (I.GT.0) ITAB=ITAB-1
IF (IABS(I).LT.10) ITAB=ITAB-1
WRITE(2,20) (' ',K=1,ITAB),EXP
FORMAT(3X,99(A1,:))
20 STR='x 10'
RETURN
60 WRITE(2,70)
70 FORMAT (' ')
STR=
VAL=A
RETURN
END
```

SUBROUTINE PAGE2

```

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, GMAG, CMAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBR1(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
LB95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBR1, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, GMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, LENLIM, ASPLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

REAL SCALE(20), DAT(3), STAND(15)
DATA SCALE/.23,.34,.5,.73,1.08,1.58,2.32,3.41,5.,7.34,10.77,
& 15.81,23.21,34.06,50.,73.4,107.7,158.1,232.1,340.6/
DATA STAND/'TM ','CM ','CD ','CQ ','CMQ ','CDQ ','UF ','AD ',
& 'AX ','ADX ','AQ ','ADQ ','AZQ ','AZZ ','AZZQ'/
CALL DATE(DAT)
105 WRITE(2,105) JOBNUM, DAT, DESC
FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,///,12X,'SAMPLE: ',60AI,///
26X,'DETAILED ANALYTICAL DATA',//)
& IF (DIL.NE.0)WRITE(2,100) (DILIFV/DILIVT)*(DIL2FV/DIL2VT)
100 FORMAT (12X,'Dilution Ratio',F32.2,:1')
115 WRITE(2,115) FILA, VOLFIL, 'mL
FORMAT (12X,'Active Area of Filter',F27.2,' sq. cm.',/,,
12X,'Final Volume Filtered',F27.2,2X,A12)
510 WRITE(2,510) GMAG
FORMAT (12X,'Magnification for Grid Measurement',I14)
520 WRITE(2,520) CMAG
FORMAT (12X,'Magnification for Fiber Counting',I16)
530 WRITE(2,530) (AREA/GRIDNO)**.5
FORMAT (12X,'Mean Dimension of Grid Square',F19.2,' micrometers')
540 WRITE(2,540) GRIDNO
FORMAT (12X,'Number of Grid Squares Counted',I18)
550 WRITE(2,550) FIBNO
FORMAT (12X,'Number of Specified Fibers Counted',I14)
553 WRITE(2,553) 8, ASPLIM
FORMAT (12X,'Aspect Ratio Limit (>',A1,'_)',I24,:1')

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557 WRITE(2,557)
      FORMAT (12X,'Fiber Lengths Exceed',24X,'0.50 micrometers')
C
C
      DO 560 L=1,CLASNO
      DO 560 K=1,6
      IF(STAND(K).EQ.CLSLIM(L)) L=98
      IF(L.EQ.99) WRITE(2,561) 'Chrysotile',2.55
      561 FORMAT(12X,'Density of ',A10,' Used in Calculations',F6.2,' g/cc')
C
      DO 562 L=1,CLASNO
      DO 562 K=7,15
      IF(STAND(K).EQ.CLSLIM(L)) L=98
      IF(L.EQ.99) WRITE(2,561) 'Amphibole ',3.2
C
      DO 567 L=1,CLASNO
      IF(CLSLIM(L).EQ.'$$$$') GOTO 567
      DO 563 K=1,15
      IF(CLSLIM(L).EQ.STAND(K)) K=98
      IF(K.GT.20) GOTO 567
      DO 564 K=1,CLSLIM
      IF(CLS(K).EQ.CLSLIM(L)) K=K+100
      WRITE(2,566) CLSLIM(L),WEIGHT(K-101)
      566 FORMAT(12X,'Density of ',A3,' Used in Mass Calculations',F8.2,' g/cc')
      567 CONTINUE
      WRITE(2,570) FIBTYP
      570 FORMAT (//12X,'Type of Fiber Counted',15X,32A1)
      580 FORMAT (/,12X,'Sample Preparation Technique',8X,A18)
      IF (PREPTC.EQ.'O2O') WRITE(2,580) 'Ozone Treating'
C
      IF (FIBNO.LT.10) RETURN
      WRITE(2,200)
200  FORMAT (///,25X,'FIBER LENGTH DISTRIBUTION'///
      & 10X,'Particle',7X,'Number',8X,'Cum',8X,'Cum No',5X,'Cum Mass'/
      & 8X,'Size Range,um Counted Number',
      & 'Percent Percent')
      WRITE(2,205) SCALE(1),SCALE(2),CUMNUM(1),CUMNUM(1),
      & 100*FLOAT(CUMNUM(1))/FLOAT(FIBNO),100*CUMMAS(1)/(CUMMAS(20)+1.E-9)
205  FORMAT(//,F12.2,' -',F7.2,I8,I13,F14.2,F12.2)
      WRITE(2,210) (SCALE(L),SCALE(L+1),CUMNUM(L)-CUMNUM(L-1),CUMNUM(L),
      & 100*FLOAT(CUMNUM(L))/FLOAT(FIBNO),
      & 100*CUMMAS(L)/(CUMMAS(20)+1.E-9),L=2,19)
210  FORMAT (I8(F12.2,' -',F7.2,I8,I13,F14.2,F12.2,/))
      RETURN
      END

```

SUBROUTINE PAGE2A

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COMMON DESC(60), SMPCom(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBR1(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAVNUM(50), RAWFIB,
LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAVNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBR1, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, LENLIM, ASPLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCom, COM, FIBTYP

```

```

REAL SCALE(20), DAT(3)
CALL DATE(DAT)
DATA SCALE/.023,.034,.05,.073,.11,.16,.23,.34,.5,.73,1.08,1.58,
& 2.32,3.41,5.,7.34,10.77,15.81,23.21,34.06/
IF (FIBNO.EQ.0) RETURN
WRITE(2,105) JOBNUM, DAT, DESC
FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,111,12X,'SAMPLE: ',6A1,111)

```

```

105
DO 10 I=1,20
KUMWID(I)=CUMWID(I)
CONTINUE
10
WRITE(2,200)
FORMAT (11,30X,'FIBER WIDTH DISTRIBUTION'///
6 19X,'Particle',7X,'Number',8X,'Cum',8X,'Cum No',/,,
& 17X,'Width Range, um Counted Number
& 'Percent')
200
WRITE(2,205) SCALE(1),SCALE(2),KUMWID(1),KUMWID(1),
& 100*FLOAT(CUMWID(1))/FLOAT(CUMWID(20))
FORMAT(11,9X,,F11.3,' -',F8.3,I8,I12,IX,F14.2)
205
WRITE(2,210)((SCALE(L),SCALE(L+1),KUMWID(L)-KUMWID(L-1),KUMWID(L),
& 100*FLOAT(CUMWID(L))/FLOAT(CUMWID(20))),L=2,19)
210
FORMAT (18(9X,F11.3,' -',F8.3,I8,I12,IX,F14.2,/))
RETURN
END

```

SUBROUTINE PAGE2B

```

C C
COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
& INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
& DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, ASHVF, ASHFA,
& ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
& MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
& GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
& FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
& NUMBRI(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
& FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
& RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
& LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DILIFV, DIL2VT, DIL2FV, SD, U95, L95,
& ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
& INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
& CUMNUM, LENLIM, ASPLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP
C C
REAL SCALE(20), DAT(3)
CALL DATE(DAT)
DATA SCALE/3.,4.4,6.46,9.49,13.92,20.44,30.,44.,64.6,94.9,139.2,
& 204.4,300.,440.,646.,949.,1392.,2044.,3000.,4403./
IF (FIBNO.EQ.0) RETURN
105 WRITE(2,105) JOBNUM, DAT, DESC
FORMAT('1',5X,2A4,47X,'DATE: ',3A4,11X,12X,'SAMPLE: ',6A1,11X)
C C
DO 10 I=1,20
KUMASP(I)=CUMASP(I)
CONTINUE
10 WRITE(2,200)
200 FORMAT(//,25X,'FIBER ASPECT RATIO DISTRIBUTION'///
& 19X,'Aspect ',7X,'Number',8X,'Cum',8X,'Cum No',/,/
& 17X,'Ratio Range Counted Number',/
& 'Percent')
WRITE(2,205) SCALE(1),SCALE(2),KUMASP(1),KUMASP(1),
& 100*FLOAT(CUMASP(1))/FLOAT(CUMASP(20))
205 FORMAT(//,9X,F12.2,' -',F7.2,I8,I12,I1X,F14.2)
WRITE(2,210)((SCALE(L),SCALE(L+1),KUMASP(L)-KUMASP(L-1),KUMASP(L),
& 100*FLOAT(CUMASP(L))/FLOAT(CUMASP(20))),L=2,19)
210 FORMAT(18(9X,F12.2,' -',F7.2,I8,I12,I1X,F14.2,/))
DO 300 L=1,19
IF(CUMASP(L)/CUMASP(20).LT.0.5) GOTO 300
K=L

```

```

    IF(CUMASP(L-1).EQ.0.0) K=L+1
    IF(CUMASP(K).EQ.CUMASP(K-1)) FIFTY=(SCALE(K)+SCALE(K+1))/2.
    IF(CUMASP(K).EQ.CUMASP(K-1)) GOTO 302
    FIFTY=SCALE(K)+(0.5-(CUMASP(K-1)/CUMASP(20)))*(SCALE(K+1)-
    &           SCALE(K))/(CUMASP(K)-CUMASP(K-1))*CUMASP(20)
    &           GOTO 302
    CONTINUE
300   DO 305 L=1,19
    &           IF(CUMASP(L)/CUMASP(20).LT.0.8413) GOTO 305
    &           K=L
    &           EIGHT4=SCALE(K)+(0.8413-(CUMASP(K-1)/CUMASP(20)))*(SCALE(K+1)-
    &           SCALE(K))/(CUMASP(K)-CUMASP(K-1))*CUMASP(20)
    &           GOTO 308
305   CONTINUE
308   DO 405 L=1,19
    &           IF(CUMASP(L)/CUMASP(20).LT.0.9773) GOTO 405
    &           K=L
    &           NINE7=SCALE(K)+(0.9773-(CUMASP(K-1)/CUMASP(20)))*(SCALE(K+1)-
    &           SCALE(K))/(CUMASP(K)-CUMASP(K-1))*CUMASP(20)
    &           GOTO 408
405   CONTINUE
408   FIBIND=FIFTY**(NINE7/EIGHT4)
    WRITE(2,400)FIFTY,NINE7/EIGHT4,FIBIND
400   FORMAT(//12X,'Median of Aspect Ratio Distribution ',F9.2,//,
    &           12X,'Slope Parameter of Distribution ',F9.2,//,
    &           12X,'Index of Fibrosity of Distribution ',F9.2)
    RETURN
    END

```

SUBROUTINE PAGE2C

```

C
C
COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
& INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
& DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
& ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
& MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
& GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
& FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
& NUMBR1(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
& FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
& RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
& LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBR1, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
& ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
& CUMNUM, LENLIM, ASPLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

C
C
REAL SCALE(20), DAT(3)
CALL DATE(DAT)
DATA SCALE/.00046,.001,.00215,.00464,.01,.0215,.0464,.1,.215,
& .464,1.,2.15,4.64,10.,21.54,46.41,100.,215.43,464.14,1000./
IF (FIBNO.EQ.0) RETURN
105 WRITE(2,105) JOBNUM, DAT, DESC
FORMAT ('1',5X,2A4,47X,'DATE: ',3A4, //,12X,'SAMPLE: ',60A1, //)
C
C
DO 10 I=1,20
MASCUM(I)=KUMMAS(I)
10 CONTINUE
WRITE(2,200)
200 FORMAT (//,35X,'FIBER MASS DISTRIBUTION'///
& 23X,'Particle',7X,'Number',8X,'Cum',8X,'Cum No',/,,
& 21X,'Mass Range, pg Counted Number',/,
& 'Percent')
WRITE(2,205) SCALE(1),SCALE(2),MASCUM(1),MASCUM(1),
& 100*FLOAT(KUMMAS(1))/FLOAT(KUMMAS(20))
205 FORMAT(//,13X,F10.4,' -',F9.4,I8,I12,1X,F14.2)
WRITE(2,210)((SCALE(L),SCALE(L+1),MASCUM(L)-MASCUM(L-1),MASCUM(L),
& 100*FLOAT(KUMMAS(L))/FLOAT(KUMMAS(20))),L=2,19)
210 FORMAT (18(13X,F10.4,' -',F9.4,I8,I12,1X,F14.2,/) )
RETURN
END

```

SUBROUTINE PAGE3

```

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, GMAG, CMAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
NODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBR1(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
LP95, UP95, IPFL, CONST

```

```
REAL LP95, UP95, CONST
```

```
REAL RAWLEN, RAWWID, RAWCLS
```

```
INTEGER RAWNUM, RAWFIB
```

```
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBR1, NUMBR2, CUMMAS, MORF
```

```
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
```

```
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
```

```
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
```

```
INTEGER DIL, GMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
```

```
CUMNUM, ASPLIM, LENLIM, CLASNO
```

```
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP
```

```
REAL DAT(3), AVAREA, GAREA, TEMP1, TEMP2
```

```
REAL*4 TEMP(3)
```

```
IF(FIBNO.EQ.0) RETURN
```

```
DO 10 I=1,3
```

```
TEMP(I)='
```

```
CALL DATE(DAT)
```

```
WRITE(2,105) JOBNUM, DAT, DESC, (TEMP(I), I=1,3)
```

```
105 FORMAT ('1', 5X, 2A4, 47X, 'DATE: ', 3A4, //, 12X, 'SAMPLE: ', 60A1, //,
, 60X, 3A4, /)
```

```
WRITE(2,110) FIBTYP, 8, ASPLIM
```

```
FORMAT (12X, 'INDIVIDUAL GRID SQUARE FIBER COUNTS: ', 32A1,
```

```
/, 12X, 'Aspect Ratio Limit >', A1, ' ', I3, ':1', 7X,
```

```
'Minimum Length Limit is 0.5 um')
```

```
WRITE(2,113)
```

```
FORMAT (//, 12X, 'Grid Square Size', I3X, 'Number of Fibers/Grid Square',
, 11X, 'Length Width Area', I3X, 'Actual Normalized',
, 13X, 'um um', //)
```

```
J=0
```

```
AVAREA=AREA/GRIDNO
```

```
DO 20 L=1, GRIDNO
```

```
J=J+1
```

```
GAREA=GRIDL(L)*GRIDW(L)
```

```
IF (J.NE.26) GOTO 20
```

```
J=0
```

```

TEMP(1)='(CON'
TEMP(2)='T''D.'
TEMP(3)='...)'
WRITE(2,105) JOBNUM,DAT,DESC,(TEMP(I),I=1,3)
WRITE(2,110) PIETYP,8,ASPLIM
WRITE(2,113)
20   WRITE(2,115) GRIDL(L),GRIDW(L),GAREA,NUMFIB(L),AVAREA/GAREA*NUMFIB(L)
115  FORMAT (8X,2F8.1,F9.0,14X,I3,9X,F7.2)
C
120  WRITE(2,120) FLOAT(FIBNO)/FLOAT(GRIDNO)
      FORMAT (/12X,'Mean Count per Average Grid Square',F6.2)
125  IF (GRIDNO.GT.2) WRITE(2,125) SD
      FORMAT (/12X,'Standard Deviation',F22.2)
130  WRITE(2,130) CHISQ
150  FORMAT (/,12X,'Total Chi-Square ',F23.2)
160  WRITE(2,160) SIG
      FORMAT (/,12X,'Significance Level of Uniformity',3X,A4,'Z')
      IF (IPFL.EQ.0) GOTO 180.
      TEMP1=(LP95/FRACT)*CONST
      TEMP2=(UP95/FRACT)*CONST
170  WRITE(2,170)
      CALL SCI(TEMP2,36,VAL,STR)
      WRITE(2,171) VAL,STR
170  & FORMAT(//,12X,'The 95% confidence limits have been determined',//,
      & ,12X,'on the basis of Gaussian statistics. If Poisson',//,12X,
      & , 'statistics were applied the upper 95% confidence')
171  & FORMAT(12X,'limit would be',F8.2,1X,A4,2X,'MFL while the lower')
      CALL SCI(TEMP1,51,VAL,STR)
      WRITE(2,175) VAL,STR
175  & FORMAT(12X,'95% confidence limit would be',F8.2,1X,A4,2X,'MFL')
      RETURN
180  & WRITE(2,190)
190  & FORMAT(//,12X,'Upper and lower 95% confidence levels have been',//,
      & ,12X,'determined on the basis of Poisson statistics.')
      RETURN
END
C
SUBROUTINE SCI(A,ISPACE,VAL,STR)
C
C
BYTE EXP(3)
IF (A.LE.0) GOTO 60
10   X=ALOG10(ABS(A))
I=INT(X+SIGN(0.499,X)-.499)
IF (I.LT.4.AND.I.GT.-2) GOTO 60
VAL=A*10.**(-I)
15   ENCODE(3,15,EXP) I
      FORMAT(I3)
      ITAB=ISPACE
      IF (I.GT.0) ITAB=ITAB-1
      IF (IABS(I).LT.10) ITAB=ITAB-1
      WRITE (2,20) (' ',K=1,ITAB),EXP

```

```
20 FORMAT(3X,99(A1,:))  
STR='x 10'  
RETURN  
60 WRITE(2,70)  
70 FORMAT(' ')  
STR=' '  
VAL=A  
RETURN  
END
```

SUBROUTINE PAGE4

```

C
C
COMMON DESC(60), SMPCom(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
& INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
& DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
& ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
& MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
& GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
& FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
& NUMBR1(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
& FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
& RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNUM(50), RAWFIB,
& LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
& ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
& CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCom, COM, FIBTYP
REAL*4 TEMP(3)

C
C
INTEGER START, FINI
C
REAL DAT(3)
C
IF (FIBNO.EQ.0) RETURN
DO 20, I=1,3
20 TEMP(I)='
CALL DATE(DAT)
FINI=0
START=1
10 FINI=FINI+99
IF (FIBNO.LT.START+99) FINI=FIBNO
C
105 WRITE(2,105) JOBNUM, DAT, DESC
FORMAT('1',5X,2A4,47X,'DATE: ',3A4,/,60X,/,12X,'SAMPLE: ',60A1//)
110 WRITE(2,110) (TEMP(I), I=1,3), FIBTYP, 8, ASPLIM
FORMAT (17X, 'ASBESTOS FIBER COUNT ANALYSIS', //,25X,
& 'SELECTED RAW DATA', 18X, 3A4, //11X,, "Fibers Classified as: ",
& ,32A1, /,11X, 'Aspect Ratio Limit >', A1, '_', I3, ':1', 7X,
& 'Minimum Length Limit is 0.5 um')
115 WRITE(2,115) (FIBLEN(L), FIBWID(L), ASP(L), L=START, FINI)
FORMAT (//,7X, 3(' Length Width Aspect'), /,6X,
& 3(' um um Ratio'), //,99(6X, 3(F8.2, F7.3, F7.1), /))
START=START+99
TEMP(1)='(CON'
TEMP(2)='T''D.'

```

TEMP(3)='...'
IF (FINI.NE.FIBNO) GOTO 10
RETURN
END

SUBROUTINE PAGES

```

C
C
COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, GMAG, CMAG, DIL, PREP(3),
& INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
& DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
& ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
& MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
& GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
& FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
& NUMBRI(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
& FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
& RAWLEN(500), RAWWID(500), RAWCLS(500), RNUM(50), RAWFIB,
& LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95
REAL ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, GMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM
INTEGER CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP
REAL*4 TEMP(3)
REAL DAT(3)
INTEGER START
C
20 DO 20 I=1,3
TEMP(I)=
CALL DATE(DAT)
NEXT=0
IST=1
ICS=1
IFLAG=0
30 START=0
WRITE(2,40) JOBNUM, DAT, DESC
40 FORMAT('1',5X,2A4,47X,'DATE: ',3A4,/,60X,/,12X,'SAMPLE: ',
& 60A1,/,/)
50 WRITE(2,50) (TEMP(I),I=1,3)
FORMAT(27X,'ASBESTOS FIBER COUNT ANALYSIS',/,33X,
& 'SAMPLE RAW DATA',12X,3A4)
55 WRITE(2,55) 27
FORMAT(1X,A1,'-')
WRITE(2,60)
60 FORMAT(/,15X,'GRID',34X,'FIBER',/,10X,'Length',
& 'Width',3(' Class Length Width'),/,
& 12X,'um',5X,'um',1X,3(12X,'um',5X,'um'),/,
& 10X,'-----',3(2X,'-----'),/)
DO 300 I=IST,GRIDNO
IF(RNUM(I).NE.0) GOTO 80
WRITE(2,70) GRIDL(I),GRIDW(I)

```

```

70      FORMAT(/,9X,F6.2,1X,F6.2,10X,'N O   F I B E R S')
START=START+2
IF(START.LT.36) GOTO 270
IST=I+1
GOTO 320
80      NUM=RAWSUM(I)+NEXT
DO 250 K=ICS,NUM,3
IF(K.GT.RAWFIB)GOTO 270
IF((K.EQ.ICS.AND.IFLAG.EQ.0)) GOTO 160
IF((K+1).GT.NUM) GOTO 100
IF((K+2).GT.NUM) GOTO 140
WRITE(2,90)(RAWCLS(J),RAWLEN(J),RAWWID(J),J=K,K+2)
90      FORMAT(24X,3(2X,A4,1X,F6.2,1X,F6.3))
GOTO 240
100     WRITE(2,130) RAWCLS(K),RAWLEN(K),RAWWID(K)
130     FORMAT(26X,A4,1X,F6.2,1X,F6.3)
START=START+1
GOTO 260
140     WRITE(2,150) (RAWCLS(J),RAWLEN(J),RAWWID(J),J=K,K+1)
150     FORMAT(24X,2(2X,A4,1X,F6.2,1X,F6.3))
START=START+1
GOTO 260
160     IF((K+1).GT.NUM) GOTO 190
IF((K+2).GT.NUM) GOTO 210
WRITE(2,180) GRIDL(I),GRIDW(I),(RAWCLS(J),RAWLEN(J),RAWWID(J),
& ,J=K,K+2)
180     FORMAT(/,9X,F6.2,1X,F6.2,2X,3(2X,A4,1X,F6.2,1X,F6.3))
GOTO 230
190     WRITE(2,200) GRIDL(I),GRIDW(I),RAWCLS(K),RAWLEN(K),RAWWID(K)
200     FORMAT(/,9X,F6.2,1X,F6.2,4X,A4,1X,F6.2,1X,F6.3)
GOTO 230
210     WRITE(2,220) GRIDL(I),GRIDW(I),(RAWCLS(J),RAWLEN(J),RAWWID(J),
& J=K,K+1)
220     FORMAT(/,9X,F6.2,1X,F6.2,2X,2(2X,A4,1X,F6.2,1X,F6.3))
230     START=START+1
240     START=START+1
IF(START.GE.36) GOTO 310
250     CONTINUE
260     ICS=NUM+1
NEXT=NUM
270     IFLAG=0
CONTINUE
300     IST=I
ICS=K+3
IFLAG=1
IF((K.GE.NUM).OR.((K+1).GE.NUM).OR.((K+2).GE.NUM)) IFLAG=0
IF((K.GE.NUM).OR.((K+1).GE.NUM).OR.((K+2).GE.NUM)) NEXT=NUM
IF((K.GE.NUM).OR.((K+1).GE.NUM).OR.((K+2).GE.NUM)) ICS=NUM+1
IF((K.GE.NUM).OR.((K+1).GE.NUM).OR.((K+2).GE.NUM)) IST=I+1
320     TEMP(1)='CON'
TEMP(2)='T''D.'
TEMP(3)='...')

```

57

```
WRITE(2,57) 27
FORMAT(1X,A1,'<')
IF(IST.LE.GRIDNO)GOTO 30
RETURN
END
```

C
C SUBROUTINE GRAPH(LIMIT)

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, GMAG, CMAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBRI(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNAM(50), RAWFIB,
LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNAM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBRI, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, GMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

C
C REAL PERCNT, DAT(3)

D
D TYPE*, ' ENTER GRAPH'
GRAPH=1

C CALL DATE(DAT)

C 27 is Code for ESCAPE

C ESCAPE sequences alter PRINTER.

C ESC ? 8 LINES/INCH

C ESC = 12 CHARS/INCH

C ESC < 10 CHARS/INCH

C ESC > 6 LINES/INCH

IF (FIBNO.GE.LIMIT) GOTO 5

100 WRITE(2,100) JOBNUM, DAT, DESC, FIBTYP, LIMIT

FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,///,12X,'SAMPLE: ',60A1,/,
12X,'Fibers Identified as ',32A,///,9X,'It was not possible',
' to plot meaningful graphical size',/,9X,'distributions',
' for this measurement since fewer than ',12,' particles',/,
,9X,'were found in the above classification.')

5 RETURN

105 WRITE(2,106) JOBNUM, DAT, DESC, 8, ASPLIM

FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,///,12X,'SAMPLE: ',60A1,
///,9X,'ASBESTOS FIBER LENGTH DISTRIBUTION',7X,
'LOG. PROBABILITY PLOT',/,10X,'Aspect Ratio Limit >',A1,
,13,:1')

```

106 FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,/,12X,'SAMPLE: ',6A1,
&           //,9X,'ASBESTOS FIBER LENGTH DISTRIBUTION',7X,
&           'LOG. PROBABILITY PLOT',/,10X,'Aspect Ratio Limit >',A1,
&           '_',I3,:1',7X,'Minimum Length Limit is 0.5 um')

C
120 WRITE(2,120) FIBTYP,FIBNO,27,27
FORMAT (/, ' Fiber Length',12X,'Fibers Classified as: ',32A1,/,
&           ' Micrometers',13X,'Number of Fibers Sized = ',I3,
&           /,1X,A1,'?',A1,'= 200+',/)

IF(GRAPH.EQ.2)GOTO 13
C
130 DO 10 L=0,57
K=L
IF(L.GT.48)K=48
10 CALL PLOT(L,100.*CUMNUM(17-K/3)/CUMNUM(20),'*',NEXT)
WRITE(2,130) 27,27
FORMAT (/, '+ + + + + + .7(' '+'),
&           6X,'+ + + +',/9X,' 0.5 ',
&           ' 1 2 5 10 20 30 40 50 60 ',
&           '70 80 90 95 98 99',A1,'<',A1,'>')
136 WRITE(2,136)
FORMAT (/,13X,'Percentage Number of Fibers Shorter',
&           ' Than Stated Length')
GRAPH=GRAPH+1
GOTO 5
15 DO 20 L=0,57
K=L
IF(L.GT.48)K=48
20 CALL PLOT(L,CUMMAS(17-K/3)/CUMMAS(20)*100,'x',NEXT)
WRITE(2,130) 27,27
WRITE(2,135)
135 FORMAT (/,13X,'Percentage Mass of Fibers Shorter',
&           ' Than Stated Length')
RETURN
END
C
C
SUBROUTINE PLOT(L,PERCNT,CHAR,NEXT)
C
C THIS SUB DOES THE PLOTING FOR THE LENGTH DISTRIBUTION GRAPHS
C
REAL PERCNT, TABLE(40), SCALE(16), SC
INTEGER LINE(16), NEXT
BYTE CHAR
DATA TABLE/.46,.53,.63,.79,.9,1.1,1.3,1.5,1.9,2.,2.5,2.9,3.4,3.8,
&           4.3,5.,5.8,6.7,7.5,8.8,10.,11.,12.,13.2,15.,16.6,18.2,20.1,
&           22.,24.,26.2,28.2,30.5,33.4,35.4,38.3,40.5,43.3,46.5,50./
DATA LINE/1,3,5,8,14,19,21,23,26,32,37,39,41,44,50,55/
DATA SCALE/'100+', '80+', '60+', '40+', '20+', '10+', '8+', '6+', '4+', '2+', '1+', '0.8+', '0.6+', '0.4+', '0.2+', '0.1+'/

```

C
IF(L.EQ.0) NEXT=1
SC='
IF(L.GT.48) PERCNT=0.0
IF(L.NE.LINE(NEXT)+2) GOTO 10
SC=SCALE(NEXT)
NEXT=NEXT+1
C
10 IF(''OD(L,3).EQ.0).AND.(PERCNT.GT.0.5).AND.(PERCNT.LT.99.9))GOTO40
15 IF(SC.EQ.' ') WRITE(2,20)
IF(SC.NE.' ') WRITE(2,30) SC
20 FORMAT(' ')
30 FORMAT(5X,A4)
RETURN
40 DO 45 K=1,40
45 IF(PERCNT.GE.TABLE(K)) I=K
DO 47 K=40,79
47 IF(PERCNT.GE.100-TABLE(80-K)) I=K
WRITE(2,50) SC,' ',K=1,I+1),CHAR
50 FORMAT(5X,A4,99(A1,:))
RETURN
END

SUBROUTINE GRAF(LIMIT)

```

COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, CMAG, CMAG, DIL, PREP(3),
& INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), CTAKEN, KUMMAS(20),
& DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
& ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
& MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
& GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
& FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
& NUMBR1(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
& FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
& RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNAM(50), RAWFIB,
& LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNAM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBR1, NUMBR2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL CTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
& ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, CMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
& CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP

```

REAL PERCNT, DAT(3)

GRAPH=1

CALL DATE(DAT)

27 is code of ESCAPE

ESCAPE sequences alter PRINTER

ESC ? 8 LINES/INCH

ESC = 12 CHARS/INCH

ESC < 10 CHARS/INCH

ESC > 6 LINES/INCH

IF (FIBNO.GE.LIMIT) GOTO 5

WRITE(2,100) JOBNUM, DAT, DESC, FIBTYP, LIMIT

```

100   FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,///,12X,'SAMPLE: ',60A1,//,
&           12X,'Fibers Identified as ',32A,///,9X,'It was not possible',
&           'to plot meaningful graphical size',/,9X,'distributions',
&           'for this measurement since fewer than ',I2,' particles',/,
&           9X,'were found in the above classification.')

```

RETURN

WRITE(2,106) JOBNUM, DAT, DESC, 8, ASPLIM

```

105   FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,///,12X,'SAMPLE: ',60A1,
&           ///,9X,'ASBESTOS FIBER ASPECT RATIO DISTRIBUTION',7X,
&           'LOG PROBABILITY PLOT',/,10X,'Aspect Ratio Limit >',A1,
&           ' ',I3,'1')

```

```

106   FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,///,12X,'SAMPLE: ',60A1,

```

```

C
&     //,9X,'ASBESTOS FIBER ASPECT RATIO DISTRIBUTION',7X,
&     'LOG. PROBABILITY PLOT',/,10X,'Aspect Ratio Limit >',A1,
&     ',I3,:1',7X,'Minimum Length Limit is 0.5 um')
C
120    WRITE(2,120) FIBTYP,FIBNO,27,27
      FORMAT (/, 'Fiber Aspect Ratio',12X,'Fibers Classified as: ',
      & 32A1,/34X,'Number of Fibers Sized = ',I3,
      & /,1X,A1,'?',A1,'= 2000+',/)

C
      DO 10 L=0,57
      K=L
      IF(L.GT.45)K=45
10      CALL PLOT2(L,100.*CUMASP(16-K/3)/CUMASP(20), '#',NEXT)
      WRITE(2,130) 27,27
130    FORMAT (/, + + + + + ' ,7(' + ),
      & 6X,'+' + + +' ,/ ,9X,' 0.5 ',,
      & ' 1 2 5 10 20 30 40 50 60 ',,
      & ' 70 80 90 95 98 99 ',A1,'<',A1,'>')

136    WRITE(2,136)
      FORMAT (/,13X,'Percentage Number of Fibers Less',
      & ' Than Stated Aspect Ratio')
      RETURN
      END

C
C
      SUBROUTINE PLOT2(L,PERCNT,CHAR,NEXT)

C
      REAL PERCNT, TABLE(40), SCALE(16), SC
      INTEGER LINE(16), NEXT
      BYTE CHAR
      DATA TABLE/.46,.53,.63,.79,.9,1.1,1.3,1.5,1.9,2.,2.5,2.9,3.4,3.8,
      & 4.3,5.,5.8,6.7,7.5,8.8,10.,11.,12.,13.2,15.,16.6,18.2,20.1,
      & 22.,24.,26.2,28.2,30.5,33.4,35.4,38.3,40.5,43.3,46.5,50./
      DATA LINE/1,3,5,8,14,19,21,23,26,32,37,39,41,44,50,55/
      DATA SCALE/'1000','800','600','400','200','100','80',
      & '60','40','20','10','8','6','4','2','1'/

C
C
      IF(L.EQ.0) NEXT=1

C
      SC=' '
      IF(L.GT.45) PERCNT=0.0
      IF(L.NE.LINE(NEXT)+2) GOTO 10
      SC=SCALE(NEXT)
      NEXT=NEXT+1

C
10      IF((MOD(L,3).EQ.0).AND.(PERCNT.GT.0.5).AND.(PERCNT.LT.99.9))GOTO40
15      IF(SC.EQ.' ') WRITE(2,20)
      IF(SC.NE.' ') WRITE(2,30) SC
      FORMAT(' ')
      FORMAT(4X,A4,'+')

```

```
40      RETURN
45      DO 45 K=1,40
45      IF(PERCNT.GE.TABLE(K)) I=K
47      DO 47 K=40,79
47      IF(PERCNT.GE.100-TABLE(80-K)) I=K
        IF(SC.EQ.' ')WRITE(2,50) SC,( ' ',K=1,I+2),CHAR
        IF(SC.NE.' ')WRITE(2,60) SC,( ' ',K=1,I+1),CHAR
50      FORMAT(4X,A4,99(A1,:))
60      FORMAT(4X,A4,'+',98(A1,:))
      RETURN
      END
```

SUBROUTINE CRAFT(LIMIT)

```
COMMON DESC(60), SMPCOM(5,60), RAW, GRAPHS, GMAG, CMAG, DIL, PREP(3),
INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFIB(50), SD, U95, L95,
GRIDL(50), GRIDW(50), FIBCLS(24), MORP(24), AREA, FIBLEN(500),
FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
NUMBR1(10), NUMBR2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
RAWLEN(500), RAWWID(500), RAWCLS(500), RAWNAM(50), RAWFIB,
LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RAWNAM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBR1, NUMBR2, CUMMAS, MORP
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, CUMMAS
INTEGER DIL, GMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCOM, COM, FIBTYP
```

REAL PERCENT, DAT(3)

GRAPH=1
CALL DATE(DAT)

27 is code of ESCAPE
ESCAPE sequences alter PRINTER
ESC ? 8 LINES/INCH
ESC = 12 CHARS/INCH
ESC < 10 CHARS/INCH
ESC > 6 LINES/INCH

IF (FIBNO.GE.LIMIT) GOTO 5
100 WRITE(2,100) JOBNUM, DAT, DESC, FIBTYP, LIMIT
FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,/,12X,'SAMPLE: ',60A1,/,
& 12X,'Fibers Identified as ',32A,/,9X,'It was not possible',
& ' to plot meaningful graphical size',/,9X,'distributions',
& ' for this measurement since fewer than ',I2,' particles',/,
& 9X,'were found in the above classification.')
5 RETURN
105 WRITE(2,106) JOBNUM, DAT, DESC, 8, ASPLIM
FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,/,12X,'AMPLE: ',60A1,
& 12X,'ASBESTOS FIBER WIDTH DISTRIBUTION',7X,
& 'LOG. PROBABILITY PLOT',/,10X,'Aspect Ratio Limit >',A1,
& 13,:1')

```

106      FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,//,12X,'SAMPLE: ',60AI,
        &           //,9X,'ASBESTOS FIBER WIDTH DISTRIBUTION',7X,
        &           'LOG. PROBABILITY PLOT',//,10X,'Aspect Ratio Limit >',AI,
        &           ' ',I3,':1',7X,'Minimum Length Limit is 0.5 um')
C
120      WRITE(2,120) FIBTYP,FIBNO,27,27
        FORMAT (/, ' Fiber Width',13X,'Fibers Classified as: ',
        & 32AI,/, ' Micrometers',13X,'Number of Fibers Sized ',I3,
C           /,1X,A1,'?',AI,'= 20.0+',/)
        DO 10 L=0,57
        K=L
        IF(L.GT.48) K=48
10       CALL PLOT3(L,100,*CUMWID(17-K/3)/CUMWID(20),'-',NEXT)
        WRITE(2,130) 27,27
130      FORMAT (/, '+ + + + + + ',7(' +'),
        &           6X,'+ + + + .,9X,' 0.5 ',
        &           ' 1 2 5 10 20 30 40 50 60 ',
        &           '70 80 90 95 98 99',AI,'<',AI,'>')
        WRITE(2,136)
136      FORMAT (/,13X,'Percentage Number of Fibers Less',
        &           ' Than Stated Width')
        RETURN
        END
C
C
C       SUBROUTINE PLOT3(L,PERCNT,CHAR,NEXT)
C
REAL PERCNT, TABLE(40), SCALE(16), SC
INTEGER LINE(16), NEXT
BYTE CHAR
DATA TABLE/.46,.53,.63,.79,.9,1.1,1.3,1.5,1.9,2.,2.5,2.9,3.4,3.8,
        &           4.3,5.,5.8,6.7,7.5,8.8,10.,11.,12.,13.2,15.,16.6,18.2,20.1,
        &           22.,24.,26.2,28.2,30.5,33.4,35.4,38.3,40.5,43.3,46.5,50./
        DATA LINE/1,3,5,8,14,19,21,23,26,32,37,39,41,44,50,55/
        DATA SCALE/'10.0',' 8.0',' 6.0',' 4.0',' 2.0',' 1.0',' 0.8',
        &           ' 0.6',' 0.4',' 0.2',' 0.10',' 0.08',' 0.06',' 0.04',' 0.02',' 0.01'/
C
C       IF(L.EQ.0) NE:=1
C
SC=' '
IF(L.GT.48) PERCNT=0.0
IF(L.NE.LINE(NEXT)+2) GOTO 10
SC=SCALE(NEXT)
NEXT=NEXT+1
C
10      IF((MOD(L,3).EQ.0).AND.(PERCNT.GT.0.5).AND.(PERCNT.LT.99.9))GOTO40
15      IF(SC.EQ.' ') WRITE(2,20)
IF(SC.NE.' ') WRITE(2,30) SC
20      FORMAT(' ')

```

```
30 FORMAT(4X,A4,'+')
RETURN
40 DO 45 K=1,40
45 IF(PERCNT.GE.TABLE(K)) I=K
DO 47 K=40,79
47 IF(PERCNT.GE.100-TABLE(80-K)) I=K
IF(SC.EQ.' ')WRITE(2,50) SC,( ' ',K=1,I+2),CHAR
IF(SC.NE.' ')WRITE(2,60) SC,( ' ',K=1,I+1),CHAR
FORMAT(4X,A4,99(A1,:))
FORMAT(4X,A4,'+',98(A1,:))
RETURN
END
```

SUBROUTINE GRAF3(LIMIT)

C C

```
COMMON DESC(60), SMPCom(5,60), RAW, GRAPHS, GMAG, CMAG, DIL, PREP(3),
& INST, SMPTYP, CLS(24), SEQNUM(2), JOBNUM(2), GTAKEN, KUMMAS(20),
& DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, ASHVF, ASHFA,
& ASHAT, ASHDIS, VOLFIL, FILA, VOLAIR, VOLWAT, PREPTC, CUMWID(20),
& MODE, BLANK, GRIDNO, FIBNO, CHISQ, SIG, NUMFLB(50), SD, U95, L95,
& GRIDL(50), GRIDW(50), FIBCLS(24), MORF(24), AREA, FIBLEN(500),
& FIBWID(500), CLASS(500), ASP(500), COUNT(3), ENTRY, CUMASP(20),
& NUMBER1(10), NUMBER2(10), NUMBRO, CLSNUM, CUMNUM(20), CUMMAS(20),
& FIBTYP(32), WEIGHT(24), FRACT, ASPLIM, LENLIM, CLSLIM(24), CLASNO,
& RAWLEN(500), RAWWID(500), RAWCLS(500), RNUM(50), RAWFIB,
& LP95, UP95, IPFL, CONST
REAL LP95, UP95, CONST
REAL RAWLEN, RAWWID, RAWCLS
INTEGER RNUM, RAWFIB
REAL FIBLEN, FIBWID, CLASS, ASP, INST, NUMBER1, NUMBER2, CUMMAS, MORF
REAL GRIDL, GRIDW, CHISQ, SIG, FIBCLS, MODE, SEQNUM, JOBNUM, CLSLIM
REAL GTAKEN, DISVOL, DILIVT, DIL1FV, DIL2VT, DIL2FV, SD, U95, L95,
& ASHVF, ASHFA, ASHAT, ASHDIS, VOLFIL, FILA, WEIGHT, FRACT, KUMMAS
INTEGER DIL, GMAG, CMAG, NUMBRO, FIBNO, GRIDNO, BLANK, NUMFIB, CLSNUM,
& CUMNUM, ASPLIM, LENLIM, CLASNO
BYTE RAW, GRAPHS, DESC, SMPCom, COM, FIBTYP
```

C C

```
REAL PERCNT, DAT(3)
```

C C

```
GRAPH=1
CALL DATE(DAT)
C 27 is code of ESCAPE
C ESCAPE sequences alter PRINTER
C ESC ? 8 LINES/INCH
C ESC = 12 CHARS/INCH
C ESC < 10 CHARS/INCH
C ESC > 6 LINES/INCH
```

C

```
IF (FIBNO.GE.LIMIT) GOTO 5
WRITE(2,100) JOBNUM, DAT, DESC, FIBTYP, LIMIT
100 FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,///,12X,'SAMPLE: ',60A1,//,
& 12X,'Fibers Identified as ',32A,///,9X,'It was not possible',
& 'to plot meaningful graphical size',//,9X,'distributions',
& 'for this measurement since fewer than ',I2,' particles',/,,
& ,9X,'were found in the above classification.')
      RETURN
5   WRITE(2,105) JOBNUM, DAT, DESC, 8, ASPLIM
105 FORMAT ('1',5X,2A4,47X,'DATE: ',3A4,///,12X,'SAMPLE: ',60A1,
& ///,17X,'ASBESTOS FIBER MASS DISTRIBUTION',7X,
& 'LOG. PROBABILITY PLOT',/,10X,'Aspect Ratio Limit >',A1,
& ',I3,'1 )
106 FORMAT ('T',5X,2A4,47X,'DATE: ',3A4,///,12X,'SAMPLE: ',60A1,
```

```

&     //,17X,'ASBESTOS FIBER MASS DISTRIBUTION',7X,
&     'LOG. PROBABILITY PLOT',/,10X,'Aspect Ratio Limit >',AI,
&     ',I3,:1',7X,'Minimum Length Limit is 0.5 um')
C
120   WRITE(2,120) FIBTYP,FIBNO,27,27
      FORMAT (/, ' Fiber Mass          ,12X,'Fibers Classified as: ',
      & 32AI,/, ' P.cograms',21X,'Number of Fibers Sized = ',I3,
      & /,1X,A1,'?',A1,'=        ',/)

C
10    DO 10 L=0,57
10    CALL PLOT4(L,100.*KUMMAS(20-L/3)/KUMMAS(20), '**',NEXT)
130   WRITE(2,130) 27,27
      FORMAT (/, '+ + + + + + + ,7(' +'),,
      & 6X,'+ + + + ',/ ,9X,' 0.5 ',
      & ' 1   2   5   10   20   30   40   50   60   ',
      & '70   80   90   95   98   99',A1,'<',A1,'>')

136   WRITE(2,136)
      FORMAT (/,13X,'Percentage Number of Fibers Less',
      & ' Than Stated Mass')

      RETURN
      END

C
C
      SUBROUTINE PLOT4(L,PERCNT,CHAR,NEXT)
C
C
      REAL PERCNT, TABLE(40), SCALE(19), SC
      INTEGER LINE(19), NEXT
      BYTE CHAR
      DATA TABLE/.45,.53,.63,.79,.9,1.1,1.3,1.5,1.9,2.,2.5,2.9,3.4,3.8,
      & 4.3,5.,5.8,6.7,7.5,8.8,10.,11.,12.,13.2,15.,16.6,18.2,20.1,
      & 22.,24.,26.2,28.2,30.5,33.4,35.4,38.3,40.5,43.3,46.5,50./
      DATA LINE/1,4,6,10,13,15,19,22,24,28,31,33,37,40,42,46,49,51,55/
      DATA SCALE/'1000','500','300','100','50','30','10',
      & '5','3','1','0.5','0.3','0.1','0.05','0.03',
      & '0.01','0.005','0.003','0.001'/

C
C
      IF(L.EQ.0) NEXT=1
C
      SC=' '
      IF(L.EQ.57) PERCNT=0.0
      IF(L.NE.LINE(NEXT)+2) GOTO 10
      SC=SCALE(NEXT)
      NEXT=NEXT+1

10    IF((MOD(L,3).EQ.!).AND.(PERCNT.GT.0.5).AND.(PERCNT.LT.99.9))GOTO 40
15    IF(SC.EQ.' ') WRITE(2,20)
      IF(SC.NE.' ') WRITE(2,30) SC
      FORMAT(' ')
      FORMAT(4X,A4,'+')

20    30
      RETURN

```

```
40      DO 45 K=1,40
45      IF(PERCNT.GE.TABLE(K)) I=K
        DO 47 K=40,79
47      IF(PERCNT.GE.100-TABLE(80-K)) I=K
        IF(SC.EQ.' ')WRITE(2,50) SC,( ' ',K=1,I+2),CHAR
        IF(SC.NE.' ')WRITE(2,60) SC,( ' ',K=1,I+1),CHAR
50      FORMAT(4X,A4,99(A1,:))
60      FORMAT(4X,A4,'+',98(A1,:))
      RETURN
      END
```