

## APPENDIX III: SHORE-BASED LABORATORY PROCEDURES

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#### INTRODUCTION

When the sediment cores are split longitudinally into two halves on board the *Glomar Challenger*, one half is preserved untouched as an archive and the other is designated as the work half. The latter is sampled for various purposes; some analyses are carried out on board, and others which require a large amount of laboratory space and/or sophisticated equipment are retained for distribution to shore-based laboratories at the completion of each cruise.

Samples from the Atlantic Ocean and Gulf of Mexico for grain size and carbon carbonate analyses are sent to the East Coast Repository of the Deep Sea Drilling Project at Lamont-Doherty Geological Observatory; those from the Pacific Ocean are sent to Scripps Institution of Oceanography.

All samples for X-ray mineralogy are sent to the Deep Sea Drilling Project laboratory at the University of California, Riverside.

#### GRAIN SIZE ANALYSIS

##### A. Purpose:

A semi-quantitative analysis by weight of the following sediment size fractions:

- >0.062 millimeter;
- 0.004 to 0.062 millimeter; and,
- <0.004 millimeter.

##### B. Material:

A 10-gram portion of fresh wet sediment taken at those intervals down the core as specified by the chief scientist – usually one sample every 150 centimeters.

##### C. To disaggregate the sediment:

1. Extrude the sediment plugs from their plastic containers into labelled 400-milliliter beakers.
2. Place the 400-milliliter beakers into an oven and dry the samples for 24 hours at 100°C.
3. Remove the beakers from the oven and add Calgon solution (50 grams of Calgon to five gallons

distilled water) so that the solution covers the dried sediment sample. Cover the beakers with watch glasses and let the samples disaggregate for at least six hours.

4. After the initial soaking period check to see if the sediment in each beaker has been completely disaggregated. If lumps of sediment still remain, attempt to break these up by hand or with a rubber policeman. If lumps of sediment persist, an attempt should be made to disperse them in the beaker using an ultrasonic probe for one minute at a low power setting.

*Note:* There is a possibility that the ultrasonic probe will break up some of the delicate microfossils that make up some of the sand and silt fractions. Thus it is desirable to attempt to disaggregate the sample without using the ultrasonic probe.

5. If the above methods fail then proceed as follows: place sample in a 1000 milliliter plastic beaker, and add 50 milliliters of approximately 10 per cent hydrogen peroxide. Let sit for 24 hours, then add 25 milliliter portions of 130 volume H<sub>2</sub>O<sub>2</sub> (38 per cent) at 24 hour intervals until there is no more reaction of organic material as noted by only the formation of small bubbles which indicate the breaking down of hydrogen peroxide, not a soapy type of foaming. Mark label each time peroxide is added.

6. Destroy the excess peroxide in the samples by placing them on a boiling water or steam bath for one hour. Then, connect the samples to a filter candle setup (Micro-porous filter, Porosity 03, Selas No. FP-126. Selas Corp., Dresher, Pennsylvania), evacuate the fluid, and then wash with 8 portions of 500 milliliters each of distilled water. (Use the same source of distilled water for the entire sample series.) Remove samples from filter candles by back pressure either from a wash bottle or from pressure from the distilled water line.

#### D. Collecting the sand fraction:

1. Place a 62 $\mu$  screen in a large evaporating dish.
2. Take a 1000-millimeter squeeze bottle containing Calgon dispersant and carefully wash the dispersed sediment suspension from the beaker onto the sieve.
3. Take the evaporating dish containing the silt and clay fraction and wash into a 1000-milliliter cylinder and dilute or concentrate to one liter using a filter candle.
4. Take the sieve containing the sand fraction and wash the sand thoroughly with tap water and finally distilled water so that all excess Calgon is removed.
5. Invert the sieve into a large plastic funnel and wash the sand into a 1000-milliliter beaker.
6. Let the beaker stand for one hour to allow the sand to settle out.
7. Take a 62 $\mu$  sieve, turn it upside down, and carefully decant off the excess water through the sieve. Any fine sand (or floating material) that escapes during this decantation will be retained on the inverted sieve.
8. After pouring all but the last few drops of water, concentrate any sand on the sieve against the bottom lip by careful washing. Using a separate squeeze bottle containing distilled water, wash this sand into the 1000-milliliter beaker.
9. Put the beaker aside and allow sand to completely dry. If necessary, the plastic beakers can be placed in an oven and dried rapidly at about 40°C.
10. When the sand is dried, it can be brushed out of beaker and transferred into pre-labelled, pre-weighed 4-dram glass vials. The coarse, medium, and fine sand fractions can be obtained by dry sieving if desired.

#### E. Pipetting the silt and clay fraction:

1. Determine the temperature of a 1000-milliliter cylinder of water in which an accurate thermometer is kept to ascertain the temperature of fluids stored in the room.
2. Stir each sample for at least one minute, take a 25-milliliter portion of the sample at a depth of 20 centimeters at a time close to 30 seconds, as noted on the table below according to the temperature of the fluid, and release into a 50-milliliter beaker and note the sample number and beaker number on the calculation sheet. This portion contains 1/50 of that part of the sample which has a particle size of less than 62 $\mu$ .

3. On the same sample, after approximately one hour (consult the time versus temperature chart below), take a 20-milliliter portion at a depth of 5 centimeters; (this contains 1/50 of that portion of the sample which has a particle size of less than 4 $\mu$ ), release the 25-milliliter portion into an evaporating dish and record its number.

4. Place the 50-milliliter beaker into an oven whose temperature is kept at 100-105°C. Let all the samples in the oven come to dryness, wait two hours more, then remove the beakers to a desiccator, allow the temperature of the desiccator to come to equilibrium with that of the room.

5. Weigh each beaker (remove from desiccator one at a time) and record the weights. Calculate the weights of each portion as shown on Table 1.

TABLE 1

Elapsed Time for Fraction >62 microns <sup>a</sup> (seconds)	@ T°C	Elapsed Time for Fraction >4 microns <sup>a</sup> (min:sec)
34.7	15°C	65:15
33.9	16°	63:48
33.0	17°	61:14
32.1	18°	60:00
31.4	19°	58:48
30.6	20°	57:43
29.8	21°	55:33
29.1	22°	54:32
28.4	23°	53:33
27.8	24°	51:24
27.2	25°	50:51

<sup>a</sup>Begin pipetting so that the middle of the withdrawal is approximately as the time above. Usually place pipette into the cylinder 10 seconds beforehand. The total withdrawal time will be 5 to 10 seconds.

#### CARBON CARBONATE ANALYSIS

##### A. Purpose:

To determine and calculate the percentage of total carbon, organic carbon, and calcium carbonate in each sediment sample.

##### B. Material:

Dried samples obtained from sediment on which water content determinations were made on board ship.

C. Procedure:

1. Open the sample vial and determine the color of the sediment. Compare the estimated calcium carbonate content in the Hole Summary lithology descriptions (prepared by the shipboard scientists) and the sample at hand. In most cases, a sediment sample either has a high or a low calcium carbonate content. This should be relatively easy to determine by reference to the color of the sediment. Red or brown colors usually indicate low calcium carbonate, white or cream colors indicate high calcium carbonate, and green or gray colors usually indicate intermediate values. However, in some cases, green sediments have a low calcium carbonate content. The smear slide descriptions should be a useful guide in determining the amount of calcium carbonate present. Classify the sediment according to its calcium carbonate content into one of the three classifications listed in Table 2. This provides a basis for estimating the sample size needed to produce good results in the LECO analyzer. By color coding the vial with a colored pen, according to the table below, the proper amount of sediment can be weighed out at a later time.

TABLE 2

Approximate CaCO <sub>3</sub> Content	Color Code	Weight of Total Carbon Sample (mg)	Weight of Organic Carbon Sample (mg)
High CaCO <sub>3</sub> (50-100%)	Yellow	50	300
Medium CaCO <sub>3</sub> (25-50%)	Blue	100	500
Low CaCO <sub>3</sub> (0-25%)	Red	500	500

2. The sample is then dried. After drying grind the sample to homogeneity with a mortar and pestle, being sure there are no discernible differences in particular size or color. The ground material should be like a fine talc.

3. Redry the sediment. Remove the sample from the oven and place in a desiccator until it has cooled to ambient temperature. Mix the sample well before weighing out into a preweighed and marked (with laboratory sample number) crucible a portion weighing from 0.050 to 0.500 grams, depending upon the estimated total carbon content (see Table 2). After the sample is weighed, dampen it with 4 to 6 drops of distilled water<sup>1</sup>, then dry at

100 to 110°C for at least 12 hours. Run on carbon analyzer. (Consult the LECO 70 Second Carbon Analyzer Manual for operation of the analyzer.) Note: the sample size should be regulated so that the digital readout reads between 1.000 and 0.050, with a maximum sample weight of 0.500 gram. The analyzer is most accurate between those readouts, hence the reason for the regulation of the sample size.

4. Calculate the percentage of total carbon as follows:

$$\frac{\text{Digital readout}}{\text{Sample wt in g}} = \% \text{ Total Carbon}$$

5. Weigh out a second sample (according to the size indicated in Table 2) into a crucible marked with a laboratory number for acidized samples. Warm a hot plate to 55°C under a hood, and place a number of samples on it. Add a solution of concentrated hydrochloric acid and distilled water, 1 part acid to 7 parts distilled water, dropwise to each crucible taking care to barely wet the sample. If the sample fizzes vigorously, add 4 to 6 drops of distilled water and then continue acidification with 1 part hydrochloric acid to 7 parts distilled water, or even 1 part hydrochloric acid to 14 parts distilled water, if necessary. When all fizzing ceases, add 2 to 4 drops more of acid solution to ensure thorough acidification.

6. Place crucibles in Walter rubber filtering crucible holders (28 milliliter in size) which are fitted into 250-milliliter flasks, supported in a rack to avoid spilling. Attach at least one extra filter flask on the vacuum side (between the pump and the crucible line) to use as an overflow safeguard. Wash the samples within the crucibles with 3 portions of the distilled water, each 5 milliliters in size. Dry samples at 100 to 110°C for at least 12 hours. Place in a desiccator for about 2 hours to allow sample to come to ambient laboratory temperature, and then run on analyzer.

7. Calculate the percentage of organic carbon as follows:

$$\frac{\text{Digital readout}}{\text{Sample wt in g}} = \% \text{ Organic carbon}$$

8. Calculate the percentage of calcium carbonate as follows:

$$(\% \text{ Total carbon} - \% \text{ Organic carbon}) \times 8.33 = \% \text{ CaCO}_3$$

9. In the tables of total carbonate percentages in all volumes of the Initial Core Descriptions it is assumed that all of the carbonate occurs in the form of calcium carbonate. However, in a few places where a sample is known to contain dolomite [CaMg(CO<sub>3</sub>)<sub>2</sub>] or rhodocrosite (MnCO<sub>3</sub>) then an

<sup>1</sup>Use the same source of distilled water for all parts of the determinations.

adjustment should be made to the standard calculations as follows:

For dolomite: (% Total carbon - % Organic carbon) x 15.02 = % CaMg(CO<sub>3</sub>)<sub>2</sub>

For rhodocrosite: (% Total carbon - % Organic carbon) x 9.57 = % MnCO<sub>3</sub>

## X-RAY MINERALOGY

### Analytical Methods

The analytical methods used are similar to those described in Legs 1 and 2. Details of the X-ray data processing employed are given in the following sections. Continuous refinement of our computer programs and processing details occur and will be reported with each of the Leg Reports.

### Analytical Accuracy

True accuracy of the X-ray powder diffraction data is probably highly variable. Relative abundances appear to be excellent. Analytical precision based on replicate runs is dependent both on abundances and the degree of preferred orientation encountered. The standard deviations range from 20 per cent of the amount measured at 1 per cent abundance; 10 per cent at 50 per cent abundance; 5 per cent error at 90 per cent abundance; to 1 per cent error at 99 per cent abundance. Sensitivities are usually better than 1 per cent, but the concentration *threshold* used is given with the data table.

The *factor* given in the data table is the mass absorption coefficient ratio of the phase in question to quartz for the optical slit system used. The details of the calculation are given under the section on the theory of the Minlog.

### Amorphous Scattering

Crystalline and amorphous material both scatter X-rays. Bragg diffraction results from the scattering of large crystallites with dimensions over several hundred Angstroms in extent. Small crystallites show X-ray Bragg line broadening while large crystallites (over 1000 Angstroms in size) show sharp diffraction lines. The degree of line broadening can be used to estimate crystallite size. Material that contains ordered elements smaller than about a hundred Angstroms or highly disordered structures will produce diffuse scattering bands. These bands are characteristic of the liquid, gel and glass states as well as the ultra-microcrystalline state and are indicative of the X-ray amorphous state.

X-ray powder diffraction with a diffracted beam monochromator is free of fluorescent radiation, and it is possible to separate the diffracted X-ray energy by computer stripping techniques into Bragg scattering, diffuse scattering, and a low angle optical correction for direct

beam-air scattering. The variable given as diffuse scattering in earlier reports is simply the uncorrected percentage of the total energy present as non-Bragg scattering. Approximately two-thirds of the total scattering is attributable to the optical correction. The excess diffuse scattering above two-thirds is attributable to amorphous matter. For very small and very large values, it closely approximates the weight per cent of amorphous material in the samples. For intermediate values it would be necessary to know the mass absorption coefficient of the bulk sample, identify all crystalline components, and know their mass absorption coefficients to calculate the true weight per cent of amorphous matter in the samples. Work is underway to expand our capability to permit this determination; however, it will not be available for several legs. The scatter plots permit some interpretation of the amorphous scattering.

The great abundance of amorphous material in samples from Leg 5 is striking. Even the calcareous sections encountered contain considerable quantities of amorphous silica, water, iron and manganese oxides, volcanic glass and amorphous clays.

### X-ray Data Smoothing

Raw X-ray diffraction data contains much background and random noise which must be removed before calculations can be performed.

Subroutine SMOOTH is designed to eliminate much of the random noise in the raw X-ray intensity data. This is accomplished by passing the entire array of intensities from each sample through a "filter," a mathematical function which averages each intensity with respect to its neighboring values. A mathematical expression of the filter is

$$\bar{x}_i = \frac{\sum_{j=1}^N C_j x_{i+j} - \left[ \frac{N+1}{2} \right]}{\sum_{j=1}^N C_j}$$

where (C<sub>j</sub>) are the weighting coefficients,  
 (x<sub>j</sub>) are the raw intensities,  
 (x<sub>j</sub>) are the smoothed intensities, and  
 N is the number of points in the filter.

For example, if N = 5, i.e. a five-point filter is to be used, the coefficients of which are C<sub>1</sub> = 2, C<sub>2</sub> = 3, C<sub>3</sub> = 5, C<sub>4</sub> = 3, C<sub>5</sub> = 2, then the 52nd smoothed intensity would be:

$$\bar{x}_{52} = \frac{2x_{50} + 3x_{51} + 5x_{52} + 3x_{53} + 2x_{54}}{2 + 3 + 5 + 3 + 2}$$

An exception must be made to reduce the  $\frac{N-1}{2}$  points at each end of the array since the full filter cannot be used. In these cases, that portion of the filter that can be used is applied, associating the particular intensity being reduced with the central coefficient. For example, using the same 5-point filter as above.

$$x_1 = \frac{5x_1 + 3x_2 + 2x_3}{5 + 3 + 2} \quad \text{and}$$

$$x_2 = \frac{3x_1 + 5x_2 + 3x_3 + 2x_4}{3 + 5 + 3 + 2}$$

Selection of smoothing filter coefficients is based on experience. There are usually an odd number of coefficients, and the values are usually "symmetric" about the central coefficient, although neither condition is necessary for the algorithm. These values are chosen to eliminate as much noise as possible and to help guarantee single maximum peaks, while maintaining resolution of multiplets and shoulder peaks.

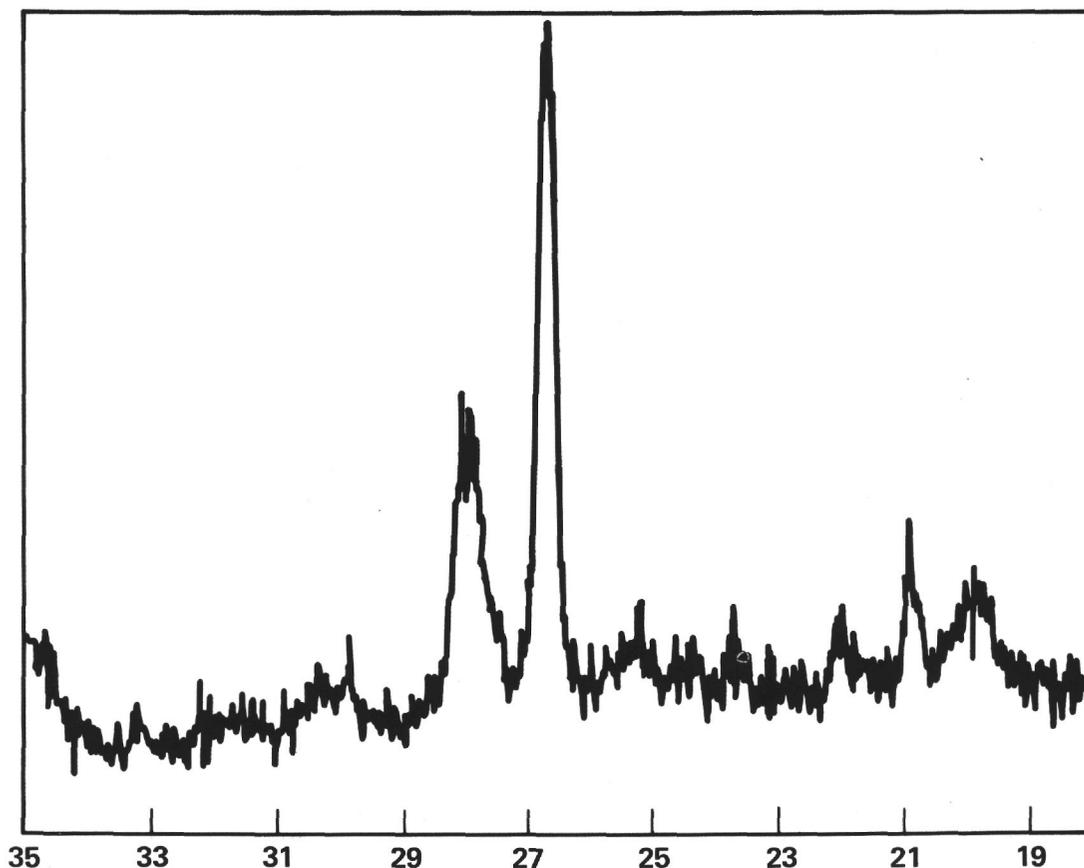
The filter being used currently consists of 13 coefficients, the value of which are:

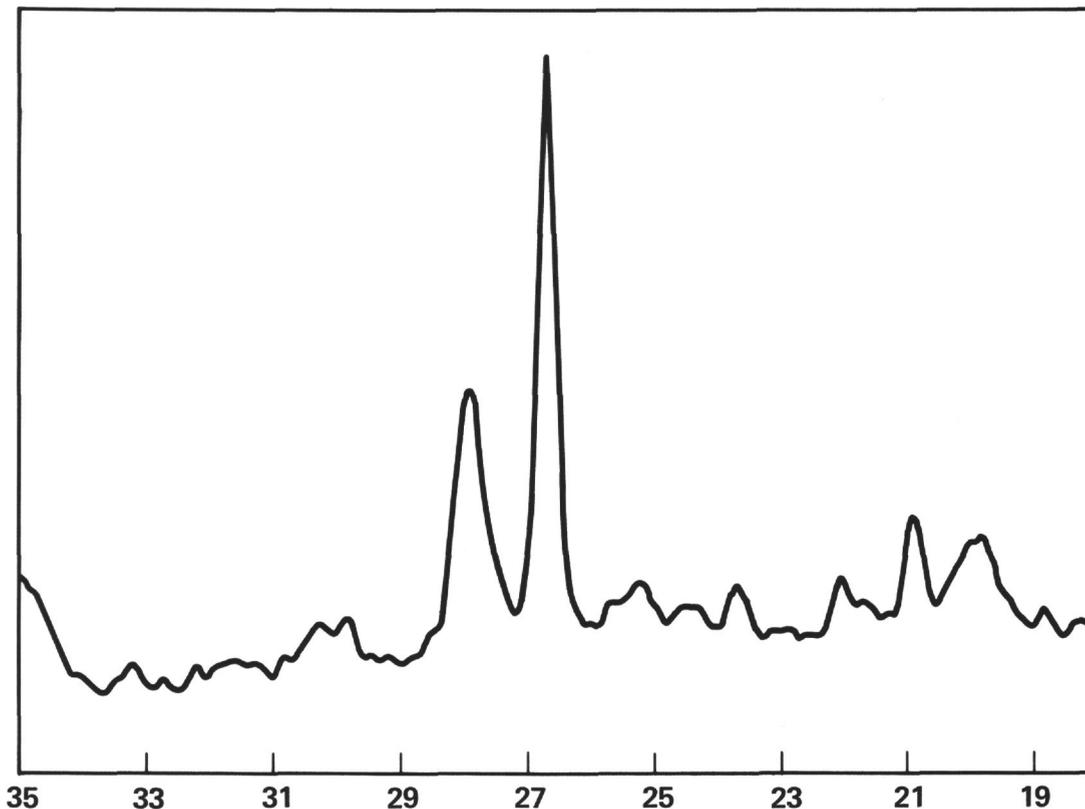
1.0, 3.4, 5.0, 5.8, 6.5, 6.8, 7.0, 6.8, 6.5, 5.8, 5.0, 3.0, 1.0.

### Background Noise Removal

After X-ray data has been smoothed, the intensity values still contain part signal and part background noise. To determine the amount of "signal" in a given datum, it is only necessary to subtract out the background noise. However, in general this noise is not a constant; rather, it is a function of the independent variables and random effects. A method of graphically approximating this noise function has evolved which consists of drawing, by hand, a baseline tangent to the lowest points of the data curve and then assuming that this line is the zero line for signal.

Subroutine BGRND simulates this hand technique of drawing a baseline. The procedure is outlined as follows: The slope is calculated from the first point to the second, then from the first point to the third, then from the first point to the fourth, and so on for all points within a designated range, called a search interval. The smallest of these slopes is selected and the first segment of the baseline is "drawn" from the first point as a starting value, slopes are calculated to each successive point within a search interval and again the minimum slope is selected. The next segment of the baseline is "drawn" from the starting value to the point where the smallest slope was found, and this point is used as the starting value for the next search. The entire array is scanned in this manner, forming a set of slopes and a





set of points connected by lines having these slopes. Mathematically, this is stated as:

$$M_i = \frac{I_i - \bar{I}_j}{x_i - x_j} \quad \text{for all } i \text{ such that } 0 < x_i - \bar{x}_j \leq SI$$

where SI is the length of the search interval and  $I_i$  are the values of the digitized data.

$$\bar{M}_j = \min(M_i)$$

$\langle \bar{x}_{j+1}, \bar{I}_{j+1} \rangle$  is the point to which the  $j^{\text{th}}$  minimum slope was calculated, and

$$\langle \bar{x}_1, \bar{I}_1 \rangle = \langle x_1, I_1 \rangle.$$

The equation of this base line is then

$$Y(x) = \sum_{j=1}^{\bar{N}} (M_j(x - x_j) + I_j)$$

where N is the number of elements in  $[(M_j, \bar{x}_j, \bar{I}_j)]$ .

In order to increase accuracy, the same scanning procedure is repeated from right to left, that is, backwards through the array calculating slopes from the starting

value to points lying to the left of it and storing, this time, the maximum slope and the points at which this maximum slope was calculated. The two lines found by scanning forward and backward are averaged together, and the averaged line is taken to be the true baseline.

After the baseline has been used to determine background noise, some random noise is still present in the data, sufficient to make peak identification difficult. A formula is used to remove as much of the random noise as possible. A "band" is formed along the baseline which has the equation:

$$B(x) = Y(x) \left[ 1 + \frac{2k}{I(x)} \right]$$

where Y is the function describing the baseline, I(x) is the function for the data, and k is a constant chosen to increase or decrease the width of the band.

The data are then adjusted to remove background noise and random noise as follows:

$$I(x) = \begin{cases} 0 & \text{if } I(x) \leq B(x) \\ I(x) - Y(x) \left[ 1 + \frac{k}{\sqrt{I(x)}} \right] & \text{if } I(x) > B(x). \end{cases}$$

It will be noted that this reduction scheme assumes that as the value of the dependent variable increases, the amount of random noise decreases.

Presently, the search interval value is 5 degrees, and the noise removal band constant is 1.5.

### Minlog Computation

After removal of random and background noise, relative weight percentage of located minerals is computed.

The program first scans the X-ray pattern and selects peaks. A peak is determined as at least a certain number of successive ascending intensity values, one on top, and then at least this same number of successive descending values. Presently this peak criterion number is two.

Included in the information pertaining to each mineral under investigation is its so-called "search window," the values of  $2\theta$  between which the location of a peak must fall in order for that mineral to be present. Mathematically, the  $2\theta$  value corresponding to a peak must satisfy the following relationship:

$$2\theta_1 < 2\theta \leq 2\theta_2$$

where  $2\theta_1$  and  $2\theta_2$  are the lower and upper bounds of the window.

The locations of all detected peaks are compared to the windows of the activated minerals for peak identification.

After identification, the peak intensities of several selected minerals are adjusted to remove interference by secondary and tertiary peaks of other minerals. The equation used is:

$$I_j^* = I_j - F_j \cdot I_i$$

where  $I_j^*$  is the adjusted intensity of the peak of mineral in question,

$I_j$  is the initial intensity of the peak,

$I_i$  is the intensity of the primary peak of the interfering mineral, and

$F_j$  is the appropriate adjustment factor.

The equation used in Minlog is:

$$PC_i = \frac{K_i I_i}{\sum_{j=1}^N K_j I_j} \times 100$$

where  $PC_i$  is the weight concentration percentage of the  $i^{\text{th}}$  mineral,

$I_i$  is the intensity of the primary peak of the  $i^{\text{th}}$  mineral component,

$K_i$  is the calibration factor of the  $i^{\text{th}}$  mineral component, and

$N$  is the number of mineral components.

### Theory of the Minlog

Powdered samples of crystalline materials are observed to diffract X-rays in accordance with the Bragg equation:

$$n\lambda = 2d \sin \theta$$

where:  $n$  is the order of the diffracted line ( $n = 1, 2, 3, \dots$  i.e., an integer)

$\lambda$  is the spacing of the planes of atoms in the crystal structure in Angstroms

$\theta$  is the angle of incidence and reflection of the diffracted X-ray beam.

In the particular arrangement that we are using, we consider Bragg diffraction of powdered rocks over a range of  $\theta$  and hold  $\lambda$  constant. This gives us variations in intensity of X-rays diffracted, in accordance with Bragg conditions, as a function of  $\theta$ . From the value of  $\theta$ , we compute, according to the Bragg equation, values of  $d/n$  or the spacings of crystal structural planes. From the intensities of the X-ray beam diffracted from the planes, we can evaluate the amount of diffracting substance present assuming one knows the absorption of X-rays by the matrix. The reasons for variations in the relative intensities of different X-ray diffraction lines from any one substance need not concern us here. However, in polyphase systems, such as we find in rocks, we are concerned with the problem of understanding X-ray bulk absorption conditions. Klug and Alexander (1948) have shown that it is possible to quantitatively analyze pellets of powdered crystalline substances according to the following reasoning.

Assume a uniform mixture of  $n$  components with particle sizes below 16 microns (obtained by grinding) so that extinction and microabsorption effects are negligible and infinitely thick (greater than 1 millimeter for sediments). In this sample, the total intensity of X-rays diffracted by the  $i^{\text{th}}$  component of the mixture of  $n$  components by some selected crystal plane (hkl) is given by

$$I_i = \frac{K_i f_i}{\mu}$$

where  $K_i$  is dependent on the nature of component  $i$  and the geometry of the apparatus,  $f_i$  is the volume fraction of  $i^{\text{th}}$  component, and  $\mu$  is the linear absorption coefficient of the powder mixture. If  $x_i$  is the

weight fraction and  $\rho_i$  the density of the  $i^{\text{th}}$  component, it then follows from the geometry that

$$f_i = \frac{x_i/\rho_i}{\sum_1^n (x_i/\rho_i)}$$

and that

$$\mu = \frac{\sum x_i(\mu_i/\rho_i)}{\sum (x_i/\rho_i)} = \frac{\sum x_i(\mu_i^*)}{\sum (x_i/\rho_i)}$$

where  $\mu_i$  is the linear absorption coefficient of the  $i^{\text{th}}$  component and  $\mu_i/\rho_i = \mu_i^*$  or its corresponding mass absorption coefficient. Substituting (3) and (4) in (2) gives

$$I_i = K_i \frac{x_i/\rho_i}{\sum \mu_i^* x_i}$$

If we consider a sample with numerous mineral components 1, 2, 3, ...,  $i, j$  of differing mass absorption coefficients and densities we see from equation (5) that the *ratio* of a peak height or area of mineral 1 to a peak of mineral 2 is only dependent on the concentration ratio of 1 to 2 and not on any of the other 3, ...,  $i, j$  components present. That is,

$$I_1 = K_1 \cdot x_1/\rho_1 \cdot 1/\sum \mu_i^* x_i$$

$$I_2 = K_2 \cdot x_2/\rho_2 \cdot \sum \mu_i^* x_i$$

$$\frac{I_1}{I_2} = \frac{K_1}{K_2} \cdot \frac{\rho_2}{\rho_1} \cdot \frac{\sum (\mu_i^* x_i)}{\sum (\mu_i^* x_i) x_2} = \text{const } 12 \frac{x_1}{x_2}$$

Experimentally, we evaluate constants 12, ...,  $i, j$ , by preparing equal weight mixtures of  $i$  and  $j$  and determining  $I_i/I_j$ . A table of these data permit the conversion of peak height ratios into weight ratios and are the basis of most of the Petro-log calibration.

Absolute analysis of any component is possible by adding a constant proportion of a known substance (aluminum metal powder) and solving equation (6). This is a true quantitative analysis and not considered under the name "Minlog analysis"

The basis for the Minlog calculation is the concept that the whole is equal to the sum of the parts. X-ray diffraction shows us all the crystalline components in a rock. We then consider those components of interest and define the rock as made up of 100 per cent of these crystalline phases. We thereby ignore moisture, organic

matter, glass, and even any minerals we so choose (e.g., a secondary cement or mud contaminant). This is a great time and cost saver as we no longer have to dry and weigh samples.

The arithmetic operation of the Minlog computation consists of recording the diffraction peak intensity ratios of all minerals to the most intense peak of  $I_1/I_2$  in equation 6. This is converted to weight per cent  $x_i$  by equation 7.

$$\frac{100x_i(\%)}{x_1+x_2+\dots+x_i+x_j} = \frac{\frac{I_i}{I_1} K_{1i} \cdot 100}{\sum \frac{I_j}{I_1} K_{1j} + \frac{I_2}{I_1} K_{12} + \dots + \frac{I_i}{I_1} K_{1i} + \frac{I_j}{I_1} K_{1j}}$$

TABLE 3  
Minerals Currently Contained in X-ray Diffraction-Data Reduction Program

ID	Name	Window	Factor	Threshold
1	Quartz	26.45 26.95	1.00	1.00
2	Calcite	29.00 29.60	1.96	1.00
3	Dolomite	30.80 31.15	1.00	1.00
4	Halite	31.65 31.90	0.83	1.00
5	Anhydrite	25.15 25.75	0.91	1.00
6	Gypsum	11.60 11.80	0.64	1.00
7	K-Feldspar	27.35 27.79	1.50	1.00
8	Plagioclase	27.80 28.15	1.50	1.00
9	Kaolinite	12.00 12.85	4.00	1.00
10	Mica	8.50 9.20	8.20	1.00
11	Chlorite	5.70 6.49	2.65	1.00
12	Mixed Layer Clay	6.50 8.19	2.65	1.00
13	Montmorillonite	4.50 5.40	17.80	1.00
14	Sylvite	28.25 28.45	1.05	1.00
15	Pyrite	56.20 56.45	2.27	1.00
16	Apatite	32.20 32.40	7.08	1.00
17	Barite	28.65 28.85	3.04	1.00
18	Siderite	31.90 32.40	1.10	1.00
19	Palygorskite	8.20 8.50	12.50	1.00
20	Phodochrosite	31.26 31.40	1.46	2.00
21	Clinoptilolite	9.71 9.99	3.33	1.00
22	Phillipsite	17.50 17.80	17.80	1.00
23	Cristobalite	21.50 22.50	10.60	2.00
24	Hematite	33.20 33.30	3.00	1.00
25	Aragonite	45.65 46.00	5.88	1.00
26	Corrensite	2.50 2.99	1.32	1.00

**TABLE 3 – Continued**

ID	Name	Window		Factor	Threshold
27	Rectorite	3.00	3.70	1.32	1.00
29	Sepiolite	7.00	7.40	16.30	1.00
30	Diffuse Scattering	0.00	0.00	0.00	0.00

**TABLE 4  
Current Set of Correction Factors**

Affected Mineral ID	Name	Interfering Mineral ID	Name	Factor
1	Quartz	10	Mica	0.90
7	K-Feldspar	19	Palygorskite	0.45
8	Plagioclase	19	Palygorskite	0.40
16	Apatite	19	Palygorskite	0.09
18	Siderite	19	Palygorskite	0.10
23	Cristobalite	19	Palygorskite	0.12
22	Phillipsite	11	Chlorite	0.75
7	K-Feldspar	22	Phillipsite	1.95
8	Plagioclase	22	Phillipsite	5.26
9	Kaolinite	22	Phillipsite	3.90
10	Mica	22	Phillipsite	0.16
23	Cristobalite	22	Phillipsite	1.63
24	Hematite	22	Phillipsite	1.42

**TABLE 4 – Continued**

Affected Mineral ID	Name	Interfering Mineral ID	Name	Factor
25	Aragonite	22	Phillipsite	0.26
27	Rectorite	22		
8	Plagioclase	23	Cristobalite	0.35
9	Kaolinite	11	Chlorite	1.00
2	Calcite	7	K-Feldspar	0.08
3	Dolomite	7	K-Feldspar	0.08
15	Pyrite	2	Calcite	0.04
20	Rhodochrosite	2	Calcite	0.03
18	Siderite	21	Clinoptilolite	0.19
24	Hematite	21	Clinoptilolite	0.08
25	Aragonite	10	Mica	0.60
25	Aragonite	1	Quartz	0.06
24	Hematite	25	Aragonite	0.42
24	Hematite	3	Dolomite	0.10

**TABLE 5  
Current Set of Alternate Peak Checks**

ID	MINERAL	ALTERNATE WINDOW		FACTOR
16	Apatite	31.9	32.19	1.25