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OPTICAL PROPERTIES
OF A
RANDOM SMALL-PARTICLE COMPOSITE

DISSERTATION

Presented in Partial Fulfillment of the Requirements
for the Degree Doctor of Philosophy in the Graduate
School of the Ohio State University

By
Kevin David Cummings, B.S.

* * * * *

The Ohio State University

1982

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CHAPTER I

INTRODUCTION

This work deals with the study of the optical properties of a 3-dimensional composite system of silver (Ag) particles and potassium chloride (KCl). This material serves as a model random inhomogeneous medium. The electronic properties are interesting because of the difference between the highly conducting Ag spheres and the insulating KCl host. Depending on the amount of metal, the composites show either metallic or insulating behavior. This change is observable in the optical properties of the system.

Despite the variety of randomly inhomogeneous systems, relatively few attempts have been made to correlate their optical properties with their constituent parts. Optical transmission measurements on dielectrics containing very small amounts of conducting particles have been made\(^1\)-\(^5\). However, sample characterization was difficult since the metal particles were generally grown in situ. Discontinuous films\(^6\)-\(^10\) and granular metal films\(^11\)-\(^13\) have received considerable amount
of attention. These systems are relatively easy to produce and the concentration of metal can be varied over a wide range. The weakness of using such systems is that they are inherently 2-dimensional and the study of the optical properties of the films can be seriously hampered by the substrate material necessary for film deposition. Optical measurements on free standing metal particles produced by gas evaporation have been made. These "smoke" samples can be made thick enough to be clearly 3-dimensional. Sample control and characterization in this system is easily obtainable, however, the particles are highly correlated and therefore do not model a random system well.

The composite system chosen in this work alleviates many of the problems discussed above. The small Ag particles can be made nearly uniform in size and can be randomly embedded in the insulating dielectric KCl to produce a truly 3-dimensional sample. The volume fraction of metal can be varied from 0 to 1 and the Ag and KCl have well characterized optical and electrical properties. We feel this system has many advantages over previous systems and is a good model for randomly inhomogeneous materials.
The organization of this thesis is as follows. Chapter II gives an overview of the theories used to describe composite systems. Chapter III explains the procedures for making the samples and characterizes the samples which were made. Chapter IV discusses the experimental techniques used to measure the reflectance of the samples. Chapter V is devoted to the handling and analysis of the data. Chapter VI presents the results of the measurements and data analysis along with a discussion of these results.
CHAPTER II

THEORY

Introduction

If the scale over which spatial fluctuations occur is small compared to the wavelength of the incident electromagnetic fields, then it is possible to view the inhomogeneous medium as uniform in its response to external fields and to describe the medium by an effective dielectric function. The problem is then to determine the effective dielectric function of the entire medium.

Most theories begin by simplifying the inhomogeneous composite system. The local dielectric function of the composite is assumed to take discrete values rather than being allowed to vary continuously. The composite is characterized by the volume fraction ($f$), dielectric function ($\varepsilon$) and geometrical information ($g$) of each grain type. The grains are then assumed to be polarized by a combination of an externally applied electric field and by the electric fields from the polarization of the background medium. From this point, two historically
different treatments of the way to handle the material outside the grain developed.

The Maxwell–Garnett theory (MGT)

The first model of this system was a molecular field model, which was originally worked out by Clausius and Mossotti and which was applied to the optical properties of small metal particles by Maxwell Garnett. According to the MGT, an isolated grain of dielectric function $\varepsilon_G$ is placed in the background host of dielectric function $\varepsilon_H$. The grains are not allowed to contact each other. The electric field acting to polarize each grain will therefore include a contribution from the polarization of the host medium. If we assume the grains can be described as aligned ellipsoids, the relationship between the internal electric fields and the applied external field can be calculated by the equations of electrostatics. The average dielectric constant of the composite, expressed in terms of the volume average of the fields, is

$$
\varepsilon_{\text{MGT}} = \varepsilon_H + \frac{\varepsilon_H f (\varepsilon_G - \varepsilon_H)}{(1-f)g (\varepsilon_G - \varepsilon_H) + \varepsilon_H}
$$

In equation (1), $g$ is the grain depolarization factor that contains the geometrical information. Values for $g$ can range from 0 (long needles) to 1 (flat plates),...
however we will assume spherical grains throughout this thesis and set $g=1/3$ in all the following discussions.

Equation (1) illustrates two properties which characterize the MGT approach to composite systems. First, the equation is inherently asymmetric in the treatment of the two materials of the system. Different answers will be obtained for the case of metal grains embedded in an insulating background and for insulating grains in a metal background, even if the volume fraction of metal is the same in both cases. Second, the equation predicts that $\varepsilon_{\text{MGT}}$ will vary smoothly from the host value to the grain value. In real systems however, the composites may display a rapid transition known as the "percolation" transition\textsuperscript{19}. The percolation transition is not predicted by MGT. In fact such effects are specifically excluded because the grains are not allowed to come into contact. Despite these problems, the MGT has been applied to numerous systems\textsuperscript{1-5} and is generally accepted as a description of dilute inhomogeneous mixtures.
The Effective Medium Approximation (EMA)

The second model of a composite system was a symmetrical effective medium approach, proposed originally by Bruggeman\textsuperscript{20} and studied quantitatively by Landauer\textsuperscript{21}. According to the EMA, a single grain of either material is embedded in a background having the average properties of the mixture. In the presence of an applied external field, the grain will be polarized and the dipole moment can be obtained by the equations of electrostatics. The induced dipole moment will produce a deviation of the external field near the grain and the spatial average of the deviation summed over all grains must equal zero. This self consistency condition gives a quadratic equation for the average dielectric constant

\[
\frac{3f(\varepsilon_G - \varepsilon_{EMA})}{\varepsilon_G + 2\varepsilon_{EMA}} + \frac{3(1-f)(\varepsilon_H - \varepsilon_{EMA})}{\varepsilon_H + 2\varepsilon_{EMA}} = 0 \quad (2)
\]

where we have assumed spherical particles.

Equation (2) illustrates two features of the EMA. First, the equation treats each material symmetrically. Second, the EMA allows for the possibility of a percolation transition. For metal spheres in an insulating host, the percolation transition occurs at
the critical volume fraction, \( f_c = 1/3 \). Like the MGT, the EMA has been applied to some systems and has been generalized to optical frequencies by many investigators\(^{19,22,23}\).

**Eddy current absorption**

Stroud\(^{24}\) has pointed out that small metal particle composites can interact with the magnetic part of an externally applied field. We incorporate this interaction into the theories by assuming eddy currents can be induced in the metallic grains and solving for the magnetic polarizability of a spherical particle. The polarizability is then related to the particle's permeability, and the average permeability of the composite can be determined in a way completely analogous to the calculation of the dielectric function. The resulting expressions are identical in form to the dielectric functions, i.e. for EMA,

\[
\frac{3f(\mu S - \mu_{\text{EMA}})}{\mu S + 2\mu_{\text{EMA}}} + \frac{3(1-f)(1-\mu_{\text{EMA}})}{1+2\mu_{\text{EMA}}} = 0 \tag{3}
\]

In equation (3), \( \mu S \) is the permeability of the spherical metal particle and we have set the permeability of the host to one.
Models for the constituent materials

As mentioned in chapter I, we chose Ag-KCl composites as a model of an inhomogeneous material. We use a simple classical picture for the dielectric response of each material. Ag is represented by a free-electron Drude model. The form for $\varepsilon_{Ag}$ is

$$\varepsilon_{Ag} = \varepsilon_{\infty}^A - \frac{\omega_p^2}{\omega^2 + i\omega/\tau}$$

(4)

where $\varepsilon_{\infty}^A$ is the high frequency value of the dielectric function for bulk Ag and $\omega_p$ is the unscreened plasma frequency for Ag. Because the Ag particles are small ($r=125 \, \AA$), the scattering time ($\tau$) is dominated by collisions with the surface. Therefore, we add a term to the scattering rate that assumes electrons are traveling at the Fermi velocity ($v_F$) in a particle of radius $r$

$$\frac{1}{\tau} = \left(\frac{1}{\tau_{Ag}}\right) + \left(\frac{v_F}{r}\right)$$

(5)

Using the scattering time of bulk Ag we calculate $1/\tau = 740 \, \text{cm}^{-1}$ for our Ag particles. The Drude model works well for frequencies below 31500 \, cm$^{-1}$, however above this frequency there is an additional contribution to $\varepsilon_{Ag}$ from interband transitions. The interband contribution was added to the Drude model from tabulated
data\textsuperscript{25}. Figures 1-3 show the reflectance, conductivity and real part of the dielectric function for this model of Ag.

The KCl is represented by a Lorentz oscillator model. There is a transverse optic (TO) phonon mode in KCl at 150 cm\textsuperscript{-1} which we represent as a Lorentz oscillator. \( \varepsilon_{\text{KCl}} \) is then

\[
\varepsilon_{\text{KCl}} = \varepsilon_\infty + \frac{\omega_L^2}{(\omega_{T0}^2 - \omega^2 - i\gamma\omega)} \tag{6}
\]

In equation (6), \( \omega_L^2 \) is the oscillator strength of KCl, \( \omega_{T0} \) is the pole of \( \varepsilon_{\text{KCl}} \) and \( \gamma \) is the full width at half maximum for the oscillator. Figures 4-6 show the reflectance, conductivity and real part of the dielectric function for this model of KCl.

Now that we have models for our composite system, we can point out one more feature that characterizes the MGT. If we neglect any contributions from the KCl (i.e. \( \varepsilon_{\text{KCl}} = 1 \)), let \( \tau \rightarrow \infty \) and substitute eq. (4) into eq. (1) for \( \varepsilon_G \), we get

\[
\varepsilon_{\text{MGT}} = 1 + \frac{3f((\varepsilon_\infty^A - 1)\omega^2 - \omega_p^2)}{(1-f)((\varepsilon_\infty^A - 1)\omega^2 - \omega_p^2) + 3\omega^2} \tag{7}
\]
Figure 1. Reflectance of bulk silver calculated by Drude model.
Figure 2. Conductivity of bulk silver calculated by Drude model.
Figure 3. Dielectric function of bulk silver calculated by Drude model.
Figure 4. Low frequency reflectance of KCl calculated by Lorentz oscillator.
Figure 5. Low frequency conductivity of KCl calculated by Lorentz oscillator.
Figure 6. Low frequency dielectric function of KCl calculated by Lorentz oscillator.
It is evident from equation (7) that $\varepsilon_{\text{MGT}}$ exhibits a strong resonance absorption when the denominator vanishes. This occurs at the frequency

$$\omega_0 = \omega_p \left( \varepsilon^\infty \frac{(f+2)}{(f-1)} \right)^{1/2}$$

This absorption peak is a characteristic feature of MGT and arises physically from the fact that the real part of the dielectric function of the metallic particles is negative below the plasma frequency and can cancel the positive dielectric constant of the medium. In contrast, the EMA has a very broad absorption peak in the optical response.

Computer calculations

The computer program EDDYCRNT was written to calculate both the EMA and MGT for composite systems. The program is written in IBM H-extended FORTRAN and runs on the Amdahl 470 computer located on the OSU campus. EDDYCRNT appears in the appendix at the end of this thesis and the operation of the program is documented in the program itself. EDDYCRNT takes in information that represents the models for the dielectric function of the two materials in the composite, calculates the dielectric function for each material and then supplies this information to calculations for the
EMA and MGT. The program solves for the average
dielectric function and permeability of the particles.
EDDYCRNT then calculates all the usual optical functions.

An interesting comparison can be made for
differences in particle sizes. A larger particle will
decrease the scattering rate as calculated by
equation (5). Figures 7-10 show a comparison of several
scattering rates without any contribution from eddy
current absorption. Notice that as the particle size
decreases (or the scattering rate increases), the
structure associated with the plasmon in Ag (at
31500 cm$^{-1}$) becomes less and less distinct.

Sum rules

Stroud$^{26}$ has derived sum rules for composite
systems. The optic sum rules, expressed for a Drude metal
composite, are

$$4\pi \int_0^{\infty} \sigma_1(\omega) \, d\omega = \frac{(\pi f \omega_p^2)}{2}$$  \hspace{1cm} (9)

$$-\int_0^{\infty} \omega \text{Im}(1/\varepsilon(\omega)) \, d\omega = \frac{(\pi f \omega_p^2)}{2}$$  \hspace{1cm} (10)

$$c \int_0^{\infty} \alpha(\omega) \, d\omega = \frac{(\pi f \omega_p^2)}{2}$$  \hspace{1cm} (11)

where $f$ is the volume fraction of the metal, $\sigma_1$ is
the real conductivity, $-\text{Im}(1/\varepsilon)$ is the loss function,
$\alpha$ is the absorption coefficient and $c$ is the speed of
Figure 7. EMA Conductivities without magnetic dipole for 3 radii, f=20%.
Figure 8. EMA Conductivities without magnetic dipole for 3 radii, $f=80%$. 

**Figure 8. EMA Conductivities without magnetic dipole for 3 radii, $f=80%$.**
Figure 9. MGT Conductivities without magnetic dipole for 3 radii, f=20%.
Figure 10. MGT Conductivities without magnetic dipole for 3 radii, f=80%.
light. The sum rule on \( \sigma_1 \) is related to the rate of energy absorption by transverse fields and the sum rule on the loss function is related to the rate of energy absorption by longitudinal fields. Using our model for Ag and neglecting any small contributions from the KCl, we are able to write equations (9)-(11) as partial sum rules for the Ag-KCl composites.

\[
(8/\omega_p^2) \int_0^{\omega} \sigma_1(\omega) \, d\omega = N_e m/m^* \tag{12}
\]

\[
-(2/\pi \omega_p^2) \int_0^{\omega} \omega \text{Im}(1/\varepsilon(\omega)) \, d\omega = N_e m/m^* \tag{13}
\]

\[
(2c/\pi \omega_p^2) \int_0^{\omega} \alpha(\omega) \, d\omega = N_e m/m^* \tag{14}
\]

From the free-electron model for Ag we expect the sum rule from eq. (12) to rise rapidly at low frequencies and saturate at a value near 1, the number of valence-conduction electrons per atom. A further discussion applying these sum rules to the Ag-KCl composites is given in chapter VI.

Stroud also derived a sum rule for the second moment of the conductivities. Again using our model for the composite, Stroud's expression may be written as a partial sum rule

\[
f(1-f) = (24/\omega_p^2) \int_0^{\omega} \omega^2 \sigma_1(\omega) \, d\omega \tag{15}
\]
We can now use equations (9) and (15) to obtain additional information about the broad peak in the EMA shown in Fig. 7 and 8 at approximately 20000 cm\(^{-1}\). This peak arises from absorption by standing modes excited by incident electromagnetic radiation in the small metal particles and is called the "impurity band" by Stroud. The square of the center of gravity for the impurity band can be calculated by dividing eq. (15) by eq. (9). (The "center of gravity" of the band (\(\omega_{\text{imp}}\)) is the location of the band if it were of zero width.) The calculation of \(\omega_{\text{imp}}\) for the composites and a comparison with the EMA predictions appears in chapter VI.
CHAPTER III

SAMPLE PREPARATION

The composites studied consisted of small Ag metal particles embedded randomly in a KCl host. We chose this system to represent the 3-dimensional inhomogeneous materials described by the theories in chapter II. Ag was chosen as the conducting element of the composite because the optical dielectric function is easily separated into free electron and bound electron behavior\textsuperscript{27} and the procedure of suspending samples in salt (KCl) for infrared analysis has been used for many years\textsuperscript{28}. The composites were made by mixing the Ag particles with KCl powder and pressing the mixture into 1/4 in. pellets. Sufficient pressure was used to let the KCl flow and form a solid pellet. Care had to be taken to insure that the Ag particles were randomly distributed throughout the composite and that the KCl did not contain water vapor. The samples were then polished flat for reflection measurements. The rest of this chapter describes the procedure and the materials to produce and characterize the samples.

25
Ag smoke preparation

The Ag metal particles were produced by the method of evaporation in a noble gas. A diagram of the equipment is shown in Figure 11. The aluminum oxide coated molybdenum boat from which the Ag was evaporated was produced by the R.D. Mathis Co. (52B-AO-MO). With the system evacuated to $10^{-6}$ Torr, the boat was decontaminated by heating it slowly with a current of approximately 5 A. It was important to inspect the ceramic at a point where it began to glow red. If sections of the ceramic appeared much darker (cooler) in color than the rest of the boat, that boat was discarded. After baking the boat for about a minute the current was slowly dropped to zero and the system returned to atmospheric pressure with nitrogen.

The boat was filled with about 0.7 g of Ag shot and was surrounded by a small glass cylinder. The bell jar was evacuated to $10^{-6}$ Torr and the boat heated very slowly. The Ag melted at about a 3 A current. As soon as the Ag melted to a single drop, the current was reduced to about 2.5 A. The Ag was kept molten for about 30 seconds. The current was then reduced slowly to zero and the bell jar was returned to atmosphere.
**Figure 11. Inert gas evaporation apparatus.**
The glass chimney on which the Ag smoke collected was 6 in. in diameter and 12 in. long. The chimney was cleaned first with a 20% solution of nitric acid, second with distilled water, third with acetone, and finally with freon. The chimney was placed over the boat and the system evacuated to \(10^{-5}\) Torr. A mixture of 75% argon and 25% oxygen was allowed to flow into the system at a rate of 35 cc/min and the system was stabilized at a pressure of 1 Torr by adjusting the pumping speed. The Ag was heated very slowly until it melted. After the Ag melted, the current was quickly raised to 4.2-4.4 A for approximately 2 minutes or until the Ag was evaporated from the boat. During the evaporation time both the current and flow rate were adjusted to keep the current and pressure at the desired values. After 2 minutes the current was lowered to zero and the system was allowed to cool for an extra minute before it was returned to atmosphere with nitrogen.

The Ag vapor loses energy to the noble gas atoms causing the Ag to cool and coalesce into small, nearly spherical particles. These particles then collect on the walls of the chimney as a black smoke. The small amount of oxygen produces an oxide coating on the particles. This coating helps insure that individual particles are isolated from one another and not clumped.
together. The smoke was collected from the chimney by brushing the powder from the glass and collecting the smoke on paper. The smoke was vortex mixed and probes from a voltmeter were placed into the powder to establish the resistance of the smoke. Only smoke with a resistance greater then 1 Mohm was used in the composite samples. The results of the smoke production are listed in Table 1.

KCl powder production

The powdered KCl was produced by grinding KCl single crystals in a liquid nitrogen immersed mill. The resulting grain size was several microns.

Composite production

The composite samples were prepared by mixing the Ag and KCl powders. Usually two samples were produced at the same time. To allow for losses during the preparation process, a 50% excess of KCl necessary for the two samples was used. To this KCl enough Ag powder was added to make the volume fraction (f) 1%. This material was vortex mixed and pressed in an evacuated (1 mTorr) 5/8 in. diameter die at 9 kbar.
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<th>Final wt. (mg.)</th>
<th>Yield (%)</th>
<th>Resistance (Mohm)</th>
<th>Evaporation time (min.)</th>
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The die was disassembled and the pellet removed. The pellet was carefully broken into smaller fragments which were then weighed. This new weight was used to recalculate the total amount of Ag and KCl left in the material after mixing and pressing. We assumed that both KCl and Ag were lost in the same proportion as their volume fractions. More Ag was added to this material; the mixture was then ground at liquid nitrogen temperature and repressed under vacuum into a 5/8 inch pellet. This cyclic procedure continued by adding more Ag, grinding and pressing until the final volume fraction was obtained.

The volume fraction was increased in this stepwise fashion to allow the Ag to mix uniformly throughout the KCl powder. The sample was increased in 1% steps for 0%<f<5% and then by 5% steps until the powder was 5% below the final volume fraction. The material was then increased by 1% steps to the final volume fraction. The mixture was then ground and pressed 4 more times to complete the mixing. The pellet was ground for a fifth time and the amount of material necessary for the first sample was removed. The remaining powder was used for the second sample.
Final sample production

The powder to be used for the sample was placed in a vacuum and left overnight at a temperature of 150°C in order to remove the water vapor which the KCl absorbed during the grinding and pressing process. The powder was removed from the warm oven and pressed under vacuum in a 1/4 in. die. The final sample was 1/4 in. in diameter and approximately .1 in. thick. The samples were stored in vacuum until they were prepared for reflection measurements.

Surface polishing

To obtain accurate reflection measurements of the samples, the surface had to be smooth and flat. The pellet was epoxied onto a 1/4-20 screw and placed in a protective form. The sample was then ground flat with 600 grit emery paper and polished using 5, 1 and 0.3 micron alumina powder. The samples were wetted with isopropanol throughout the polishing process. Using this procedure most samples could be made quite shiny. However, the sample surface still showed signs of diffuse scattering. The scattering increased as the sample was exposed to air and the water vapor attacked the KCl in the sample. The rough surface scattered the high frequency light and caused the reflectance to decrease
with increasing frequency. To compensate for this rough surface scattering, many samples were coated with 3000 Å of Au immediately after the reflectance was measured. The reflectance of the Au coated surface was then measured. A comparison between the Au coated surface and the uncoated surface allowed correction of the reflection spectrum for scattering. Table 2 lists the samples that were corrected in this manner.

Characterization

The first step to characterizing the composites was to determine the particle size. Scanning electron microscope (SEM) pictures were taken of several samples. Plate I shows examples of the Ag particles at the surface of the composites. The Ag particles are spherical in shape and measure approximately 250 Å in diameter. The second step in the characterization of the samples was to inspect the distribution of Ag in the sample. Plate II shows examples of the distribution of the Ag particles at the surface of the sample. The small white dots are the Ag particles. Notice that although there are some clumps of particles, the Ag is clearly not isolated into large islands. Instead, it is distributed across the entire surface of the sample.
Table 2. Summary of sample investigations

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<tr>
<th>f (cm⁻¹) by f (cm⁻¹) by f (cm⁻¹)</th>
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<th>500-45000</th>
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<tr>
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</table>
Plate I. SEM pictures showing Ag particle size and shape.

- For $f = 0.085$, 1000 Å
- For $f = 0.334$, 1000 Å
Plate II. SEM pictures showing Ag particle distribution.

\[ f = 0.085 \quad 1 \mu \]  

\[ f = 0.334 \quad 1 \mu \]
To determine the amount and distribution of the elements present in the samples, X-ray elemental analysis was performed in the SEM. X-rays are generated when the electron beam strikes the sample surface. These X-rays are collected and energy analyzed. An example of a spectrum is shown in Figure 12. This spectrum was analyzed and the atomic percent of each element was calculated. Quantitative analysis in the SEM is accomplished using well known correction procedures. A modified version of Frame-C, a NBS program developed for energy dispersive X-ray analysis, provides a basis for correcting inter-elemental effects. These effects are called ZAF corrections where Z=atomic number, A=absorption and F=fluorescence. Table 3 and 4 display the results of the X-ray analysis of the samples. Most samples had regions which appeared darker or lighter than the majority of the surface. However X-ray analysis of these regions found that the Ag concentration differed (in atomic percent) from the normal surface by 5% or less. The only exception was the large deviation found in the f=20% (by weight) sample #2. The regions that appeared darker tended to have small amounts of Fe contamination from the die. However these dark regions were a small fraction of the total surface area and differed in Ag concentration by small amounts. This
**Figure 12.** X-ray spectra from SEM.
Table 3. Summary of X-ray analysis on 800 μ scale

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<td></td>
<td>12; dark</td>
</tr>
<tr>
<td>0.20 #2</td>
<td>30.84 35.68 31.94 0.15 0 1.39</td>
<td></td>
<td>12; dark</td>
</tr>
<tr>
<td>0.20 #2</td>
<td>46.78 27.85 25.38 0 0 0</td>
<td></td>
<td>12; light</td>
</tr>
<tr>
<td>0.24</td>
<td>27.50 38.50 33.07 0.94 0 0</td>
<td></td>
<td>8; dark</td>
</tr>
<tr>
<td>0.24</td>
<td>30.32 36.01 32.17 1.54 0 0</td>
<td></td>
<td>8; normal</td>
</tr>
<tr>
<td>0.50</td>
<td>57.54 18.59 15.76 6.91 0 1.21</td>
<td></td>
<td>5; dark</td>
</tr>
<tr>
<td>0.50</td>
<td>60.09 18.91 14.57 7.14 0 0 5; normal</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.76</td>
<td>95.63 3.88 0 0.49 0 0</td>
<td></td>
<td>10; dark</td>
</tr>
<tr>
<td>0.76</td>
<td>90.49 7.80 1.71 0 0 0</td>
<td></td>
<td>12; normal</td>
</tr>
<tr>
<td>0.80 #3</td>
<td>52.35 22.13 15.48 7.94 0 2.09</td>
<td></td>
<td>3; dark</td>
</tr>
<tr>
<td>0.80 #3</td>
<td>53.89 22.37 17.34 6.40 0 0</td>
<td></td>
<td>12; normal</td>
</tr>
</tbody>
</table>
analysis indicates that in general the variation in Ag concentration was small and on average should have little effect on the optical properties of the system.

Table 3 and 4 also indicate many samples had sulfur (S) contamination on the Ag particles. Ag will tarnish when S in the air contacts it forming Ag₂S. Also notice that the atomic percent of Cl is consistently less than that of K. This difference occurs in the analysis because the weak Cl line lies very close to the Ag and S lines. The Ag volume fraction of each sample was calculated from the atomic percent by assuming bulk densities for the constituents. The metallic volume fraction was corrected for the S contamination by assuming each S atom is bonded to 2 Ag atoms. The K concentration was used in the calculation of the volume fraction of KCl and any other contaminant found was included in the calculation. A summary of volume fractions calculated by this analysis is included in Table 2 along with the other investigations that were performed on the samples. In all following discussions, f will be the calculated volume fraction and not the volume fraction determined by weight.
Another possible contaminant is the amount of oxide coating on each particle. A thick oxide on the particles would change the diameter and volume fraction. There are presently no quantitative measurements of the oxide thickness. However, in the production of the particles, care was taken to consistently produce the same amount of oxide on all particles. Sum rule calculations, discussed in chapter VI, indicate that for the majority of the samples the oxide coating reduces the volume fraction by only small amounts.

An experiment to determine the resistivity of the samples was conducted on many of the composites. However, all samples tested were either too resistive or too conductive to obtain reliable values. This was an expected result since the insulator-to-metal transition occurs rapidly and the investigation of this transition takes great care. However, the samples did show consistent behavior with DC conductivities extrapolated from the optical measurements discussed in the next chapters. In all cases studied, the samples were either very resistive and indicated extremely small conductivities or so conductive that they could not be accurately measured.
CHAPTER IV

EXPERIMENTAL TECHNIQUES

The monochromator

A vacuum spectrometer built around a Perkin-Elmer model 16U grating monochromator was used to measure the reflectance in the 500 to 45000 cm\(^{-1}\) region. Figure 13 is a diagram of this instrument. The entire instrument can be evacuated to pressures below 1 Torr to reduce the absorption by atmospheric water vapor in the infrared region. All surfaces within the vacuum box were covered with 3M.Nextel\textsuperscript{®} flat black paint to reduce stray light. Long-pass and bandpass filters eliminated unwanted orders of diffraction. A large spherical mirror imaged the exit slit of the monochromator onto the composite sample. A second spherical mirror focused the reflected light onto the detector. Three sources, four gratings, and three detectors were used to cover the infrared, visible, and ultraviolet regions with moderate resolution, \(\Delta\omega/\omega=10^{-3}\).
Figure 13. Schematic of the Perkin-Elmer grating monochromator.
The gratings were calibrated by passing the light from a HeNe laser ($\lambda=6328$ angstroms or $15803$ cm$^{-1}$) through the monochromator and observing the different orders of diffraction. The data were fit with a third degree polynomial. Table 5 lists the values obtained for the gratings. These parameters were used to calculate the wavenumbers from the drum numbers on the grating monochromator.

The resolution of Perkin-Elmer grating monochromators has been calculated. The resolution of a grating monochromator, the portion of the continuous spectrum thrown across the exit slit which gets through to the detector depends on the effects of a finite slit width and the diffraction of a limiting aperture. With reference to Figure 14, the grating equation can be written as

$$m\lambda=d(\sin(i)+\sin(D))$$

where $m$ is the order, $d$ is the grating constant (cm/line), $i$ is the angle of incidence and $D$ is the angle of diffraction. Writing this equation for two wavelengths, converting to wavenumbers ($\omega=1/\lambda$) and defining $\Delta\omega=\omega_1-\omega_2$ (the spectral width), we find
Table 5. Drum to wavenumber parameters

Wavenumber (cm\(^{-1}\)) = A + B \times DRUM + C \times DRUM^2 + D \times DRUM^3

<table>
<thead>
<tr>
<th>Grating (lines/mm)</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>170.351</td>
<td>16.017</td>
<td>-0.0107</td>
<td>-0.000245</td>
</tr>
<tr>
<td>40</td>
<td>231.345</td>
<td>21.533</td>
<td>0.0272</td>
<td>-0.00068</td>
</tr>
<tr>
<td>101</td>
<td>584.203</td>
<td>54.418</td>
<td>0.0508</td>
<td>-0.00124</td>
</tr>
<tr>
<td>240a</td>
<td>1387.533</td>
<td>130.572</td>
<td>0.0776</td>
<td>-0.00159</td>
</tr>
<tr>
<td>640b</td>
<td>3696.487</td>
<td>347.897</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>1440b</td>
<td>8280.0</td>
<td>789.4</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2880</td>
<td>16560.0</td>
<td>1578.8</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

\(^a\)Data fit with first degree polynomial.

\(^b\)Data from Perkin-Elmer.
Figure 14. Schematic ray diagram for a grating.
\[ \Delta \omega = \frac{\omega S \text{ctn}(\phi) \, d \omega h(\alpha)}{2f} + \frac{d \omega h(\alpha)}{Wm} \]  

(17)

where \( S \) is the slit width (cm), \( f \) is the focal length of the collimator mirror (26.7 cm), \( \phi \) is the angle of the grating, \( W \) is the width of the collimated beam (3.4 cm), \( h(\alpha) \) is an error function for the slits and \( \alpha = SW_\omega / f \). The angle of the grating is related to the wavenumber by the equation

\[ \csc(\phi) = 2d\omega \]  

(18)

The error function \( h(\alpha) \) is shown in Figure 15.32. The first term in equation (17) is from the physical slits and the second term is the contribution from the ultimate resolving power of the grating. In general the ultimate resolving power is not reached, since the second term depends on the physical slit width through the term \( h(\alpha) \).

Solving equation (17) for \( S \) we get

\[ S = \frac{2f}{\sqrt{(2d\omega)^2 - 1}} \left( \frac{\Delta \omega}{\omega} - \frac{d \omega h(\alpha)}{Wm} \right) \]  

(19)

Figures 16-23 show the maximum slit width for a spectral resolution \((\Delta \omega / \omega)\) of .1% for each grating including the second order of the 1440 lines/mm grating. These Figures
Figure 15. Graph of $h(\alpha)$ vs $\alpha$ based on calculations of Schuster.\textsuperscript{32}
Figure 16. Maximum slit width for resolution of 0.1% for 30 lines/mm grating vs wavenumber.
Figure 17. Maximum slit width for resolution of .1% for 40 lines/mm grating vs wavenumber.
Figure 18. Maximum slit width for resolution of 0.1% for 101 lines/mm grating vs wavenumber.
Figure 19. Maximum slit width for resolution of 0.1% for 240 lines/mm grating vs wavenumber.
Figure 20. Maximum slit width for resolution of .1% for 640 lines/mm grating vs wavenumber.
Figure 21. Maximum slit width for resolution of .1% for 1440 lines/mm grating vs wavenumber.
Resolution = 0.1%
2880 lines/mm grating

Figure 22. Maximum slit width for resolution of 0.1% for 2880 lines/mm grating vs wavenumber.
Figure 23. Maximum slit width for resolution of .1% for average grating vs drum number.
were calculated by self consistently solving for S using an iteration on h(α). In each of these calculations, S has been determined to better than 1/2 micron, which was the maximum resolution of the slit width controller on the grating monochromator.

Equation (17) can also be solved to determine the interval between data points. In these calculations it was assumed that the frequency could be accurately determined from the drum number by a linear equation and that two data points should be taken for each Δω. The grating controller allowed accurate steps of 0.005 (of the drum number) for each impulse sent to the controller. The impulses per step (IPS, the change in the drum number between points) is then given by

\[
\text{IPS}(\text{2pts/Δω}) = \frac{100\omega}{B} \left( S(\omega) \sqrt{(2d\omega)^2 - 1} + \frac{dh(\alpha)}{Dm} \right) \tag{20}
\]

where B is the linear term relating the drum number to the wavenumber and the slit width S is now a function of frequency given by equation (19). Figures 24-31 show the IPS necessary to obtain two points/Δω and to obtain a resolution of 0.1%. In practice the slit width should be changed according to Figure 23 and the IPS according to Figure 31 to obtain two points/Δω and a resolution of 0.1%.
Figure 24. IPS per step necessary to resolve structure at resolution of 0.1% for 30 lines/mm grating vs wavenumber.
Figure 25. IPS per step necessary to resolve structure at resolution of .1% for 40 lines/mm grating vs wavenumber.
Figure 26. IPS per step necessary to resolve structure at resolution of .1% for 101 lines/mm grating vs wavenumber.
Figure 27. IPS per step necessary to resolve structure at resolution of .1% for 240 lines/mm grating vs wavenumber.
Figure 28. IPS per step necessary to resolve structure at resolution of 0.1% for 640 lines/mm grating vs wavenumber.
Figure 29. IPS per step necessary to resolve structure at resolution of .1% for 1440 lines/mm grating vs wavenumber.
Figure 30. IPS per step necessary to resolve structure at resolution of .1% for 2880 lines/mm grating vs wavenumber.
Figure 31. IPS per step necessary to resolve structure at resolution of .1% for average grating vs drum number.
Operation of the monochromator

Table 6 list the parameters used to cover the 500-45000 cm\(^{-1}\) region with the monochromator. The three sources used were a globar, which was provided with the spectrometer, a quartz tungsten bulb and a deuterium arc lamp. The three detectors, all provided with the spectrometer, were a KBr window thermocouple, an ambient temperature PbS cell and an end-on multiplier phototube. The regions which used the photomultiplier tube were run at atmospheric pressure and all other regions were run in a vacuum of 1 Torr or better. All three detectors were connected to the input of an Ithaco model 393 lock-in amplifier. The source was chopped (approximately 17 Hz) and the lock-in output signal was fed into an integrating digital voltmeter (DVM). The DVM transmitted its data to a card punch where the data were placed on computer cards.

Figure 32 is a flow diagram of a typical data collecting session. The session started by mounting the samples to be studied and an aluminum mirror which was used as a reference. The Perkin-Elmer stepping motor controller (PESMC) was initialized by setting the digital read out of the controller equal to the drum position.
Table 6. Monochromator parameters

<table>
<thead>
<tr>
<th>Wavenumbers (cm⁻¹)</th>
<th>Drum Numbers</th>
<th>Grating Numbers (lines/mm)</th>
<th>Slit Width (microns)</th>
<th>Filters &amp; Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>510-710</td>
<td>13-22</td>
<td>40</td>
<td>1750</td>
<td>221-2009 Thrm/Glo</td>
</tr>
<tr>
<td>690-970</td>
<td>2-7</td>
<td>101</td>
<td>1750</td>
<td>221-1790 Thrm/Glo</td>
</tr>
<tr>
<td>910-1525</td>
<td>6-17</td>
<td>101</td>
<td>1500</td>
<td>221-1789 Thrm/Glo</td>
</tr>
<tr>
<td>1460-1920</td>
<td>16-24</td>
<td>101</td>
<td>1500</td>
<td>221-1788 Thrm/Glo</td>
</tr>
<tr>
<td>1780-2440</td>
<td>3-8</td>
<td>240</td>
<td>1750</td>
<td>221-1788 Thrm/Glo</td>
</tr>
<tr>
<td>2300-4280</td>
<td>7-22</td>
<td>240</td>
<td>1250</td>
<td>221-1787 Thrm/Glo</td>
</tr>
<tr>
<td>3700-4740</td>
<td>0-3</td>
<td>640</td>
<td>50</td>
<td>221-1787 PbS/W</td>
</tr>
<tr>
<td>4390-8570</td>
<td>2-14</td>
<td>640</td>
<td>20</td>
<td>301-1308 PbS/W</td>
</tr>
<tr>
<td>8280-13000</td>
<td>0-6</td>
<td>1440</td>
<td>50</td>
<td>1R80 PbS/W</td>
</tr>
<tr>
<td>12200-15400</td>
<td>5-9</td>
<td>1440</td>
<td>100</td>
<td>2-64/HA30 PbS/W</td>
</tr>
<tr>
<td>14600-20700</td>
<td>8-16</td>
<td>1440</td>
<td>15</td>
<td>3-71 Photo/W</td>
</tr>
<tr>
<td>19300-25000</td>
<td>14-21</td>
<td>1440</td>
<td>20</td>
<td>B460 Photo/W</td>
</tr>
<tr>
<td>24000-27000</td>
<td>20-24</td>
<td>1440</td>
<td>100</td>
<td>U330 Photo/W</td>
</tr>
<tr>
<td>26000-32000</td>
<td>6-10</td>
<td>2880</td>
<td>450</td>
<td>U360 Photo/D2</td>
</tr>
<tr>
<td>31000-38700</td>
<td>9-14</td>
<td>2880</td>
<td>450</td>
<td>U330 Photo/D2</td>
</tr>
<tr>
<td>37000-47000</td>
<td>13-19</td>
<td>2880</td>
<td>850</td>
<td>2467 Photo/D2</td>
</tr>
</tbody>
</table>
Figure 32. Flow diagram for operation of Perkin-Elmer grating monochromator.
We set the rate at which the controller sent impulses to the motor to 200 impulses/sec. and we set the impulses/step (IPS) to 20. This value of IPS allowed 10 points to be taken for every drum revolution. In the same manner, we initialized the slit width controller and filter controllers. The grating which covered the desired frequency range was inserted into the monochromator and the corresponding detector was mounted and aligned to obtain the maximum signal. After we obtained the maximum signal, data collection could begin.

The initial and final drum numbers were entered into the PESMC and the filters and slit width were set. We used the filters to absorb unwanted orders of radiation from the grating. We chose the slit width to give maximum signal while remaining in the linear region of the detector (<10 mV). The spectral region was scanned quickly to find the proper gain setting of the lock-in amplifier. We typically ran the amplifier with the internal time constant set to 125 msec. Once we set the gain, the PESMC took the data automatically.
A discussion of the operation and control of the PESMC is given in the appendix of this thesis. Once the start button is pushed on the PESMC, the drum is slewed to the initial drum number and the DVM is allowed to integrate the signal for a predetermined time (2 sec). The digital number is stored on a computer card and the PESMC holds the DVM from collecting more data. The PESMC then indexes the drum by IPS and the DVM is released to obtain another data point. This procedure continues until the present position equals the final drum number, at which point the PESMC stops and returns control to its front panel. A blank computer card was inserted to indicate the end of that data set. The procedure was continued for all spectral regions of interest for this detector and grating combination. The next sample (or mirror) was then positioned and the procedure continued until all samples (and mirror) had been investigated as indicated in Table 6. The analysis of the data will be discussed in the next chapter.
The interferometer

A Michelson interferometer was used to measure the reflectance in the 10 to 700 cm\(^{-1}\) region. Figure 33 is a diagram of this instrument. The interferometer and its operation have been described previously.\(^{33,34}\) The signal at the detector as a function of path difference between the two arms of the interferometer is the Fourier transform of the spectral intensity distribution. By computing the inverse Fourier transform of this signal, one obtains the signal intensity as a function of frequency (the spectrum). Problems occur from the finite distances involved in taking the data. However, well established corrections can be used to compensate for these errors.\(^{35}\) With beamsplitters of 2.5 and 12 micron thickness, the 10-700 cm\(^{-1}\) region was examined with a resolution of \(\Delta \omega / \omega = 10^{-2}\). A liquid cooled bolometer was used for detection of the far infrared radiation. The detector was a doped germanium semiconductor held at 1.2K by pumping on liquid helium. A set of filters was used to cut off unwanted higher frequency radiation. The detector was biased by a battery and the voltage (signal) across the detector was
Figure 33. Schematic of the Michelson interferometer.
supplied to the Ithaco lock-in amplifier. The amplifier, DVM and card punch worked as before with a controller moving the mirror instead of turning a grating. The analysis of this data will be discussed in chapter V.
CHAPTER V

DATA ANALYSIS

Initial data preparation

This chapter briefly describes the procedures and software used to determine the optical properties of the samples from the measured data. A detailed description of the hardware and software is given in the appendix at the end of this thesis. Both the instruments punch the digital voltmeter (DVM) data onto computer cards. These cards contain 16 points of 5 digits each and each set of data (run) was separated by a blank card. The initial processing was done on a DEC MINC-23 laboratory minicomputer; however, the cards had to be placed into a form that the MINC could interpret. A card reader was used to place card images into a General Automation GA-16/460 (SPC) computer located in the same building as our experiments. The GA-16 was then connected to the MINC computer via a RS-232 serial port (at 4800 baud) and the card images were transferred to the MINC.

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The MINC BASIC program SPECOM allowed communication between the MINC and GA-16 computers. This BASIC program emulates a GA-16 terminal. All the procedures which can be accomplished by a GA-16 terminal can also be done by the MINC computer running the program SPECOM. Additional features allow the transfer of files between the MINC and GA-16. The symbol ""]" allows access to the file transfer features. There is no check of the data sent or received; however, there has been no evidence of errors arising from the transfer of files by SPECOM.

The card reader, in contrast, often inserts errors into the data file. Once the data file is transferred to the MINC, the file should be checked for errors. The MINC BASIC program VERIFY checks the data card images which were placed into a file by the program SPECOM. VERIFY also finds all card images containing only a single point. These points are not used in the spectrum analysis and should be deleted. VERIFY also finds card images which have characters other than a number and cards that do not contain the correct number of characters. These errors should be corrected in the MINC file by using the MINC editor. The VERIFY program also indicates the largest number of cards in one run, a number which will be used in a later program.
After the data file is corrected, the informational header cards used for converting the data to spectra are placed into the file. The MINC FORTRAN program PEHEDR is used to place header cards on data taken on the Perkin-Elmer instrument and MCHEDR is used for data from the Michelson interferometer. These programs take raw data, put header cards on the runs and place the modified data in a sequential file. The information needed to run these programs is listed in the appendix at the end of this thesis. After the runs have the header information, they are ready to be sorted into order for the programs which will compute the spectrums. The MINC BASIC program FILSRT is used for the sorting process. FILSRT produces a virtual array that stores a card image in each element of array, allowing the single sequential data file to be broken into runs and these runs to be sorted into any order necessary. The runs are sorted into the appropriate order (see appendix) and the data necessary for plotting are placed at the beginning of the file. The file is then transferred back to the GA-16 with SPECOM. The data are now ready to be converted into spectra.
Computing spectra

After the procedures discussed in the previous section are finished, the data are ready to be submitted to the Amdahl 470 computer located on the OSU campus. All the following programs are written in IBM H-extended FORTRAN. The programs appear in the appendix at the end of this thesis.

The program PERKELMR reduces data from the Perkin-Elmer grating monochromator. The operation of the program is documented in the program itself. PERKELMR takes the data for a run and converts it into a spectrum. The program also corrects the background spectra for errors which occur due to small structure in the reflectance of the Al background mirror and calculates the ratio of sample spectra to background spectra (the reflectance). Finally, the individual reflectances are sorted together to obtain a single average reflectance spectrum over the entire frequency range studied; this final average reflectance may be plotted or put in a file for further analysis. This procedure was used to calculate the reflectance of the sample from 500 to 45000 cm\(^{-1}\).
The program FOURTRNS reduces data from the Michelson interferometer. The operation of this program is documented in the program itself. FOURTRNS takes the data for a run, converts it into an interferogram and Fourier transforms the interferogram yielding a spectrum. Individual runs may be averaged together in the program, but FOURTRNS does not have a sorting procedure for runs that cover different frequency regions. The program corrects the background spectrum by reading another file that contains the reflectance of the background material (Al mirror) and dividing out any structure that is due to the mirror. FOURTRNS then calculates the reflectance and allows the creation of a file which contains the final average reflectance for further analysis. This procedure was used to calculate the reflectance of the samples from 10 to 140 cm\(^{-1}\) and from 100 to 700 cm\(^{-1}\).

The program SORTFREQ combines the reflectance files produced by PERKELMR and FOURTRNS. The operation of the program is documented in the program itself. The individual files were sorted and averaged together to produce a single reflectance spectrum covering the frequency range of 10 to 45000 cm\(^{-1}\). SORTFREQ produces a final file that contains the complete reflectance spectrum for further Kramers-Kronig analysis. The
reflectance data are discussed in chapter VI and all the reflectances are given in the appendix of this thesis.

Kramers-Kronig transform

After carrying out the procedures in the previous section, the data are ready for Kramers-Kronig analysis. Kramers-Kronig dispersion relations can be derived on purely mathematical grounds. However a simple picture for the kind of relationship that must exist between the real and imaginary parts of the optical response function (\( \epsilon(\omega) \) = dielectric constant) will be presented. This picture follows the one presented by Wooten. Suppose a single pulse of radiation is incident on a sample at \( t=0 \). We assume the sample can absorb only a very narrow band of frequencies. This frequency is a Fourier component of the pulse and naturally should extend from \( t=-\infty \) to \( t=\infty \). Of course these components interfere destructively at times \( t<0 \) to produce no impulse until \( t=0 \). However, since our system has absorbed this component the destructive interference is incomplete and the result is radiation (not canceled by the absorbed component) at times \( t<0 \). The result is clearly unphysical since no system can respond before the impulse arrives at time \( t=0 \). Therefore causality implies that absorption of
one frequency must be accompanied by a compensating shift of phase of the other frequencies. This required phase shift is the relation prescribed by the Kramers-Kronig dispersion relation.

There are numerous ways to determine the optical constants. The one used for this work was to measure the reflectance at near normal incidence and to use the Kramers-Kronig relation to determine the optical properties. The reflectance at frequency $\omega$ is given by

$$R(\omega) = r(\omega)r^*(\omega)$$  \hspace{1cm} (21)

where the amplitude reflectivity is

$$r(\omega) = \frac{n(\omega) - 1 + ik(\omega)}{n(\omega) + 1 + ik(\omega)}$$  \hspace{1cm} (22)

In equation (22), $n(\omega)$ is the refractive index and $k(\omega)$ is the extinction coefficient. We can write the complex reflectance as

$$r(\omega) = \rho(\omega)e^{i\theta}(\omega)$$  \hspace{1cm} (23)

where now

$$R(\omega) = \rho^2(\omega).$$  \hspace{1cm} (24)
We assume $r(\omega)$ can be continued into the complex plane and that a contour integral is possible over the appropriate semicircle. This allows us to write a Kramers-Kronig relation between $\rho(\omega)$ and $\Theta(\omega)$. Eq. (23) can be rewritten as

$$\ln(r(\omega)) = \ln(\rho(\omega)) + i\Theta(\omega)$$  \hfill (25)

and the Kramers-Kronig dispersion relations are

$$\ln(\rho(\omega)) = -\frac{1}{\pi} \operatorname{p.v.} \int_{-\infty}^{\infty} \frac{\Theta(\omega')}{\omega' - \omega} d\omega'$$  \hfill (26)

$$\Theta(\omega) = -\frac{1}{\pi} \operatorname{p.v.} \int_{-\infty}^{\infty} \frac{\ln(\rho(\omega'))}{\omega' - \omega} d\omega'$$  \hfill (27)

Since the input and output functions must be real we have

$$r(-\omega) = r^*(\omega)$$  \hfill (28)

and we can rewrite (27) as

$$\Theta(\omega) = -\frac{2}{\pi} \operatorname{p.v.} \int_{0}^{\infty} \frac{1}{\omega' + \omega} \ln(\rho(\omega')) (\omega')^2 d\omega' - \omega^2$$  \hfill (29)

We now have the desired expression for $\Theta(\omega)$. The reflectivity $\rho(\omega)$ is determined experimentally and the
integral must be done numerically. Once $\phi(\omega)$ (the phase shift upon reflection at the surface) is determined $n(\omega)$ and $k(\omega)$ can be determined from equation (22). All the usual optical functions can now be calculated:

\[ \alpha(\omega) = \frac{2\omega k(\omega)}{c} \quad (30) \]

$\alpha(\omega)$ is the absorption coefficient and $c$ is the speed of light.

\[ \epsilon_1(\omega) = \frac{(n(\omega)^2 - k(\omega)^2)}{\mu} \quad (31) \]
\[ \epsilon_2(\omega) = \frac{2n(\omega)k(\omega)}{\mu} \quad (32) \]

$\epsilon_1(\omega)$ is the real part of the dielectric function and $\epsilon_2(\omega)$ is the imaginary part. $\mu$ is the magnetic permeability and is assumed to be one in all the calculations.

\[ \sigma_1(\omega) = \omega \epsilon_2(\omega) / 4\pi \quad (33) \]

$\sigma_1(\omega)$ is the real part of the conductivity

\[ \text{loss}(\omega) = -\text{Im}\left(\frac{1}{\epsilon(\omega)}\right) \quad (34) \]

Loss($\omega$) is the loss function. The sum rules discussed in chapter II can also be calculated by numerical integration. They are
\[ \int_0^\infty \sigma(\omega) \, d\omega = \frac{\omega_p^2}{8} \]

\[ \int_0^\infty \alpha(\omega) \, d\omega = \frac{\omega_p^2}{2c} \]

\[ \int_0^\infty \omega \text{loss}(\omega) = \frac{\omega_p^2}{2} \]

and the reflectance can be recalculated by

\[ R(\omega) = \frac{(n(\omega)-1)^2 + k(\omega)^2}{(n(\omega)+1)^2 + k(\omega)^2} \]

The reflectance was calculated as a check on the Kramers-Kronig transformation and always agreed with the experimental value.

Notice the integral in equations (26 and 27) must be carried to all frequencies, requiring assumptions about the reflectance in regions where data do not exist. In the Kramers-Kronig transformations three regions had to be treated in this manner. The first was the 0 to 10 cm\(^{-1}\) region. Samples which displayed low DC conductivities (below percolation), were assumed to have a constant reflectance from the last few points around 10 cm\(^{-1}\) to DC. This approximation assumed the lowest
Data points are a good estimate of the DC value of the reflectance. This extrapolation was checked with the low frequency values of pure KCl and found to be in good agreement. Samples which displayed large DC conductivities (above percolation) were assumed to continue to one with the Hagen-Reubens relation

\[ R(\omega) = 1 - A\omega^{1/2} \]  
(39)

where \( A \) was chosen to make the data fit the first few data points.

The second extrapolation was done in the region just above the last data point (45000 cm\(^{-1}\)). This region was assumed to contain contributions from interband transitions and was approximated by the reflectance

\[ R(\omega) = R_i(\omega_i/\omega)^s \]  
(40)

where \( R_i \) is the average of the last few points at frequency \( \omega_i, \omega > \omega_i \) and \( s \) is some fitted parameter. In this case the parameter \( s \) was chosen to give values close to those of bulk Ag obtained by other investigators\(^{37}\). The value for \( s \) was chosen to be .8.
The third extrapolation was done for still higher frequencies and continues to $\omega = \infty$. In this region, the electrons can be assumed to be a free electron gas so that the reflectance goes as $\omega^{-4}$. The crossover frequency (from interband to free electron) was chosen to be 400,000 cm$^{-1}$.

The program KRAMKROG transforms the data produced by the program SORTFREQ and calculates the optical functions described above. The operation of the program is documented in the program itself. KRAMKROG has several features which allow the correction of the reflectance before the transformation is performed. The program can simply transform the reflectance or it can take the sample reflectance, divide it by another reflectance and then multiply it by a third reflectance. The second feature was used to correct for surface scattering from the samples. The sample data was divided by data taken from the same surface but coated by Au. This quotient was then scaled by the bulk reflectance of Au to get rid of the Au structure. In this way the reflectance of the sample was transformed with the effects of surface scattering divided out. The results of these computations are given in chapter VI and in the appendix at the end of this thesis.
CHAPTER VI

RESULTS AND DISCUSSION

This chapter presents the data obtained in this investigation. All figures are given at the end of the chapter. A discussion of the results follows the presented data.

Reflectance data

Figures 34-39 show the reflectance of several samples. Notice that the low frequency reflectance increases with increasing volume fraction of Ag and the plasma minimum of Ag (at 31500 cm⁻¹) is apparent in all the samples. The sharp rise in the reflectance after the plasma minimum is due to interband transitions of electrons in Ag. The structure at 29500 cm⁻¹ in Fig. 39 is a surface plasmon which was excited in the rough Ag film. Figures 40-42 show the low frequency behavior of several samples. The structure at 150 cm⁻¹ in Fig. 40 and Fig. 41 is the transverse optic...
(TO) phonon mode of the KCl. This structure disappears when the volume fraction of Ag is increased above percolation (Fig. 42).

Figures 43-52 show the calculated reflectance for several volume fractions obtained from the EMA and the MGT. The MGT is asymmetric in its view of the two materials; one is viewed as a host and the other is viewed as grains. To obtain more accurate results from the MGT, the calculations were divided into two regions: For samples with volume fractions of metal less than 50% the model assumed Ag grains embedded in a KCl host while above 50% KCl grains were assumed to be mixed in a Ag host. This switch from an insulating host to a conducting host artificially produced a percolation transition for the MGT calculations. This transition occurs automatically in the EMA for volume fractions above 1/3. It is clear that the EMA predicts the rising low frequency reflectance and increasing sharpness of the plasma minimum (at 31500 cm\(^{-1}\)) with increasing volume fraction of Ag. The MGT in contrast predicts a sharp resonance at 25000 and 30000 cm\(^{-1}\) that is not seen in our data.
Figures 53-57 show the reflectance calculations for low frequencies. Although the EMA does predict the disappearance of the TO phonon of KCl with increasing volume fraction, the disappearance occurs at higher Ag concentrations in the theory. This discrepancy arises because the EMA has a higher critical volume fraction \( f_c \) than the experimental system. The experimental system has its percolation transition at \( f=20\% \) whereas the EMA predicts it should occur at \( f=1/3 \) for spherical metal particles. A comparison of the EMA and experimental reflectances in this low frequency region indicate the similarity between the two systems for volume fractions above and below the critical volume fraction. In this low frequency region, the KCl host MGT calculations have values similar to the EMA below \( f=1/3 \) and the Ag host have values similar to the EMA above \( f=1/3 \).

Data from Kramers-Kronig transformation

Figures 58-63 show the conductivity \( (\sigma_1) \) for the same six samples as the reflectance. Notice the very large change in the low frequency values of the conductivity as the volume fraction of Ag increases. There is a minimum in the conductivity that corresponds to the plasma minimum in the reflectance and a sharp
rise in the conductivity after this minimum from the
interband transitions. Figures 64-66 show the low
frequency conductivity in more detail. The peak in the
figures is from the TO phonon in KCl. This structure
is swamped by the conductivity of Ag as the volume
fraction is increased.

Figures 67-76 are the conductivities calculated
from the EMA and MGT. The broad low resonance at
20000 cm\(^{-1}\) of the impurity band is evident in the EMA.
Notice the width of the zero frequency peak (in samples
above \(f_c\)) in the calculations increases in a fashion
similar to the experimental values. The MGT, however,
has the very strong Maxwell Garnett resonance at 25000
\(\text{cm}^{-1}\) that we do not see in our data. Figures 77-79
show the low frequency values for several volume
fractions. Both theories are similar in this region so
only the EMA has been plotted. With increasing
concentration of Ag, the TO phonon of KCl is enhanced.
The magnitude of the TO phonon peak is in good agreement
for filling fractions up to 20 percent. Above this
point, however, the experimental system shows a very large
enhancement over the EMA. Again we believe the rapid
increase in the experimental system is due to the onset
of percolation which is not present in the EMA until
\(f=1/3\).
Figures 80-85 show the real part of the dielectric function ($\varepsilon_1$). Notice that at low frequencies $\varepsilon_1$ is positive for samples below percolation and has large negative values for samples above percolation. The frequency where $\varepsilon_1$ crosses zero increases with increasing volume fraction of Ag. Examples of both free and bound electron behavior can be seen (Fig. 85). The sharp decrease toward $-\infty$ at low frequencies is from the free electrons which give Ag high reflectivity and conductivity at low frequencies. The peak above zero at 32000 cm$^{-1}$ is from the electrons of the d states which lie 4 eV below the Fermi surface in Ag. These two effects combine to fix the plasma minimum at 31500 cm$^{-1}$. Figures 86-88 show the low frequency behavior of several samples.

Figures 89-98 are the calculations for the real part of the dielectric function. The EMA describes the experimental data better than the MGT. Figures 99-101 show the low frequency calculations in greater detail.

Figures 102-107 are examples of the absorption coefficient ($\alpha$) and Figures 108-113 show the loss function. They are shown here as examples of the functions which are integrated for the sum rule calculations discussed in chapter II. The strong minimum in the
absorption coefficient and the large peak in the loss function are from the plasmon in Ag. Notice that both the structures become more pronounced with increasing volume fraction of Ag.

Figures 114-119 show details of the low frequency low volume fraction \( \alpha \). The structure at 150 cm\(^{-1} \) is the TO phonon of the KCl. For low frequencies the absorption coefficient can be written as

\[
\alpha = K \omega^2
\]  

(41)

where \( K \) depends upon the particle radius and DC conductivity. Previous work\(^{38} \) on 800 \( \AA \) diameter Ag particles indicate \( K \) is between 1.1 and 1.4 \((f=0.003 \text{ and } 0.01 \text{ with } \omega < 100 \text{ cm}^{-1})\). In our lowest volume fraction sample (Fig. 114, \( f=0.057 \)) we see an \( \omega^2 \) type dependence, however the \( K \) for this region is approximately 0.03 which is closer to the theoretical value. We conclude that the anomalously large absorption found by many investigators\(^{39-41} \) does not exist in our system for the extended frequency range beyond the TO phonon of KCl. Figures 114-119 also indicate that as the volume fraction is increased \( \alpha \) changes from an \( \omega^2 \) type dependence to a dependence which is linear in \( \omega \). This has been observed by previous investigators\(^{37} \) and has been explained by theories that deal with clustering effects\(^{42} \).
Figures 120-127 show the EMA calculations for the low frequency region of the absorption coefficient ($\alpha$). Notice the scale of the calculations is $1/10$ the scale of the data in Figs. 114-118. The TO phonon absorption increases with increasing volume fraction of Ag. Figs. 120 and 121 show the effect of particle size on $\alpha$. The increased absorption with increasing particle size is due to the magnetic dipole absorption in the larger particles. The small low frequency peak at $50 \text{ cm}^{-1}$ in $\alpha$ also comes from the magnetic dipole absorption. Notice the small particles have a rapid increase in absorption as the frequency increases. This rise in $\alpha$ comes from the electric dipole absorption of the smaller particles. Figures 122-127 compare the magnetic and electric absorption for several particle sizes. The particle size must be quite large before eddy current effects increase $\alpha$ by an appreciable amount.

Sum rules

Figure 128 shows the effective number of electrons per silver atom calculated from $\sigma_1$. Notice the sharp rise as the volume fraction of Ag is increased. Figures 129 and 130 show the effective number of electrons
calculated from $\alpha$ and the loss function, respectively. All three partial sum rules will reach the same values if the integration is carried to high enough frequencies. The sum rules for Ag do not obtain equivalent values until 100 eV ($800,000 \text{ cm}^{-1}$)\textsuperscript{43}. Fig. 128 shows the large plateau between the regions of free electron behavior and interband transitions. We stopped the partial sum rules, discussed in detail in chapter II, at the plasma minimum of bulk Ag and assumed the oscillator strength of bulk Ag was one at this frequency (Ag has one free electron per atom).

Equations (9)-(11) predict a linear relationship between the volume fraction ($f$) and oscillator strength ($Ne/m^* m$). Figures 131-133 plot the calculated oscillator strength versus volume fraction for the surface corrected samples. The line in Fig. 131 is the expected result from the above discussions. Notice that the simple assumptions of this model are not quite correct. The value of bulk Ag ($f=1$) is slightly higher than one. The increased strength could come from a small interband contribution at this frequency. Within the scatter, the low volume fraction data fit the expected results quite well. In Figs. 132 and 133 the line is the expected results scaled by the value obtained from
bulk Ag. The sum rule is shown in Fig. 132. Again the low volume fraction data fit the expected results well. However, the loss function sum rule (Fig. 133) does not show a good fit. The scatter at this low value of the loss function sum rule is large and we would expect the data to fit the predicted results if the integration could be carried to much higher frequencies. At this time there is no explanation for the behavior of the points between 50% and 80% in Figs. 131 and 132.

Figure 134 plots the ratio of the center frequency of the impurity band ($\omega_{imp}$), discussed in chapter II, to the plasma frequency ($\omega_p$) versus volume fraction of Ag. The line is the expected result for spherically symmetric composites below percolation as described by Stroud\textsuperscript{26}. The fit of the data to the theory is quite good. We see the impurity band decreasing in frequency with increasing volume fraction.
In summary, the optical properties of Ag-KCl composite systems are well described by the EMA. The optical sum rules are obeyed for low volume fraction samples and the concentration dependence of the impurity band center agrees with the theory for spherically symmetric composite systems.
Figure 34. Measured reflectance of $f=0.008$ sample.
Figure 35. Measured reflectance of $f=0.057$ sample.
Figure 36. Measured reflectance of $f=0.192$ sample.
Figure 37. Measured reflectance of $f=0.547$ sample.
Figure 38. Measured reflectance of $f=0.656$ sample.
Figure 39. Measured reflectance of f=0.987 sample.
Figure 40. Low frequency reflectance of $f=0.057$ sample.
Figure 41. Low frequency reflectance of f=0.218 sample.
Figure 42. Low frequency reflectance of $f=0.334$ sample.
Figure 43. EMA reflectance for $f=0.057$. 

**Figure 43.** EMA reflectance for $f=0.057$. 

*Note:* The plot shows the EMA reflectance as a function of frequency (cm$^{-1}$) with a peak at around 15,000 to 30,000 cm$^{-1}$.
Figure 44. EMA reflectance for $f=0.192$. 

Figure 44. EMA reflectance for $f=0.192$. 

$E = 0.192$
Figure 45. EMA reflectance for $f=0.547$. 

$E M A$ Reflectance 

Frequency (cm$^{-1}$) 

$0 1 2 3 4 5 6 7 8 9 10$
Figure 46. EMA reflectance for $f = 0.656$. 

Frequency (cm$^{-1}$)
Figure 47. EMA reflectance for $f = 0.987$. 

Frequency (cm$^{-1}$)
Figure 48. MGT reflectance for $f = 0.057$. 

Figure 48. MGT reflectance for $f = 0.057$. 

$MGT \text{ Reflectance}$

$\text{Frequency (cm}^{-1}\text{)}$
Figure 49. MGT reflectance for $f=0.192$. 

$\text{MGT Reflectance}$

$\text{Frequency (cm}^{-1}\text{)}$

$\text{f = 0.192}$
Figure 50. MGT reflectance for $f=0.547$. 

$MGT$ Reflectance

Frequency (cm$^{-1}$)

$0$ $15000$ $30000$ $45000$
Figure 51. MGT reflectance for $f = 0.656$. 
Figure 52. MGT reflectance for $f = 0.987$. 
Figure 53. Low frequency EMA reflectance for $f=0.057$. 

**Figure 53.** Low frequency EMA reflectance for $f=0.057$. 

**f = 0.057**
Figure 54. Low frequency EMA reflectance for $f=0.218$. 

*Figure 54. Low frequency EMA reflectance for $f=0.218$.***
Figure 55. Low frequency EMA reflectance for $f=0.334$. 

[Graph showing EMA reflectance vs. frequency (cm$^{-1}$).]
Figure 56. Low frequency EMA reflectance for $f = 0.547$. 
Figure 57. Low frequency MGT reflectance for $f=0.334$. 

$f = 0.334$
Figure 58. Conductivity of $f=0.008$ sample.
Figure 59. Conductivity of $f=0.057$ sample.
Figure 60. Conductivity of f=0.192 sample.
Figure 61. Conductivity of f=0.547 sample.
Figure 62. Conductivity of f=0.656 sample.
Conductivity (ohm-cm),

Figure 63. Conductivity of $f=0.987$ sample.
Figure 64. Low frequency conductivity of $f=0.057$ sample.
Figure 65. Low frequency conductivity of $f=0.192$ sample.
Figure 66. Low frequency conductivity of f=0.218 sample.
Figure 67. EMA conductivity for $f=0.057$. 

**EMA Conductivity (ohm-cm)$^{-1}$**

**Frequency (cm$^{-1}$)**
Figure 68. EMA conductivity for $f=0.192$. 
Figure 69. EMA conductivity for $f = 0.547$. 

EMA Conductivity (ohm-cm$^{-1}$) vs Frequency (cm$^{-1}$)
Figure 70. EMA conductivity for $f = 0.656$. 

EMA Conductivity (ohm-cm$^{-1}$) vs. Frequency (cm$^{-1}$)
Figure 71. EMA conductivity for $f = 0.987$. 

**Frequency (cm$^{-1}$)**

**EMA Conductivity (ohm-cm)$^{-1}$**
Figure 72. MGT conductivity for $f=0.057$. 
Figure 73. MGT conductivity for $f=0.192$. 
Figure 74. MGT conductivity for $f=0.547$. 

MGT Conductivity (ohm-cm)$^{-1}$

Frequency (cm$^{-1}$)
Figure 75. MGT conductivity for $f = 0.656$. 

MGT Conductivity (ohm-cm$^{-1}$) vs. Frequency (cm$^{-1}$)
Figure 76. MGT conductivity for $f=0.987$. 

**MGT Conductivity (ohm-cm)$^{-1}$**

**Frequency (cm$^{-1}$)**

- $f = 0.987$
Figure 77. Low frequency EMA conductivity for f=0.057.
Figure 7.8. Low frequency EMA conductivity for $f=0.192$. 
Figure 79. Low frequency EMA conductivity for $f=0.218$. 
Figure 80. Real part of the dielectric function of \( f = 0.008 \) sample.
Figure 81. Real part of the dielectric function of $f=0.057$ sample.
Figure 82. Real part of the dielectric function of $f=0.192$ sample.
Figure 83. Real part of the dielectric function of f=0.547 sample.
Figure 84. Real part of the dielectric function of \( f=0.656 \) sample.
Figure 85. Real part of the dielectric function of \( f=0.987 \) sample.
Dielectric Function

Figure 86. Low frequency dielectric function of f=0.057 sample.
Figure 87. Low frequency dielectric function of f=0.192 sample.
Figure 88. Low frequency dielectric function of \( f = 0.218 \) sample.
Figure 89. EMA dielectric function for $f = 0.057$.
Figure 90. EMA dielectric function for $f=0.192$. 

Frequency (cm$^{-1}$)
Figure 91. EMA dielectric function for $f = 0.547$. 

Figure 91. EMA dielectric function for $f=0.547$. 

$\text{EMA Dielectric Function}$ 

$\text{Frequency (cm}\text{-1})$
Figure 92. EMA dielectric function for $f=0.656$. 

$E M A \text{ Dielectric Function}$

$\text{Frequency (cm}^{-1}\text{)}$

$f = 0.656$
Figure 93. EMA dielectric function for $f=0.987$. 
Figure 94. MGT dielectric function for $f=0.057$. 

*Figure 94. MGT dielectric function for $f=0.057$.**
Figure 95. MGT dielectric function for $f=0.192$. 

Frequency (cm$^{-1}$)

MGT Dielectric Function
Figure 96. MGT dielectric function for $f = 0.547$. 

$\eta$
Figure 97. MGT dielectric function for $f = 0.656$. 

MGT Dielectric Function

Frequency (cm$^{-1}$)
Figure 98. MGT dielectric function for $f = 0.987$. 
Figure 99. Low frequency EMA dielectric function for $f = 0.057$. 

Frequency (cm$^{-1}$)
Figure 100. Low frequency EMA dielectric function for $f = 0.192$. 

$E M A$ Dielectric Function

Frequency (cm$^{-1}$)

$f = 0.192$
Figure 101. Low frequency EMA dielectric function for $f=0.218$. 
Figure 102. Absorption coefficient of \( f = 0.008 \) sample.
Absorption Coefficient (microns$^{-1}$)

Figure 103. Absorption coefficient of $f=0.057$ sample.
Figure 104. Absorption coefficient of $f=0.192$ sample.
Figure 105. Absorption coefficient of $f=0.547$ sample.
Figure 106. Absorption coefficient of $f=0.656$ sample.
Figure 107. Absorption coefficient of $f=0.987$ sample.
Figure 108. Loss function of $f=0.008$ sample.

$f = 0.008$
not corrected
Figure 109. Loss function of $f=0.057$ sample.
Figure 110. Loss function of $f=0.192$ sample.
Figure 111. Loss function of $f=0.547$ sample.
Figure 112. Loss function of f=0.656 sample.
Figure 113. Loss function of $f=0.987$ sample.
Figure 114. Low frequency absorption coefficient for $f=0.057$ sample.
Figure 115. Low frequency absorption coefficient for $f=0.085$ sample.
Figure 116. Low frequency absorption coefficient for f=0.172 sample.
Figure 117. Low frequency absorption coefficient for $f=0.186$ sample.
Figure 118. Low frequency absorption coefficient for $f=0.192$ sample.
Figure 119. Low frequency absorption coefficient for $f=0.334$ sample.
Figure 120. Low frequency EMA absorption with magnetic dipole for 3 radii; $f = 0.057$. 

- $r = 25 \text{ Å}$
- $r = 125 \text{ Å}$
- $r = 500 \text{ Å}$

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Bulk KCl
Figure 121. Low frequency EMA absorption with magnetic dipole for 3 radii; $f=0.192$. 

![Graph showing EMA absorption with magnetic dipole at different radii](image-url)
Figure 122. Low frequency EMA absorption, comparing magnetic dipole; r=25 Å, f=0.057.
Figure 123. Low frequency EMA absorption, comparing magnetic dipole: $r = 25 \, \text{Å}, f = 0.192$. 

- $f = 0.192$
- $r = 25 \, \text{Å}$

- mag. & elec. dipole
- elec. dipole only
Figure 124. Low frequency EMA absorption, comparing magnetic dipole; $r=125 \, \text{Å}$, $f=0.057$. The graph shows the EMA absorption coefficient against frequency (cm$^{-1}$) with two lines: one for magnetic and electric dipole combined, and another for electric dipole only.
Figure 125. Low frequency EMA absorption, comparing magnetic dipole; \( r = 125 \, \text{Å}, \, f = 0.192 \).
Figure 126. Low frequency EMA absorption, comparing magnetic dipole; \( r = 500 \text{ \AA} \), \( f = 0.057 \).
Figure 127. Low frequency EMA absorption, comparing magnetic dipole; $r=500 \text{ Å}$, $f=0.192$. 

- mag. & elec. dipole
- elec. dipole only
Conductivity

\( f = 0.987 \)

\( f = 0.767 \)

\( f = 0.330 \)

\( f = 0.192 \)

\( f = 0.057 \)

Figure 128. Oscillator strength vs frequency from conductivity sum rule.
Figure 129. Oscillator strength vs frequency from absorption sum rule.
Figure 130. Oscillator strength vs frequency from loss function sum rule.
Figure 131. Oscillator strength vs volume fraction from conductivity data.
Figure 132. Oscillator strength vs volume fraction from absorption coefficient data.
Figure 133. Oscillator strength vs volume fraction from loss function data.
Figure 134. Center frequency of impurity band divided by plasma frequency vs volume fraction.
This appendix contains a manual of the terms used in the operation of the controller. It contains a description of all the buttons, connectors and lights that exist on the controller. The commands which the IEEE bus controller will relay to the microprocessor in the controller are also listed along with a brief listing and description of IEEE commands which are contained in the MINC basic program language.
PERKIN-ELMER STEPPING MOTOR CONTROLLER MANUAL

B  IEEE code

Usage: SEND("Bx",1) x=0-7

Assigns PARALLEL POLL bit position. Default position is bit 7.

BLANK  Term

A display will be BLANKed if an improper number has been entered into its memory. (see appropriate term)

C  IEEE code

Usage: SEND("C",1)

Same as: pushing CONT key.

CLEARING INSTRUMENTS  IEEE function

Usage: ALL_INSTR_CLEAR
Useage: INSTR_CLEAR(1)

Either command has the same effect as pressing the RESET button.

Usage: IEEE_BUS_CLEAR

This command clears the instrument independent part of all instruments on the IEEE bus.
CLR DISP  
CLeaRs out the GENERIAL/IPS DISPlay and memory.

CONT    
The controller CONTinues the action before it was stopped. (START etc.)

DI  
IEEE code

Usage: SEND("DI",1) 
FOR I=1 TO 10
RECEIVE(S$(I),6,1) 
NEXT I
RECEIVE(S$(11),8,1)

The command is used to transfer data from the controller to the IEEE bus. The first 10 numbers are sent in an 16 field with leading zeros sent as blanks. The values are

1) PRESENT POSITION 
2) Last digit of above 
3) INITIAL POSITION 
4) Last digit of above 
5) FINAL POSITION 
6) Last digit of above 
7) IMPULSES PER STEP 
8) Number of impulses given so far in this STEP. 
9) IMPULSES PER SEC 
10) CRATING #.

A last 8 bit binary status word is sent as a sequence of '0' and '1'. They are

Bit #1  Space sent as '0'  
#2  Space sent as '0'  
#3  '1' => STEP IN PROGRESS  
#4  '1' => HALF STEP mode; '0' => Full STEP mode 
#5  Space sent as '0'  
#6  '1' => REVerse DIREction; '0' => ForWarD DIREction  
#7  Space sent as '0'  
#8  '1' => WAVE mode; '0' => DRUM mode.
**DIR F/R Key toggle**

Sets the DIRECTION that impulses will drive the motor.

**DISP Key**

The DISPLAY key is used in sequence with the numeric keys to inspect the memory locations of the controller.

- **DISP, 1** places the number of IMPULSES PER STEP in the GENERAL/IPS display.
- **DISP, 2** places the GRATING # in the GENERAL/IPS display. (see WAVE/DRUM)
- **DISP, 3** places the IMPULSES PER SEC in the GENERAL/IPS display.

**DR IEEE code**

Usage: SEND("DR",1)

Sets DRUM mode.

**DRUM (WAVE/) Key toggle**

Sets the mode in which data on the digital displays are presented. WAVE mode (without decimal pts.) gives numbers in wavenumbers (cm⁻¹) where DRUM mode (with decimal pts.) gives numbers as they correspond to the drum connected to the stepping motor.

**DVM HOLD Light**

The controller is HOLDing the Digital VoltMeter from collecting data.

**DVM J3 Cannon plug**

Connects the Digital VoltMeter to the controller.
ENT Key

The ENTer key is used in sequence with the numeric keys to enter data into the controllers memory. First place the number you want entered into the GENERAL/IPS display by pressing the numeric keys (5.5=550 etc.).

ENT, 1 places the number in the PRESENT POSITION.
ENT, 2 places the number in the last digit of the PRESENT POSITION. This number must be 0, 25, 50 or 75 where only 0 and 50 are allowed in full STEP mode.
ENT, 3 places the number in the INITIAL POSITION.
ENT, 4 places the number in the last digit of the INITIAL POSITION.
ENT, 5 places the number in the FINAL POSITION.
ENT, 6 places the number in the last digit of the FINAL POSITION.
ENT, 7 places the number in IMPULSES PER STEP.
ENT, 8 places the number in GRATING #
ENT, 9 places the number in IMPULSESE PER SEC.

If the number is incorrect then the display will be BLANKed and will remain empty until a correct number is ENTERed.

FINAL POSITION Display

Indicates the FINAL POSITION of the START sequence. (limits = 0 - 2400)

FO IEEE code

Usage: SEND("FO",1)

Sets ForWarD DIRection.

FP IEEE code

Usage: SEND("FPxxxx",1) xxxx=0-2400

Sets FINAL POSITION.
 FS  
 IEEE code  
 Usage: SEND("FS",1)  
 Sets Full STEP mode.

FWD  
 IEEE code  
 Light

Impulses will drive the motor in the Forward DIRECTION.

G  
 IEEE code  
 Usage: SEND("Gxxxx",1) xxxx=30,40,101,240,640,1440,2880  
 Sets GRATING #.

GENERAL/IPS  
 IEEE code  
 Display  
 Indicates the number of impulses sent to the motor during a STEP, a number ENTERed from the keyboard or the number stored in memory when used with DISPLAY.

GRATING #  
 IEEE code  
 Term  
 The number of lines per mm for that grating. It is used in calculating the WAVEnumbers. (limited to 30, 40, 101, 240, 640, 1440, 2880)

HA  
 IEEE code  
 Usage: SEND("HA",1)  
 Same as pushing the STOP key.
HALF Light

The motor is set to run in HALF step mode. (see STEP H/F)

--------

HS       IEEE code

Usage: SEND("HS",1)

Sets HALF STEP mode.

--------

IM       IEEE code

Usage: SEND("IMxxx",1) xxx=1-32768

Sets the IMPULSES PER STEP. The default is 20.

--------

IM PULSES PER SEC        Term

The number of IMPULSES PER SECond the controller sends to the motor while STEPPing. (limits = 1 - 350)

--------

IM PULSES PER STEP        Term

The number of impulses which are sent to the motor in one STEP. (limits = 1 - 32768)

--------

INITIAL POSITION Display

Indicates the starting position of the START sequence. (Limits = 0 - 2400)

--------

IP       IEEE code

Usage: SEND("IPxxxx",1) xxxx=0-2400

Sets the INITIAL POSITION.
**LIMIT J2**  
Cannon plug  
Connects the mechanical LIMIT SWITCHEs to the controller.

**LIMIT SWITCH**  
Term  
A mechanical switch set to stop the motor from running the drum beyond its limit.

**LL**  
Light  
Mechanical Lower LIMIT SWITCH has been activated.  
(see MOTOR OVERRIDE)

**MANUAL**  
Push button  
Executes one STEP.

**MOTOR J1**  
Cannon plug  
Connects the stepping motor to the controller.

**MOTOR OVERRIDE**  
Push button  
Moves the motor when one of the mechanical LIMIT SWITCHEs are activated. The DIREction is determined logically and the distance is determined by the distance needed to deactivate the LIMIT SWITCH. After using this switch the PRESENT POSITION must be reset.
PARALLEL POLL IEEE function

Usage: ENABLE_PAR_POLL(0 or 1, 0-7, 1)

0=> sets line if status bit is clear; 1=> sets line if status bit is set.
0-7=> the data line (bit) which is set in response to a PARALLEL POLL.
This command must proceed any PARALLEL POLL which might follow.

Usage: PAR POLL(R)

This command conducts a PARALLEL POLL as instructed by the above command. R is the response (number) to the PARALLEL POLL. If 3 instruments set bits 0, 1 and 3 but no other instruments set the rest then R=1+2+8=11.

Usage: DISABLE_PAR_POLL(1)
Usage: DISABLE_ALL_PAR_POLL

These commands disable the ENABLE_PAR_POLL command. In the controller when the PARALLEL POLL status bit is
0=> START sequence is finished; 1=> START sequence is not finished.
The controller has a default that sets data line bit 7 (see B) which the MINC will override in ENABLE_PAR_POLL.

PM IEEE code

Usage: SEND("PMxx", 1) xx=0, 25, 50, 75
Sets the last digit of PRESENT POSITION. (see ENT)

POWER Switch

Applies power to logic and stepper motor. After power up an automatic RESET is executed.
PP IEEE code
Usage: SEND("PPxxxx",1) xxxx=0-2400
Sets the PRESENT POSITION.

PRESENT POSITION Display
Indicates the current position of the grating,
limits = 0 - 2400

RA IEEE code
Usage: SEND("RAxxx",1) xxx=1-350
Sets the IMPULSES PER SEC. Default is 250.

RE IEEE code
Usage: SEND("RE",1)
Sets REVerse DIRection.

REMOTE AND LOCAL IEEE function
Usage: LOCAL_INSTR(1)
Usage: DISABLE_REMOTE
These commands puts the controller in the LOCAL state
where the front panel controls the instrument.

Usage: ENABLE_REMOTE
This command puts all instruments in the REMOTE state.
The first SEND statement automatically places the
instruments in REMOTE.

Usage: TEST_REMOTE(R)
If any instrument is in REMOTE then R=-1, if they are
in LOCAL mode then R=0.
RESET Push button

The RESET will set the INITIAL POSITION, PRESENT POSITION and FINAL POSITION to 0.0, the IMPULSES PER STEP to 20, the GRATING # to 2880, the IMPULSES PER SEC to 250, the DIRECTION to FORWARD and will set the controller to the following modes; DRUM, full STEP, cancels any BLANKing displays and applies DVM HOLD.

---

REV Light

Impulses will drive the motor in the Reverse DIRECTION.

---

RUN Term

A set of STEPS from INITIAL POSITION to FINAL POSITION. (see START)

---

SERIAL POLL IEEE function

Usage: SERIAL_POLL(S,,1)

This command conducts a SERIAL POLL on the controller. S is the status byte of the controller. It is an 8 bit byte and is in the range 0-255. Each bit has the following meaning:

- Bit #0 1 => WAVE mode; 0 => DRUM mode
- #1 1 => PRESENT POSITION is 2400
- #2 1 => REV; 0 => FWD DIRECTION
- #3 1 => PRESENT POSITION is 0
- #4 1 => HALF; 0 => Full STEP mode
- #5 1 => LIMIT SWITCH is on
- #6 1 => SERVICE REQUEST (SRQ) on
- #7 1 => a BLANK display
SERVICE REQUEST  

IEEE function

Usage: SRQ_SUBROUTINE(line #)

If this statement is in a program and a SERVICE REQUEST occurs the program will start executing at line # as soon as it comes to a point inbetween statements in the program. A SERIAL_POLL statement must be included in the subroutine to allow the instrument to return to active state and allow the program to continue.

Usage: TEST_SRQ(R)

If the SRQ line is set by any instrument when this statement is executed then R=-1, if the SRQ line is not set then R=0. The controller sets the SRQ line if BLANKing occurs or if a LIMIT SWITCH is turned on.

SL  

IEEE code

Usage: SEND("SL",1)

Same as pushing the SLEW push button.

SLEW  

Push toggle

Supplies continuous impulses to the stepping motor.

SPEED  

Push button

Supplies a manual STEP signal. This is the same type signal which comes automatically from the DVM when RUNning. STEP signals are accepted only after the START sequence. The STEP signal supplies a STEP, HOLDS the DVM during the step, updates the PRESENT POSITION, checks if the RUN is over and then releases the DVM. (see START)
SS  IEEE code
Usage: SEND("SS",1)
Same as pushing the MANUAL button.

ST  IEEE code
Usage: SEND("ST",1)
Begins the START sequence.

START  Push button
Begins the START sequence. The controller will move the motor to the INITIAL POSITION and release the DVM. The controller will now accept STEP signals (see SPEED) until the PRESENT POSITION equals the FINAL POSITION. This STEP signal terminates the START sequence, HOLDS the DVM and returns control to the front panel. During the START sequence the front controls are inactive except during a short time after the STEP signal is received. If a button or key is pushed during the RUN it will not be executed until the next STEP signal. If the button or key changes the way a START sequence is executing the DVM HOLD will come on (SLEW, CLR DISP, STEP H/F etc.); if it does not effect the START sequence the DVM HOLD is not turned on (STOP, WAVE/DRUM. DISP etc.) and the sequence may be CONTinued without error.

STEP  Term
A set of impulses sent to the motor to move it a given distance.
STEP H/F

Key toggle

Sets the motor to move in Half STEP mode. In Half STEP mode the IMPULSES PER STEP is set to 1 and cannot be changed. When an impulse is sent to the motor it will turn 1/2 the distance (400 impulses/revolution) as in Full STEP mode (200 impulses/rev.). When returning to Full STEP the IMPULSES PER STEP is set to 20.

STEP IN PROGRESS Light

Impulses are being sent to the motor.

STOP Key

STOPs the controller. This may be in opposition (SLEW etc.) to the toggle sequence of some switches so it may cause toggles to be out of sequence until CONTinue is pressed. This key is designed to be used to STOP the START sequence.

SYNC BNC connector

The impulses which are sent to the stepping motor appear at this connector.

TEST FOR LISTENERS IEEE function

Usage: TEST_LISTENERS(R,1)

If the controller is listening (on IEEE bus) then R=-1, if it is not listening then R=0.

TRIGGER INSTRUMENTS IEEE function

Usage: TRIGGER_INSTR(1)

This command will begin the START sequence.
Has no function.

Mechanical upper LIMIT SWITCH has been activated. (see MOTOR OVERRIDE)

Usage: SEND("W",1)

Sets the WAVE mode.

Sets the mode in which data on the digital displays are presented. WAVE mode (without decimal pts.) gives numbers in wavenumbers (cm⁻¹) where DRUM mode (with decimal pts.) gives numbers as they correspond to the drum connected to the stepping motor.
This appendix contains an outline of the operation of the hardware and software necessary to analyze the data taken on either the Michelson interferometer or the Perkin-Elmer grating monochromator. The appendix also contains useful information on the GA-16 computer and TSO system.
I. How To Get a Line Connected To the GA-16

The GA-16 computer is located on the second floor of Smith Lab. The connector SWITCH BOARD is located on the front panel of the first module of the computer. A diagram of a connector block appears below.

```
+--------
|       | This is the top part of the
|       | connector that allows
|       | connection TO a port or
|       | IRCC SWITCH.
+--------
|       | This is the middle part of
|       | the connector that allows
|       | connection FROM a terminal.
|       |
+--------
|       | This is the lower part of
|       | the connector that allows
|       | a monitor to observe the
|       | connections above.
+--------
```

The average baud rate is 1200, however some ports have rates of 2400, 300 etc. All devices that are not labeled are assumed to have a 1200 baud rate. The baud rate of a GA-16 port can be controlled with software by logging on as the SYSTEM USER. Type a RETURN on the terminal opposite the GA-16. The GA-16 will respond with

```
INVALID USER NAME
ENTER USER NAME
?```
To this answer

SYSTEM

the GA-16 will then type

ENTER PASSWORD

?

The password to type is

HEP

You are now logged on as the system controller. To change the baud rate of a port type

$BAUD PORT BAUDNO

where PORT is the port number (51) you want changed and BAUDNO is the baud rate you wish (300, 1200 etc.). After you change the baud rate you must type "LOGOFF" and then logon the system as yourself to have access to your files.

NOTE: Any changes should be corrected immediately after your use.

The SWITCH BOARD has default connections which are indicated on the front panel. When connections are made to the front, the default connections are broken. It is important to determine which default connections are in use.

1. To make a connection to the GA-16, one must LOGON to the system at a console which is already connected. The command

USERS

will list the following information:
<table>
<thead>
<tr>
<th>Port</th>
<th>User</th>
<th>State</th>
<th>Part</th>
<th>Prty</th>
<th>Logged on at</th>
<th>User Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>TY</td>
<td>System</td>
<td>Blocked</td>
<td>0</td>
<td>0</td>
<td>Date Time</td>
<td>Mibs System Console</td>
</tr>
<tr>
<td>50</td>
<td>RJE</td>
<td>Blocked</td>
<td>1</td>
<td>7</td>
<td>Date Time</td>
<td>Hasp/RJE Console</td>
</tr>
<tr>
<td>51</td>
<td></td>
<td>Blocked</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>52</td>
<td>Tanner</td>
<td>Run</td>
<td>0</td>
<td>0</td>
<td>Date Time</td>
<td>David Tanner X6267</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ETC.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Each port will have a line of data. The port numbers without names (51) are not currently in use and a connection may be made to that port. The port labeled RUN is the one which you are using at the time USER is typed. Notice that only the last digit of the port number is used as a label for the connectors.

2. To make a connection to the IRCC SWITCH one must look at the lights on the box labeled OSU MODEM on the shelf behind the computer. There are 4 lights per channel:

- TXD => TRANSMIT DATA (TD)
- RXD => RECEIVE DATA (RD)
- DCD => DATA CARRIER DETECT (CD)
- DTR => DATA TERMINAL READY (TR)

A connection CAN be made to an IRCC line whenever the DCD light is OFF. There are a total of 8 IRCC lines, however IRCC 8 is a line that comes FROM the SWITCH only. The other 7 lines go TO the SWITCH only.
II. Placing Card Images Onto the GA-16

The DECWRITER opposite the GA-16 is the console terminal for connections, via the 9600 baud line, to the IRCC Amdahl computer. The CARD READER (CR) beside the GA-16 is normally dedicated to the REMOTE JOB ENTRY (RJE), and must be disconnected for use with the GA-16.

1. The RJE cannot be submitting a program to the Amdahl. To insure this, simply read in the small deck of cards for a job called UTILITY. It is usually located in storage behind the card reader. Check that the last card in the deck has "/^E0F" on it. Load the cards into the CR, push the POWER and then the RESET button. After the cards are read, the DECWRITER will type out a message which indicates that the program UTILITY is being submitted to the Amdahl. When it is finished the message

"RD01 NOT READY"

will be printed. This message indicates the card reader is ready to be disconnected from RJE.

2. To disconnect the card reader type onto the DECWRITER

```
^R.Z RD01
^R.LUI=NO
```

where "/^R" indicates that you depress the CTRL key when you type the "R". Notice the spaces in the first line and the use of "0" and "0"; the lines must be typed exactly. Each line is entered into the system by pressing the RETURN key at the end of that line.

3. LOGON to a terminal connected to the GA-16. Place a card with "/^*" (in the first 2 columns) as the last card in the deck, load your cards into the reader and hit the RESET button (just as you would do to read in the UTILITY-job cards). If everything has been working correctly (and sometimes RJE can get confused) the card reader will sit in the ready mode without reading any cards. You then type on the terminal you logged onto

```
COPY CR filename
```

where "filename" is the name of the file where the card images will be stored (limited to 8 alpha-numeric characters). The CR will begin to read the cards. If no errors are detected in the reading process, the CR will continue till it reads the "/^*" or "END" card which will close
the file. If an error is detected, then an error message will be printed on the terminal and the CR will stop. There will be 3 options to enter:

A. "C" => CONTINUE the copy, but do not worry about the error. In general the entire card with the error will not be added to the file and the card must be added later by some edit procedure.

B. "K" => KILL the copy, do not save what has been read into the file and return to MIBS to start over again.

C. "R" => RETRY to read the card. Take the last card read and insert it as the first card to be read when the CR starts. Press the RESET key on the reader, enter "R" on the terminal and hit the RETURN key. The CR will re-read that card and if there is no error the file will be identical to the cards.

4. More files may be entered by simply loading in the cards and entering another COPY command.

NOTE: If you copy to a filename that already exists the old file will be deleted and replaced by the new file.

5. Reconnect the CR to RJE by typing on the DECRYTER

```
^R.LUI=CR
^R.S RD01
```

The CR is now connected to RJE and jobs which were submitted while the CR was disconnected can now be sent to the Amdahl.

6. To obtain a copy of the file on the LINE PRINTER (LP) type on the terminal

```
$PRINT filename
```

This will start a PROCEDURE (PROC), on the GA-16, that copies filename to LP. LOGOFF the GA-16 by typing

```
LOGOFF
```
III. Transfer of Files Between the GA-16 and Minc Computers

The MINC must be connected to the GA-16.

NOTE: Make all connections with the MINC OFF. If connections are made and the programs do not work, check the micro fuse on the serial port board. This fuse is sensitive and supplies the DTR signal necessary for some devices.

The connection to the MINC should be made to the second serial port from the bottom (port SLU1). The connection to the GA-16 should be made as described in I.

The software necessary to communicate with the GA-16 is the BASIC program SPECOM. The features and conventions of SPECOM are:

1. The GA-16 OPERATING SYSTEM (MIBS) symbol for "ready for input" is a "?". This symbol is represented by " <=" on the MINC.

2. A command for the GA-16 is typed when the " <=" appears. The command will write over the " <=" as it is typed.

3. If several "^C" (CTRL C's) are entered, the program SPECOM will be stopped and MINC will return to READY. However, the status of the GA-16 remains unchanged. You may leave SPECOM (and the GA-16) whenever the " <=" appears, do any MINC manipulations and then return to the GA-16 by running SPECOM. The program will begin at the point you left the GA-16.

NOTE: If you leave the GA-16 in this manner you have NOT logged off the system. You must end the use of the GA-16 by "LOGOFF" or "BYE" only.

4. If you wish to send ^C's to the GA-16, enter " )" at the " <=". This will send ^C's to the GA-16 (causing **CONSOLE INTERRUPT) without affecting the SPECOM.

5. If a " ]" is entered the program will list a menu of items which it can perform. At present SPECOM can transfer files to and from the GA-16 (at 4800 baud).

A. Files transferred from the GA-16 to the MINC are made in sets of 22 lines. 22 lines are transferred into MINC's memory from the GA-16 and then MINC places these lines into a file. The lines are written on the terminal at the time they are placed into the file. This continues until the end of the file is reached.
B. Files transferred from the MINC to the GA-16 are made one line at a time. The lines are written onto the terminal after they have been received by the GA-16.

NOTE: There is no check on the accuracy of the data sent or received. However, there is no evidence of errors arising from the transfer of files by SPECOM.

C. The conventions for ending a file on the MINC and GA-16 are different. However, SPECOM will correctly end the files; no "special" endings are needed for transferred files. The conventions are:

   a. A MINC file must have the END OF FILE MARKER (EOFM) as the first character of the last line in the file. The EOFM is represented by the ~Z symbol on the VT105. If the file's last line ends with a FORM FEED (FF or ~L) then a blank line must be inserted between the FF and EOFM.

   b. A GA-16 file is ended by a line starting with the symbols "/*" or a line with at least one space and the word "END". If either appear in a file, the file will be stopped at that line and any lines that follow will be lost.

When a file is transferred from the GA-16, the MINC file is closed when either a "/*" or "END" line is encountered. The "/*" will NOT be placed at the end of the MINC file, however the "END" WILL be placed at the end of the file. When a file is transferred from the MINC, the GA-16 file is closed by a "/*" line when the EOFM is encountered. The "/*" is the last line in the GA-16 file. However, if the next to last line in the MINC file is "END", this will be the last line in the GA-16 file and the "/*" will be lost.

6. To LOGOFF the GA-16 type either "LOGOFF" or "BYE" at "<=". This will disconnect the GA-16 from the MINC and stop SPECOM.

NOTE: The program SPECOM is designed to accomplish all the functions of a terminal connected to the GA-16 (including the special edit functions) EXCEPT transfer TAB characters. If a TAB appears in a file or is typed in a line, the program will NOT work correctly and should be restarted.
IV. Software to Place Header Cards on Data Files

NOTE: The runs must be SEPARATED by at least ONE BLANK CARD. There must be ONE BLANK CARD at the END (before the "/*") of the last run and there CANNOT be any cards before the first data card.

1. BASIC program VERIFY. This program:
   A. Finds all card images with only one point on it. These cards should be deleted from the file.
   B. Finds cards which have characters other than numbers on them. CR errors will sometimes change the numbers to characters.
   C. Finds cards which do not have the correct number of characters on them. Cards must have some multiple of 5 characters.
   D. Prints the above errors on the terminal and MINC LP. It also prints the largest number of cards in one run and the total number of card images in the file.

The errors found by VERIFY should be corrected before proceeding.

2. FORTRAN programs PEHEDR and MCHEDR. These programs:
   A. Take unheadered data (default DY1:filspc.RAW), puts header cards on the runs and places the headered data in a sequential file (default DY1:filspc.DAT).
   B. Have the formats, written in parentheses, beside the input remarks. The formats can be followed by filling with spaces or the read field may be terminated by commas. For example:

   IPD DRUM1 DRUM2 . . .
   (I2) (F6.3) (F6.3) . . .
   0109.00015.000 . . . or
   1,9.,15., . . .

   The two lines above are input to the program identically. Yes and no questions have the answer which is checked in parentheses. For example the question "More data (Y)?" means that a "Y" will allow more data to be entered and anything else will cause the program to continue to the next step.
C. Program PEHEDR is used to place header cards on data taken on the Perkin Elmer grating monochromator. MCHEDR is used to place header cards on data taken on the big Michelson interferometer.

**NOTE:** As the programs are now written, a blank line is produced at the beginning of the output file. This line should be deleted before going to the next step.

3. **BASIC program FILSRT.** This program:

A. Produces a virtual array (default DY1:filspc.VRT) that stores a card image in each element of the array. This allows the single file DY1:filspc.DAT to be broken into runs and then these runs can be sorted into any order to produce another file.

B. Stores all files names it has sorted (up to 50) in a catalog with the number of runs in that file and the number of cards in the largest run (the number given by VERIFY +2).

C. After the program has the information from "B", (either from the catalog or from the terminal) FILSRT opens the array and lists a menu of tasks it can perform. These include:

   a. Placing the DY1:filspc.DAT file into the DY1:filspc.VRT virtual array.

   b. Display or modify the elements of the virtual array.

   c. Write the runs (along with other lines of data) from the virtual array to another file in the order necessary for the Amdahl programs PERKELMR or FOURTRNS.

**NOTE:** The program FILSRT CHANGES NAMES while running and therefore it is necessary to run FILSRT from disk each time a new file is sorted. If an ERROR should occur and the program stops (or C's are entered) then the FIRST COMMAND typed should be CLOSE. If this is not done the virtual array, and any file being written, may be LOST. The array name and dimensions will remain in the catalog and do not need to be re-entered.

4. The header card images used by PERKELMR and FOURTRNS for plots should be added to the beginning of the files and the files are sent to the GA-16 using section III.

   A source listing of each program is given at the end of this outline.
V. How to submit Programs from the GA-16 to the IRCC Amdahl computer

The following describe conditions necessary to submit a job from the GA-16 to the Amdahl computer system.

1. The SOURCE programs are placed into files on the GA-16. Each program and subroutine will be in a separate file on the GA-16.

2. The data file may be on either the GA-16 or stored on disc at the Amdahl.

3. The JOB CONTROL LANGUAGE (JCL) card images are placed in a separate file from the SOURCE. Examples of JCL are given at the end of the outline. Some JCL cards require a "/*" at their beginning, therefore a PROC is used to translate the JCL in the GA-16 file to a file which can be submitted to the Amdahl computer. The conventions are:

   A. A "/*" in the first two columns of JCL is written as "@@".
   B. The line "=filename" in the JCL instructs the PROC to insert the file "filename" at this point in the submittal file.
   C. A "/*" must be the last card in the JCL file.

4. The PROC that submits the JOB to the Amdahl is called SUBMIT. To submit a JOB type

   SUBMIT filejcl

where "filejcl" is the file of JCL as described in 3. The SUBMIT PROC will

   A. Build another file with the JCL cards, source cards and data cards.
   B. Transfer this file (by the RJE) to the Amdahl for batch processing.
   C. Act as traffic cop allowing only one SUBMIT to occur at any one time.
   D. Print a statement on the DECWRITER which indicates the JOB is being submitted. The statement will look like

   HH.MM.SS JOB 1234 $HASP100 JOBNAME ON R13.RD01 NAME
where HH.MM.SS is the hours, minutes and seconds the JOB was submitted, JOB 1234 is the job number given by the Amdahl, JOBNAME is the name you gave the program in the JCL file and NAME is your name as given on the first JCL card. When the line

```
  . RD01 NOT READY
```

is printed, the submitting is over and the next SUBMIT command will be executed.

5. A JOB submitted to the Amdahl from the GA-16 HIGH ENERGY PHYSICS computer (HEP) will have its output routed to the LP on the second floor. However the LP will not print JOBS with more than 3000 lines. Any output with more lines will be "hung" and the output must be routed to another LP. The ROUTE console command will be discussed in the section on useful console commands. When a JOB output has been RECEIVED by the GA-16 the DECWRITER will type

```
  . JOB JOBNAME RECEIVED -- X.XXX LINES --Y.YYY CARDS
```

The CARDS are card images which were "punched" to the GA-16. This is discussed in more detail in the section on useful TSO commands.

6. Sometimes the SUBMIT PROC or the RJE or both may be left in a state that is improper and this will "hang" the system (the SUBMIT will not end). There may be several problems and therefore there are many solutions that should be discussed. This section contains solutions to the problems with the SUBMIT PROC and should be tried first. The next section deals with the errors and solutions to the RJE.

A. When the CR has been disconnected (as in II) the RJE will sometimes not give the SUBMIT PROC the line necessary to submit a file. To clear this problem, submit the deck of cards UTILITY as described in II. The CR should read the cards, submit UTILITY and then be ready to execute the SUBMIT PROC.

B. If someone has submitted a file which has an incorrect first JCL card the following message is typed on the DECWRITER

```
HH.MM.SS $HASP125 R13RD01 SKIPPING FOR JOB CARD
```

If the submitted file does not end correctly (a "/*" for a submit file or a "/*EOP" for a deck of cards) the SUBMIT PROC will not end and any new JOBS will not be executed. If your JOB takes a long time to be submitted (> 10 minutes) then check the DECWRITER. If the DECWRITER has a JOB being submitted (or many JOBS that were submitted) then everything is probably OK and the submitting is just busy. If however the DECWRITER is not busy, then you should
a. Run a "/*EOF" card through the CR. This may clear the problem and the DECRITER will indicate that it is proceeding with the next submit file.

b. If "a" does not work then you must run a PROC that clears the submit file. Copy the submit file of the last JOB by typing on a terminal

```
COPY :SUBMFILE XX
```

Only the first 3 or 4 lines will be written, however the name of the last JOB and the person responsible should appear in the first line. Check the DECRITER for this job or contact the person to check on the status of that JOB (e.g. did he submit it recently or 20 minutes ago etc.). If there was an error in the submit JCL, the SUBMIT PROC can be cleared by typing

```
$CLRSUBM
```

on a terminal.

NOTE: If the $CLRSUBM PROC is executed during someones correctly running submittal, that program will be ended abnormally and the Amdahl will not be able to run the program.

C. You cannot exit the SUBMIT PROC by entering ^C's. If someone leaves the SUBMIT by ^C's, the PROC is left in an unended state and will not transmit the file to the Amdahl. This problem is corrected by clearing the submit file as described in the above section.

7. Sometimes the problem is in the RJE itself. If the steps in 6 did not satisfactorily clear the problem, it may be corrected by the following:

A. Plug the 9600 baud line monitor (section I) into the LED lights on the SWITCH BOARD. Both the TD and RD lights should blink quickly at regular intervals. If the TD light is not blinking then the RJE is not working correctly. If the RD light is not blinking then the Amdahl may not be working correctly.

B. Check to see if the Amdahl is working by calling the computer status number (2-3140). If the Amdahl is not connected to the GA-16 (but working) the DECRITER will have typed the message
This indicates a TIME OUT has occurred at the given time. It is natural to get several time outs in a day and they should not last more than a few seconds. When the message

**OK HHMMSS**

appears, the Amdahl should be ready to communicate with the GA-16.

If the LED's indicate the RJE is disconnected from the Amdahl, try getting a response from the Amdahl over the DECWRITER by typing in one of the commands given in the section on useful console commands. If there is a response, the RJE is connected and the problem is probably in the SUBMIT PROC. However, if there is no response (and the Amdahl is working) the RJE should be restarted. To restart RJE type on the DECWRITER

```
^C ^C
```

The DECWRITER will write

**CONSOLE INTERRUPT
MIBS 4.3 - OSU/HEP
?

At the "?" type

```
$RJE
```

This will start a PROC that will link the Amdahl and the GA-16. The DECWRITER will type

```
ENTER
JOB
SET SI=CR SO=:SYSOUTB LO=LP. . . :RJOSU
.MIBS RJE REV J4
```

Next type

```
^R.X
```

where "^R" is "CTRL R". The DECWRITER will type

```
. ON-LINE
. RD01 NOT READY
```

At this point the RJE is ready to submit JOBS.
NOTE: When you restart the RJE, the Amdahl is disconnected from the GA-16. Therefore any programs being transmitted or received will be lost. One should wait until the DECWRITER shows no activity and the LP is not printing before restarting the RJE.
VI. Software to Analyze and Transfer Data with the Amdahl Computer

At present there are three major programs that will analyze data on the Amdahl. Only one program is necessary to transfer data from the GA-16 to the Amdahl.

1. PERKELMR - Reduces data from the Perkin Elmer grating monochromator. The LP output is sent to the second floor HEP LP. However, the plots are sent to the Versatec plotter which is on the fifth floor of Baker Systems Engineering. The operation of the program is documented in the program itself. The JCL file which submits PERKELMR to the Amdahl is PERKJCL. There is a PROC which will edit the JCL file and then submit it to the Amdahl. To use this PROC type

$PERKSUB NAME1 NAME2

where NAME1 is the name of the data file on the GA-16 and NAME2 is the name of the file to be placed on the TIME SHARING OPERATION (TSO) account. If the data file is NOT going to produce a file on TSO then a "TRASH" name should be used. Even though the file will be empty, a file gets produced. If the data file DOES produce a TSO file, NAME2 is the name of this file (which contains the frequencies, ratios and number of points averaged together of the combined plot).

2. FOURTRNS - Reduces data from the big Michelson interferometer. Both plots and LP output are sent to the fifth floor of Baker Systems Engineering. The JCL file which submits FOURTRNS to the Amdahl is FOURJCL. There is a PROC which will edit the JCL file and then submit it to the Amdahl. To use this PROC type

$FOURSUB NAME1 NAME2 NAME3

where NAME1 is the name of the data on the GA-16, NAME2 is the name of the file to be placed on TSO (as in 1 above, the TRASH filename) and NAME3 is the name of a TSO file which has data that is used to correct the reflectance of the background sample. At present the background materials available are

A. MIRROR - No correction (default)
B. ALUMINUM
C. ALUMGOLD - Aluminum / gold
D. GOLD
E. OVERGOLD - 1 / gold
F. SILVER
3. KRAMKROG - Transforms data from TSO files produced by PERKELMR or FOURTRNS. The operation of KRAMKROG is described in the program. The LP output is sent to the GA-16 and the plots to Baker. The JCL file which submits KRAMKROG to the Amdahl is KRAMJCL. There is a PROC which will edit the JCL file and then submit it to the Amdahl. To use this PROC type

$KRAMSUB NAME1 NAME2 NAME3 NAME4

where NAME1 is the name of the data TSO file, NAME2 is the name of a divisor data file (on TSO) for NAME1, NAME3 is the name of the TSO file which has data that is used to correct the quotient of NAME1 and NAME2, and NAME4 is the name of the file to be written on TSO (the TRASH filename) that will contain the output data in a form similar to the LP output.

NOTE: Do not use the same name of TRASH filenames for TSO files until you have deleted the old files from TSO. The multiple use of the same name will eventually lead to problems which are not easily corrected.

4. SCOPY - Is a program that transfers files from the GA-16 to a TSO account on the Amdahl. The JCL file which submits SCOPY is called COPYJCL. There is a PROC which will edit the JCL and submit it to the Amdahl. To use this PROC type

$COPYSUB NAME1 NAME2

where NAME1 is the filename of the file on the GA-16 to be copied to the TSO account and NAME2 is the name the file will have on the TSO account.

NOTE: At present all files written from the GA-16 to a TSO account have the FILE TYPE ".DATA" which is automatically added to the name by the submit JCL.
VII. Useful MIBS Commands

The following is a list and short description of commands which are available on the GA-16.

**NOTE:** CR= CARD READER, DW= DECWRITER on the far wall from the GA-16, LP= LINE PRINTER and XX= the TERMINAL which you have logged onto the GA-16.

1. **ACCESS filename (READ)** - The ACCESS command is a method of protecting a file from being altered or erased. The command

   ACCESS filename READ

   protects "filename" from being altered. The command

   ACCESS filename

   unprotects "filename" and allows the file to be edited or erased.

2. **COPY file1 file2** - The COPY command places the contents of "file1" into "file2". The "file" can also be a device. This allows you to COPY to DW or from the CR etc. If you type the command

   COPY filename XX

   "filename" will be copied to your terminal. 22 lines will be placed on the terminal and then "PAUSE" will be typed. You can enter 3 types of answers at the PAUSE.

   **A.** RETURN KEY => continue to the next 22 lines and pause.

   **B.** "S" => STOP and return to MIBS.

   **C.** NUMBER => print NUMBER amount of lines and pause. NUMBER can be between 1-99 and once used resets the number of lines printed in "A" above.

3. **$EDIT filename** - Starts a PROC that will allow editing of "filename". When the terminal types "EDIT" the editor is ready to accept any of the following commands

   **A.** "B" => Go to the BOTTOM of filename and enter INPUT mode (see RETURN KEY).
B. "C /old/new/ n" => CHANGE any set of characters matching "old" to the characters "new". Do this CHANGE for a total of n times and stop. The CHANGE command will only search DOWN a file for a match to "old".

C. "CL" => Print the position of the COLUMNS on the terminal. They appear as

****.****1****.****2****.****3 . . .

where 1,2 etc. are the position of the 10th, 20th etc. columns and the "." is the fifth column from the last number.

D. "D n" => DELETE the next n lines down in the file starting at the pointer. The pointer is at the last line typed on the terminal.

E. "F /model/ n" => FIND the characters in the file that match "model", move the pointer to that line and print that line onto the terminal. If n is present FIND "model" n times. The FIND command will only search DOWN filename for a match to "model".

F. "I n" => INSERT the next n lines of text that is entered after "I" (on the next lines) into the file after the pointer. If n is present index the pointer 1 after each line so the following INSERT will be placed below.

G. "M" => MODIFY the line at the pointer. "M" will retype the line to be modified and then place the cursor under that line. The symbols used to MODIFY a line are

a. "/" => Delete the character above this symbol.

b. ":" => Make the character above this symbol a space (" ").

c. " " => Make no change to the above character.

d. ":" => Insert all symbols after the ":" into the line starting one character before the ":" symbol. The insert is stopped by a space (" ") in the modifying line.

e. "Any Other Symbol" => Replace this symbol with the character above it.

TH LINEEEWILL EB MODIEIED
@E /^ //@BE F
THE LINE WILL BE MODIFIED.
H. "N n" => Move down the NEXT n lines without printing the lines inbetween.

I. "P n" => PRINT the next n lines down in the file starting at the pointer.

J. "Q" => QUIT the EDIT and return to MIBS.

K. "R" => REPLACE the line at the pointer with the line of text that is entered after the "R" (on the next line).

L. RETURN KEY => Change from EDIT mode to INPUT mode. In EDIT mode the commands in this section are used; in INPUT everything typed is inserted into the file at the pointer. Another RETURN KEY will change from INPUT to EDIT again.

M. "T" => Go to the TOP of the file.

N. "U n" => Go UP n lines in the file from the pointer without printing the lines inbetween.

NOTE: If n is not present it is assumed to be 1. In all cases n= "*" indicates the command should be continued to the end of the file.

4. ENTER & RETURN - Are the first and last lines for a file that is to be executed as a PROC on the GA-16.

5. FILES - Will usually cause the message

MIBS FILES REV3
UNIT LO NOT DEFINED

After this message type "XX" and a listing of all the files in your directory will be printed in the same manner as COPY command (2). The command

FILES :

will list all the global files (files which are available to all users).

6. JOB - Will reset the port to its initial conditions.

7. MENU - produces a list of commands that MIBS will execute.

8. PACK - Will move all free sectors to the end of your disk area. It does the same manipulations as COLLECT in BASIC or SQUEEZE in RT-11.
9. $PRINT filename - Will produce a copy of "filename" on the GA-16 LP.

10. PURGE filename - Will delete "filename" from your disk.

NOTE: PURGE WITHOUT A FILENAME will attempt to ERASE ALL PROGRAMS on your disk area!

11. SET X=Y - Is used to set certain logic lines equal to other lines or to devices.

12. USERS - Will list the ports which are currently in use.

NOTE: In these "filename"s a "*" is a wildcard which stands for any characters that may appear in that spot within a file name.
VIII. Use of the Magnetic Tape With the GA-16 Computer

This section describes PROC's, commands and methods of storing and retrieving files from magnetic tapes. The tape drive on the left is device MO and the one on the right is M1. At present M1 is not working well and drive MO should be used.

1. Tapes can be obtained through Central Stores on campus with 100-W forms. To load a tape, place it onto the top hub and push the toggle in the hub so that it is flat. This will secure the tape to the hub. The tape is fed through MO as shown on the lower left corner schematic. Wrap the tape onto the lower take up reel several times to secure it. Close the cover, press the POWER switch and the LOAD switch. The tape will advance till it "sees" the metallic strip that marks the beginning of the tape. The tape is now ready to be controlled from a terminal connected to a GA-16 port.

NOTE: A small plastic ring must be inserted into the grove in the back of tape reel to be able to write onto the tape. If the ring is missing, the tape will be protected and you can only read from the tape.

2. To REWIND a tape to the beginning type

   REWIND MO

3. The PROC to find the beginning of a file present on a tape is

   DFIN MO filename

where "filename" is the name of the file on the tape.

NOTE: All operations on a tape search down the tape until the end is found.

4. To COPY a file from a tape to the disk type

   DFIN MO filename
   COPY MO filename D

The "D" in the COPY command tells the GA-16 that the file has been stored in a DISK format.
5. To copy a file from the disk to a tape type

```
DFIND MO nofile
K
:BACK MO
COPY filename MO D
COPY nextfile MO D

EOFM MO
REWIND MO
```

where "nofile" is a file that does NOT exist on the tape (this finds the end of the tape), "K" is the answer to the error that occurs when you do not find "nofile", BACK is a PROC that backs the tape one file (after BACK the tape is at the beginning of the old EOFM) and EOFM is a PROC that writes the new EOFM on the tape after all the files are placed on the tape.

NOTE: A new tape without any files should be started at the COPY commands in the sequence above.

6. To list all the files on a tape to the terminal type

```
DLIST MO
R
```

where the "R" is the answer to the error message that occurs when the end of the tape is reached.

7. To list all the files on a tape to LP type

```
JOB
SET 5=LP
DLIST MO
R
:EOF LP
JOB
```

where EOF sends the END OF FILE to the LP after the list in complete.
8. To make a backup copy of every file on your disk, run the PROC

TAPEUSER MO S

where "S" implies you want the files SORTED (BLANK => nosort) and placed on the tape in alphabetical order. This PROC will start at the beginning of the tape (so any old files on the tape will be erased), place the files (from your section of disk space) on the tape and check the files to insure they are correct. The PROC will also place files in your file list with the names

99999999
DD$MM$YY

where DD is the day, MM is the month and YY is the year the PROC TAPEUSER was used. Any new files produced will be placed after these files and hence they serve as a marker for which files are on tape and which are not.

NOTE: Some of files will not be copied correctly (WC, WS etc.). These are special files which are used by the PROC's and should not cause concern. Only if one of the files you produced shows an error should the PROC be rerun or the tape replaced.

9. To remove a tape, type the REWIND command on a terminal, press the RESET button on the tape reader and then hold the REWIND button down. The tape should be removed after its use and stored.
IX. Useful Console Commands for the Amdahl Computer

The following is a list of commands (JES2) that must be typed on the DECWRITER across from the GA-16. JES2 commands communicate directly with the Amdahl and help control JOBS submitted to it.

NOTE: Precede all lines with "^R" (CTRL R). This gets the REJ's attention and will print a "?" on the DECWRITER.

1. \$C 'jobname' - Will cancel the JOB "jobname". (The single quotes are necessary for this command.)

2. \$D 'jobname' - Print the status of "jobname".

3. \$DN - Display the names of all JOBS which are to be sent (ROUTED) to the GA-16.

4. \$DN,R=RO-R99,Q=XEQX - Display the names of all the CLASS X (X= A-O) JOBS in the computer. (This can become a very long list!)

5. \$LQ - List the print and punch QUE for the GA-16 computer.

6. \$R ALL,J=XXXX,D=DISTAN - ROUTE a JOB output to another site. XXXX is the JOB number (found by 2 above) and DISTAN is the site for output (DISTAN= HEP, ROBLAB, CENTRAL etc.).

NOTE: In the above commands, the entries between commas can be added to other commands. So the command \"$LQ,R=RO-R99,Q=XEQX\" is a valid command which lists the QUE for JOB class X (and so on). If you make a mistake in typing the commands the DECWRITER will type

\$HASPO000 'mistake' INVALID COMMAND

where "mistake" is the incorrect command that you typed.
X. Useful TSO Commands

The following is a short list of PROCs and procedures which are available for a HEP USER with a TSO account. All commands are typed onto a terminal logged onto a TSO line.

1. $PRINT DA(filename) ROUTE(DISTAN) - COPY "filename" (including the extension, e.g. ".DATA") to the LP at site DISTAN (=HEP, ROBLAB, CENTRAL etc.). If you are transferring a file that is not listed under the TSO number (TSNUM) that the terminal is logged on as (i.e. someone else's file), the "filename" becomes

   'TSNUM.filename.extn'

where the "" is part of the "filename" that goes between the parenthesis.

2. $PUNCH DA(filename) ROUTE(DISTAN) - COPY "filename" to the CARD PUNCH (CP) at site DISTAN. If you are transferring someone else's file "filename" becomes

   ' 'TSNUM.filename.extn'

where the " " are part of the "filename". If DISTAN= HEP then the file is transferred from TSO file to the GA-16 global file ":SYSOUTB". The file ":SYSOUTB" should be copied to a file in your disk area.

NOTE: All files transferred by $PUNCH are placed in the same file ":SYSOUTB". It is important to copy this file soon after transfer because the next person to use the $PUNCH command will erase the file you placed in ":SYSOUTB".

3. If you create a file with a file name that already exists on your TSO account, that file will not be cataloged and therefore it cannot be deleted. To find all uncataloged files use the TSO PROC

   $SPACE

This will list all uncataloged files which you have created. To catalog uncataloged files use the PROC
$CATLG file1,file2,... VOLID

where file1, file2... are the files to be cataloged and VOLID is the disk pack that holds the files (e.g. IRCC83). The VOLID is obtained from the $SPACE command along with the file names.
This appendix contains the software programs that were written for the Digital Equipment Corporation MINC-23 laboratory mini computer. The programs SPECOM, VERIFY and FILSRT are written in BASIC and must be run with MINC BASIC (Version 2.0). The programs PEHEDR and MCHEDR are written in RT-11 FORTRAN and must be run under the RT-11 system (Version 3B). The subroutines that follow MCHEDR are the subroutines necessary for the programs PEHEDR and MCHEDR. The description and operation of these programs appear in chapter V.
10 REM *****************************************************************
20 REM SPECOM
30 REM Program by Kevin Cummings
40 REM *****************************************************************
50 DIM D$(24)
60 DISPLAY CLEAR | MOVECURSOR(24,1)
70 Q$='?' | P$=' ENTER PASSWORD:' | B$='/' | C0$=':' | L$=CHR$(10)
80 Z$=CHR$(3)+CHR$(3) | S$=' ' | E9$=' /* ' | E8$=' END' | P9$=' PAUSE'
90 CIN(,M$, ,1,-1)
100 PRINT M $
110 PRINT ' <=24;1H';
120 LINPUT //0,C$
130 IF C$=')' THEN COUT(,Z$,,1) | GO TO 180
140 IF C$=']' GO TO 230
150 IF C$='BYE' GO TO 700
160 IF C$='LOGOFF' GO TO 700
170 COUT(,C$,,1)
180 CIN('RETRIEVE',M$,1,1)
190 IF M0$=Q $ THEN M0$=B$ | GO TO 110
200 IF M0$=P$ THEN PRINT P$; | M0$=B$ | GO TO 120
210 IF SEG$(M$,1,1)$ L$ THEN M0$=M0$+M$ | GO TO 180
220 PRINT SEG$(M$,2,LEN(M$)) | M0$=SEG$(M$,2,LEN(M$)) | GO TO 180
230 PRINT 'Menu for mine controlled spec functions.'
240 PRINT ' 1=> Return to command instructions.'
250 PRINT ' 2=> Copy from spec to mine file.'
260 PRINT ' 3=> Copy from mine to spec file.'
270 PRINT 'Which function'; | INPUT F % | PRINT
280 IF F % >0 THEN IF F%<4 GO TO 300
290 GO TO 230
300 ON F% GO TO 110,310,540
310 PRINT 'What is the name of the file to be copied from the spec,'
320 INPUT S9$
330 PRINT 'What is the file spec for the file to be stored on the mine,'
340 INPUT M9$
350 OPEN M9$ FOR OUTPUT AS FILE #1 DOUBLE BUF
360 C9$='COPY '+S9$+' XX' | J=1
370 PRINT C9$
380 COUT(,C9$,1)
390 CIN('RETRIEVE',M$,1,1)
400 IF M0$=P9$ GO TO 460
410 IF M0$=E9$ GO TO 470
420 L9=LEN(M0$) | L9$=SEG$(M0$,L9-2,L9)
430 IF L9$=E8$ THEN D$(J)=M0$ | J=J+1 | GO TO 470
440 IF SEG$(M$,1,1)$ L$ THEN M0$=M0$+M$ | GO TO 390
450 D$(J)=M0$ | M0$=SEG$(M$,2,LEN(M$)) | J=J+1 | GO TO 390
460 CIN('RETRIEVE',M$,1,1) | CIN('RETRIEVE',M$,1,1)
470 FOR K=2 TO J
480 D9$=SEG$(D$(K),2,LEN(D$(K)))
490 PRINT #1,D9$ | PRINT D9$
500 NEXT K
510 IF SEG$(M0$,1,3)=E9$ THEN CLOSE | M0$=B$ | GO TO 180
520 IF L9$=E8$ THEN CLOSE | M0$=B$ | GO TO 180
530 J=1 | M0$=B$ | COUT(,CHR$(13),,1) | GO TO 390
540 PRINT 'What is the name of the file to be stored on the spec';
550 INPUT S9$
560 PRINT 'What is the filespec of the file to be copied from the minc';
570 INPUT M9$
580 OPEN M9$ FOR INPUT AS FILE #1 DOUBLE BUF
590 C9$='ROVA '+S9$ | PRINT C9$
600 COUT(,C9$,,1)
610 CIN('RETRIEVE',M$,1,,1)
620 IF M0$=Q$ THEN M0$=B$ | GO TO 660
630 IF SEG$(M$,1,1)<L$ THEN M0$=M0$+M$ | GO TO 610
640 IF M0$=S$ THEN M0$=SEG$(M$,2,LEN(M$)) | GO TO 610
650 PRINT SEG$(M0$,2,LEN(M0$) | M0$=SEG$(M$,2,LEN(M$)) | GO TO 610
660 IF END #1 THEN CLOSE | GO TO 690
670 LINPUT //1,L9$ | PRINT L9$
680 COUT(,L9$,,1) | GO TO 610
690 COUT('/*',,1) | GO TO 180
700 COUT(C$,,1)
710 FOR I=1 TO 3
720 CIN('RETRIEVE',M$,1,1)
730 PRINT M$
740 NEXT I
750 END
REM **************************************************************
20 REM VERIFY
30 REM Program by Kevin Cummings
40 REM **************************************************************
50 DIM P$(82)
60 PRINT 'Which filespec do you wish verified';
70 INPUT F$
80 PRINT | PRINT 'This program will verify about 12 1/2 blocks/minute.'
90 FOR J=1 TO 82 | P$(J)=' ' | NEXT J
100 PRINT | PRINT
110 OPEN 'LP:' FOR OUTPUT AS FILE #2 DOUBLE BUF
120 PRINT #2,' VERIFY for ' ;F$;' ' ;DAT$;' | PRINT #2 | PRINT #2
130 OPEN F$ FOR INPUT AS FILE #1 DOUBLE BUF
140 IF END #1 THEN GO TO 410
150 LINPUT | IF L$='' THEN L=0
160 K=K+1
170 IF K>K0 THEN K0=K
180 C=C+1
190 L=LEN(L$)
200 FOR I=1 TO L
210 C$=SEG$(L$,1,1)
220 A=ASC(C$)
230 IF A>47 THEN IF A<58 GO TO 260
240 IF L=5 THEN GO TO 350
250 IF L=5 THEN PRINT 'CARD #;C; has only one point on it.'
260 NEXT I
270 T%=INT(L/5) | T=L/5
280 IF T%<T THEN IF L>O THEN PRINT 'CARD #;C; has digits.'
290 IF T%>T THEN IF L>0 THEN PRINT #2,'CARD #;C; has digits.'
295 IF T%>T GO TO 350
300 IF L=5 THEN PRINT 'CARD #;C; has only one point on it.'
310 IF L=5 THEN PRINT #2,'CARD #;C; has only one point on it.'
315 IF L=5 GO TO 350
320 IF F>1 GO TO 140
330 PRINT 'CARD #';C
340 PRINT #2,'CARD #';C
350 PRINT L$
360 PRINT #2,L$
370 FOR J=1 TO L | PRINT P$(J); | PRINT #2,P$(J); | NEXT J
380 PRINT | PRINT #2
390 FOR J=1 TO 82 | P$(J)=' ' | NEXT J | F=0
400 GO TO 140
410 PRINT | PRINT 'The largest number of cards in one run is';K0;'.'
420 PRINT #2 | PRINT #2,'The largest number of cards in one run is';K0;
430 PRINT 'Last card processed was CARD #';C
440 PRINT #2,'Last card processed was CARD #';C
450 CLOSE
460 END
PROGRAM PEHEDR

C This program takes raw data in the form of card images and
C creates a file of data with header images.
C
C Program by Kevin Cummings
C
DIMENSION IPD(99),DRUM1(99),DRUM2(99),IPS(99)
DIMENSION VOLT(99),GRAT(99),IDATA(81)
DIMENSION FILLAM(15),NEWFIL(15)
DIMENSION TITLE(30,99)
REAL IPS
LOGICAL*1 TITLE,FILLAM,NEWFIL,ERR,NO
C
C Initialize arrays.
C
10 DO 20 I=1,15
   FILNAM(I)=''
   NEWFIL(I)=''
20 CONTINUE
C
C Set up initial names and number of runs, open in and out files.
C
30 TYPE 40
40 FORMAT(//$Enter filespec of existing data file (DY1:*.*.RAW). '$)
   ACCEPT 50,NCHAR,(FILNAM(J),J=1,NCHAR)
50 FORMAT(Q,14A1)
   FILNAM(NCHAR+1)="000"
   CALL FIlSPCE(FILNAM,'DY1: ','.RAW',ERR)
   IF (ERR.EQ..FALSE.) GO TO 90
60 TYPE 70,FILLAM
70 FORMAT($ Error detected, filespec = '$,15A1,'.*/
I'*$Do you wish to change the filespec (Y)? '$)
   ACCEPT 80,NO
80 FORMAT(A1)
   IF (NO.EQ.'Y') GO TO 30
90 TYPE 100
100 FORMAT($Enter filespec of output data file with headers
1 (DY1:*.*.DAT). '$)
   ACCEPT 50,NCHAR,(NEWFIL(J),J=1,NCHAR)
   NEWFIL(NCHAR+1)="000"
CALL FILSPC(NEWFIL,'DY1:','.DAT',ERR)
IF (ERR.EQ..FALSE.) GO TO 120

110 TYPE 70,NEWFIL
ACCEPT 80,NO
IF (NO.EQ.'Y') GO TO 90

120 TYPE 130
130 FORMAT(/'What is the run number for this set of runs (F4.0)? ')
ACCEPT 140,RUNNUM

140 FORMAT(F4.0)
TYPE 150

150 FORMAT(/'What is the total number of runs in this data file 1 (I3)? ')
ACCEPT 160,ITOTAL

160 FORMAT(I3)
CALL RUNTTL(ITOTAL,RUNNUM,TITLE)
CALL PE2HED(ITOTAL,RUNNUM,IPD,DRUM1,DRUM2,IPS,VOLT,GRAT)
OPEN (UNIT=2,NAMEN=NEWFIL,CARRIAGECONTROL='FORTRAN')

C
C**** * * * * * * * * * * * * * * * * * * * * * * * * * A** A  A* * * * * * * * * * * * * * * *  * * * **
C  Write a new file of data with header information.
C**** * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * A * * A * * * * * * * * * * * * * * * * * * * * * * * * * *

C

DO 520 I=1,ITOTAL
WRITE(3,431) RUNNUM+I*.01,(TITLE(J,I),J=1,29)
TYPE 430,RUNNUM+I*.01,(TITLE(J,I),J=1,29)

430 FORMAT(1H,F6.2,29A1)

431 FORMAT(F6.2,29A1)
WRITE(3,441) IPD(I),DRUM1(I),DRUM2(I),IPS(I),VOLT(I),GRAT(I)
TYPE 440,IPD(I),DRUM1(I),DRUM2(I),IPS(I),VOLT(I),GRAT(I)

440 FORMAT(1H,1I,F9.3,2F10.3,2F10.4)
441 FORMAT(1I,F9.3,2F10.3,2F10.4)
450 READ(2,460,END=530) (IDATA(J),J=1,80)
460 FORMAT(80I1)
470 WRITE(3,481) (IDATA(J),J=1,80)
TYPE 480,(IDATA(J),J=1,80)
480 FORMAT(1H,80I1)
481 FORMAT(80I1)

JDATA=0
DO 490 J=1,10
JDATA=JDATA+IDATA(J)

490 CONTINUE
IF (JDATA) 500,500,450

500 READ(2,501,END=530) DATA

501 FORMAT(F6.2)
IF (DATA) 500,500,510

510 BACKSPACE 2
520 CONTINUE

530 TYPE 540,I,ITOTAL
540 FORMAT(/' End of file. ','I2',' runs written out of ','I2','.')
CLOSE (UNIT=2,DISPOSE='SAVE')
CLOSE (UNIT=3,DISPOSE='SAVE')

C*****************************************************************************
C  Sequence for starting the program with new files.
C*****************************************************************************
C
TYPE 920
920 FORMAT('Do you wish to start with a new "raw" data file (Y)?')
ACCEPT 80,NO
IF (NO.EQ.'Y') GO TO 10
STOP 'PROGRAM PEHEDR'
PROGRAM MCHEDR

C***************************************************************************
C
This program takes raw data in the form of card images and creates a file of data with header images.

C
C Program by Kevin Cummings

C***************************************************************************

DIMENSION IPD(99),NPOINT(99),IPS(99)
DIMENSION VOLT(99),IDATA(81)
DIMENSION FILNAM(15),NEWFIL(15)
DIMENSION TITLE(30,99)
REAL IPS
LOGICAL*1 TITLE,FILNAM,NEWFIL,ERR,NO

C***************************************************************************
C Initialize arrays.
C***************************************************************************

10 DO 20 I=1,15
   FILNAM(I)=''
   NEWFIL(I)=''
20 CONTINUE

C***************************************************************************
C Set up initial names and number of runs, open in and out files.
C***************************************************************************

30 TYPE 40
40 FORMAT(/'Enter filespec of existing data file (DY1:*_.RAW).'
   ACCEPT 50,NCHAR,(FILNAM(J),J=1,NCHAR)
50 FORMAT(Q,14A1)
   FILNAM(NCHAR+1)="000"
   CALL FILSPC(FILNAM,'DY1.*_RAW',ERR)
   IF (ERR.EQ..FALSE.) GO TO 90
60 TYPE 70,FILNAM
70 FORMAT(/'Error detected, filespec = ',15A1,'.'/
   1'$Do you wish to change the filespec (Y)?'
   ACCEPT 80,NO
80 FORMAT(A1)
   IF (NO.EQ.'Y') GO TO 30
90 TYPE 100
100 FORMAT(/'Enter filespec of output data file with headers
   1 (DY1:*_.DAT).'
   ACCEPT 50,NCHAR,(NEWFIL(J),J=1,NCHAR)
   NEWFIL(NCHAR+1)="000"
CALL FILSPC(NEWFIL,'DY1:','DAT',ERR)
IF (ERR.EQ.FALSE.) GO TO 120
110 TYPE 70,NEWFIL
ACCEPT 80,NO
IF (NO.EQ.'Y') GO TO 90
120 TYPE 130
130 FORMAT(/'What is the run number for this set of runs (F4.0)?'

ACCEP 140,RUNNUM
140 FORMAT(F4.0)

Type 150
150 FORMAT(/'What is the total number of runs in this data file 1 (I3)?'

ACCEP 160,ITOTAL
160 FORMAT(I3)

CALL RUNTTL(ITOTAL,RUNNUM,TITLE)
CALL MC2HED(ITOTAL,RUNNUM,IPD,NPOINT,IPS,VOLT)
OPEN (UNIT=2,NAME=FILNAM,TYPE='OLD',READONLY)
OPEN (UNIT=3,NAME=NEWFIL,TYPE='NEW')

C* Write a new file of data with header information.
C* Write a new file of data with header information.

DO 520 I=1,ITOTAL
WRITE(3,431) RUNNUM+I*.01,(TITLE(J,I),J=1,29)
TYPE 430,RUNNUM+I*.01,(TITLE(J,I),J=1,29)
430 FORMAT(1H6,F6.2,29A1)
431 FORMAT(F6.2,29A1)
WRITE(3,441) IPD(I),NPOINT(I),IPS(I),VOLT(I)
TYPE 440,IPD(I),NPOINT(I),IPS(I),VOLT(I)
440 FORMAT(1H1,I4,F10.3,F10.4)
441 FORMAT(I1,'1',I4,F10.3,F10.4)
450 READ(2,460,END=530) (IDATA(J),J=1,80)
460 FORMAT(80I1)
470 WRITE(3,481) (IDATA(J),J=1,80)
TYPE 480,(IDATA(J),J=1,80)
480 FORMAT(1H80I1)
481 FORMAT(80I1)
JDATA=0
DO 490 J=1,10
JDATA=JDATA+IDATA(J)
490 CONTINUE
IF (JDATA) 500,500,450
500 READ(2,501,END=530) DATA
501 FORMAT(F6.2)
IF (DATA) 500,500,510
510 BACKSPACE 2
520 CONTINUE
530 TYPE 540,I,ITOTAL
540 FORMAT(/' End of file. ',I2,' runs written out of ',I2,'. ')
CLOSE (UNIT=2,DISPOSE='SAVE')
CLOSE (UNIT=3,DISPOSE='SAVE')

C******************************************************************************
C Sequence for starting the program with new files.
C******************************************************************************
C
TYPE 920
920 FORMAT(/'$Do you wish to start with a new "raw" data file (Y)?'/)
      ACCEPT 80,NO
      IF (NO.EQ.'Y') GO TO 10
      STOP 'PROGRAM MCHEDR'
SUBROUTINE FILSPC(FILNAM,DEVICE,TYPE,ERR)

C******************************************************************************
C This subroutine takes in a file name and insures a proper filspec for
C the MINC. If a ":" does not exist in FILNAM then DEVICE is
C concatenated on the left. If a ":" does not exist in FILNAM then
C TYPE is concatenated on the right. If ERR is passed back by the
C subroutine as ":.TRUE." then the string FILNAM has been truncated.
C
C Typical values are DEVICE='DY1:" & TYPE=':DAT'.
C NOTE: FILNAM is in ASCIZ and needs a null character as terminator.
C
C Program by Kevin Cummings
C******************************************************************************

LOGICAL*1 FILNAM(15),TEMPFL(15),ERR
DO 10 I=1,15
   TEMPFL(I)=''
10 CONTINUE
ERR=.FALSE.
IDOT=0
CALL INDEX(FILNAM,':',',IDOT)
IF (IDOT.EQ.0) CALL CONCAT(FILNAM,TYPE,TEMPFL,14,ERR)
IF (IDOT.NE.0) CALL SCOPY(FILNAM,TEMPFL,14,ERR)
IDOT=0
CALL INDEX(TEMPFL,':',',IDOT)
IF (IDOT.EQ.0) CALL CONCAT(DEVICE,TEMPFL,FILNAM,14,ERR)
IF (IDOT.NE.0) CALL SCOPY(TEMPFL,FILNAM,14,ERR)
RETURN
SUBROUTINE MC2HED(ITOTAL,RUNNUM,IPD,NPOINT,IPS,VOLT)

C ******************************************************
C This subroutine fills arrays that produce the second header card for
C each individual run from the Big Michelson. ITOTAL is the total
C number of runs (<99) and RUNNUM is the number for that days set
C of runs.
C
C Program by Kevin Cummings
C ******************************************************
DIMENSION IPD(99),NPOINT(99),VOLT(99)
REAL IPS(99)
LOGICAL*1 NO
DO 10 I=1,99
   IPD(I)=0
   NPOINT(I)=0
   IPS(I)=0.0
   VOLT(I)=0.0
10 CONTINUE
20 TYPE 30
30 FORMAT(/' $Enter run number (<1) for second header card (F4.2).ˈ)
ACCEPT 40,RUN
40 FORMAT(F4.2)
IF (RUN) 420,420,100
RUNN=RUNNUM+RUN
210 FORMAT(A1)
220 TYPE 230
230 FORMAT(//' Enter the following data for this run number.ˈ)
TYPE 240
240 FORMAT(/ˈ RUN # IPD NPOINT IPS VOLTˈ)
   1ˈ (12) (15) (F5.1) (F7.3)ˈ)
TYPE 250,RUNN
250 FORMAT(/1H$,F6.2,ˈˈ)
ACCEPT 260,JPD,MPOINT,SIPS,SVOLT
260 FORMAT(I2,I5,F5.1,F7.3)
TYPE 270,RUNN,JPD,MPOINT,SIPS,SVOLT
270 FORMAT(/1H $F6.2,ˈ IPD=(' ,I1,ˈ) NPOINT=(' ,I4,ˈ) IPS=(' ,F5.1,ˈ)
   1ˈ VOLT=(' ,F7.3,ˈ)ˈ)
TYPE 280
280 FORMAT(/ˈ$Is this correct (N)? ˈ)
ACCEPT 210,NO
IF (NO.EQ.'N') GO TO 220
290 J=(RUN+.001)*100
IPD(J)=JPD
NPOINT(J)=MPOINT
IPS(J)=SIPS
VOLT(J)=SVOLT
TYPE 300,RUNN
252
300 FORMAT(//' Please enter an associated run with run ' , F6.2, ' . ' )
320 FORMAT(' Enter the run (e.g. .35); a zero or no entry ends the
1 loop (F4.2). ' )
330 ACCEPT 40,RUN
340 TYPE 350
350 IF (RUN) 420,420,340
360 TYPE 380
370 ACCEPT 360, IPD
380 IF (IPD.EQ.0.0) 440,440,380
390 FORMAT(F7.3)
400 IF (TVOLT.GT.0.0) SVOLT=TVOLT
410 GO TO 290
420 TYPE 430
430 FORMAT(//' Number of unheadered runs appear below. ' )
440 DO 450 I=1,ITOTAL
450 UNHEAD=I/100.
460 IF (IPS(I).EQ.0.0) TYPE 440,UNHEAD
470 FORMAT(1H ,F4.2)
480 CONTINUE
490 FORMAT(//' Do you wish to enter more data (Y)? ' )
500 IF (NO.EQ.'Y') GO TO 20
510 TYPE 490
520 FORMAT(//' Would you like to inspect the arrays (N)? ' )
530 IF (NO.EQ.'N') GO TO 520
540 DO 510 I=1,ITOTAL
550 RUNN=RUNNUM+(I*0.01)
560 TYPE 500 , RUNN, IPD(I), NPOINT(I), IPS(I), VOLT(I)
570 FORMAT(1H ,F6.2, ' ',I1, ' ',I4,F10.3,F10.4)
580 CONTINUE
590 GO TO 460
600 CONTINUE
610 RETURN
SUBROUTINE PE2HED(ITOTAL,RUNNUM,IPD,DRUM1,DRUM2,IPS,VOLT,GRAT)
C
C*****************************************************************************
C This subroutine fills arrays that produce the second header card for
C each individual run from the Perkin Elmer. ITOTAL is the total
C number of runs (>99) and RUNNUM is the number for that days set
C of runs.
C
C Program by Kevin Cummings
C*****************************************************************************
C
DIMENSION IPD(99),DRUM1(99),DRUM2(99),VOLT(99),GRAT(99)
REAL IPS(99)
LOGICAL*1 NO
DO 10 I=1,99
IPD(I)=0
DRUM1(I)=0.0
DRUM2(I)=0.0
IPS(I)=0.0
VOLT(I)=0.0
GRAT(I)=0.0
10 CONTINUE
20 TYPE 30
30 FORMAT(/'$Enter run number (<1) for second header card (F 4.2).'')
ACCEPT 40,RUN
40 FORMAT(F4.2)
RUNN=RUNNUM+RUN
210 FORMAT(A1)
220 TYPE 230
230 FORMAT(/' Enter the following data for this run number.' )
TYPE 240
240 FORMAT(/' RUN # IPD DRUM1 DRUM2 IPS VOLT GRAT' )
1 /' (I2) (F6.3) (F6.3) (F5.1) (F7.3) (F7.2)' )
TYPE 250,RUNN
250 FORMAT(/'HI$F6.2,' )
ACCEPT 260,JPD,SDRUM1,SDRUM2,SIPS,SVOLT,SGRAT
260 FORMAT(I2,2F6.3,F5.1,F7.3,F7.2)
TYPE 270,RUNN,JPD,SDRUM1,SDRUM2,SIPS,SVOLT,SGRAT
270 FORMAT(/'HI$F6.2,' IPD=(' ,I1,' ) DRUM1=(' ,F6.3,' ) DRUM2=(' ,F6.3,
1')/' IPS=(' ,F5.1,' ) VOLT=(' ,F7.3,' ) GRAT#=(' ,F7.2,' )'
TYPE 280
280 FORMAT(/'$Is this correct (N)? ' )
ACCEPT 210,NO
IF (NO.EQ.'N') GO TO 220
290 J=(RUN+.001)*100
IPD(J)=JPD
DRUM1(J)=SDRUM1
DRUM2(J)=SDRUM2
IPS(J)=SIPS
VOLT(J)=SVOLT
GRAT(J)=SGRAT

300 FORMAT(//' Please enter an associated run with run ',F6.2,'.')

310 FORMAT( ' Example: mirror run .01 may be associated with sample
1 runs .11 and .21.')

320 FORMAT( ' Enter the run (e.g. .35); a zero or no entry ends the
1 loop (F4.2).')

330 ACCEPT 40,RUN
IF (RUN) 420,420,340

340 TYPE 350
350 FORMAT( '$IPD=(I1)? ')
ACCEPT 360,JPD

360 TYPE 370
370 FORMAT(I1),SVOLT

380 FORMAT( '$VOLT=(' ,F7.3,')? ')
ACCEPT 390,TV0LT

390 FORMAT(F7.3)
IF (TV0LT.GT.0.0) SV0LT=TV0LT
GO TO 290

420 TYPE 430
430 FORMAT(/' Number of unheaded runs appear below.')
DO 450 I=1,ITOTAL
UNHEAD=I/100.
IF (IPS(I).EQ.0.0) TYPE 440,UNHEAD

440 FORMAT(1H,F4.2)
CONTINUE

460 TYPE 470

470 FORMAT(//' Do you wish to enter more data (Y)? ') Accept 210,NO
IF (NO.EQ.' Y') GO TO 20
TYPE 490

490 FORMAT(//' Would you like to inspect the arrays (N)? ') Accept 210,NO
IF (NO.EQ.' N') GO TO 520
DO 510 I=1,ITOTAL
RUNN=RUNNUM+(I*0.01)
TYPE 500,RUNN,IPD(I),DRUM1(I),DRUM2(I),IPS(I),VOLT(I),GRAT(I)

500 FORMAT(1H,F6.2,' ',I1,F9.3,2F10.3,2F10.4)
CONTINUE
GO TO 460

520 CONTINUE

RETURN
SUBROUTINE RUNITL(ITOTAL,RUNNUM,TITLE)

C*******************************************************************************
C This subroutine fills an array with titles for each run. The total
C number of runs is ITOTAL which must be less than 99. RUNNUM is the
C run number for that day's set of runs. The array TITLE should be
C printed as follows; (TITLE(J,I),J=1,29) where I is the individual
C run. The format is 29A1.
C
C Program by Kevin Cummings
C*******************************************************************************

LOGICAL*1 TITLE(30,95),"TITLE(30),NO
DO 20 I=1,30
  TITLE(I)="'
DO 10 J=1,99
  TITLE(I,J)="'

10 CONTINUE
20 CONTINUE

90 TYPE 100
100 FORMAT(/' Enter a title for a set of runs. ')
110 ACCEPT 100,NCARR, (' TITLE(J), J=1,NCARR)

TYPE 120
120 FORMAT(/' Enter individual runs (e.g., .35) that have this
1 title. ')/' Zero or no entry ends the loop (F4.2). ')
130 TYPE 131
131 FORMAT( 'RUN #')
140 ACCEPT 140, RUN
150 FORMAT(F4.2)
160 IF (RUN) 170,170,150
150 DATA=(-30,-95)@100.
160 TITLE(I,100)=STITLE(I)
GO TO 120

170 TYPE 171
171 FORMAT(/' Numbers of untitled runs appear below. ')
180 IF (TITLE(I,1),EQ.,' ALL.TITLE(2,1),EQ.,') TYPE 190, IUNTITL
160 FORMAT(HE ,F4.2)
190 CONTINUE
195 TYPE 200
200 FORMAT(/' Do you wish to title more runs (Y)? ')
210 ACCEPT 200, Y
210 IF (Y(1:4,1)) GO TO 90.
TYPE 220
220 FORMAT('/$Would you like to inspect the array of titles (N)?')
ACCEPT 210,NO
IF (NO.EQ.'N') GO TO 250
DO 240 I=1,ITOTAL
TYPE 230,RUNNUM+I*,.01,(TITLE(J,I),J=1,29)
230 FORMAT(1H ,F6.2,29A1)
240 CONTINUE
GO TO 195
250 CONTINUE
RETURN
10 REM ##################################################################
20 REM                  FILSRT.BAS
30 REM                    Program by Kevin Cummings
40 REM ##################################################################
50 DISPLAY CLEAR
60 OPEN 'ARYFIL.CAT' AS FILE #1
70 DIM #1,C$(50,2)=14
80 PRINT 'The following arrays have been catalogued:' | PRINT
90 FOR I=0 TO 50 STEP 3
100 IF C$(I,0)='' GO TO 170
110 PRINT C$(I,0),
120 IF C$(I+1,0)='' GO TO 170
130 PRINT C$(I+1,0),
140 IF C$(I+2,0)='' GO TO 170
150 PRINT C$(I+2,0)
160 NEXT I
165 PRINT
170 PRINT 'What is the name of the virtual array (DY1:*.VRT) you wish'
180 PRINT 'to work with'; | LINPUT A$
190 IF POS(A$, ',',1)=0 THEN A$='DY1:'+A$
200 IF POS(A$, '.',1)=0 THEN A$=A$+'.VRT'
210 FOR I=0 TO 50
220 IF C$(I,0)=A$ THEN D1$=C$(I,1) | D2$=C$(I,2)
225 IF C$(I,0)=A$ THEN D3$=STR$(VAL(D1$)+1) | GO TO 245
230 NEXT I
240 GO TO 300
245 PRINT
250 PRINT 'File '+A$+' is catalogued with dimensions of '+D3$+' runs'
260 PRINT 'with a maximum of '+D2$+' cards in each run.'
270 PRINT 'Is this the correct file (Y)'; | INPUT Y$
280 IF Y$='Y' GO TO 450
290 GO TO 80
300 PRINT | PRINT 'File '+A$+' is not catalogued.'
310 PRINT 'Do you wish to catalogue a file with this name (Y)';
315 INPUT Y$
320 IF Y$='Y' GO TO 340
330 GO TO 80
340 FOR I=0 TO 50
350 IF C$(I,0)='' GO TO 380
360 NEXT I
370 PRINT 'Catalogue is full, please create a new catalogue.'
375 GO TO 1450
380 PRINT | PRINT 'What is the total number of runs in this new array';
390 INPUT D1 | D1=D1-1
400 PRINT 'What is the maximum number of cards that a run may have
410 PRINT '(total number of run cards +2, for header cards.)';
420 INPUT D2
430 C$(I,0)=A$ | D1$=STR$(D1) | D2$=STR$(D2)
440 C$(I,1)=D1$ | D3$=STR$(VAL(D1$)+1) | C$(I,2)=D2$
450 CLOSE #1 | U=CTRLC
460 OPEN 'DIMFIL.BAS' FOR OUTPUT AS FILE #2
470 PRINT #2,'540 COMMON AS,D1$ ,D2$,D3$'
480 PRINT #2,'550 OPEN ""+AS+"" AS FILE #3'
490 PRINT #2,'560 DIM #2,F$("+D1$+","+D2$+")=80'
500 PRINT #2,'570 OVERLAY "FILEST.BAS" LINE 540'
510 CLOSE #2
520 COMMON AS,D1$,D2$,D3$
530 CHAIN 'DIMFIL.BAS' LINE 540
540 |
550 |
560 |
570 |
580 KILL 'DIMFIL.BAS'
590 PRINT | PRINT | PRINT ' Menu for virtual arrays'
600 PRINT ' 1=> End work with this virtual array.'
610 PRINT ' 2=> Write from a sequential file to the virtual array.'
620 PRINT ' 3=> Write from the virtual array to a sequential file.'
630 PRINT ' 4=> Display and/or modify the virtual array.'
640 PRINT | PRINT 'Which function do you wish?'; | INPUT S
650 IF S>0 THEN IF S<5 GO TO 670
660 GO TO 540
670 GO TO 1450,680,690,770
680 PRINT
690 PRINT 'What is the name (DY1:*.DAT) of the sequential file?'
700 INPUT SS
710 IF POS(SS,$' $,1)=0 THEN SS='DY1:4S$
720 PRINT SS AS FILE #4 DOUBLE BUF
730 ON SS-1 GO TO 740,840
740 FOR I=0 TO VAL(D1$)
750 FOR J=0 TO VAL(D2$)
760 IF E$ THEN GO TO 950
770 LINPUT #4,LS
780 F$(I,J)=LS
790 IF SEC$(LS,1,10)="0000000000" GO TO 810
800 NEXT J
810 NEXT I
820 PRINT | PRINT I+1;'runs out of '+F$+" were placed in the array.'
830 CLOSE #4 | GO TO 520
840 PRINT | PRINT 'Please enter the run numbers (<1) in order.'
850 PRINT 'A zero will end the loop.'
860 PRINT "RUN #"; | INPUT P | IF P<6 GO TO 951
870 R$=R$106,2-1 | IF P<VAL(11$) GO TO 900
880 PRINT "The array '+AS+ does not have a run';R$+1;'. The largest'
890 PRINT 'run number is';VAL(P$)/100;'' | PRINT | GO TO 760
900 FOR J=0 TO VAL(E$)
910 IF SEC$(F$(I$),1,10)="0000000000" GO TO 840
920 IF F$(I$,J)="" GO TO 770
930 PRINT #4,F$(I$,J)
940 NEXT J
950 GO TO 960
951 PRINT 'To add a line of text to the file type the line at the "?".'
952 PRINT 'A null line will close the file.'
953 LINPUT L$ | IF LEN(L$)=0 GO TO 960
954 PRINT #4,L$ | GO TO 840
956 CLOSE #4 | GO TO 590
970 PRINT | PRINT ' The modifying commands are:'
980 PRINT ' C => Display the list of commands.'
990 PRINT ' D => Display an element of array '+A$+'("RETURN" also).'
1000 PRINT ' DR => Display a run in array '+A$+'.'
1010 PRINT ' M => Modify an element of array '+A$+'.'
1020 PRINT ' " " under a character makes no change.'
1030 PRINT ' "" under a character deletes it.'
1040 PRINT ' "" replaces a character with a space.'
1050 PRINT ' "@" inserts characters between two @s, in front of'
1055 PRINT ' first @.'
1060 PRINT ' Any other character replaces the one above it.'
1070 PRINT ' Q => Quit modifying and return to main menu.'
1080 PRINT ' R => Replace the entire element of array '+A$+'.'
1090 PRINT | PRINT 'Command'; | INPUT C $
1100 IF C$='C' GO TO 970
1110 IF C$='Q' GO TO 590
1120 IF C$='DR' THEN PRINT 'What is the run number (<1)'; | INPUT R
1130 IF C$='DR' THEN PRINT ' E=0'; | GO TO 1150
1130 PRINT 'What is the run number (<1) and element (run,element):'
1140 INPUT R,E | PRINT
1150 R%=R*100.2-1 | IF R%>=0 THEN IF R%<=VAL(D1$) GO TO 1180
1160 PRINT 'The array '+A$+' does not have a run';R%+1';. The largest'
1170 PRINT 'run number is';VAL(D3$)/100;';.' | PRINT | GO TO 1090
1180 E%=E | IF E%>=0 THEN IF E%<=VAL(D2$) GO TO 1210
1190 PRINT 'The array '+A$+' does not have element';E%:' The largest'
1200 PRINT 'element number is '+D2$+' (0 included).'; | PRINT
1205 GO TO 1090
1210 IF C$='R' THEN PRINT ' ';F$(R%,E%) | LINPUT F$(R%,E%) | GO TO 1090
1220 IF C$='M' GO TO 1300
1230 IF C$='DR' GO TO 1250
1240 PRINT F$(R%,E%) | GO TO 1090
1250 FOR J=0 TO VAL(D2$)
1260 IF SEG$(F$(R%,J),1,10)='0000000000' GO TO 1290
1270 PRINT F$(R%,J)
1280 NEXT J
1290 PRINT | GO TO 1090
1300 PRINT ' ';F$(R%,E%) | LINPUT M$
1310 F=LEN(F$(R%,E%)) | F$=' ' | K=0 | F9=0
1320 M=LEN(M$)
1330 IF F$='M THEN M$=M$+'' | GO TO 1320
1340 FOR L=1 TO M
1350 K=K+1
1360 IF SEG$(M$,K,K)=' ' THEN F$=F$+SEG$(F$(R%,E%),L,L) | GO TO 1430
1370 IF SEG$(M$,K,K)='}' GO TO 1430
1380 IF SEG$(M$,K,K)='~' THEN F$=F$+'' GO TO 1430
1390 IF SEG$(M$,K,K)='@' THEN K=K+1 | F9=1
1400 IF SEG$(M$,K,K)='@' THEN F9=0 | GO TO 1430
1410 IF F9=1 THEN F$=F$+SEG$(M$,K,K) | K=K+1 | GO TO 1400
1420 F$=F$+SEG$(M$,K,K)
1430 NEXT L
1440 F$(R%,E%)=F$ | PRINT F$ | GO TO 1090
1450 CLOSE
1460 END
APPENDIX D

COMPUTER PROGRAMS WRITTEN FOR DATA ANALYSIS ON THE AMDAHL 470 COMPUTER

This appendix contains the programs EDDYCRNT, PERKELMR, FOURTRNS, SORTFREQ, KRAMKROG and all the subroutines necessary for these programs. All the programs were written in IBM H-extended FORTRAN and were run on the Amdhal 470 computer on the OSU campus. A discussion of the operation of these programs is given in chapter II and V.

261
**Program EDDYCRNT**

This program calculates the optical functions for both the effective medium approximation and the Maxwell Garnett theory in composite systems. The program treats the depolarisation factor of the particles as a parameter equal to the percolation threshold of the particular class of the composite. The program includes the effects of magnetic dipole absorption.

```plaintext
DIMENSION IDENT(15),JDENT(15),LDENT(15),RUN(4),RUD(4)
DIMENSION V(550),VLOG(550),ISTR(3),X9(50),Y9(50),DY9(50),A0(50)
DIMENSION SIGMA(550),EP1(550),DATA(550),A1(50),A2(50),A3(50)
DIMENSION X8(50),Y8(50),DY8(50),A5(50),A6(50),A7(50),A8(50)
REAL IDENT,JDENT,LDENT
REAL M1EMA,M2EMA,M1MCT,M2MCT,M1MET,M2MET
DOUBLE PRECISION X9,Y9,DY9,A0,A1,A2,A3,X8,Y8,DY8,A5,A6,A7,A8
COMPLEX*16 UNIT,CPX,DCMPLX,CFREQ,EPSA,EPSC,EPSMET,EPSINS,
*A,AKA,MAGPOL,MUMET,MUMG1,M1,M2,MUMA,MUMGT,CN1,CN2,
*CD81,COSH,PSED,EPSE,
*A,B,C,E1,E2,CD8,EPSEMA,EPSEMGT,CNDXEM,REF,DCONJG,CNDXMG
LOGICAL*1 CO
DATA CO,'/','/
DATA ISTR,'EMA0','MGTO',' /
1 FORMAT(15A4)
2 FORMAT(1H1)
3 FORMAT (1X,
* F8.2,2X,
* F9.1,1X,
* F8.5,2X,
* F8.2,2X,
* F8.4,2X,
* F8.1,2X,
* F8.2,2X,
* F8.5,2X,
* F9.2,1X,
* F9.2,1X,
* F9.2,1X,
* F8.2,2X,
* F8.4)
4 FORMAT (1X,'FREQUENCY ',
* ' ALPHA ',
* ' REFLECTAN',
* ' EPSILON1 ',
```
**EPSILON2**
* CONDUCT *
* MU1 *
* MU2 *
* EPSILON1 *
* EPSILON2 *
* CONDUCT *
* MU1 *
* MU2 *

*1X)
5 FORMAT(1X,'WP=' ,F6.0,1X,'WO=' ,F6.1,1X,'WR=' ,F6.1,1X,'EC=' ,F6.2/
*1X,
* 'WL=' ,F6.1,1X,'W2=' ,F6.1,1X,'G=' ,F6.1,
*1X,'EB=' ,F6.2)
6 FORMAT (1X,16X,'EFFECTIVE MEDIUM',50X,'METAL ITSELF')
7 FORMAT (1X,16X,'MAXWELL GARNET',50X,'METAL ITSELF')
8 FORMAT(1X,'DC CONDUCTIVITY=' ,F10.0,' OHM-CM-1')
9 FORMAT (15)
10 FORMAT (1X,'RESISTIVITY=' ,F10.5,' MICROOHM-CM')
11 FORMAT (1X,'FF=' ,F6.4,'2X,'DEPOLF=' ,
*F6.4,2X,'R (A)=' ,F7.0)
12 FORMAT(11,1012,12)
13 FORMAT (1X,'MAX VALUE OF IMAG(KA) EXCEEDED.')
14 FORMAT (1X,F9.2,2X,15A4)
23 FORMAT (8F10.0)
24 FORMAT (F6.0,15A4)
25 FORMAT (10F10.2)
160 FORMAT(3X,'FREQ',7X,'E1',8X,'E2',8X,'S1',6X,'ALPHA',6X,'REFL')
161 FORMAT(3X,'FREQ',7X,'N',9X,'K',8X,'LOSS',6X,'SUMS',6X,'SUMA',
*6X,'SUML')
165 FORMAT('/**')
410 FORMAT(2A4)
411 FORMAT(1X,3(A4,1X)/)

C************************************************************************************************************************
C INPUT HEADERS FOR THE TWO CALCULATIONS (EMA AND MGT).
C************************************************************************************************************************
C
READ(5,1) (JDENT(K),K=1,15)
READ(5,1) (LDENT(K),K=1,15)
UNIT=DCMPLX(1.0D0,0.0D0)
CPX=DCMPLX(0.0D0,1.0D0)
PI=3.14159
CC=3.0E+10

C************************************************************************************************************************
C READ PLOTTING AND PUNCHING PARAMETERS
C Y AXIS IS 10 INCHES LONG. LOGS ARE TO BASE 10.
CARD #3  I FORMAT
C  1:  1=> LINEAR PLOTS; 0=> NO PLOTS
C  2-3: 1=> LOG PLOTS; 0=> NO PLOTS
C  4-5: 1=> PLOT CONDUCTIVITY; 0=> NO PLOT
C  6-7: 1=> PLOT REAL DIELECTRIC FUNCTION; 0=> NO PLOT;
C  8-9: 1=> PLOT REFLECTANCE; 0=> NO PLOT
C  10-11: 1=> PLOTS HAVE LINES AND SYMBOLS.; 0=> LINES ONLY
C -1=> SYMBOLS ONLY.
C  12-13:  A NUMBER WHICH SPECIFIES THE SYMBOL (3=+)
C  14-15: 1=> PUNCH EMA DATA IN A TSO FILE; 0=> NO PUNCH
C  16-17: 1=> PUNCH MGT DATA IN A TSO FILE; 0=> NO PUNCH
C  18-19: 1=> SWITCH HOST AND GRAIN IN CALCULATION

CARD #4  F FORMAT
C  1-10: LENGTH OF X-AXIS
C  11-20: STARTING WAVE NUMBER FOR X-AXIS
C  21-30: ENDING WAVE NUMBER FOR X-AXIS
C  31-40: STARTING WAVE NUMBER FOR LOG X-AXIS
C  42-50: ENDING WAVE NUMBER FOR LOG X-AXIS

CARD #5  F FORMAT
C  1-10: STARTING NUMBER FOR CONDUCTIVITY ON Y-AXIS
C  11-20: ENDING NUMBER FOR CONDUCTIVITY
C  21-30: STARTING NUMBER FOR DIELECTRIC FUNCTION ON Y-AXIS
C  31-40: ENDING NUMBER FOR DIELECTRIC FUNCTION
C  41-50: STARTING NUMBER FOR REFLECTANCE ON Y-AXIS
C  51-60: ENDING NUMBER FOR REFLECTANCE

CARD #6  MIXED FORMAT
C  1-6: IDENTIFYING RUN NUMBER
C  7-35: HEADER FOR CALCULATION

READ(5,12)LINEAR,LOG,ISIG,IEPS,IDATA,JLN,LSY,IEMA,IMGTL,IFLAG
READ(5,23)XAXIS,VLO,VHI,VLOGL,VLOGH
READ(5,23)SIGLO,SIGHI,EPSL,EPSH,DATALO,DATAHI
DELS=(SIGHI-SIGLO)/10.
DELEPS=(EPSHI-EPSL)/10.
DELAT=(DATAHI-DATALO)/10.
DELLOG=(VLOGH-VLOGL)/XAXIS
DELLIN=(VHI-VLO)/XAXIS
NSETS=1000
DO 301 NS=1,NSETS

READ PARAMETERS FOR THE DIELECTRIC FUNCTION MODEL
C F= FILLING FRACTION OF THE SAMPLE.
C G= DEPOLARIZATION FACTOR FOR PARTICLES (SPHERES=.33333).
C AR= THE RADIUS OF PARTICLES IN ANGSTROMS.
C THE FOLLOWING PERTAIN TO THE METAL
C ECORE= OPTICAL DIELECTRIC CONSTANT FOR THE METAL.
C WP= PLASMA FREQUENCY FOR THE METAL (UNSCREENED).
C W0= CENTER OF THE CONDUCTIVITY PEAK ( =0 FOR DRUDE).
C WR= 1/TAU WHERE TAU IS THE RELAXATION TIME IN CM.
C THE FOLLOWING PERTAIN TO THE HOST MATERIAL.
C EBCORE= OPTICAL DIELECTRIC CONSTANT OF THE HOST MATERIAL.
C WL=SQR(EBCORE*(W0**2-W2**2)) WHERE W0 IS THE 2ND PT. WHERE E1 IS 0
C W2=Wt; THE FREQUENCY AT WHICH E1(W) GOES THROUGH 0 (POLE).
C GAMMA=FULL WIDTH AT HALF MAX FOR INSULATOR MODE
C WRITE THESE.
C******************************************************************************

CWRITE( 6,2)
CALL GOPARM (LEN,ISTR(3))
IF (LEN.NE.4) GO TO 302
IF (IEMA.EQ.1) WRITE(9,410) ISTR(1),ISTR(3)
IF (IMGT.EQ.1) WRITE(10,410) ISTR(2),ISTR(3)
WRITE(6,411) ISTR
READ(5,24) RUN(1),(IDENT(K),K=1,15)
WRITE(6,14) RUN(1),(IDENT(K),K=1,15)
IF (RUN(1).LT. 0.) GOTO 302
IF (IEMA.EQ.1) WRITE(9,14) RUN(1),(IDENT(K),K=1,15)
IF (IMGT.EQ.1) WRITE(10,14) RUN(1),(IDENT(K),K=1,15)
READ(5,23) F,G,AR
WRITE(6,11) F,G,AR
IF (IEMA.EQ.1) WRITE(9,11) F,G,AR
IF (IMGT.EQ.1) WRITE(10,11) F,G,AR
RUN(2)=F
RUN(3)=G
RUN(4)=AR
RADIUS=AR*1.E-8
READ(5,23) ECORE,WP,W0,WR,EBCORE,WL,W2,GAMMA
WRITE(6,5) WP,W0,WR,ECORE,WL,W2,GAMMA,EBCORE
IF (IEMA.EQ.1) WRITE(9,5) WP,W0,WR,ECORE,WL,W2,GAMMA,EBCORE
IF (IMGT.EQ.1) WRITE(10,5) WP,W0,WR,ECORE,WL,W2,GAMMA,EBCORE
IF (WR.EQ.0.0) GO TO 30
SIG0=(WP**2)/(60.*WR)
RHO=1.66/SIG0
WRITE(6,8) SIG0
WRITE(6,10) RHO
30 CONTINUE
IF (IFLAG.EQ.1) WRITE(6,1021)
1021 FORMAT(’F=1-F CALCULATION’)
WX=WP
IF (IFLAG.EQ.1) WX=WL
CALL CUBFIT(NCUBE,0.,X9,Y9,DY9,A0,A1,A2,A3,WX)
CALL CUBEIT(NCUBE,0.,X8,Y8,DY8,A5,A6,A7,A8)
RUD(1)=WP/1000.
RUD(2)=WR/100.
RUD(3)=ECORE
RUD(4)=EBCORE

C*********************************************************************
C CALCULATE THE EMA ABSORPTION.
C*********************************************************************
C
WRITE(6,2)
WRITE(6,4)
WRITE(6,6)
N=250
XN=N
IF (IEMA.EQ.1) WRITE(9,160)
IF (IEMA.EQ.1) WRITE(9,161)
DO 101 I=1,N
AI=I
AI=AI/XN
FREQ=VHI*AI
CFREQ=FREQ*UNIT
IF (I.EQ.1) GO TO 1000
BI=I-1
BI=BI/XN
FREQ0=VHI*BI
1000 CONTINUE
C
C*********************************************************************
C DIELECTRIC FUNCTION EQUATION FOR EPSMET AND EPSINS.
C*********************************************************************
C
EPSD=(0.D0,0.D0)
EPSA=(0.D0,0.D0)
EPSINS=(0.D0,0.D0)
IF (IFLAG.EQ.1) EPSA=EBCORE*UNIT
IF (IFLAG.EQ.1) GO TO 1100
CALL CBAND(FREQ,CAND,X8,Y8,DY8,A5,A6,A7,A8)
EPSA=CAND*CPX
1100 EPS=(W P**2)*UNIT/((W0*UNIT)**2-CPFX**2-CFREQ*WR)
IF (IFLAG.EQ.1) GO TO 1101
CALL DBAND(FREQ,BAND,X9,Y9,DY9,A0,A1,A2,A3)
EPSD=BAND*UNIT
1101 EPSMET=EPSA+EPSD+EPS
E1MET=DR EAL(EPSMET)
E2MET=DI MAG(EPSMET)
SIMET=FR EQ*E2MET/60.
IF (IFLAG.EQ.1) CALL CBAND(FREQ,CAND,X8,Y8,DY8,A5,A6,A7,A8)
IF (IFLAG.EQ.1) CALL DBAND(FREQ,BAND,X9,Y9,DY9,A0,A1,A2,A3)
IF (IFLAG.EQ.1) EPSINS=CAND*CPX
IF (IFLAG.EQ.1) EPSINS=EPSINS+BAND*UNIT
IF (IFLAG.EQ.1) GO TO 52
EPSINS=EBCORE*UNIT
IW L=WL
IF (IWL) 51,51,52
52 CONTINUE
EPSC=(WL**2)*UNIT/((W2*UNIT)**2-CFREQ**2-CPX*CFREQ*GAMMA)
EPSINS=EPSINS+EPSC
51 CONTINUE
C
********************************************************************
C 'PERMEABILITY' FUNCTION EQUATION FOR MUMET AND MUINS.
C********************************************************************
C IF (RADIUS.EQ.0.0) MUMET=UNIT
IF (RADIUS.EQ.0.0) GO TO 80
AKA=(2.D0)*PI*CFREQ*CDSQRT(EPSMET)*RADIUS
C=CDCOS(AKA)/CDCSIN(AKA)
MAGPOL=(0.375D0/PI)*(3.0D0/(AKA)**2-(3.0D0/AKA)*C-1.0D0)
MUMET=(UNIT+(PI/0.375D0)*MAGPOL)/(UNIT-(PI/0.75D0)*MAGPOL)
80 CONTINUE
M1MET=DREAL(MUMET)
M2MET=DIMAG(MUMET)
MUINS=UNIT
C
********************************************************************
C CALCULATE EMA DIELECTRIC FUNCTION.
C********************************************************************
C
A=(1.—G)*UNIT
B=-EPSMET*(F-G)-EPSINS*(1.-F-G)
C=-G*EPSMET*EPSINS
E1=(-B+CDSQRT(B*B-4.*A*C))/(2.*A)
E2=(-B—CDSQRT(B*B-4.*A*C))/(2.*A)
IF (DIMAG(E1) .GE. 0.0) EPSEMA=E1
IF (DIMAG(E2) .GE. 0.0) EPSEMA=E2
C
********************************************************************
C CALCULATE EMA PERMEABILITY.
C********************************************************************
C
A=(1.—G)*UNIT
B=-MUMET*(F-G)-MUINS*(1.-F-G)
C=-G*MUMET*MUINS
M1=(-B+CDSQRT(B*B-4.*A*C))/(2.*A)
M2=(-B—CDSQRT(B*B-4.*A*C))/(2.*A)
IF (DIMAG(M2) .GE. 0.0) MUEMA=M2
IF (DIMAG(M1) .GE. 0.0) MUEMA=M1
C
********************************************************************
C CALCULATE OPTICAL CONSTANTS FOR EMA.
C********************************************************************
C
CN1=CDSQRT(EPSEMA*MUEMA)
C N 2 = - C D S Q R T ( E P S E M A * M U E M A )
IF ( D I M A G ( C N 1 ) . G E . 0 . 0 ) C N D X E M = C N 1
IF ( D I M A G ( C N 2 ) . G E . 0 . 0 ) C N D X E M = C N 2
R E F = ( U N I T - C N D X E M / M U E M A ) / ( U N I T + C N D X E M / M U E M A )
R E F L E M = R E F * D C O N J G ( R E F )
E 1 E M A = D R E A L ( E P S E M A )
E 2 E M A = D I M A G ( E P S E M A )
M 1 E M A = D R E A L ( M U E M A )
M 2 E M A = D I M A G ( M U E M A )
S 1 E M A = F R E Q * E 2 E M A / 6 0 .
A L O S S = E 2 E M A / ( E 1 E M A * * 2 + E 2 E M A * * 2 )
E M A N = ( 1 2 * P I * S 1 E M A ) / ( 1 0 0 0 * . * A L P E M A )
E M A K = ( 1 0 0 0 0 . * A L P E M A ) / ( 4 * P I * F R E Q )
I F ( I . E Q . 1 ) G O T O 1 0 0 1
Q = Q + 3 0 . * ( S 1 E M A + P 1 ) * ( F R E Q - F R E Q 0 )
Q 1 = Q 1 + . 5 * ( A L O S S + B L O S S ) * F R E Q * ( F R E Q - F R E Q 0 )
Q 2 = Q 2 + . 5 * ( A L P E M A + B L P ) * ( F R E Q - F R E Q 0 )
1 0 0 1 P 1 = S 1 E M A
B L O S S = A L O S S
B L P = A L P E M A
I F ( I . E Q . 1 ) G O T O 1 0 0 2
S U M M = Q * 1 7 . 1 * ( 7 . 1 E - 1 2 )
S U M S O L = Q 1 * 1 7 . 1 * ( 7 . 1 E - 1 2 )
S U M L A P = Q 2 * 1 7 . 1 * ( 1 . 1 4 E - 8 )
1 0 0 2 C O N T I N U E
* E I M E T , E 2 M E T , S 1 M E T , M 1 M E T , M 2 M E T
I F ( I E M A . E Q . 1 ) W R I T E ( 9 , 1 5 0 ) F R E Q , C O , E 1 E M A , C O , E 2 E M A , C O , S 1 E M A , C O ,
* A L P E M A , C O , R E F L E M
V ( I ) = F R E Q
V L O G ( I ) = A L O G I 0 ( F R E Q )
S I G M A ( I ) = S 1 E M A
E P 1 ( I ) = E 1 E M A
D A T A ( I ) = A L P E M A
D A T A ( I ) = R E F L E M
C
C******************************************************************************
C DATA MAY BE CHOSEN AS ANY OF THE CALCULATED OPTICAL FUNCTIONS
C******************************************************************************
C
1 0 1 C O N T I N U E
I F ( I E M A . E Q . 1 ) W R I T E ( 9 , 1 6 5 )
W R I T E ( 6 , 4 )
W R I T E ( 6 , 6 )
C
C******************************************************************************
C PLOT DATA AS DESIRED.
C******************************************************************************
C
111 CONTINUE
   IF(LINEAR) 139,139,130
130 IF(ISIG) 133,133,131
131 CONTINUE
   CALL IRPLOT(SIGMA,SIGLO,DELS,V,VLO,DELLIN,XAXIS,N,
      * 'SIGMA (OHM-CM)-1',16,'FREQUENCY (CM-1)',16,JLN,LSY,
      *RUN,4,IDENT,RUD,4,JDENT,1)
133 IF (IEPS) 136,136,134
134 CONTINUE
   CALL IRPLOT(EP1,EPSLO,DELEPS,V,VLO,DELLIN,XAXIS,N,
      * 'EPSILON 1',9,'FREQUENCY (CM-1)',16,JLN,LSY,
      *RUN,4,IDENT,RUD,4,JDENT,1)
136 IF(IDATA) 139,139,137
137 CONTINUE
   CALL IRPLOT(DATA,DATALO,DELDAT,V,VLO,DELLIN,XAXIS,N,
      * ' ',1,'FREQUENCY (CM-1)',16,JLN,LSY,
      *RUN,4,IDENT,RUD,4,JDENT,1)
139 IF(LOG)200,200,140
140 IF(ISIG)143,143,141
141 CONTINUE
   CALL IRPLOT(SIGMA,SIGLO,DELS,VLOG,VLOGLO,DELLIN,XAXIS,N,
      * 'SIGMA (OHM-CM)-1',16,'LOG10 FREQUENCY',15,JLN,LSY,
      *RUN,4,IDENT,RUD,4,JDENT,2)
143 IF (IEPS)146,146,144
144 CONTINUE
   CALL IRPLOT(EP1,EPSLO,DELEPS,VLOG,VLOGLO,DELLIN,XAXIS,N,
      * 'EPSILON 1',9,'LOG10 FREQUENCY',15,JLN,LSY,
      *RUN,4,IDENT,RUD,4,JDENT,2)
146 IF(IDATA)200,200,147
147 CONTINUE
   CALL IRPLOT(DATA,DATALO,DELDAT,VLOG,VLOGLO,DELLIN,XAXIS,N,
      * ' ',1,'LOG10 FREQUENCY',15,JLN,LSY,
      *RUN,4,IDENT,RUD,4,JDENT,2)
200 CONTINUE
C******************************************************************************
C  CALCULATE THE MGT ABSORPTION.
C******************************************************************************
C
WRITE (6,2)
WRITE (6,7)
WRITE (6,4)
N=250
IF (IMGT.EQ.1) WRITE(10,160)
IF (IMGT.EQ.1) WRITE(10,161)
DO 201 I=1,N
   AI=I
   AI=AI/XN
FREQ=VHI*AI
CFREQ=CFREQ*UNIT
IF (I.EQ.1) GO TO 1003
BI=I-1
BI=BI/XN
FREQO=VHI*BI
1003 CONTINUE
C
********************************************************************************
C DIELECTRIC FUNCTION EQUATION FOR EPSMET AND EPSINS.
********************************************************************************
C
EPSD=(0.D0,0.D0)
EPSA=(0.D0,0.D0)
EPSINS=(0.D0,0.D0)
IF (IFLAG.EQ.1) EPSA=ECORE*UNIT
IF (IFLAG.EQ.1) GO TO 1102
CALL CBAND(FREQ,CAND,X8,Y8,DY8,A5,A6,A7,A8)
EPSA=CAND*CPX
1102 EPSE=(WP**2)*UNIT/((W0*UNIT)**2-CFREQ**2-CPX*CFREQ*WR)
IF (IFLAG.EQ.1) GO TO 1104
CALL DBAND(FREQ,BAND,X9,Y9,DY9,A0,A1,A2,A3)
EPSD=BAND*UNIT
1104 EPSMET=EPSA+EPSD+EPSE
E1MET=DREAL(EPSMET)
E2MET=DIMAG(EPSMET)
S1MET=FREQ*E2MET/60.
IF (IFLAG.EQ.1) CALL CBAND(FREQ,CAND,X8,Y8,DY8,A5,A6,A7,A8)
IF (IFLAG.EQ.1) CALL DBAND(FREQ,BAND,X9,Y9,DY9,A0,A1,A2,A3)
IF (IFLAG.EQ.1) EPSINS=CAND*CPX
IF (IFLAG.EQ.1) EPSINS=EPSINS+BAND*UNIT
IF (IFLAG.EQ.1) EPSINS=EPSINS+BAND*UNIT
IWL=WL
IF (IWL) 151,151,152
152 CONTINUE
EPSC=(WL**2)*UNIT/((W2*UNIT)**2-CFREQ**2-CPX*CFREQ*GAMMA)
EPSINS=EPSINS+EPSC
151 CONTINUE
RUD(4)=EPSINS
C
********************************************************************************
C 'PERMEABILITY' FUNCTION EQUATION FOR MUMET AND MUISN.
********************************************************************************
C
IF (RADIUS.EQ.0.0) MUMET=UNIT
IF (RADIUS.EQ.0.0) GO TO 180
AKA=(2.D0)*PI*CFREQ*CDSQRT(EPSMET)*RADIUS
C=CDCOS(AKA)/CDOS(AKA)
MAGPOL=(0.375D0/PI)*(3.0D0/(AKA)**2-(3.0D0/AKA)**2-(C-1.0D0)
MUMET = \( (UNIT+ (\pi /0.375D0) \times MAGPOL) / (UNIT- (\pi /0.75D0) \times MAGPOL) \)

180 CONTINUE
M1MET = DREAL (MUMET)
M2MET = DIMAG (MUMET)
MUINS = UNIT

C*********************************************************************
C CALCULATE MGT DIELECTRIC FUNCTION.
C*********************************************************************

EPSMGT = EPSINS + EPSINS \times F \times (EPSMET - EPSINS) / 
          \left[ (1.-F) \times G \times EPSMET + (1.-G+F\times G) \times EPSINS \right]

C*********************************************************************
C CALCULATE MGT PERMEABILITY.
C*********************************************************************

MUMGT = MUINS + MUINS \times F \times (MUMET - MUINS) / 
          \left[ (1.-F) \times G \times MUMET + (1.-G+F\times G) \times MUINS \right]

C*********************************************************************
C CALCULATE OPTICAL CONSTANTS FOR MGT.
C*********************************************************************

CN1 = CDSQRT (EPSMGT \times MUMGT)
CN2 = -CDSQRT (EPSMGT \times MUMGT)
IF (DIMAG (CN1) \geq 0.0) CNDXMG = CN1
IF (DIMAG (CN2) \geq 0.0) CNDXMG = CN2
REF = (UNIT - CNDXMG/MUMGT) / (UNIT + CNDXMG/MUMGT)
REFLMG = REF \times DCONJG (REF)
E1MGT = DREAL (EPSMGT)
E2MGT = DIMAG (EPSMGT)
M1MGT = DREAL (MUMGT)
M2MGT = DIMAG (MUMGT)

SMGT = FREQ \times E2MGT / 60.
ALPMGT = 4. \times PI \times FREQ \times DIMAG (CNDXMG)
ALOSSM = E2MGT / (E1MGT \times 2 + E2MGT \times 2)
MCTK = (12 \times PI \times SMGT) / (10000. \times ALPMGT)
MGTK = (10000. \times ALPMGT) / (4 \times PI \times FREQ)

IF (I.EQ.1) GO TO 1004
Q1M = QM + 30. \times (S1MGT + P1M) \times (FREQ - FREQ0)
Q1M = Q1M + 5. \times (ALOSSM + BLOSSM) \times FREQ \times (FREQ - FREQ0)
Q2M = Q2M + 5. \times (ALPMGT + BLM) \times (FREQ - FREQ0)

1004 P1M = SMGT
BLOSSM = ALOSSM
BLPM = ALPMGT
IF (I.EQ.1) GO TO 1005
SUM = QM * 17.1 * (7.1E-12)
SUMLOS = Q1M * 17.1 * (7.1E-12)
SUMALP = Q2M * 17.1 * (1.14E-8)
CONTINUE
WRITE(6,3) FREQ,ALPMGT,REFLMG,E1MGT,E2MGT,S1MGT,M1MGT,M2MGT,
* E1MET,E2MET,S1MET,M1MET,M2MET
IF (IMGT.EQ.1) WRITE(10,150) FREQ,CO,E1MGT,CO,E2MGT,CO,S1MGT,CO,
*ALPMGT,CO,REFLMG
IF (IMGT.EQ.1) WRITE(10,155) FREQ,CO,MGTN,CO.MGTK,CO,ALOSSM,CO,
*SUM,CO,SHMLO,CO,SUMLAP
V(I)=FREQ
VLOG(I)=ALOG10(FREQ)
SIGMA(I)=S1MGT
EP1(I)=E1MGT
DATA(I)=ALPMGT
DATA(I)=REFLMG
CONTINUE
IF (IMGT.EQ.1) WRITE(10,165)
WRITE(6,4)
WRITE(6,7)
C**-----------------------------------------C
C PLOT DATA AS DESIRED.
C*-----------------------------------------C
C
CONTINUE
IF(LINEAR) 239,239,230
IF(ISIG) 233,233,231
CONTINUE
CALL IRPLOT(SIGMA,SIGLO,DELS,V,VLO,DELLIN,XAXIS,N,
* 'SIGMA (OHM-CM)-1',16,'FREQUENCY (CM-1)',16,JLN,LSY,
*RUN,4,IDENT,RUD,4,LDENT,1)
233 IF (IEPS) 236,236,234
CONTINUE
CALL IRPLOT(EP1,EPSLO,DELEPS,V,VLO,DELLIN,XAXIS,N,
* 'EPSILON 1',9,'FREQUENCY (CM-1)',16,JLN,LSY,
*RUN,4,IDENT,RUD,4,LDENT,1)
236 IF(IDATA) 239,239,237
CONTINUE
CALL IRPLOT(DATA,DATALO,DELDAT,V,VLO,DELLIN,XAXIS,N,
* 'DATA',1,'FREQUENCY (CM-1)',16,JLN,LSY,
*RUN,4,IDENT,RUD,4,LDENT,1)
239 IF(LOG)300,300,240
IF(ISIG)243,243,241
CONTINUE
CALL IRPLOT(SIGMA,SIGLO,DELS,VLOG,VLOGLO,DELLOG,XAXIS,N,
* 'SIGMA (OHM-CM)-1',16,'LOG10 FREQUENCY',15,JLN,LSY,
*RUN,4,IDENT,RUD,4,LDENT,2)
243 IF(IEPS)246,246,244
CONTINUE
CALL IRPLOT(EP1,EPSLO,DELEPS,VLOG,VLOGLO,DELLOG,XAXIS,N,
* 'EPSILON 1',9,'LOG10 FREQUENCY',15,JLN,LSY,
*RUN,4,IDENT,RUD,4,LDENT,2)
246 IF(IDATA)300,300,247
247 CONTINUE
    CALL IRPLOT(DATA,DATALO,DELDAT,VLOG,VLOGLO,DELLOG,XAXIS,N,
        *' ',1,'LOG10 FREQUENCY',15,JLN,LSY,
        *RUN,4,IDENT,RUD,4,LDENT,2)
300 CONTINUE
    WRITE(6,2)
301 CONTINUE
302 CONTINUE
STOP
COMMON W,R,AB,S,NPTOT
REAL IDENT,IPS,NOISE,NOISE
DIMENSION VR(38),RAL(38),RZU(15),IDNT(15),RUI(15),CEN(15),
*Y(1000),PSA(1000),V(1000),VLCG(1000),CEACT(8),YY(1000),
*SAO(I000),INSOT(1000),ALPHA(1000),A(4),M(1000),S(1000),C(1000),
*AV(5000),RS(8000),VNP(15)
DATA $VR/0.0,5.55,0.25,0.71A,7.00,0.30?,0.00,1.000,1.125,1.429,0.1007,
2000,2500,3333,5000,7500,11425,1705,2121,2500,2803,3333,4286,5385,
$1667,13162,20000,22222,25000,30000,33333,50000/,$RL/1.0,0.45,$
$3.556,3.596,8.678,8.761,8.536,8.976,8.927,8.932,8.961,9.076,$
$9.101,9.106,9.105/ 2 FORMAT (111) 3 FORMAT (15) 4 FORMAT (11)
5 FORMAT (11(9.0,5F10.0,F12)
6 FORMAT (1X,11,2X,5I,13,6I POINTS,4X,5IPREC=,F9.4,2X,4IP=,F4.1,2X,
*5VOLT=,F9.4,1X,6I V OLTS,4X,10THICKNESS=,F8.5,1X,2IP=,4X,
*SHRAT=,F6.0,SHLINES/83) 7 FORMAT (16F5.5) 8 FORMAT (16(1X,F6.5))
9 FORMAT (F9.2,1X,F8.6,2X,F5.2) 11 FORMAT (11,10D2)
14 FORMAT (//27,9(1.0(G=1),2X,INTENSITY (CVOLTS)),3X,5RATIO,
*14X,5ALPHA,7X,REX(C=1),7X,13INTENSITY (CVOLTS),3X,5RIO10,14X,
*5ALPHA,/) 15 FORMAT (///3,9(1.0(G=1),3X,13IN TENSITY (CVOLTS),34X,2ND(G=1),
*3X,13INTENSITY (CVOLTS) /)
16 FORMAT (23X2(F9.2,6X,S16.5,38))
17 FORMAT (1X,9(F9.2,3X,F10.5,3X,F7.4,4X,F7.4,5X,F8.3,6X))
18 FORMAT (1X,9X,"SPECTRUM RANGE IS ':F8.3,' AT 'F9.2,' C=1")
19 FORMAT (1X,9X,"SPECTRUM RANGES BETWEEN 'F9.2,' C=1 & 'F9.2,
* C=1 ST ',F4.0," OF PARAMETERS")
20 FORMAT (14X)
22 FORMAT (8F10.6) 24 FORMAT (6.0,1.5A8)
25 FORMAT (17,F6.2,1X,17A4)
26 FORMAT (1X,18F7.2)
27 FORMAT (F6.2,15A4)
28 FORMAT (/2X,8HNU(CM-1),4X,15HPOINTS AVERAGED,4X,5HRATIO,14X,*
      5HALPHA,7X,8HNU(CM-1),4X,15HPOINTS AVERAGED,4X,5HRATIO,14X,5HALPHA
      *)
1001 FORMAT(3H3 0)
1002 FORMAT(26H9. 0. 4 5000.)
1003 FORMAT(53H0. 6000. -20. 20. 0. 1.0)
1004 FORMAT(53H0. 50. 0. 300. 0. 1.0)
1005 FORMAT(53H0. 50. 0. 0.7 0. 0.1)
1007 FORMAT(53H400000. 0.8 17.094 1.00 10. -1.)
1008 FORMAT(9H -1.0)
1009 FORMAT(4H-99.)
1010 FORMAT(3HO-1)
1011 FORMAT(2H/*)
C
C******************************************************************************
C READ CONTROLS FOR PLOTTING, PUNCHING OF RATIO AND PUNCHING OF
C SMOOTHED RATIO. Y AXIS IS 10 INCHES LONG. LOGS ARE TO BASE 10.
C
C CARD#1   I FORMAT
C  1: 1=> PLOT SPECTRUM; 0=> SKIP SPECTRUM PLOT.
C  3: 1=> PLOTS HAVE SYMBOLS & LINES; 0=> PLOTS HAVE LINES;
C    -1=> PLOTS HAVE SYMBOLS ONLY. (SEE IRPLOT FOR JLN)
C  5: A NUMBER FROM 0-14 THAT SPECIFIES SYMBOL TO BE DRAWN.
C    (SEE IRPLOT FOR LSY)
C  7: 0=> PLOT INDIVIDUAL GRAPHS AND COMBINED GRAPHS.
C    1=> PLOT ONLY COMBINED GRAPHS.
C  9: N=> PUNCH EVERY N TH POINT OF RATIO; 0=> NO PUNCHING
C 11: N=> PUNCH EVERY N TH POINT OF SMOOTHED RATIO; 0=> NO
C    PUNCHING.
C
C CARD#2   F FORMAT
C  1-10: LENGTH OF X-AXIS IN INCHES.
C 11-20: STARTING WAVE NUMBER ON X-AXIS.
C 21-30: ENDING WAVE NUMBER ON X-AXIS. (0 => NO COMMON PLOTS)
C 31-40: STARTING LOGARITHMIC WAVE NUMBER ON X-AXIS.
C 41-50: ENDING LOGARITHMIC WAVE NUMBER ON X-AXIS. 0 => NO PLOT
C
C CARD#3   F FORMAT
C  1-10: STARTING NUMBER FOR RATIO ON Y-AXIS.
C 11-20: ENDING NUMBER FOR RATIO ON Y-AXIS. 0 => NO PLOT
C 21-30: STARTING NUMBER FOR SMOOTHED RATIO ON Y-AXIS.
C 31-40: ENDING NUMBER FOR SMOOTHED RATIO ON Y-AXIS. 0 => NO
C 41-50: STARTING NUMBER FOR ALPHA ON Y-AXIS.
C 51-60: ENDING NUMBER FOR ALPHA ON Y-AXIS. 0 => NO PLOT
C
C CARD#4   F FORMAT
C  1-10: GAIN FOR SAMPLE #1.
C 11-20: GAIN FOR SAMPLE #2.
**THIS CARD CAN BE FILLED FOR A TOTAL OF 8 GAINS.**

**GAIN = 1 WHENEVER COLUMNS ARE LEFT BLANK (0).**

C

C******************************************************************************************************************

DO 401 NTIMES=1,100
DO 29 K=1,1000
W(K)=0.0
R(K)=0.0
RS(K)=0.0
AL(K)=0.0
S(K)=1.0
29 CONTINUE
NPTOT=0
N=1
1PD=0
WRITE(6,2)
READ(5,11) ISP,JLN,LSY,NAVE,IPKREG,IPNSHO
IF(NAVE.LT.0) GOTO 502
READ(5,23) XAXIS,VLO,VHI,VLOGLO,VLOGHI
READ(5,23) RATLO,RATHI,RSMLO,RSMHI,ALPLO,ALPHI
DELL1N=(VHI-VLO)/XAXIS
DELLOG=(VLOGHI-VLOGLO)/XAXIS
DELR=(RATHI-RATLO)/10.
DELSMO=(RSMHI-RSMLO)/10.
DELALP=(ALPHI-ALPLO)/10.
READ(5,23) (GFAC(K),K=1,10)
DO 30 NK=1,10
IF (GFAC(K).EQ.0.0) GFAC(K)=1.0
30 CONTINUE
C

C******************************************************************************************************************

C START BIG LOOP.

C******************************************************************************************************************

C

NSETS=1000
DO 301 NR=1,NSETS
IF (1PD.NE.0) WRITE(6,2)
C

C******************************************************************************************************************

C HEADER CARDS FOR EACH RUN.

C . CARD#1 F FORMAT
C 1-6: RUN NUMBER
C 7-25: RUN TITLE IN ALPHA NUMERICS.
C

C CARD#2 MIXED FORMAT
C 1: 0=> BACKGROUND; 1-7=> SAMPLE # 1-7. (I FORMAT)
C 2-10: INITIAL RUN NUMBER (F FORMAT)
C 11-20: FINAL RUN NUMBER (F FORMAT)
C 21-30: IMPULSES PER STEP (F FORMAT)
31-40: VOLTAGE SETTING FROM AMPLIFIER IN MILLIVOLTS. \(3=3.162\) (F FORMAT)

41-50: GRATING NUMBER. NOTE 2ND ORDER OF 1440=2880. (F FORMAT)

51-60: THICKNESS OF SAMPLE IN CM. = 1 IF UNKNOWN (F FORMAT)

61-62: # OF POINTS TO LOOSE AT BEGINNING OF RUN. (I FORMAT)

THE ABSORPTION COEFFICIENT IS CALCULATED FROM:

\[ \text{ALPHA} = -\left(\frac{1.0}{\text{THICK}}\right) \ln(\text{RATIO}) \]

READ IN THESE AND THE SPECTRUM.

PRINT THE FIRST HEADER CARD.

READ (5,24) RUN(HD),IDNT(K),K=1,15
WRITE (6,25) RUN(KL),IDNT
IF (RUN(HD).LT.0.0) GO TO 302
RUNN=IFIX(RUN(HD))
RUNNUM=FLOAT(RUNN)
DO 50 111=1,15
SAVDE(111)=IDNT(111)
50 CONTINUE
READ(5,5) IPD,DRUM1,DRUM2,IPS,VOLT,GRAT,THICK,LOOSE
DRUM=DRUM2-DRUM1
NP=DRUM*200/IP5
IF (VOLT .EQ. 0.003) VOLT=0.003165
IF (VOLT .EQ. 0.030) VOLT=0.03165
IF (VOLT .EQ. 0.300) VOLT=0.3165
IF (VOLT .EQ. 3.000) VOLT=3.165
IF (VOLT .EQ. 30.000) VOLT=31.65
IF (THICK .EQ. 0.0) THICK=1.0
WRITE (6,6) IPD,NP,DRUM1,IPS,VOLT,THICK,GRAT
WRITE (6,20)
34 READ(5,7) (YY(K),K=1,NP)
WRITE (6,6)(YY(K),K=1,NP)
IF (1PP.EQ.0) GFACT=1.
IF (1PP.EQ.0) GO TO 33
IF (1PP.GT.0) 1PP=1PP
GFACT=GFACT(1.P)
33 CONTINUE
DO 35 1=1,NP
Y(K)=YY(K)*VOLT/GFACT
C IF (RUN(ID).GE.304.24.AND.RUN(ND).LT.304.99) Y(K)=Y(K)/.9626
C IF (RUN(ID).GE.278.51.AND.RUN(ND).LT.278.99) Y(K)=Y(K)/1.01
C IF (RUN(ID).GE.250.75.AND.RUN(ND).LT.250.76) Y(K)=Y(K)*.97782
C IF (RUN(ID).GE.304.36) Y(K)=Y(K)/1.014
35 CONTINUE
IF (LOOSE.EQ.0) GO TO 40
LNP=NP-LOOSE
DO 36 K=1,LNP
LK=K+LOOSE
Y(K)=Y(LK)
36 CONTINUE
NP=MP
DRUM1=DRUM1+LOOSE*IPS/200.
WRITE(6,20)
WRITE(6,6)IPS,DRUM,IPN,NP,NP,IPS,VOLT,THICK,GRAT
40 CONTINUE
NP=NP/2
NP=NP*2

C
C SELECT CONSTANTS FOR THE FREQUENCY CALCULATION.
C
C
IF (GRAT.EQ. 2880.) AC=16560.
IF (GRAT.EQ. 2880.) B=1578.6
IF (GRAT.EQ. 2880.) C=0.0
IF (GRAT.EQ. 2880.) D=0.0
IF (GRAT.EQ. 1440.) AC=8280.
IF (GRAT.EQ. 1440.) B=769.4
IF (GRAT.EQ. 1440.) C=0.0
IF (GRAT.EQ. 1440.) D=0.0
IF (GRAT.EQ. 640.) AC=3696.437
IF (GRAT.EQ. 640.) B=347.897
IF (GRAT.EQ. 640.) C=0.0
IF (GRAT.EQ. 640.) D=0.0
IF (GRAT.EQ. 240.) AC=1387.533
IF (GRAT.EQ. 240.) B=120.572
IF (GRAT.EQ. 240.) C=0.0776
IF (GRAT.EQ. 240.) D=-0.0159
IF (GRAT.EQ. 161.) AC=594.263
IF (GRAT.EQ. 161.) B=54.418
IF (GRAT.EQ. 161.) C=0.0568
IF (GRAT.EQ. 161.) D=-0.0124
IF (GRAT.EQ. 40.) AC=231.345
IF (GRAT.EQ. 40.) B=21.533
IF (GRAT.EQ. 40.) C=0.0272
IF (GRAT.EQ. 40.) D=-0.0066
IF (GRAT.EQ. 30.) AC=170.351
IF (GRAT.EQ. 30.) B=16.017
IF (GRAT.EQ. 30.) C=-0.0107
IF (GRAT.EQ. 30.) D=-0.00245

C
C CALCULATE FREQUENCIES
C
SAIAX=0.0
KMAX=0
DO 140 K=1,NP
XK=K-1
DRUM=DRUM1+IPS/200.*XK
V(K)=AC+B*DRUM+C*DRUM*2+D*DRUM*3
VLOG(K)=ALOG10(V(K))
IF(Y(K)-SAMAX)140,140,135
135 SAMAX=Y(K)
KMAX=K
140 CONTINUE
WRITE (6,20)
WRITE(6,18) SAMAX,V(KMAX)
NOISE=0.25
NOISE=0.10
SACUT=SAMAX*NOISE
NOTSPC=NOISE*100.
IF(IPD)172,172,180
C
C******************************************************************************
C OUTPUT BACKGROUND AND LOAD BACKGROUND ARRAY.
C******************************************************************************
C
172 call STON(Y,NP,KMAX,SACUT,KFIRST,KLAST) WRITE(6,19) V(KFIRST),V(KLAST),NOTSPC
SAZERO=0.0
MX=NP/2
WRITE(6,20)
WRITE(6,20)
DO 175 L=1,MX
LN=L+NX
C WRITE(6,16) V(L), Y(L), V(LN), Y(LN)
PSA(L)= Y(L)
PSA(LN)= Y(LN)
175 CONTINUE
PSZERO=SAZERO
NDECKS=10
DO 177 J=1,15
JDENT(J)=11*EST(J)
177 CONTINUE
DO 178 J=1,NDECKS
RUN(J)=RUN(J)
178 CONTINUE
GO TO 190
C
C******************************************************************************
C CALCULATE RATIO AND ALPHA AND OUTPUT THEM WITH SPECTRUM.
C******************************************************************************
C
CALL STON(Y, NP, KMAX, SACUT, KF, KL)
WRITE(6,19) V(KF), V(KL), NOISP
SAZERO=0.0
MX=NP/2
WRITE(6,14)
WRITE(6,13)
NPTOT=NPTOT+(KL-1-KFIRST+1)
DO 191 K=1, NP
RATIO(K)=(Y(K)-SAZERO)/(PSA(K)-PSZERO)
C
C**********************************************************************
C RAL(N)=REFLECTANCE OF ALUMINUM AT SELECTED FREQUENCIES.
C THIS ROUTINE INTERPOLATES A VALUE FOR REFLECTANCE OF ALUMINUM AT THE
C FREQUENCIES AT WHICH DATA WAS SAMPL ED, AND THEN MULTIPLIES THE
C RATIO OF SAMPLE/MIRROR BY THE INTERPOLATED VALUE, RALV.
C**********************************************************************
C
C N=1
181 IF(V(K)-VR(N)) 183,183,182
182 N=N+1
GO TO 181
183 SLOPE=(RAL(N)-RAL(N-1))/(VR(N)-VR(N-1))
RALV=RAL(N-1)+SLOPE*(V(K)-VR(N-1))
RATIO(K)=RATIO(K)*RALV
191 CONTINUE
RSMOT(1)=RATIO(1)
RSMOT(2)=RATIO(2)
RSMOT(NP-1)=RATIO(NP-1)
RSMOT(NP)=RATIO(NP)
MX=NP/2
DO 193 K=3, NP
RSMOT(K)=(RATIO(K-2)+3.*RATIO(K-1)+6.*RATIO(K)+3.*RATIO(K+1)+
*RATIO(K+2))/14.
193 CONTINUE
DO 188 K=1, NP
IF (KSMOT(K)) 185,185,187
185 ALPHA(K)=0.0
GO TO 188
187 ALPHA(K)=(-1./THICK).*ALOG(RSMOT(K))
188 CONTINUE
MX=NP/2
DO 190 K=1, MX
N=K
WRITE(6,17) V(K), Y(K), RATIO(K), RSMOT(K), ALPHA(K), V(M), Y(M),
*RATIO(M), RSMOT(M), ALPHA(N)
190 CONTINUE
IF (GAVL,NCT,0) GOTO 561
IF (TSP) 220,220,200
C
C**********************************************************************
C PLOT SPECTRUM.

```
C 260 CONTINUE
ZMAX=0.
   DO 224 K=1,NP
      IF( Y(K)-ZMAX) 224,224,223
   223 ZMAX= Y(K)
   224 CONTINUE
   A(1)=ZMAX
   A(2)=0.0
   CALL SCALE(A,10.0,2,1)
   SALO=A(3)
   DELSA=A(4)
   CALL IRPLOT(Y,SALO,DELSA,V,VLO,DELLIN,XAXIS,NP,
      * 'INTENSITY (HVOLTS)',18,'FREQUENCY (CM-1)',16,JLN,LSY,
      *RUN,NDECKS,IDENT,RUD,-15,IDENT,0)
   220 IF(IPD) 301,301,221
   221 IF(VI11) 240,240,230
      IF(RAT11) 233,233,221
   C PLOT RATIO.
   C 230 CONTINUE
      CALL IRPLOT(RATIO,RATLO,DELR,V,VLO,DELLIN,XAXIS,NP,
         * 'RATIO',5,'FREQUENCY (CM-1)',16,JLN,LSY,
         *RUN,NDECKS,IDENT,RUD,IDENTS,IDENT,1)
   233 IF(ALP11) 230,230,234
   C PLOT ABSORPTION COEFFICIENT.
   C 234 CONTINUE
      CALL IRPLOT(ALPHA,ALPLO,DELA,L,V,VLO,DELLIN,XAXIS,NP,
         * 'ALPHA (CM-1)',12,'FREQUENCY (CM-1)',16,JLN,LSY,
         *RUN,NDECKS,IDENT,RUD,IDENTS,IDENT,1)
   236 IF(RS11) 239,239,237
   C PLOT SMOOTHED RATIO.
   C 237 CONTINUE
      CALL IRPLOT(RSMOT,RSML,DFLSM,XLO,DELLIN,XAXIS,NP,
         * 'RATIO SMOOTHED',14,'FREQUENCY (CM-1)',16,JLN,LSY,
         *RUN,NDECKS,IDENT,RUD,IDENTS,IDENT,1)
   229 IF(VL0CHT) 249,249,260
```
240 IF (RATHI) 243,243,241

C

C********************************************************************************************************
C PLOT RATIO, LOGARITHMIC
C********************************************************************************************************
C
241 CONTINUE
CALL TRPLOT(RATIO,RATLO,DELR,VLOGO,DLOLOGO,XAXIS,NP,
        *'RATIO',5,'LOG10 FREQUENCY',15,JLY,LSY,
        *RUN,NDECKS,IDENT,RUD,NDENTS,IDENT,2)
243 IF (ALPHI) 246,246,244

C

C********************************************************************************************************
C PLOT ABSORPTION COEFFICIENT, LOGARITHMIC
C********************************************************************************************************
C
244 CONTINUE
CALL TRPLOT(ALPHA,ALPLO,DELA,LOGO,DELLOGO,XAXIS,NP,
        *'ALPHA (CM-1)',12,'LOG10 FREQUENCY',15,JLY,LSY,
        *RUN,NDECKS,IDENT,RUD,NDENTS,IDENT,2)
246 IF (KSHOT) 249,249,247

C

C********************************************************************************************************
C PLOT SMOOTHED RATIO, LOGARITHMIC
C********************************************************************************************************
C
247 CONTINUE
CALL TRPLOT(KSHOT,KSHLO,DELS,LOGO,DELLOGO,XAXIS,NP,
        *'RATIO SMOOTHED',14,'LOG10 FREQUENCY',15,JLY,LSY,
        *RUN,NDECKS,IDENT,RUD,NDENTS,IDENT,2)
249 CONTINUE
501 CONTINUE
IF (IP10) 301,301,250

C

C********************************************************************************************************
C END PLOT. SORT
C********************************************************************************************************
C
250 CALL RURDLR(V,RATIO,ALPHA,KFIRST,KLAST)
341 CONTINUE

362 CONTINUE
RS(1)=I(1)
RS(2)=I(2)
RS(IPTOT-1)=I(NPTOT-1)
RS(IPTOT)=R(IPTOT)
NS=KPTOT
DO 406 K=3,NS
406 RS(K)=(RS(K-2)+3.*RS(K-1)+6.*RS(K)+3.*RS(K+1)+R(K+2))/14.
WRITE (6,2)
WRITE (6,26)
WRITE (6,13)
MX=NPTOT/2
DO 600 K=1,IX
M=K+IX
WRITE (6,17) W(K),S(E),R(E),RS(E),AB(E),W(M),S(M),R(M),RS(M),
*AI(M)
600 CONTINUE

C
C***********************************************************************
C PUNCH RATIOS
C***********************************************************************
C
IF (IPNREG) 195,195,194
194 CONTINUE
C WRITE(9,1001)
C WRITE(9,1002)
C WRITE(9,1003)
C WRITE(9,1004)
C WRITE(9,1005)
WRITE(9,27) RUNNUM,SAVINT
C WRITE(9,1007)
DO 196 K=1,NPTOT,IPNREG
WRITE(9,9) W(K),R(K),S(K)
196 CONTINUE
C WRITE(9,1008)
C WRITE(9,1009)
C WRITE(9,1010)
WRITE(9,1011)
195 CONTINUE
IF (IPNSHO) 198,198,199
199 CONTINUE
C WRITE(9,1001)
C WRITE(9,1062)
C WRITE(9,1003)
C WRITE(9,1004)
C WRITE(9,1005)
WRITE(9,27) RUNNUM,SAVINT
C WRITE(9,1007)
DO 197 K=1,NPTOT,IPNSHO
WRITE(9,9) W(K),RS(K),S(K)
197 CONTINUE
WRITE(9,1008)
C WRITE(9,1009)
C WRITE(5,1010)
WRITE(9,1011)
198 CONTINUE
C
C***********************************************************************
C PLOT COMBINED RUNS
C***********************************************************************
IF (VIII) 409,409,402
402 IF (RATHI) 404,404,403
403 CALL IRPLOT(R, RATLO, DELR, M, VLO, DELLIN, XAXIS, NPTOT,
   * 'RATIO', 5, 'FREQUENCY (CM^-1)', 16, JLN, LSY, RUN, NDECKS, IDENT,
   * RUD, NDENTS, JDENT, 1)
404 IF (RSIII) 407,407,405
405 CONTINUE
   CALL IRPLOT(RS, RMSLO, DELSLO, M, VLO, DELLIN, XAXIS, NPTOT,
   * 'RATIO SMOOTHED', 14, 'FREQUENCY (CM^-1)', 16, JLN, LSY, RUN,
   * NDECKS, IDENT, RUD, NDENTS, JDENT, 1)
407 IF (ALPHI) 409,409,408
408 CALL IRPLOT(AB, ALPLO, DELAP, M, VLO, DELLIN, XAXIS, NPTOT,
   * 'ALPHA (CM^-1)', 12, 'FREQUENCY (CM^-1)', 16, JLN, LSY, RUN,
   * NDECKS, IDENT, RUD, NDENTS, JDENT, 1)
409 IF (VLOGHI) 401,401,420
420 DO 425 K=1,NPTOT
   VLOC(K)=ALOC10(W(K))
425 CONTINUE
410 IF (RATHI) 411,411,410
411 CALL IRPLOT(R, RATLO, DELR, VLOG, VLOGLO, DELLOG, XAXIS, NPTOT,
   * 'RATIO', 5, 'LOG10 FREQUENCY', 15, JLN, LSY,
   * RUN, NDECKS, IDENT, RUD, NDENTS, JDENT, 2)
412 CALL IRPLOT(RS, RMSLO, DELSLO, VLOG, VLOGLO, DELLOG, XAXIS, NPTOT,
   * 'RATIO SMOOTHED', 14, 'LOG10 FREQUENCY', 15, JLN, LSY,
   * RUN, NDECKS, IDENT, RUD, NDENTS, JDENT, 2)
413 IF (ALPHI) 401,401,414
414 CALL IRPLOT(AB, ALPLO, DELAP, VLOG, VLOGLO, DELLOG, XAXIS, NPTOT,
   * 'ALPHA (CM^-1)', 12, 'LOG10 FREQUENCY', 15, JLN, LSY,
   * RUN, NDECKS, IDENT, RUD, NDENTS, JDENT, 2)
401 CONTINUE
502 CONTINUE
STOP
**PROGRAM FOURTRNS**

4096 POINT FAST FOURIER TRANSFORM

REAL IDENT, JDE

INTEGER PWP

DIMENSION YY(8200)

DIMENSION Y(4100), PSA(4100), SIGMA(4100), PSIGMA(4100), 
THETA(4100), PTHETA(4100), PATH(4100), V(4100), VLOG(4100)

DIMENSION RATIO(4100), ALPHA(4100), ALLOC(4100), PHI(4100), 
SIGMA(4100), SIGALP(4100), SIGALG(4100), DATA(4100), RNORM(4100)

DIMENSION SA2(4100,10), PRATTO(4100), VR(1000), RMISS(1000)

DIMENSION K(4), A(4), IDENT(15), JDE(15), RUN(10), PRD(10), GFACT(10)

EQUIVALENCE (SA2(1,1), PHI(1)),
* (SA2(1,2), RATIO(1)),
* (SA2(1,3), VLOG(1)),
* (SA2(1,4), V(1)),
* (SA2(1,5), ALPHA(1)),
* (SA2(1,6), ALLOC(1)),
* (SA2(1,7), SIGMA(1)),
* (SA2(1,8), SIGALP(1)),
* (SA2(1,9), SIGALG(1)),
* (SA2(1,10), DATA(1))

EQUIVALENCE (YY(1), SA(1)), (YY(4101), SIGMA(1))

1 FORMAT(11,10I2)
2 FORMAT(1HI)
3 FORMAT (11, I4)
4 FORMAT (11,12,12,15,15)
5 FORMAT (11,11,14,14,15)
6 FORMAT (1X, 11,12,12,15,15, POINTS, STF, =', P, 9.4, ' MICRON', ',
* AMPLIFIER=', 'F9,4', ' V', ' THICKNESS=', 'F8,5', ' MICRON', R=', 'F4,2, 
* SLOPE=', 'F6,4', ' CAL=', 'F6,3)
7 FORMAT (1X, 'S/R (K ABOVE', 'F9.3', ' FREQUENCIES BETWEEN ', 'F7.2, 
* AND', 'F7.2', ' CM-1')
8 FORMAT (1X, 'S/R (K ABOVE', 'F9.3', ' FREQUENCIES BETWEEN ', 'F7.2, 
* AND', 'F7.2', ' CM-1')

10 FORMAT (1X, 'S/R (K ABOVE', 'F9.3', ' FREQUENCIES BETWEEN ', 'F7.2, 
* AND', 'F7.2', ' CM-1')
11 FORMAT (1X, 'S/R (K ABOVE', 'F9.3', ' FREQUENCIES BETWEEN ', 'F7.2, 
* AND', 'F7.2', ' CM-1')
12 FORMAT (1X, 'S/R (K ABOVE', 'F9.3', ' FREQUENCIES BETWEEN ', 'F7.2, 
* AND', 'F7.2', ' CM-1')
13 FORMAT (1X, 'S/R (K ABOVE', 'F9.3', ' FREQUENCIES BETWEEN ', 'F7.2, 
* AND', 'F7.2', ' CM-1')
14 FORMAT (1X, 'S/R (K ABOVE', 'F9.3', ' FREQUENCIES BETWEEN ', 'F7.2, 
* AND', 'F7.2', ' CM-1')
15 FORMAT (1X, 'S/R (K ABOVE', 'F9.3', ' FREQUENCIES BETWEEN ', 'F7.2, 
* AND', 'F7.2', ' CM-1')
16 FORMAT   *(2X,2(F7.2,6X,F8.3,6X,F8.4,6X,F8.5,12X))
17 FORMAT   *(2X,F7.2,6X,F8.3,6X,F8.4,6X,F8.5,6X,F8.5,8X,F8.3,8X,F10.3,
*8X,F8.5)
18 FORMAT   (/1X, ‘INTERFEROGRAM’)
19 FORMAT   (1X,F10.4,5X,F10.7)
20 FORMAT   (1X,‘TH POINT WAS TOO BIG. IT IS NOW ’,F7.0)
21 FORMAT   (/1X,’RUN ’,F7.2,’ HAS MIN VAL ’,F9.3,’ AND MAX VAL ’,F9.3)
22 FORMAT   (/1X,11,’ SIDED DATA. MAX VALUE= ’,F7.0,’ AT THE’,15,
*’ TH POINT. FFT WILL START AT THE’,15,’ TH POINT.’)
23 FORMAT   (BF10.0)
24 FORMAT   (F6.0,15A4)
25 FORMAT   (1H ,F6.2,1X,15A4)
26 FORMAT   (F6.2,15A4)
27 FORMAT   (F9.2,1X,F8.6)
601 FORMAT   (5H  -1.0)
PI= 3.1415927
ALZERO=0.
MULT=0
DO 39 K=1,4100
PRATIO(K)=1.0
39 CONTINUE
WRITE(6,2)
READ(5,1) NORM.IPN
IF (NORM.EQ.0) GO TO 37
READ(10,24) RNULL,(IDENT(K),K=1,15)
WRITE(6,25) RNULL,IDENT
DO 36 K=1,1000
READ(10,23) VK(K),RMIR(K)
WRITE(6,19) VK(K),RMIR(K)
IF (VK(K).LT.0.0) GO TO 37
36 CONTINUE
37 NMIR=K-1
CALL PLOTS(0,0,0)
C
C******************************************************************************
C CARD#1  I FORMAT
C 1:  1=> CORRECT REFL OF BACKGROUND MATERIAL; 0=> NONE
C C READ PLOTTING PARAMETERS
C Y AXIS IS 10 INCHES LONG. LOGS ARE TO BASE 10.
C CARD#2  I FORMAT
C 1:  1=> PLOT INTERFEROGRAM; 0=> NO PLOT
C 2-3:  1=> PLOT SPECTRUM; 0=> NO PLOT; -1=> END PROGRAM
C 4-5:  1=> PLOT PHASE; 0=> NO PLOT
C 6-7:  1=> SYMOL AND LINE; 0=> LINE ONLY; -1=> SYMOL ONLY
C 8-9:  A KINDER (OF THE PLOT SYMBOL) 0-14
C  10-11:  1=> PUNCH RATIO IN FILE; 0=> NO PUNCH
C
C  CARD#3  F FORMAT
C  1-10:  LENGTH OF X-AXIS IN INCHES
C  11-20:  STARTING WAVENUMBER ON X-AXIS
C  21-30:  ENDING WAVENUMBER ON X-AXIS (0=> NO COMMON PLOTS)
C  31-40:  STARTING LOGARITHMIC WAVENUMBER ON X-AXIS
C  41-50:  ENDING LOGARITHMIC WAVENUMBER ON X-AXIS (0=> NO PLOT)
C
C  CARD#4  F FORMAT
C  1-10:  STARTING NUMBER FOR RATIO ON Y-AXIS
C  11-20:  ENDING NUMBER FOR RATIO ON Y-AXIS (0=> NO RATIO PLOT)
C  21-30:  STARTING NUMBER FOR ALPHA ON Y-AXIS
C  31-40:  ENDING NUMBER FOR LOG10 ALPHA ON Y-AXIS (0=> NO PLOT)
C  41-50:  STARTING NUMBER FOR LOG10 ALPHA ON Y-AXIS
C  51-60:  ENDING NUMBER FOR LOG10 ALPHA ON Y-AXIS (0=> NO PLOT)
C
C  CARD#5  F FORMAT
C  1-10:  GAIN FOR SAMPLE #1
C  11-21:  GAIN FOR SAMPLE #2
C  22-31:  THIS CARD CAN BE FILLED FOR A TOTAL OF 8 GAINS
C  32-41:  GAIN=1 WHENEVER COLUMNS ARE LEFT BLANK (0)
C
C  CARD#6  1 FORMAT
C  1:  1=> AVERAGE THE DATA SETS; 0=> NO AVERAGE
C  2-3:  0=> NO; 1=> LIGHT; 2=> MEDIUM; 3=> HEAVY;
C  4:  0=> TRIANGULAR APODIZATION
C  5-6:  0=> SUBTRACT COMPUTED ZERO FROM INTER; 1=> NO SUB
C  6-10:  NUMBER OF POINT FOR SHORTENED INTEGRATION
C  11-15:  NUMBER OUTPUT POINTS TO BE USED (0=> NEXT POWER OF 2)
C
C**************************************************************************************
C
C DO 461 NTIM=1,100
C READ(5,1) LITER,ISP,IPHAS,ILS,LSY,IPN
C IF (ISP .LT. 0 ) GO TO 501
C LSY=LSY+1
C READ(5,22) XAXIS,VL0,VHI,VLOG10,VLOG11
C DELX=(VHI-VLO)/XAXIS
C DELLOG=(VLOG10-VLOG11)/XAXIS
C READ (5,23) RAT0,RATHI,ALPH1,ALPH1,ALOCH1,ALOG11
C DELALP=(ALPH1-ALPH1)/10.
C DELALG=(ALOG11-ALOG11)/10.
C PI0:=P1=-2.14159
C PI0H=-2.14159
C PI0L=(PI0H-PI0L)/10.
C READ (5,23) (GFACT(E),E=1,8)
C DO 20 K=1,3
C IF (GFACT(E) .EQ. 0.0) GFACT(E)=1.0
30 CONTINUE
READ(5,4) NAVE, IAPOD, NZERO, NPTS, NLPTS
C
C***************************************************************************
C START BIG LOOP.
C***************************************************************************
C
NDECKS=1
NSETS=1000
DO 301 NS=1,NSETS
C
C***************************************************************************
C READ MULT IN COL 1 OF CARD, IF NAVE=1, 0=> NO CHANCE;
C 1=> PRATIO(K)=RATIO(K)/PRATIO(K) BEFORE OUTPUT OF RATIO;
C 9=> PRATIO(K)=1. SET AFTER BACKGROUND OUTPUT
C #=> CALL MIRROR CORRECTIONS
C READ NDECKS WHICH DETERMINES HOW MANY INTERFEROCGRAMS WILL BE
C AVERAGED. THIS CARD MUST PRECEDE EACH BLOCK OF INTERFEROCGRAMS WHICH
C ARE AVERAGED. THE READ FORMAT IS IA (COLS 3-5).
C***************************************************************************
C
CALL AZERO(THETA, 4100)
35 IF (NAVE .NE. 0) READ(5,3) MULT, NDECKS
NDECK=NDECKS
C
C***************************************************************************
C HEADER CARDS FOR EACH INTERFEROCGRAM
C
C CARD#1  F FORMAT
C 1-6: RUN NUMBER (-99= END INTERFEROCGRAM READ LOOP)
C 7-35: RUN TITLE IN ALPHA NUMERICS
C
C CARD#2  MIXED FORMAT
C 1:  0=> BACKGROUND; 1-C=> SAMPLE NUMBER
C 2:  0=> STEP IN MICRON; 1=> BIG MICH; 2=> ASYM MICH;
C 2=>LAMELLAR
C 3-6: 0=> SEARCH FOR WHITE LIGHT; #=> POINT OF WHITE LIGHT
C 7-10: HIGHER OF POINTS TO BE READ
C 11-20: IF COL. 2=0 THEN STEP IN MICRONS; OTHERWISE IPS HERE
C 21-30: VOLTAGE SETTING IN MILLIVOLTS
C 31-40: THICKNESS OF SAMPLE USED TO CALCULATE ALPHA
C 41-50: HIGHER SUBTRACTED F0R COMPUTED SPECTRUM IF NZERO=1
C 51-60: REFLECTANCE OF SAMPLE TO CORRECT BASELINE OF ALPHA
C 61-70: CORRECTION OF THE SLOPE OF THE PHASE
C 71-90: THE RESULT FROM THE DIVIDE WHICH WAS OVER 100000
C***************************************************************************
C
DO 114 NAVE=1,NDECKS
33 READ(5,24) EN(EAVEC), (TENV(K),K=1,15)
   IF (EN(ECASE)) 302, 32, 34
34 WRITE(1,2)
WRITE(6,25) RUN(NAVERG),IDENT
READ(5,5) IPD,INST,KP,NP,STEP,VOLT,THICK,ZERO,REFN,SLOPE,TOOBIC
IF (NP .EQ. 0) NP=PNP
PNP=NP
IF (STEP .EQ. 0.) STEP=PSTEP
PSTEP=STEP
IF (INST .EQ. 1) STEP=STEP*0.3164
IF (INST .EQ. 2) STEP=STEP*0.512
IF (INST .EQ. 3) STEP=STEP*2.466
IF (VOLT .EQ. 0.0) VOLT=1.0
IF (VOLT .EQ. 0.03) VOLT=.03162
IF (VOLT .EQ. 0.3) VOLT=.03162
IF (VOLT .EQ. 3.0) VOLT=3.162
IF (VOLT .EQ. 30.0) VOLT=31.62
IF (THICK .EQ. 0.0) THICK=-2.3026
IF (IPD .NE. 0) GAIN=GFLECT(1)
WRITE (6,6) IPD,NP,STEP,VOLT,THICK,REFN,SLOPE,GAIN
XH=NP
STEP=STEP/(10000.0)
CUTOFF=.0/(4.0*STEP)
RES=.0/(100*STEP*4.)
CALL INTIO(Y,NP,1)
IF (TOOBIC .NE. 0) Y(KF)=TOOBIC
32 CONTINUE
IF (TOOBIC .NE. 0) WRITE(6,20) KF,TOOBIC
KF=1
WRITE(6,18)
CALL INTIO(Y,NP,2)

C*************************************************************************
C FIND VALUE AND INDEX OF THE WHITE LIGHT POSITION.
C*************************************************************************
C
CALL MAXIN: (Y,NP,Y,KF,YMAX,PMAX)
KF=KMAX
NSIDES=1
IF (KMAX .GT. 1) NSIDES=2
IF (NSIDES .NE. 2) .AND. (Y(KMAX+1) .GT. Y(KMAX-1)) KF=KMAX+1
WRITE(6,22) NSIDES,YMAX,KMAX,KF

C*************************************************************************
C FIND AND SUBTRACT AVERAGE VALUE OF INTERFEROGRAM.
C CALCULATE THE NOISE OF THE INTERFEROGRAM.
C*************************************************************************
C
IF (NSIDES .NE. 1) CALL AVVAL1(Y,NP,NSPTS,RES)
IF (NSIDES .NE. 2) CALL AVVAL2(Y,NP,NSPTS,KF,RES)
IF (INTER .EQ. 0) GOTO 70

C

C PLOT INTERFEROGNAM

C

DO 69 K=1,NP
XK=K-KF
PATH(K)=XK*STEP*2.0
69 CONTINUE

NP2=NP+2
CALL SCALE(Y,10.,NP,1)
CALL SCALE(PATH,7.,NP,1)
YLO=Y(NP+1)
DELY=Y(NP+2)
PL0=PATH(NP+1)
DELPAT=PATH(NP+2)
CALL WINDOW(-1.,7.05,-5.10.)
CALL PLOTS(0.,0.,0.)
CALL TRPLOT(Y,YLO,DELY,PATH,PL0,DELPAT,7.0,NP,
'SIGNAL',6,'PATH DIFFERENCE (CM)',20,10,10,
'SIGNAL',6,'PATH DIFFERENCE (CM)',20,10,10,
'PATH',15,'PATH',15)
70 CONTINUE

C

C APODIZE INTERFEROGRAM. SELECT DEGREE OF APODIZATION ACCORDING
C TO IAPOP. APODIZE SYMMETRICALLY ABOUT MAX POINT.

C CALL APODIZ(Y,NP,KMAX,IAP0P,RES,EP5)

C

C FIND THE POWER OF TWO WHICH IS JUST LARGER THAN NP.

C CALL N2POW(NP,MP,11LPTE,NU)

C SETUP INTERFEROGRAM FOR FOURIER TRANSFORM.

C

C

HP2=NP*2
IF (NEILES .EQ. 2) MP2=MP
IF (NEILES .EQ. 1) CALL SETUP1(Y,YY,NP,MP2)
IF (NEILES .EQ. 2) CALL SETUP2(Y,YY,NP,MP,KF)
WRITE(6,10) IPD,IP,IAP0P,CUTOFF,RES
WRITE (6,11)
CALL INTO(YY,IP2,2)

C
CNORMALIZE INTERFEROGRAM.
C CALL FOURIER TRANSFORM SUBROUTINE.
C THE FOURIER COEFFICIENTS ARE RETURNED IN YY. THE COSINE TRANSFORM'S
C ARE IN ODD NUMBERED LOCATIONS AND THE SINE TRANSFORMS ARE IN EVEN
C NUMBERED LOCATIONS.

C*****************************************************************************

DO 99 K=1,MP2
YY(K)=YY(K)*VOLT/(100.*CATH)
99 CONTINUE
MP1=2+2*MP+4
CALL TRANSF(YY,MP1,NU)
IF (NSIDES .EQ. 2) GOTO 106
XMP=MP
DO 105 J=1,MP
SA2(J,NAVELG)=YY(2*J-1)*XMP
105 CONTINUE
GOTO 112
106 CONTINUE
MP=MP/2
XMP=MP
DO 108 J=1,MP
XJN=J-1
ACOS=YY(2*J-1)*XMP
BJS=YY(2*J)*XMP
SA2(J,NAVELG)=SORT(ACOS**2+BSIN**2)
PHI12=1.*ATAN2(BJS,ACOS)+PI*EPS*XJN/1.00001/XMP
THETA(J)=THETA(J)+PHI12/XMP
108 CONTINUE
112 CONTINUE

C*****************************************************************************

C FIND THE LARGEST AND SMALLER VALUES OF THE SPECTRUM (EXCEPTING THE
C LOWEST FREQUENCY POINTS).

C*****************************************************************************

IZ=NP/16
DO 126 J=1,IZ
Y(J)=SA2(J,NAVELG)
126 CONTINUE
CALL MAX16 (Y,IZ,MP,MIN,YMIN,MXMAX)
WRITE(6,21) EPS(YAVREG),YMIN,YMAX
114 CONTINUE
C*****************************************************************************

C AVERAGE SPECTRUM AND PHASE AND CALCULATE STANDARD DEVIATION.
C*****************************************************************************

CALL AZERO(SIGMA,MP)
CALL AZERO(SA,MP)
DO 131 K=1,MP
DO 130 J=1,NDECKS
SA(K)=SA2(K,J)/XNDF,CK +SA(K)
130 CONTINUE
131 CONTINUE
IF (NDECKS .LT. 2) GOTO 134
DO 133 K=1,MP
VARA=0.
DO 132 J=1,NDECKS
VARA=VARA+(SA2(K,J)-SA(K))**2/(XNDF,K-1.)
132 CONTINUE
SIGMA(K)=SORT(VARA)
133 CONTINUE
134 CONTINUE
C
C********************************************************************************
C CALCULATE THE FREQUENCIES.
C FIND THE MAX, MIN, ZERO, AND NOISE OF THE AVERAGED SPECTRUM.
C********************************************************************************
C
V(1)=0.
RES=1.00001/(4.*XM*STEP)
DO 141 M=2, MP
XI=M
V(M)=(XI-1.)*RES
VLOG(M)=ALOG10(V(M))
141 CONTINUE
VLOG(1)=VLOG(2)-1.
SZ=MP/16
CALL MAXMIN (SA,MZ,MP,ZMIN,ZMAX,NMAX)
JJ=MP-MP/16
CALL AVEHEV(SA,JJ,JM,JMP,SAZERO,VARA)
SA=SORT(VARA)
SLAPC=SA*K100./(ZMAX-SAZERO)
IF (SAZERO .NE. 0) WRITE (6,11) ZMAX,ZMIN,SAZERO
IF (SAZERO .NE. 0) WRITE (6,12) ZMAX,ZMIN,SAZERO,ZERO
IF (SAZERO .NE. 0) SAZERO=ZMAX
WRITE (6,13) SPA,SLAPC
V(MP+1)=VLOG
V(MP+2)=BELLIN
IF (NSIDES .LE. 1) GOTO 155
C
C********************************************************************************
C PUT IN A PHASE CORRECTION FACTOR WITH SLOPE AND YCEPT AND ZEROFF,
C ROTATE PHASE BACK TO -PI TO PI
C********************************************************************************
C
YCEPT=0.
DO 152 K=1,MP
\[ \theta(k) = \theta(k) - (\text{slope} \cdot v(k) + \text{ycept}) \]

153 CONTINUE

IF (ABS(\theta(k)) \leq 3.1415927) GO TO 152
IF (\theta(k) < 0.0) \theta(k) = \theta(k) + 6.2831854
IF (ABS(\theta(k)) \leq 3.1415927) GO TO 152
IF (\theta(k) > 0.0) \theta(k) = \theta(k) - 6.2831854

GOTO 153

152 CONTINUE

155 CONTINUE

WRITE(6,1)

RIGHT = XAXIS + 0.05
MP2 = MP + 2
IF (ISP.EQ.0) GOTO 170

C
C******************************************************************************
C PLOT SPECTRUM.
C******************************************************************************
C
A(1) = XMAX
A(2) = 0.0
CALL SCALE(A, 10.0, 2, 1)
SALO = A(3)
DELSA = A(4)
SIGMA(HP+1) = 0.
SIGMA(MP+2) = DELSA
CALL WISDOM(-1., RIGHT, -5.10)
CALL PLOTS(0, 0, 0)
IF (NDECKS.EQ.1) CALL LIKE(V, SIGMA, MP, 1, JLNX, LS)
CALL IPLPLOT(THETA, PHSLO, DELPU, V, VLO, PELLIN, XAXIS, HP,
  * 'INTENSITY', 0, 'FREQUENCY (cm-1)', 16, JLNX, LSY,
  * 'PHASE (radians)', 15, 'FREQUENCY (cm-1)', 16, JLNX, LSY,
  * RANG, NDECKS, IDENT, RUB, -15, IDENT, 1)
IF (NDECKS.EQ.1) GOTO 170
IF (ISP.EQ.0) GOTO 170

C
C******************************************************************************
C PLOT PHASE.
C******************************************************************************
C
CALL WISDOM(-1., RIGHT, -5.10)
CALL PLOTS(0, 0, 0)
CALL IPLPLOT(THETA, PHSLO, DELPU, V, VLO, PELLIN, XAXIS, HP,
  * 'PHASE (radians)', 15, 'FREQUENCY (cm-1)', 16, JLNX, LSY,
  * RANG, NDECKS, IDENT, RUB, -1, IDENT, 1)
170 IF (IPP.EQ.0) GOTO 180

SACUT = 0.10
CALL SION(SA, LP, XMAX, SACUT, KEFIRST, KLAST)
LP = KLAST - KEFIRST + 1
WRITE(6, 9) SACUT, V(KEFIRST), V(KLAST)

C
C******************************************************************************
C OUTPUT BACKGROUND AND LOAD BACKGROUND ARRAY.

C***********************************************************************

C
WRITE(6,15)
MX=MP/2
DO 175 L=1,MX
LN=L+MX
WRITE(6,16) V(L),SA(L),SIGMA(L),THETA(L),V(LN),SA(LN),SIGMA(LN),
*THETA(LN)
175 CONTINUE
DO 176 L=1,MP
PSA(L)=SA(L)-SAZERO
IF (PSA(L) .EQ. 0.0) PSA(L)=0.00001
PSIGMA(L)=SIGMA(L)
PTHETA(L)=THETA(L)
176 CONTINUE
DO 177 J=1,15
JDEMT(J)=I.DENT(J)
177 CONTINUE
DO 170 J=1,NDECKS
RUJ(J)=RUN(J)
170 CONTINUE
NDENTS=NDECKS
IF (NL.LT.NE.9) GO TO 301
DO 179 L=1,NP
PATIO(L)=1.
179 CONTINUE
GO TO 301
C
C***********************************************************************

C CALCULATE RATIO AND ALPEA AND OUTPUT THEM WITH SPECTRM.

C***********************************************************************

C
160 WRITE(6,14)
ALZERO=(2./THICK)**ALOG(1.-THICK)
DO 165 K=1,MP
SIN(K)=THETA(K)-PTHETA(K)
RATIO(K)=(SA(K)-SAZERO)/PSA(K)
SPECT=SIGMA(K)/SA(K)
PSPECT=PSIGMA(K)/PSA(K)
SIGMAT(K)=RATIO(K)**(SP*C**2+PSPECT**2)
ALPHA(K)=0.
IF (RATIO(K) .GT. 0.) ALPHA(K)=-ALOG(RATIO(K))/THICK-ALZERO
ENOM(K)=RATIO(K)/PRATIO(K)
165 CONTINUE
IF (BUILT.NE.1) GO TO 167
DO 166 K=1,MP
PRATIO(K)=ENOM(K)
166 CONTINUE
167 CONTINUE
IF (NURM.NE.0) CALL MTRROR(v,RNORM,MP,VR,RMIR,NMIR)
DO 190 K=1,LP
WRITE(6,17)V(K),SA(K),SIGMA(K),THETA(K),PHI(K),RATIO(K),ALPHA(K),
*RNORM(K)
V(K)=V(K+KFIRST-1)
PHI(K)=PHI(K+KFIRST-1)
RATIO(K)=RATIO(K+KFIRST-1)
RNORM(K)=RNORM(K+KFIRST-1)
SIGMAT(K)=SIGMAT(K+KFIRST-1)
ALPHA(K)=ALPHA(K+KFIRST-1)
SIGALP(K)=SIGMAT(K)/RATIO(K)/ABS(TICK)
ALLOG(K)=0.0
IF(ALPHA(K) .GT. 0.0) ALLOG(K)=ALOG10(ALPHA(K))
SIGALG(K)=0.
IF(ALPHA(K) .GT. 0.0) SIGALG(K)=SIGALP(K)/ALPHA(K)
190 CONTINUE
LP1=LP+1
DO 192 K=LP1,UP
WRITE(6,17)V(K),SA(K),SIGMA(K),THETA(K),PHI(K),RATIO(K),ALPHA(K),
*RNORM(K)
192 CONTINUE
IF(IPN .EQ. 0) GOTO 201
IF (MULT.EQ.1) GO TO 201
WRITE(9,27) RUN(1), IDENT
DO 196 K=1,LP
WRITE(9,28) V(K), RNORM(K)
196 CONTINUE
WRITE(9,601)
201 CONTINUE
LP2=LP+2
IF (DELLIN .EQ. 0) GOTO 251
IF ((ISP .EQ. 0) .OR. NSIDES .EQ. 1) GOTO 206
IF (IPHAS .EQ. 0) GO TO 206
C
C********************************************************************************************************
C PLOT PHASE DIFFERENCE.
C********************************************************************************************************
C
CALL WINDOW(-1.,RIGHT,-5,10.)
CALL PLOTS(0,0,0)
CALL IPLOT(PHI,PHASLO,DELPHS,V,VLG,DELLIN,XAXTS,LP,
* 'PHASE DIFFERENCE (RADIANS)', 26, 'FREQUENCY (CM^{-1})', 16, JLN, LSY,
* RUN, CHECKS, IDENT, RUN, XAXTS, IDENT, 1)
206 CONTINUE
IF (DELR .EQ. 0) GOTO 211
C
C********************************************************************************************************
C PLOT RATIO.
C********************************************************************************************************
C
SIGRAT(LP1)=RATLO
SIGRAT(LP2)=DELR
CALL WINDOW(-1.,RIGHT,-.5,10.)
CALL PLOTS(0,0,0)
IF (NDECKS .GT. 1) CALL LINE(V,SIGRAT,LP,1,JLN,LS)
CALL IRPLOT(RATIO,RATLO,DELR,V,VLO,DELLIN,XAXIS,LP,
 '*RATIO',5,'FREQUENCY (CM-1)',16,JLN,LSY,
 *RUN,NDECKS,IDENT,RUD,NDENTS,JIDENT,1)
IF (NORMAL .EQ. 0) GO TO 211
CALL WINDOW(-1.,RIGHT,-.5,10.)
CALL PLOTS(0,0,0)
IF (NDECKS .GT. 1) CALL LINE(V,SIGRAT,LP,1,JLN,LS)
CALL IRPLOT(RNORM,RATLO,DELR,V,VLO,DELLIN,XAXIS,LP,
 '*CORRECTED RATIO',15,'FREQUENCY (CM-1)',16,JLN,LSY,
 *RUN,NDECKS,IDENT,RUD,NDENTS,JIDENT,1)
211 CONTINUE
IF (DELALP .EQ 0 . ) GOTO 216
C
C**********************************************************************
C PLOT ABSORPTION COEFFICIENT.
C**********************************************************************
        CALL WINDOW(-1.,RIGHT,-.5,10.)
        CALL PLOTS(0,0,0)
        CALL IRPLOT(ALPHA,ALPLO,DELALP,V,VLO,DELLIN,XAXIS,LP,
         '*ALPHA (CM-1)',12,'FREQUENCY (CM-1)',16,JLN,LSY,
         *RUN,NDECKS,IDENT,RUD,NDENTS,JIDENT,1)
216 CONTINUE

C**********************************************************************
C PLOT LOG OF ABSORPTION COEFFICIENT
C**********************************************************************
        CALL WINDOW(-1.,RIGHT,-.5,10.)
        CALL PLOTS(0,0,0)
        CALL IRPLOT(ALLOG,ALLOGLO,DELALG,V,VLO,DELLIN,XAXIS,LP,
         '*LOG10 ALPHA',11,'FREQUENCY (CM-1)',16,JLN,LSY,
         *RUN,NDECKS,IDENT,RUD,NDENTS,JIDENT,3)
251 CONTINUE

C**********************************************************************
C PLOT RATTO.
C**********************************************************************
        CALL WINDOW(-1.,RIGHT,-.5,10.)
        CALL PLOTS(0,0,0)
        CALL IRPLOT(RATIO,RATLO,DELR,VLOG,VLOGLO,DELLOG,XAXIS,LP,
CONTINUE
   IF (DELaP .EQ. 0 .)  GOTO 266
   CALL WINDOW(-1.,RIGHT,-.5,10.)
   CALL PLOTS(0,0,0)
   CALL IRPLOT(ALPHA,ALPLO,DELaP,VLOG,VLOGLO,DELLOC,XAXIS,LP,
   *'ALPHA (CM-1)',12,'LOG10 FREQUENCY',15, JLN,LSY,
   *RUN,NDECKS,IDENT,RUD,NDENTS,IDENT,2)
266 CONTINUE
   IF (DELaG .EQ. 0 .)  GOTO 301
   CALL WINDOW(-1.,RIGHT,-.5,10.)
   CALL PLOTS(0,0,0)
   CALL IRPLOT(ALOG,ALOGLO,DELaG,VLOG,VLOGLO,DELLOC,XAXIS,LP,
   *'LOG10 ALPHA',11,'LOG10 FREQUENCY',15, JLN,LSY,
   *RUN,NDECKS,IDENT,RUD,NDENTS,IDENT,4)
301 CONTINUE
302 CONTINUE
401 CONTINUE
501 CONTINUE
STOP
C
C **ắng programmes SORTFREQ
C
C THIS PROGRAM WILL COMBINE (SORT) UP TO THREE SEPERATE FILES STORED
C ON AN TSO ACCOUNT AND WRITE THEM FOR INPUT TO PROGRAM KRAMKROC.
C
C
COMON W,RA,L,S,NPTOT
          REAL IDENT
*W(8000),VLOC(8000),R(8000),S(8000),AB(8000)
10 FORMAT (I1,10I2)
20 FORMAT (6F10.0)
30 FORMAT (F6.0,15A4)
40 FORMAT (1H1)
50 FORMAT (1X,F6.2,1X,15A4)
60 FORMAT (1X,'THE NUMBER OF DATA POINTS IS ',I4,/) 
70 FORMAT (1X,5(F8.2,1X,F8.5,1X,F3.0,2X))
80 FORMAT (/2X,8HINT(CM-1),4X,15HINTS AVERAGED,4X,5HRATIO,14X,
*SHALPHA,7X,8HINT(CM-1),4X,15HINTS AVERAGED,4X,5HRATIO,14X,
*SHALPHA,/) 
90 FORMAT (26X,'REGULAR',5X,'SMOOTH',44X,'REGULAR',5X,'SMOOTH')
100 FORMAT (1X,2(F9.2,3X,F10.3,3X,F7.4,16X,F8.3,6X))
110 FORMAT(3H3)
120 FORMAT(26H10. 0. 50000.)
130 FORMAT(53H0. 10000. -50. 50. 0. 1.5)
140 FORMAT(53H0. 50. 0. 500. 0. 2.0)
150 FORMAT(0. 50. 0. 2.0 0. 0.20)
160 FORMAT (F6.2,15A4)
170 FORMAT(52H40000. 0.8 17.094 1.00 10. -1.0)
180 FORMAT (F9.2,1X,F8.6,2X,F5.2)
190 FORMAT(9H -1.0)
200 FORMAT(4H99.)
210 FORMAT(3H0-1)
220 FORMAT(2H/#)
C
C
C*****************************************************************************
C
C
C
CARD#1 I FORMAT
C
1: 1=> READ TSO FILE FROM READ(10,...; 0=> SKIP
C 2-3: 1=> READ TSO FILE FROM READ(11,...; 0=> SKIP
C 4-5: 1=> READ TSO FILE FROM READ(12,...; 0=> SKIP
C 6-7: 1=> PUNCH A RESULT FILE ON WRITE(9,...; 0=> SKIP
C 8-9: A NUMBER FROM 1-14 THAT SPECIFIES SYMBOL TO BE USED
C 10-11: 1=> SYMBOLS & LINES; 0=> LINES; -1=> SYMBOLS
C
C
CARD#2 F FORMAT
C
1-10: LENGTH OF X-AXIS IN INCHES.
11-20: STARTING WAVELENGTH ON X-AXIS.
21-30: ENDING WAVELENGTH ON X-AXIS. (0=> NO COMMON PLOTS)
31-40: STARTING LOGARITHMIC WAVELENGTH ON X-AXIS.
41-50: ENDING LOGARITHMIC WAVELENGTH ON X-AXIS, 0=> NO PLOTS

CARD#3 F FORMAT
1-10: STARTING NUMBER FOR DATA ON Y-AXIS.
11-20: ENDING NUMBER FOR DATA ON Y-AXIS. 0=> NO RATIO PLOTS

CALL AZERO(W,8000)
CALL AZERO(R,8000)
CALL AZERO(AB,8000)
CALL AZERO(RUN,4)
DO 230 K = 1,0000
    S(K) = 1.0
230 CONTINUE
NPTOT=0

I=1
READ(5,10) ITIN,IEVK,ITTV,IPCHI,LSY,JLN
READ(5,20) XAXIS,VLO,VIH,VLOCHL,VLOCHI
READ(5,20) RATLO,PARI
DELI=(VIH-VLO)/XAXIS
DELLOC=(VLOCHL-VLOCHI)/XAXIS
DEL=(RATHI-RATLO)/10.

C HEADER CARDS FOR EACH RUN SHOULD BE STORED IN THE TSO FILE
CARD#1 F FORMAT
1-6: RUN NUMBER
7-35: RUN TITLE IN ALPHANUMERICS.
CARD#2 F FORMAT
1-10: GAIN WHICH WILL DIVIDE THE ENTIRE FILE.

IF (ITIN) 300,300,240
240 CALL AZERO(V,2000)
CALL AZERO(RA,2000)
DO 250 K = 1,2000
    SG(K) = 1.0
250 CONTINUE
READ(10,30) RUN(1),(IEVT(K),K=1,15)
READ(10,20) GFACT
K=1

260 READ(10,20) V(K),RA(K),SG(K)
   IF (V(K)) 280,270,270
270 IF (SG(K).EQ.0.0) SG(K)=1.0
    RA(K)=RA(K)/GFACT
K = K + 1
GO TO 260

280 NPTEN = K - 1
WRITE(6,40)
WRITE(6,50) RUN(I), (IENNT(K), K = 1, 15)
I = I + 1
WRITE(6,60) NPTEN
NX = NPTEN/5
NX = NX/2
NX = NX*2
DO 290 K = 1, NX
J = K + NX
L = J + NX
M = L + NX
WRITE(6,70) V(K), RA(K), SG(K), V(J), RA(J), SG(J), V(L), RA(L), SG(L),
* V(N), RA(N), SG(N), V(M), RA(M), SG(M), V(K), RA(K), SG(K)
290 CONTINUE
CALL BUBBLE(V, RA, RA, SG, 1, NPTEN)

300 IF (IEVN) 370, 370, 310
310 CALL AZERO(V, 2000)
CALL AZERO(RA, 2000)
DO 320 K = 1, 2000
SG(K) = 1.0
320 CONTINUE
READ(11,30) RUN(I), (IENNT(K), K = 1, 15)
READ(11,20) CFACT

330 READ(11,20) V(K), RA(K), SG(K)
IF (V(K)) 350, 350, 360
340 IF (SG(K) . EQ. 0.0) SG(K) = 1.0
RA(K) = RA(K)/CFACT
K = K + 1
GO TO 330
350 NPEV = K - 1
WRITE(6,40)
WRITE(6,50) RUN(I), (IENNT(K), K = 1, 15)
I = I + 1
WRITE(6,60) NPEV
NX = NPEV/5
NX = NX/2
NX = NX*2
DO 360 K = 1, NX
J = K + NX
L = J + NX
M = L + NX
WRITE(6,70) V(K), RA(K), SG(K), V(J), RA(J), SG(J), V(L), RA(L), SG(L),
* V(N), RA(N), SG(N), V(M), RA(M), SG(M), V(K), RA(K), SG(K)
360 CONTINUE
    CALL BUBLE(V,RA,RA,SC,1,NPEVN)
C
370 IF (1TWV) 440,440,380
380 CALL AZERO(V,2000)
    CALL AZERO(RA,2000)
    DO 390 K=1,2000
       SG(K)=1.0
390 CONTINUE
    READ(12,30) RUN(I),(IDENT(K),K=1,15)
    READ(12,20) GFACT
    K=1
400 READ(12,20) V(K),RA(K),SG(K)
    IF (V(K)) 420,410,410
410 IF (SG(K).EQ.0.0) SG(K)=1.0
    RA(K)=RA(K)/GFACT
    K=K+1
    GO TO 400
420 NPTWV=K-1
    WRITE(6,40)
    WRITE(6,50) RUN(I),(IDENT(K),K=1,15)
    WRITE(6,60) NPTWV
    MX=NPTWV/5
    MX=MX/2
    MX=MX*2
    DO 430 K=1,MX
       J=K+MX
       L=J+MX
       N=L+MX
       WRITE(6,70) V(K),RA(K),SG(K),V(J),RA(J),SG(J),V(L),RA(L),SG(L),
                  V(N),RA(N),SG(N)
430 CONTINUE
    CALL BUBLE(V,RA,RA,SC,1,NPTWV)
C
C***********************************************************
C OUTPUT CONTAINED DATA
C***********************************************************
C
440 WRITE(6,40)
    WRITE(6,50)
    WRITE(6,60)
    MX=NPTOT/2
    MX=MX/2
    MX=MX*2
    DO 450 K=1,MX
       M=K+MX
       WRITE(6,100) V(K),S(K),R(K),AE(K),M(N),S(H),R(H),AE(M)
450 CONTINUE
C
C PUNCH DATA

C IF (IPNCH) 480,480,460
460 WRITE(9,110)
   WRITE(9,120)
   WRITE(9,130)
   WRITE(9,140)
   WRITE(9,150)
   WRITE(9,160) RUN(I),(IDENT(K),K=1,15)
   WRITE(9,170)
   DO 470 K=1,NPTOT
   WRITE(9,180) W(K),R(K),S(K)
470 CONTINUE
   WRITE(9,190)
   WRITE(9,200)
   WRITE(9,210)
   WRITE(9,220)
480 CONTINUE

C PLOT COMBINED DATA

C IF (VI) 510,510,490
490 IF (VLOG) 510,510,500
500 CALL IRPLOT(R,RATIO,DELIN,W,VLOG,DELLOG,XAXIS,NPTOT,
   *'RATIO',5,'FREQUENCY (CM-1)',16,JLN,LSY,NUM,NDECKS,IDENT,
   *RUN,IDENT,1)
510 IF (VLOGH) 550,550,520
520 DO 530 K=1,NPTOT
   VLOG(K)=ALOG10(W(K))
530 CONTINUE
      IF (VLOG) 550,550,540
540 CALL IRPLOT(R,RATIO,DELIN,W,VLOG,DELLOG,XAXIS,NPTOT,
   *'RATIO',5,'LOG10 FREQUENCY',15,JLN,LSY,
   *RUN,NDECKS,IDENT,NUM,IDENT,2)
550 CONTINUE
STOP
C PROGRAM KRAMKROC

REAL IDENT
REAL LOSS,LOSSLO,LOSSHI

DIMENSION W(3000),R(3000),SIGMA(3000),EPS(3000),DATA(3000),
*WLOG(3000),IDENT(15),RUN(2),EXIT(1000),SUMALP(3000),
*WEACK(3000),WPACK(3000),ISTR(2)

DATA IDENT/'PER ','CENT',' * P ','OINT','S = ','SMOO','THIN',
* 'G ',' ',' ',' ',' ',' ',' ',', '/

1 FORMAT(F6.0,15A4)
2 FORMAT (111)
3 FORMAT (8F10.0)
4 FORMAT (1X,F7.3,15A4)
5 FORMAT(1X,'FREE ELECTRON BEHAVIOR STARTS AT',F10.2,'CM-1',
* AND INTERBAND REGION GOES AS 1/W**',F5.2/
*1X,'UNIT CELL VOLUME IS',F7.1,'A**3')
6 FORMAT(4(2X,F8.2,1X,F8.5,1X,F8.5))
7 FORMAT(11,312)
8 FORMAT(5F10.0)
9 FORMAT(I5)
30 FORMAT(1X,'DATA SMOOTHED, NSM=',15)
405 FORMAT('FREE E STARTS',F10.2,'CM-1',/INTERBAND = 1/W**'
* ,F5.2,'CELL VOLUME IS',F7.1,'A**3')
410 FORMAT(2A4)
411 FORMAT(1X,2A4/)
WRITE (6,2)

C

C ******************************************************************************************
C THIS PROGRAM HAS TWO LOOPS. THE OUTER LOOP (DO 201 ...) ALLOWS THE
C CHANGE OF PLOTTING PARAMETERS. THE INNER LOOP (DO 101 ...) ALLOWS
C DIFFERENT RUNS TO BE PLOTTED WITH THE SAME PLOTTING PARAMETERS.
C THE INNER LOOP IS ENDED WITH A NEGATIVE RUN NUMBER, WHILE THE OUTER
C IS ENDED BY 0-1.
C
C HEADER CARDS FOR PLOTTING PARAMETERS
C
C CARD #1 I FORMAT
C
1: NUMBER WHICH SPECIFIES THE SYMBOL TO BE USED IN PLOTS
C 0=> END OUTER LOOP (SEE IRPLOT FOR LSY)
C
2-3: 1=> BOTH LINES AND POINTS WILL APPEAR ON GRAPHS;
C 0=> LINES ONLY; -1=> POINTS ONLY WILL APPEAR.
C
4-5: 0=> THE PROGRAM WILL DO THE INTEGRAL ON THE DATA AS
C GIVEN IN THE FILE; 1=> THE PROGRAM WILL DIVIDE THE
C DATA BY THE DATA WHICH IS SET AS FILE #8 BEFORE THE
C INTEGRAL. THEN IT WILL CORRECT FOR THE DIVIDED DATA
BY INTERPOLATING A CORRECT VALUE FOR THE REFLECTANCE
OF THE DIVIDED DATA AND THEN SCALE THE QUOTIENT;
2=> THE CORRECTION ONLY WILL BE DONE.
6-7: 1=> PUNCH THE FILE WITH KKTF; 0=> NO FILE.

CARD #2  F FORMAT
1-10: LENGTH OF X-AXIS IN INCHES
11-20: STARTING WAVEVECTOR ON X-AXIS
21-30: ENDING WAVEVECTOR ON X-AXIS (0=> NO LINEAR PLOTS)
31-40: STARTING LOGARITHMIC WAVEVECTOR ON X-AXIS
41-50: ENDING LOGARITHMIC WAVEVECTOR ON X-AXIS; 0=> NO PLOT

CARD #3  F FORMAT
1-10: STARTING NUMBER FOR SIGMA ON Y-AXIS
11-20: ENDING NUMBER FOR SIGMA ON Y-AXIS (0=> NO PLOTS)
21-30: STARTING NUMBER FOR EPSILON ON Y-AXIS
31-40: ENDING NUMBER FOR EPSILON ON Y-AXIS (0=> NO PLOTS)
41-50: STARTING NUMBER FOR REFLECTANCE ON Y-AXIS
51-60: ENDING NUMBER FOR REFLECTANCE (0=> NO PLOT)

NOTE: THE FOLLOWING ARE NOT SET TO PLOT WITH LOG FREQUENCY

CARD #4  F FORMAT
1-10: STARTING NUMBER FOR ALPHA ON Y-AXIS
11-20: ENDING NUMBER FOR ALPHA (0=> NO PLOTS)
21-30: STARTING NUMBER FOR EPSILON 2 ON Y-AXIS
31-40: ENDING NUMBER FOR EPSILON 2 (0=> NO PLOT)
41-50: STARTING NUMBER FOR LOSS FUNCTION ON Y-AXIS
51-60: ENDING NUMBER FOR LOSS FUNCTION (0=> NO PLOTS)

CARD #5  F FORMAT
1-10: STARTING NUMBER FOR EXTINCTION COEFFICIENT ON Y-AXIS
11-20: ENDING NUMBER FOR EXTINCTION COEFFICIENT; 0=> NO
21-30: STARTING NUMBER FOR THE SUM RULE ON Y-AXIS
31-40: ENDING NUMBER FOR SUM RULE (0=> NO PLOTS)
41-50: STARTING NUMBER FOR LOSS FUNCTION SUM RULE ON Y-AXIS
51-60: ENDING NUMBER FOR LOSS FUNCTION SUM RULE; 0=> NO
61-70: STARTING NUMBER FOR ALPHA SUM RULE ON Y-AXIS
71-80: ENDING NUMBER FOR ALPHA SUM RULE (0=> NO PLOT)

HEADER CARDS FOR EACH RUN

CARD #1
1-6: RUN NUMBER
7-35: RUN TITLE IN ALPHA NUMERICS

CARD #2
1-10: WAVEVECTOR AT WHICH FREE ELECTRON BEHAVIOR BEGINS
11-20: EXPONENT FOR W IN THE INTERBAND REGION.
21-30: VOLUME PER ELECTRON OF CFF IN CUBIC ANGSTROMS.
31-40: MULTIPLICATIVE FACTOR FOR THE REFLECTANCE.
(ASSUMED TO BE 1, IF LEFT BLANK)
41-50: % OF SMOOTHING TO BE DONE, IDEAL IS 100 (%), 0=> NONE
CHI SQ = %*(NUMBER OF POINTS).
51-60: EXTRAPOLATION PROCEDURE TO DC REFLECTANCE.
>0 => KNOWN DC CONDUCTIVITY IS HERE IN (OHM-CM)-1
=0 => REFLECTANCE IS CONSTANT FROM DC TO FIRST POINT
<0 => METALLIC CONDUCTIVITY ASSUMED. (R=1-A(W**1/2))
61-70: DC OFFSET OF REFLECTANCE, A NUMBER SUBTRACTED FROM
THE DATA.

DO 201 NTIMES=1,100
READ(5,7) LSY,JLN,IFLAG0,PUNCH
IF (IFLAG0.EQ.1) READ(8,7) III,JJJ,KKK
IF(LSY.EQ.0) GO TO 202
IF (IFLAG0,EQ.1) READ(8,8) AAA,BBB,CCC,DDD,EEE
READ(5,8) XAXIS,NLO,ULH,ULOGLO,ULOGH
IF (IFLAG0.EQ.1) READ(8,3) FFF,GGG,HHH,RRR,SSS,TTT
READ(5,3) SIGLO,SIGHI,EPSLO,EPSHI,DATA0,DATAH
IF (IFLAG0.EQ.1) READ(8,3) UUU,VVV,WWW,XXX,YYY,ZZZ
READ(5,3) ALPHLO,ALPHHI,EPS2LO,EPS2HI,LOSSLO,LOSSHI
IF (IFLAG0.EQ.1) READ(8,3) AAA,BBB,CCC,DDD,EEE
READ(5,3) EXTLO,EXTHI,SUMLLO,SUMLHI,SUMLHI,
*SUMLHI,SUMLHI
DELS=(SIGHI-SIGLO)/10.
DELEPS=(EPSHI-EPSLO)/10.
DELDAT=(DATAHI-DATALO)/10.
DELLIN=(ULH-VLO)/XAXIS
DELMLOG=(ULOGHI-ULOGLO)/XAXIS
DELALPH=(ALPHHI-ALPHLO)/10.
DELFP2=(EPS2HI-EPS2LO)/10.
DELOSS=(LOSSHI-LOSSLO)/10.
DELEXT=(EXTHI-EXTLO)/10.
DELSUM=(SUMLHI-SUMLLO)/10.
DELSUML=(SUMLHI-SUMLLO)/10.
DELSUML=(SUMLHI-SUMLLO)/10.
NSETS=1000
DO 101 NS=1,NSETS
READ(5,1) RUN(1), (1DELT(K),K=1,15)
IF (RUN(1).LT.0.0) GO TO 102
IF (IFLAG0.EQ.1) READ(8,1) RUN(1), (JDELT(K),K=1,15)
IF (IFLAG0.EQ.0) READ(10,1) RUN (FACE(K),K=1,15)
IF (IFLAG0,EQ.1) READ(8,3) SS,TT,HH,VV,WW,XX
READ(5,3) UA,DE,VC,FACTP,ASH COMB,RZEPS
ASH=ASH
IF (IFLAG0.EQ.1) PUL(1)=ASH
IF (FACTR.EQ.0.0) FACTR=1.0
*
DO 301 K=1,2990
READ(5,3) W(K),R(K)
IF(W(K).LT.0.0) GO TO 302
DATA(K)=R(K)
R(K)=(R(K)-RZERO)*FACTR
301 CONTINUE
302 N=K-1
DO 13 K=1,N
L=N-K+11
R(L)=R(L-10)
W(L)=W(L-10)
13 DATA(L)=DATA(L-10)
C
*************************************************************
C CALCULATE 10 DATA POINTS FROM LAST POINT TO DC.
C*************************************************************
C
N=11+10
W(2)=W(11)/10.
W(3)=W(11)/7.
W(4)=W(11)/5.
W(5)=W(11)/3.
W(6)=W(11)/2.
W(7)=W(11)/1.7
W(8)=W(11)/1.5
W(9)=W(11)/1.3
W(10)=W(11)/1.1
RAVE=0.
DO 14 L=11,15
14 RAVE=RAVE+R(L)/5.
A=(1.-R(11))/SQRT(W(11))
DO 15 L=1,10
DATA(L)=0.
IF (COND.GT.0.) R(L)=1.-SQRT(2.*W(L)/15./COND)
IF (COND.LE.0.) R(L)=RAVE
15 IF (COND.LT.0.) R(L)=1.-A*SQRT(W(L))
NP=N
IF (IFLAG.NE.1) GO TO 10
DO 303 K=1,2990
READ(8,3) WBACK(K),RBACK(K)
IF (WBACK(K).LT.0.0) GO TO 304
303 CONTINUE
304 WBACK=K-1
DO 305 K=1,WEACK
L=WBACK-K+11
RBACK(L)=RBACK(L-10)
305 WBACK=K-WEACK(L-10)
C
*************************************************************
C CALCULATE 10 DATA POINTS FROM LAST POINT TO DC.

C******************************************************************************

C
NEACK=NEACK+10
WBACK(1)=WBACK(11)/200.
WBACK(2)=WBACK(11)/50.
WBACK(3)=WBACK(11)/100.
WBACK(4)=WBACK(11)/50.
WBACK(5)=WBACK(11)/10.
WBACK(6)=WBACK(11)/5.
WBACK(7)=WBACK(11)/2.
WBACK(8)=WBACK(11)/1.7
WBACK(9)=WBACK(11)/1.3
WBACK(10)=WBACK(11)/1.1
RAVE=0.
DO 314 L=11,15
314 RAVE=RAVE+RBACK(L)/5.
A=(1.-RBACK(11))/SQRT(WBACK(11))
DO 315 L=1,10
IF (VW.GT.0.) RBACK(L)=1.-SQRT(2.*WBACK(L)/15./VW)
IF (VW.LE.0.) RBACK(L)=RAVE
315 IF (VW.LE.0.) RBACK(L)=1.-A*SQRT(WBACK(L))
CALL M1K0R(W.R,NP,WBACK,RBACK,NRACK,1)
10 CONTINUE
NP=N
IF (IFLAGO.EQ.0) GO TO 140
DO 120 K=1,1000
PFAD(10,3) VMIK(K),RMIR(K)
IF (VMIK(K).LT.0.0) GO TO 130
120 CONTINUE
130 RMIR=K-1
CALL M1KIR(W.R,NP,VMIR,RMIR,NHTR,0)
CALL CORRET(NP,W.R,DATA)
140 CONTINUE
IF(NSM.NE.0) GO TO 12
C
C******************************************************************************

C SMOOTH REFLECTANCE.
C******************************************************************************

C
WRITE(6,8(N=1,NP)) NSM
X:=.9P
S=ASIN(XX/100.
CALL SETUPS(W.R,NP,S)
KP:=1
12 CONTINUE
C
C******************************************************************************

C OUTPUT DATA.
C******************************************************************************
C

IF (IPUNCH.NE.1) GO TO 150
CALL GOPARM(LEN,ISTR)
IF (LEN.NE.8) GO TO 202
WRITE(9,410) ISTR
WRITE(6,411) ISTR

150 WRITE(6,4) RUN(1), IDENT(K), K=1,15
IF (IPUNCH.EQ.1) WRITE(9,4) RUN(1), IDENT(K), K=1,15
IF (IFLAGO.EQ.1) WRITE(6,4) RUD(1), IDENT(K), K=1,15
IF (IPUNCH.EQ.1.AND.IFLAGO.EQ.1) WRITE(9,4) RUD(1),
*(IDENT(K), K=1,15)
IF (IFLAGO.NE.0) WRITE(6,4) RUN,(BACK(K), K=1,15)
IF (IFLAGO.NE.0.AND.IPUNCH.EQ.1) WRITE(9,4) RUN,(BACK(K), K=1,15)
WRITE(6,5) WA,DE,VC
IF (IPUNCH.EQ.1) WRITE(9,405) WA,PE,VC
MX=N/4
NX=NX/2
MX=MX*2
DO 20 K=1,NX
L=K+MX
M=L+MX
NP=M+MX
IE (R(K).GT..999) R(K)=.999
IF (R(L).GT..999) R(L)=.999
IF (R(M).GT..999) R(M)=.999
IF (R(NP).GT..999) R(NP)=.999
WRITE(6,6) V(K),V(K),DATA(K),V(L),V(L),DATA(L),V(M),V(M),DATA(M), *
*(V(NP),V(NP),DATA(NP)
WLOG(I)=ALOG10(V(K))
WLOG(L)=ALOG10(V(L))
WLOG(M)=ALOG10(V(M))
WLOG(NP)=ALOG10(V(NP))

20 CONTINUE
WRITE(6,2)
WRITE(6,80) ESM
WRITE(6,4) RUN(1), IDENT(V), V=1,15
IF (IFLAGO.EQ.1) WRITE(6,4) RUN(1),(IDENT(V), V=1,15)
IF (IFLAGO.EQ.0) WRITE(6,4) RUN,(BACK(V), V=1,15)
CALL KITF(X,PE,WA,DE,VC SIGIA,EPS DATA,ALPHA,EPS?,LOSS,EXT,SYM
*SUNLO,SUNALP,IPUNCH)
WRITE (6,2)

C
C***********************************************************************
C PLOT DATA.
C***********************************************************************
C
IF(WIT) 40,60,30
30 IF(SIGIA) 32,33,31
31 CALL IPILOT(SIGIA,SIGLO,DELS.W,DELX.XAXIS,N,
*SIGIA (CN-CN)-1',16,'FREQUENCY (CN-1)',16,JLY,LSY,
*RUN, 1, IDENT, RUD, 1, JIDENT, 1)

33 IF (EPSH1) 36, 36, 34
34 CALL IRPLOT(EPS, EPSLO, DELEPS, W, WLO, DELLIN, XAXIS, N,
             *'EPSILON 1', 'FREQUENCY (CM-1)', 16, JLN, LSY,
             *RUN, 1, IDENT, RUD, 1, JIDENT, 1)
36 IF (DATAH1) 39, 39, 37
37 CALL IRPLOT(DATA, DATALO, DELDAT, U, WLO, DELLIN, XAXIS, N,
             *'REFLECTION', 'FREQUENCY (CM-1)', 16, JLN, LSY,
             *RUN, 1, IDENT, RUD, 1, JIDENT, 1)
39 IF (WLOGH1) 50, 50, 40
40 IF (SICHI) 43, 43, 41
41 CALL IRPLOT(SIGMA, SIGLO, DELSIG, WLOGLO, DELLOG, XAXIS, N,
             *'SIGMA (G M-CH)-1', 'LOG10 FREQUENCY', 15, JLN, LSY,
             *RUN, 1, IDENT, RUD, 1, JIDENT, 2)
43 IF (EPSH1) 46, 46, 44
44 CALL IRPLOT(EPS, EPSLO, DELEPS, WLOCLO, DELLOC, XAXIS, N,
             *'EPSILON 1', 'LOG10 FREQUENCY', 15, JLN, LSY,
             *RUN, 1, IDENT, RUD, 1, JIDENT, 2)
46 IF (DATAH1) 49, 49, 47
47 CALL IRPLOT(DATA, DATALO, DELDAT, WLOCLO, DELLOC, XAXIS, N,
             *'REFLECTION', 'LOG10 FREQUENCY', 15, JLN, LSY,
             *RUN, 1, IDENT, RUD, 1, JIDENT, 2)
49 IF (WULT) 70, 70, 50
50 IF (ALPHH1) 62, 62, 61
51 CALL IRPLOT(ALPHA, ALPHLO, DELALPHA, U, WLO, DELLIN, XAXIS, N,
             *'ALPHA (HECM)', 'FREQUENCY (CM-1)', 16, JLN, LSY.
             *RUN, 1, IDENT, RUD, 1, JIDENT, 1)
52 IF (EPS2H1) 64, 64, 63
53 CALL IRPLOT(EPS2, EPS2LO, DELEPS2, W, WLO, DELLIN, XAXIS, N,
             *'EPSILON 2', 'FREQUENCY (CM-1)', 16, JLN, LSY,
             *RUN, 1, IDENT, RUD, 1, JIDENT, 1)
56 IF (LOSSH1) 68, 68, 67
57 CALL IRPLOT(LOSS, LOSSLO, HELLOSS, W, WLO, DELLIN, XAXIS, N,
             *'LOSS FUNCTION', 'FREQUENCY (CM-1)', 16, JLN, LSY,
             *RUN, 1, IDENT, RUD, 1, JIDENT, 1)
59 IF (EXTH1) 70, 70, 50
60 IF (SULH1) 72, 72, 71
61 CALL IRPLOT(SUM, SULLO, DELSUM, U, WLO, DELLIN, XAXIS, N,
             *'SUM RULE', 'FREQUENCY (CM-1)', 16, JLN, LSY,
             *RUN, 1, IDENT, RUD, 1, JIDENT, 1)
64 IF (SUMLH1) 74, 74, 73
65 CALL IRPLOT(SUMALPHA, SUMALPHLO, DELSUMALPHA, U, WLO, DELLIN, XAXIS, N,
             *'ALPHA SUM RULE', 'FREQUENCY (CM-1)', 16, JLN, LSY,
*RUN, 1, IDENT, RUD, 1, JDENT, 1)

74 CONTINUE
101 CONTINUE
102 CONTINUE
201 CONTINUE
202 CONTINUE
STOP
FUNCTION AP0D (XK,XORIG,XNP,C0,C1,C2,C4,NEXP)
C**************************************************************************************************
  X1=XORIG-1.
  X2=XNP-XORIG
  XMMax=X2
  IF (X1.GT. X2) XMMax=X1
  UK=ABS((XK-XORIG)/XMMax)
  UPAR=1.0-UK**NEXP
  AP0D=C0+C1*UPAR+C2*UPAR**2+C4*UPAR**4
RETURN
SUBROUTINE APODIZ(Y,NP,KF,IAPOD,RES,XEPS)
C******************************************************************
C THIS ROUTINE SET THE PARAMETERS FOR APOD
C******************************************************************
C
DIMENSION Y(NP)
IA=IAPOD+1
GO TO (123,122,121,120,119),IA
119 C0=0.
   C1=1.
   C2=0.
   C4=0.
   NEXP=1
   RES=RES*2.0
   GOTO 125
120 C0=0.09
   C1=0.0
   C2=0.5875
   C4=0.3225
   NEXP=2
   RES=1.6*RES
   GOTO 125
121 C0=0.26
   C1=-0.154833
   C2=0.944838
   C4=0.0
   NEXP=2
   RES=1.4*RES
   GOTO 125
122 C0=0.548
   C1=-0.0533
   C2=0.5353
   C4=0.0
   NEXP=2
   RES=1.2*RES
   GOTO 125
123 C0=1.0
   C1=0.0
   C2=0.0
   C4=0.0
   NEXP=1
125 CONTINUE
   Y0=IC=1.
   IF (1:F .EQ. 1) GOTO 73
   XB=KF-1
   X0=KF
  XA=KF+1
   YB=Y(KF-1)
   Y0=Y(KF)
YA=Y(KF+1)
T1=Y0*(XA*XA-XB*XB)
T2=YB*(XA*XA-X0*X0)
T3=YA*(X0*X0-XB*XB)
XORIC=(T1-T2-T3)/(2.*Y0-YB-YA)/2.

73 CONTINUE
XNP=NP
DO 72 K=1,NP
XK=K
Y(K)=Y(K)*APOD(XK,XORIC,XNP,C0,C1,C2,C4,NEXP)
72 CONTINUE
IF (YA.GT.YB) KF=KF+1
XKF=KF
XEPS=XORIC-XKF
RETURN
SUBROUTINE AVEDEV (X,N1,N2,NPTS,XAVE,SUN)
C
C****************************************************************************************************************************
C THIS SUBROUTINE CALCULATES THE AVERAGE AND DEVIATION OF DATA
C****************************************************************************************************************************
C
DIMENSION X(NPTS)
XN=N2-N1+1
XAVE=0.
DO 10 M=N1,N2
XAVE=XAVE+X(M)/XN
10 CONTINUE
SUM=0.
DO 20 M=N1,N2
SUM=SUM+X(M)-XAVE)**2/XN
20 CONTINUE
RETURN
SUBROUTINE AVVAL1(Y, NP, NSPTS, RES)
C
C******************************************************************************
C CALLS AVEDEV AND CALCULATES RESOLUTION, ONE SIDED
C******************************************************************************
C
DIMENSION Y(NP)

1 FORMAT(1X,'AV VAL=','F10.3',' STD DEV=','F10.5',' STD DEV/AV VAL=','F6.3',' % UNAPODISED RESOLUTION=','F7.3',' CM-1')

XNP=NP

IF ((NSPTS .LT. NP) .AND. (NSPTS .NE. 0)) NP=NSPTS

XN=NP

RES=RLS*XNP/XN

JJ=NP-NP/8

CALL AVEDEV (Y, JJ, NP, NP, YAVE, SUM)

DO 37 K=1,NP

Y(K)=(Y(K)-YAVE)

37 CONTINUE

SDEV=SQRT(SUM)

SDPCT=SDEV/YAVE*100.

WRITE(6,1) YAVE, SDEV, SDPCT, RES

RETURN
SUBROUTINE AVVAL2 (Y,NP,NSPTS,KF,RES)

C*****************************************************************************
C CALLS AVEDEV AND CALCULATE RESOLUTION, TWO SIDED
C*****************************************************************************
C
DIMENSION Y(NP)

1 FORMAT(1X,'AV VAL=',F10.3,' STD DEV=',F10.5,' STD DEV/AV VAL=',F6.3,'% UNAPODISED RESOLUTION=',F7.3,' CM-1')
XNP=NP

IF ((NSPTS.CT. NP).OR. (NSPTS.EQ.0)) GOTO 45
KS=NP/2-NSPTS/2
DO 44 K=1,NSPTS
   Y(K)=Y(K+KS)
44 CONTINUE
KF=KF-NP/2+NSPTS/2
NP=NSPTS

45 CONTINUE
XN=NP
RES=2.*RES*XNP/XN
JJ=NP/16+1
CALL AVEDEV(Y,1,JJ,NP,YAVB,SUM)
SDEVB=SQRT(SUM)
SDPCB=SDEVB/YAVB*100.0
JJ=NP/NP/16
CALL AVEDEV(Y,JJ,NP,NP,YAVT,SUM)
SDEVT=SQRT(SUM)
SDPCT=SDEVT/YAVT*100.0
XNP=NP
DO 64 K=1,NP
   XK=K
   Y(K)=Y(K)-(YAVE+(YAVT-YAVE)*XK/XNP)
64 CONTINUE
WRITE(6,1) YAVE,SDEVB,SDPCB,RES
WRITE(6,1) YAVT,SDEVT,SDPCT,RES
RETURN

1
SUBROUTINE BUBBLE(V,RATIO,ALPHA,KFIRST,KLAST)

C******************************************************************************************
C BUBBLE SORT FOR COMBINING SMALL ARRAYS INTO ONE ARRAY.
C ALL SORTING OCCURS ON ARRAY V ONLY, RATIO AND ALPHA ARE DEPENDENT ON V.
C
C THE CONDITIONS ON THE COMBINING SORT ARE (26/JUN/81):
C 1) ONLY ELEMENTS BETWEEN KFIRST AND KLAST ARE COMBINED FROM V,
   RATIO AND ALPHA INTO W, R, AND AB.
C 2) THE ELEMENTS OF V ARE PLACED INTO ARRAY W SUCH THAT W ELEMENTS
   ARE ARRANGED FROM LOWEST VALUE TO HIGHEST VALUE.
C 3) IF THE DISTANCE BETWEEN ELEMENTS IN V ARE LESS THAN THE
   ELEMENTS OF W THEN THE ELEMENTS OF V ARE INSERTED INTO W.
C 4) HOWEVER IF AN ELEMENT OF V IS NEAR AN ELEMENT OF W THEN THE TWO
   ELEMENTS ARE AVERAGED TOGETHER. NEAR IN THIS CASE IS WITHIN
   20% OF THE DISTANCE BETWEEN ELEMENTS IN V.
C 5) IF THE DISTANCE BETWEEN ELEMENTS IN V IS GREATER THAN THE
   ELEMENTS OF W THEN THE ELEMENTS IN V ARE AVERAGED WITH THE
   NEAREST ELEMENT OF W.
C
C THE ARRAY S INDICATES THE NUMBER OF ELEMENTS AVERAGED TOGETHER IN
C THE COMBINED ARRAYS.
C V, RATIO AND ALPHA ARE DIMENSIONED ARRAYS WITH 1000 ELEMENTS.
C W, R, AB AND S ARE ARRAYS IN COMMON WITH 8000 ELEMENTS.
C NPTOT IS THE TOTAL NUMBER OF ELEMENTS IN THE COMBINED ARRAYS. NPTOT
C SHOULD BE INITIALIZED TO ZERO IN THE MAIN PROGRAM. NPTOT IS IN THE
C COMMON BLOCK ALSO.
C
C NOTE: THE ARRAYS W, R, AB AND S SHOULD BE INITIALIZED TO 0.0, S=1.0
C
C PROGRAM BY I'EVIN CUNNINGHS
C
C******************************************************************************************

COMMON W,R,AB,S,NPTOT
DIMENSION V(1000),RATIO(1000),ALPHA(1000)
SPTOT=SPTOT+(KLAST-KFIRST)+1
M=1
250 DO 200 J=KFIRST,KLAST
  S=SPTOT+1
  10 255 L=1,2:SPTOT
  I=1-1
  W(SPTOT-K)=V(SPTOT-K-1)
  R(SPTOT-K)=R(SPTOT-K-1)
  AB(SPTOT-K)=AB(SPTOT-K-1)
  255 S(SPTOT-K)=S(SPTOT-K-1)
  V(1)=V(J)
  K(1)=RATIO(J)
  200 CONTINUE
  M=M+1
\[ AB(1) = \text{ALPHA}(J) \]
\[ S(1) = 1. \]

260 IF (W(ND+1) .NE. 0.) GO TO 265
IF (J.EQ.1) \( DV = \text{ABS}(V(J+1)-V(J)) \)
IF (J.NE.1) \( DV = \text{ABS}(V(J)-V(J-1)) \)
\( BAVE = W(ND) - 2*DV \)
IF (BAVE.LE.W(ND-1)) GO TO 267
GO TO 295

265 IF (W(ND+1).GE.W(ND)) GO TO 270
\( \text{HOLD} = W(ND+1) \)
\( \text{AHHOLD} = \text{AL}(ND+1) \)
\( \text{SHOLD} = S(HD+1) \)
\( W(ND+1) = W(ND) \)
\( R(ND+1) = R(ND) \)
\( \text{AB} = \text{AL}(ND+1) \)
\( S(ND+1) = S(ND) \)
\( W(ND) = \text{HOLD} \)
\( R(ND) = \text{AHHOLD} \)
\( \text{AB} = \text{SHOLD} \)
\( \text{ND} = ND+1 \)
GO TO 260

270 IF (J.EQ.1) \( DV = \text{ABS}(V(J+1)-V(J)) \)
IF (J.NE.1) \( DV = \text{ABS}(V(J)-V(J-1)) \)
\( TAVE = W(ND) + 2*DV \)
\( BAVE = W(ND) - 2*DV \)
IF (BAVE.GE.W(ND+1)) GO TO 275
IF (BAVE.LE.W(ND-1)) GO TO 287
GO TO 285

275 \( W(ND) = (W(ND+1) + S(ND+1) + H(ND)) / (S(ND+1) + 1.) \)
\( R(ND) = (R(ND+1) + S(ND+1) + R(ND)) / (S(ND+1) + 1.) \)
\( \text{AB} = (\text{AB}(ND+1) + \text{S}(ND+1) + \text{AB}(ND)) / (S(ND+1) + 1.) \)
\( S(ND) = S(ND+1) + 1. \)
\( \text{ND} = ND+1 \)
\( \text{NPTOT} = \text{NPTOT} - 1 \)
DO 280 K = ND, NPTOT
\( W(K) = W(K+1) \)
\( R(K) = R(K+1) \)
\( \text{AB}(K) = \text{AB}(K+1) \)
280 \( S(K) = S(K+1) \)
\( W(NPTOT) = 0. \)
\( R(NPTOT) = 0. \)
\( \text{AB}(NPTOT) = 0. \)
\( S(NPTOT) = 1. \)
GO TO 295

285 IF (W(K-2).LE.0.) \( \text{WLP} = W(ND+2) - W(ND+1) \)
IF (W(K-2).EQ.0.) AND (W.K.LT.2.) \( \text{WLP} = W(K+1) - W(K) \)
IF (W(K+2).EQ.0.) AND (W.K.LT.1.) \( \text{WLP} = W+1. \)
IF (W.K.GE.3) \( \text{WLP} = W(K-1) - W(K-2) \)
IF (ND.EQ.2) DWDN=W(ND+1)-W(ND-1)
IF (ND.EQ.1) DWDN=DV+1.
WUP=W(ND+1)-W(ND)
IF (ND.GE.2) WDN=W(ND)-W(ND-1)
IF (ND.LT.2) WDN=DV
IF (DV.LE.DWUP) GO TO 295
IF (DV.LE.DWDN) GO TO 295
IF (WUP.LT.WDN) GO TO 275

287  W(ND)=(W(ND-1)*S(ND-1)+W(ND))/(S(ND-1)+1.)
R(ND)=(R(ND-1)*S(ND-1)+R(ND))/(S(ND-1)+1.)
AE(ND)=(AE(ND-1)*S(ND-1)+AE(ND))/(S(ND-1)+1.)
S(ND)=S(ND-1)+1.
NHND=ND-1
NPTOT=NPTOT-1
DO 290 K=NHND,NPTOT
  W(K)=W(K+1)
  R(K)=R(K+1)
  AE(K)=AE(K+1)
290  S(K)=S(K+1)
  W(NPTOT)=0.
  R(NPTOT)=0.
  AE(NPTOT)=0.
  S(NPTOT)=1.
295  ND=1
300  CONTINUE
NCOUNT=1
297  IF (V(NCOUNT).EQ.0.) GO TO 298
     NCOUNT=NCOUNT+1
     GO TO 297
298  NPTOT=NCOUNT-1
301  CONTINUE
RETURN
SUBROUTINE CBAND(FREQ,F,X8,Y8,DY8,A5,A6,A7,A8)
C
C*****************************************************************************************
C THIS ROUTINE INTERPOLATES A VALUE FROM A CUBIC SPLINE FIT TO DATA
C
C*****************************************************************************************
C
C PROGRAM BY KEVIN CUMMINGS
C*****************************************************************************************
C
DIMENSION X8(50),Y8(50),DY8(50),A5(50),A6(50),A7(50),A8(50)
DOUBLE PRECISION X8,Y8,DY8,A5,A6,A7,A8
J=1
10 IF (FREQ.LT.X8(J)) GO TO 20
   J=J+1
   GO TO 10
20 J=J-1
   F=A5(J)+A6(J)*(FREQ-X8(J))+A7(J)*(FREQ-X8(J))**2+A8(J)*$(FREQ-X8(J))**3
RETURN
SUBROUTINE CORRET(N,W,R,RHOLD)

C******************************************************************************
C THIS ROUTINE INSERTS A PORTION OF DATA INTO ANOTHER DATA SET.
C A LINEAR SCALE IS USED TO MATCH END POINTS.
C
C PROGRAM BY KEVIN CUMMINGS
C******************************************************************************
C
DIMENSION W(K),R(K),RHOLD(N)
DO  10 K=1,N
  IF (W(K).LE.15000.) N1 = K
  IF (W(K).LE.25000.) N2 = K
10   CONTINUE
B=R(N1)/RHOLD(N1)
A=(R(N2)-R(N1)*RHOLD(N2)/RHOLD(N1))/((W(N2)-W(N1))*RHOLD(N2))
DO 20 L=N1,N2
  R(L)=(A*(W(L)-W(N1))+B)*RHOLD(L)
20   CONTINUE
RETURN

SUBROUTINE CUBEIT(N,S,X8,Y8,DY8,A5,A6,A7,A8)
C
C*************************************************************************************************
C THIS ROUTINE INPUTS DATA, CALCULATES THE PARAMETERS TO A LINEAR
C SPLINE FIT TO THE DATA AND OUTPUTS ALL INFORMATION.
C
C PROGRAM BY KEVIN CUMMINGS
C*************************************************************************************************
C
DOUBLE PRECISION X8,Y8,DY8,A5,A6,A7,A8
DIMENSION X8(50),Y8(50),DY8(50),A5(50),A6(50),A7(50),A8(50)
WRITE(6,1)
1 FORMAT(1HO)
2 FORMAT(8F10.0)
K=1
10 READ(5,2) X8(K),Y8(K),DY8(K)
   IF (DY8(K).EQ.0.) DY8(K)=1.
   IF(X8(K)) 14,13,13
13 K=K+1
   GO TO 10
14 N=K-1
   CALL LINEAR(X8,Y8,DY8,N,S,A5,A6,A7,A8)
   DO 20 J=1,N
      WRITE(6,8) X8(J),Y8(J),DY8(J),A5(J),A6(J),A7(J),A8(J)
20 FORMAT(2X,7(E12.4,3X))
   CONTINUE
   WRITE(6,1)
RETURN
SUBROUTINE CUBFIT(N,S,X9,Y9,DY9,A0,A1,A2,A3,WP)

C THIS ROUTINE INPUTS DATA, SUBTRACTS THE DRUDE MODEL VALUE,
C FITS A LINEAR FUNCTION TO THE DATA AND OUTPUTS ALL INFORMATION
C
C PROGRAM BY KEVIN CUMMINGS

C*******************************************************************************

C
DOUBLE PRECISION X9,Y9,DY9,A0,A1,A2,A3
DIMENSION X9(50),Y9(50),DY9(50),A0(50),A1(50),A2(50),A3(50)
WRITE(6,1)
1 FORMAT(110)
2 FORMAT(8F10.0)
K = 1
READ(5,2) X9(K),Y9(K),DY9(K)
IF (LY9(K).EQ.0.) Y9(K)=1.
Y9(K)=Y9(K)+(WP**2)/(X9(K)**2)
14 K = K + 1
13 N = K-1
CALL LINEAR(X9,Y9,DY9,..,S,A0,A1,A2,A3)
DO 20 J = 1,N
WRITE(6,8) X9(J),Y9(J),DY9(J),A0(J),A1(J),A2(J),A3(J)
8 FORMAT(2X,7(E12.4,3X))
20 CONTINUE
WRITE(6,1)
RETURN
SUBROUTINE DBAND(FREQ,F,X9,Y9,DY9,A0,A1,A2,A3)

C
C***********************************************************************
C THIS ROUTINE INTERPOLATES A VALUE FROM A CUBIC SPLINE FIT TO DATA
C
C***********************************************************************
C
C PROGRAM BY KEVIN CUNNINGS
C***********************************************************************
C
DIMENSION X9(50),Y9(50),DY9(50),A0(50),A1(50),A2(50),A3(50)
DOUBLE PRECISION X9,Y9,DY9,A0,A1,A2,A3
J=1
10 IF (FREQ.LT.X9(J)) GO TO 20
    J=J+1
    GO TO 10
20  J=J-1
    F=A0(J)+A1(J)*(FREQ-X9(J))+A2(J)*(FREQ-X9(J))**2+A3(J)*$(FREQ-X9(J))**3
RETURN
SUBROUTINE GRIDLC(FVAL, DELTA, AXLEN, Y, NY, NYNUM, NINTEC)

C ************************************************************
C SUBROUTINE TO CALCULATE PARAMETERS FOR LOGARITHMIC GRAPHS IN IRPLOT
C PARAMETERS ARE USED IN VERSATEC ROUTINE GRID.
C
C PROGRAM BY CHARLES PORTER
C
C ************************************************************

DIMENSION X(100), Y(12), ARRLOG(9)
DIMENSION FNUM(12)
DATA ARRLOG / 0.30103, 0.1760913, 0.1249387, 0.09691001, 0.07918125,
* 0.06694679, 0.057991947, 0.051152522, 0.045757491 /
TVAL = FVAL + DELTA * AXLEN
SCL = 1. / DELTA
IF FVAL = EVAL
TTVAL = TVAL

C FIRST COMPUTE NO. OF WHOLE NUMBER AND NUMBER
C OF INTERVALS (CYCLES OR FRACTIONS OF CYCLES)

NINTVL = ITVAL - IFVAL
NINTEC = ITVAL - IFVAL + IFIX(SIGN(1., TVAL) - SIGN(1., FVAL)) / 2
TFRAC = TVAL - FLOAT(ITVAL)
FFRAC = FVAL - FLOAT(IFVAL)
IF (TFRAC .GT. 0.) NINTVL = NINTVL + 1
IF (FFRAC .LT. 0.) NINTVL = NINTVL - 1
IF (FFRAC .EQ. 0.) NINTEC = NINTEC + 1

C COMPUTE LARGE-SCALE OVERLAY ON INTEGRAL NUMBER
C OF CYCLES

IF (NINTVL .EQ. 1) GO TO 30
Y(1) = -SCL * FFRAC
IF (FFRAC .GE. 0.) Y(1) = Y(1) + SCL
IF (.3 .GT .0.) GO TO 20
NCRT = NINTVL - 1
DO 10 I = 2, NCRT
10 Y(I) = SCL
20 Y(NINTVL) = SCL * FFRAC
IF (TFRAC .GE. 0.) Y(NINTVL) = Y(NINTVL) + SCL
GO TO 40
30 Y(NINTVL) = SCL

C COMPUTE LOGARITHMIC GRID INTERVALS

40 IF (.3 .EQ. 1) GO TO 90
1 = I
J = 1
FTERM = -FFRAC
IF (FFRAC .GE. 0.) FTERM = FTERM + 1.
SU! = 0.
50 I = I + 1
ICTR = 10 - I
SUM = SUM + ARLLOG(ICTR)
IF (SUM .LT. FTERM) GO TO 50
SUM = SUM - ARLLOG(ICTR)
X(J) = SCL * (FTERM - SUM)
55 ICTR = ICTR + 1
IF (ICTR .GT. 10) GO TO 60
J = J + 1
X(J) = SCL * ARLLOG(ICTR)
GO TO 55
60 IF (NINTVL .EQ. 2) GO TO 75
ITEST = NINTVL - 1
DO 70 I = 2, ITEST
DO 65 K = 1, 9
J = J + 1
65 X(J) = SCL * ARLLOG(K)
70 CONTINUE
75 TTFRM = TFRAC
IF (TFRAC .LT. 0.) TTFRM = TTFRM + 1.
SU! = 0.
DO 80 I = 1, 9
J = J + 1
ICTR = 1
X(J) = SCL * ARLLOG(I)
SUM = SUM + ARLLOG(I)
IF (SUM .LE. TTFRM) GO TO 85
80 CONTINUE
85 CONTINUE
SUM = SUM - ARLLOG(ICTR)
X(J) = SCL * (TTFRM - SUM)
GO TO 120

C  DO CASE OF ONE CYCLE OR LESS AS SPECIAL
C
90 FTERM = FFRAC
IF (FFRAC .LT. 0.) FTERM = FTERM + 1.
TTFRM = TFRAC
IF (TFRAC .LT. 0.) TTFRM = TTFRM + 1.
SU! = 0.
I = 0
J = 1
95 I = I + 1
SUM = SUM + ARLLOG(1)
IF (SUM .LE. FTERM) GO TO 95
X(J) = SCL * (SUM - FTERM)
100 IF (SUM .GT. TTFRM) GO TO 110
105 I=I+1
  J=J+1
  X(J)=SCL*ARRLOG(I)
  SUM=SUM+ARRLOG(I)
  IF (SUM .LT. TTERM) GO TO 105
  SUM=SUM-ARRLOG(I)
  X(J)=SCL*(TTERM-SUM)
  GO TO 120
110 X(J)=SCL*(TTERM-FTERN)

C
C  COMPUTE NUMBERS
C

120 ANUM=IFVAL,
  IF ((FVAL .GT. 0.) .AND. (FFRAC .NE. 0.)) ANUM=ANUM+1.
  DO 125 1=1,NINTEG
    FNUM(1)=ANUM
  125 ANUM=ANUM+1.

C
NY=1000+1,NNTVL
NX=1000+J
RETURN
SUBROUTINE INTIO(ARRAY,N,ISWCH)

C***********************************************************************
C INPUTS DATA TO PROGRAM
C***********************************************************************
C
DIMENSION ARRAY(N)
GO TO (1,2), ISWCH
1 READ(5,7) ARRAY
RETURN
2 WRITE(6,8) ARRAY
RETURN
7 FORMAT(16F5.0)
8 FORMAT(1X,16F8.1)
SUBROUTINE IKPEOT(YIATA,YMIN,DELY,XDATA,XMIN,DELX,XAXIS,MP,
*YLABEL,NYCHAR,XLABEL,NXCHAR,JLN,LSY,
*RUC;ELECS,IDENT,RUD,NUMOS,IDENT,IPLOT)

C*******************************************************************************
C THIS SUBPROGRAM PLOTS ARRAY YDATA VERSUS ARRAY XDATA IN A
C STANDARD FORMAT. THE SUBPROGRAM IS DESIGNED TO WORK WITH THE
C VERSATEC PLOTTER. THE PAGE SIZE IS 8.5 BY 11 INCHES.
C
C PARAMETERS
C
C YDATA ARRAY FOR Y AXIS.
C YMIN VALUE WHICH CORRESPONDS TO THE BOTTOM OF THE PLOT.
C DELY INCREMENT WHICH CORRESPONDS TO ONE INCH OF
C VERTICAL DISTANCE.
C
C NOTE: Y AXIS IS ALWAYS TEN INCHES HIGH.
C
C XDATA ARRAY FOR X AXIS.
C XMIN VALUE WHICH CORRESPONDS TO THE LEFT EDGE OF PLOT.
C DELY INCREMENT WHICH CORRESPONDS TO ONE INCH OF
C HORIZONTAL DISTANCE.
C XAXIS LENGTH OF X-AXIS, IN INCHES.
C MP NUMBER OF POINTS IN ARRAYS XDATA AND YDATA.
C YLABEL LABEL OF Y AXIS.
C NYCHAR NUMBER OF CHARACTERS IN THE Y LABEL.
C XLABEL LABEL OF X AXIS.
C NXCHAR NUMBER OF CHARACTERS IN THE X LABEL.
C JLN DETERMINES IF DATA POINTS ARE SHOWN OR CONNECTED
C BY LINE SEGMENTS.
C =0: LINE SEGMENTS; NO POINTS.
C =1: SYMBOL DRAWN WITH LINE SEGMENTS.
C =-1: SYMBOL ONLY DRAWN.
C
C LSY SPECIFIES THE SYMBOL.
C USEFUL SYMBOLS: 0:BOX, 1:OCTAGON 2:TRIANGLE,
C 3:+, 4:X, 5:Diamond, 6:ARROW, 11:* 14:STAP.
C
C IPLOT PARAMETER SPECIFYING TYPE OF PLOT TO BE PRODUCED
C IPLOT X Y
C
C 0 LINEAR LINEAR INTERFEROGRAF
C 1 LINEAR LINEAR FREQUENCY PLOT
C 2 LOG LINEAR
C 3 LINEAR LOG
C 4 LOG LOG
C
C IF IPLOT=1, THE ABSCissa IS ASSUMED TO BE
C FREQUENCY IN CM-1 AND THE TOP OF THE PLOT IS GIVEN
C IN ENERGY UNITS OF EV.
C
C IF IPLOT=2,3,4 THEN SUBROUTINE CRIDLC IS INVOKED
C TO COMPUTE LOGARITHMIC GRID INTERVALS (MAXIMUM OF
TEN FULL CYCLES IN EITHER DIRECTION).

RUN ARRAY OF RUN NUMBERS.
NDECKS NUMBER OF POINTS IN RUN.
IDENT LABEL
RUD ARRAY OF RUN NUMBERS, USUALLY FOR BACKGROUNDS
NDENOS NUMBEROF POINTS IN RUD

IF NDENOS IS LESS THAN OR EQUAL TO ZERO, RUD AND
IDENT WILL NOT BE DRAWN. THEY MUST STILL BE
SPECIFIED, HOWEVER IN THE SUBROUTINE CALL.
IDENT LABEL FOR BACKGROUND.

NOTE: YLABEL AND XLABEL ARE READ IN AS LITERAL DATA, ENCLOSED
PARAMETERS.

REAL IDENT,IDENT
DIMENSION IDENT(15),IDENT(15),YLABEL(15),XLABEL(15),
*RUN(NDECKS),RUD(NDENOS)
DIMENSION YDATA(NP),XDATA(NP)
DIMENSION GI(160),HI(160),G2(12),H2(12)
DIMENSION FNUM(12)
DIMENSION IPL(2,4)
DATA CHIOT /1.24E-04/
DATA IPL /1,1,2,1,1,2,2,2/
DATA LMASK1,LMASK2,LMASK3 /-1,3,255/

NOTE ON LINE MASE:
LMASK1 IS USED FOR OUTSIDE BORDERS: SET AT -1 (SOLID LINE)
TO BE CONSISTENT WITH AXES.
LMASK2 IS USED FOR CHI ON LINEAR PLOTS AND FINE SPACING
ON LOG PLOTS.
LMASK3 IS USED FOR LARGE OVERLAY ON DECADES FOR LOG PLOTS.

LOGICAL INTFIL
RIGHT=FAXIS+.05
CALL WINDOW(-1.,RIGHT,-.5,10.)
CALL PLOTS(0,0.4)
YNU=0.
DO 5 K=1,NDECKS
CALL NUMBER(-.75,YNU,.14,RUN(K),90.0,2)
YNU=YNU+.9
5 CONTINUE
CALL SYMOL(-.75,6.0,0.14,IDENT,90.0,60)
IF(NDENOS)1,1,2
2 YNU=0.
DO 6 K=1,NDENOS
CALL NUMBER(-,.50,YNU,.14,RUD(K),90.0,2)
YNU=YNU+.9
6 CONTINUE
CALL SYMOL(-.50,.0,.14,IDENT,90.0,60)
1 CONTINUE
XDATA(MP+1)=XMIN
XDATA(MP+2)=DELY
YDATA(MP+1)=YMIN
YDATA(MP+2)=DELY
CALL LINE(XDATA,YDATA,MP,1,JK1,LSY)
INTER=.FALSE.
IF (IPL0T .NE. 0) GO TO 10
INTER=.TRUE.
IPL0T=1
C
C DRAW X-AXES
C
10 IX=IPL(1,1PLOT)
IX=IPL(2,1PLOT)
GO TO (20,30), IX
C
C LINEAR CASE
C
20 CALL AXIS(0.,0.,XLABEL,-NXCHAR,XAXIS,0.,XMIN,DELY)
IF (.NOT. INTER) GO TO 25
CALL HLINE(0.,XAXIS,10.,LSK1)
GO TO 40
25 XMINP=CPLOT*XMIN
DELYP=1.0E-06*DELY
XAXISP=1.24*YAXIS
CALL FACTOR(.866)
CALL AXIS(0.,12.4,'PHOTO ENERGY (EV)',-10.,YAXISP,0.,
*XAXISP,DELYP)
CALL ULINE(A1NT(XAXISP),XAXISP,12.4,LSK1)
CALL FACTOR(1.0)
GO TO 40
C
C LOGARITHMIC CASE
C
30 CALL HLINE(0.,XAXIS,0.,LSK1)
CALL HLINE(0.,XAXIS,10.,LSK1)
STARTY=XAXIST/R-.07*FLOAT(EX_CHAR)
CALL SYSTOL(STARTY,-.3,.4,.14,YLABEL,0.,NXCHAR)
C
C DRAW Y-AXES
C
40 GO TO (50,60), IY
C
C FIRST LINEAR CASE
C
50 CALL AXIS(0.,0.,YLABEL,SYCHAR,10.,50.,YMIN,DELY)
CALL VLINE(0.,10.,XAXIS,LSK1)
GO TO 70
C  NOW LOGARITHMIC CASE
C
60 CALL VLINE(0.,10.,0.,LMASK1)
   CALL VLINE(0.,10.,XAXIS,LMASK1)
   STARTY=5.-.07*FLOAT(NYCHAR)
   CALL SYMBOL(-.25,STARTY,.14,YLABEL,90.,NYCHAR)
C
C  DRAW GRID
C
70 NX=INT(XAXIS)
    GO TO (75,70,85,90), IPLLOT
75 CALL GRID(0.,0.,NX,1.,10,1.,LMASK2)
    GO TO 100
80 CALL GRIDLG(XMIN,DELX,XAXIS,C1,C2,N1,N2,FNUM,NINTEG)
   IF (XMIN .LE. AINT(XMIN)) GO TO 31
   X=0.
   JTEST=1
   GO TO 83
81 X=G2(1)
   JTEST=2
83 DO 82 J=1,NINTEG
   CALL NUMBER(X,-.2,.1,FNUM(J),0.,-1)
   X=X+G2(JTEST)
82 JTEST=JTEST+1
   CALL GRID(0.,0.,N1,C1,10,1.,LMASK2)
   CALL GRID(0.,0.,N2,C2,10,1.,LMASK3)
   GO TO 160
85 CALL GRIDLG(YMIN,DELY,10.,C1,C2,N1,N2,FNUM,NINTEG)
   IF (YMIN .LE. AINT(YMIN)) GO TO 86
   Y=0.
   JTEST=1
   GO TO 88
86 Y=G2(1)
   JTEST=2
88 DO 87 J=1,NINTEG
   CALL NUMBER(-.1,Y,.1,FNUM(J),96.,-1)
   Y=Y+G2(JTEST)
87 JTEST=JTEST+1
   CALL GRID(0.,0.,NY,1.,NX,C1,LMASK2)
   CALL GRID(0.,0.,NY,1.,NX,C2,LMASK3)
   GO TO 160
90 CALL GRIDLG(YMIN,DELY,XAXIS,C1,C2,N1,N2,FNUM,NINTEG)
   IF (YMIN .LE. AINT(YMIN)) GO TO 91
   X=0.
   JTEST=1
   GO TO 93
91 X=G2(1)
   JTEST=2
93 DO 92 J=1,NINTEG
   CALL NUMBER(X,-.2,.1,FNUM(J),0.,-1)
X=X+G2(JTEST)
92 JTEST=JTEST+1
   CALL GRIDLC(YMIN,DELY,10.,H1,H2,M1,M2,FNUM,NINTEG)
   IF (YMIN .NE. AINT(YMIN)) GO TO 96
   Y=0.
   JTEST=1
   GO TO 98
96 Y=H2(1)
   JTEST=2
98 DO 97 J=1,NINTEG
   CALL NUMBER(-.1,Y,1,FNUM(J),.1,.1,-1)
   Y=Y+H2(JTEST)
97 JTEST=JTEST+1
   CALL GRID(0.,0.,N1,G1,H1,H2,MSK2)
   CALL GRID(0.,0.,N2,G2,H2,H2,MSK3)
100 CALL PLOT(0.,0.,999)
   IF (INTERP) IPILOT=0
   RETURN
SUBROUTINE KTF(N,RE,W,VA,DE,VC,SIGMA,EPS,DATA,ALPHA,EPS2,LOSS, *EXT,SUM,SUMLOS,SUMALP,IPUNCH)
C
C**********************************************************************
C THIS SUBROUTINE PERFORMS A KRAMERS-KRONIG TRANSFORM OF REFLECTANCE
C DATA RL(I) GIVEN AT N FREQUENCIES W(I).
C
C FOR FREQUENCIES BETWEEN W(N) AND WA, A 1/W**DEPENDENCE IS
C ASSUMED SIMULATING TRANSITIONS IN HIGH FREQUENCY RANGE NOT
C Measured, and FOR FREQUENCIES ABOVE WA, A 1/W**4
C DEPENDENCE IS ADOPTED, SIMULATING FREE ELECTRON BEHAVIOR.
C
C INPUT
C N - NUMBER OF DATA POINTS.
C RE- TABLE OF BULK REFLECTANCE VALUES, N POINTS LONG.
C W - TABLE OF FREQUENCY VALUES, N POINTS LONG.
C VA- FREQUENCY AT WHICH FREE ELECTRON BEHAVIOR SETS IN.
C DE- FREQUENCY DEPENDENCE OF REFLECTANCE IN INTERBAND REGION
C VC- VOLUME OF UNIT CELL, IN CUBIC ANGSTROMS.
C
C OUTPUT
C SIGMA - TABLE OF CONDUCTIVITY
C EPS - TABLE OF DIELECTRIC FUNCTION.
C DATA - TABLE OF REFLECTANCE
C ALPHA - TABLE OF ABSORPTION COEFFICIENT
C EPS2 - TABLE OF IMAGINARY DIELECTRIC FUNCTION
C LOSS - TABLE OF LOSS FUNCTION
C EXT - TABLE OF EXTINCTION COEFFICIENT
C SUM - TABLE OF CALCULATED SUM RULE
C SUMLOS - TABLE OF CALCULATED LOSS SUM RULE
C SUMALP - TABLE OF CALCULATED ALPHA SUM RULE
C
C UNITS AND CAUTIONS
C ALL FREQUENCIES IN CM^-1
C SIGMA IN (OHM-CM)**-1.
C ABSORPTION COEFFICIENT IN (MICRON)**-1.
C SUM RULE CALCULATION GIVES M0/M* NFF
C !RE MUST NOT EQUAL ZERO.
C
C PROGRAM WRITTEN BY C.S.JACOBS.
C
C**********************************************************************
C
REAL LOSS
DIMENSION RL(3000),W(3000),U(3000),EXT(3000),EXT1(3000)
DIMENSION SIGMA(3000),EPS(3000),DATA(3000),SUMLOS(3000)
*ALPHA(3000),EPS2(3000),LOSS(3000),SUM(3000),EXT(3000)
*SUMALP(3000)
COMPLEX CMPLX,CEXP,A,B,D
LOGICAL@1 C
DATA C'/"','/
100 FORMAT (III)
101 FORMAT (1X,'KRAMERS KRONIG TRANSFORM OF REFLECTANCE DATA')
102 FORMAT (IX,'FREQ',EPS1, EPS2, SIGNAL, *XT COEF SUMPL')
35 FORMAT (1H,2X,F8.1,4X,F8.2,6X,F8.2,2X,F10.2,5X,F7.4,5X,F5.3,4X,F6
*2,5X,F6.3,5X,F5.3,5X,F5.2,5X,F5.2,4X,F6.3)
36 FORMAT (F10.1,F10.3)
198 FORMAT(3X,'FREQ',7X,'E1',8X,'E2',6X,'S1',6X,'ALPHA',6X,'REFL')
199 FORMAT(3X,'FREQ',7X,'N',9X,'K',8X,'LOSS',6X,'SUMS',6X,'SUMA',
*6X,'SUML')
202 FORMAT('*/')
Y(X,Z)=1./(Z**2-X**2)
WRITE (6,101)
N=N-1
PI=3.141592
DO 10 I=1,N

H(I)=W(1+1)-W(1)
ENT(I)=AL0G(RL(1))
10 CONTINUE
EN(T(I))=AL0G(REC(I))
WRITE (6,102)
IF (JPLEQ.EQ.0) GO TO 60
WRITE (9,199)
WRITE (9,199)
60 CONTINUE
C
C************************************************************************************
C KRAMERS-KRONIG INTEGRAL IS PERFORMED AT EACH OF THE FREQUENCIES.
C************************************************************************************
C
LO 95 K=2,N
DO 15 I=1,N

ENT(I)=ENT(I)-ENT(I)
15 CONTINUE
C
C************************************************************************************
C ACCUMLATE INTEGRAL
C************************************************************************************
C
S=0.
DO 17 I=1,N
C
C************************************************************************************
C AVOID DIVIDING BY ZERO.
C************************************************************************************
C
IF(I.EQ.K-1) GOTO 16
IF(I.EQ.K) GOTO 17
S=S+0.5*(ENT1(I)*Y(W(I),W(K))+ENT1(I+1)*Y(W(I+1),W(K)))
GO TO 17
16 S=S+0.5*(H(I)*ENT1(I)*Y(W(I),W(K))+ENT1(I+1)*Y(W(I+1),W(K))*)
17 CONTINUE

C******************************************************************************
C CALCULATE PHASE WITH EXTRAPOLATION AT HIGH AND LOW FREQUENCIES.
C******************************************************************************
C
TH1=W(K)*S/PI
TH1=TH1+ENT1(I)*ALOG((W(K)+W(1))/(W(K)-W(1)))/(2.0*PI)
TH1=TH1-ENT1(N)*ALOG((W(N)+W(K))/(W(N)-W(K)))/(2.0*PI)
*+(1.0/PI)*W(K)*((N-1)+DE/WA)+(1.9)*DE*((W(K)/W(N))*3)
TH1=TH1/(1.0+1.0)
A=SQRT(REFT(K))+CEXP(I)
B=(1.0+A)/(1.0-A)

C******************************************************************************
C CALCULATE OPTICAL CONSTANTS.
C******************************************************************************
C
REFR=REAL(B)
EXT1=AIMAG(B)
E1=REFR*2-EXT1**2
E2=2.0*REFR*EXT1
S1=W(K)*REFR*EXT1/30.
S2=-W(K)*E1/60.
ALOSS=E2/(E1+2*E2)**2
ALP=4.0*PI*W(K)*EXT1/10000.
IF(K.KO,2) GOTO 40
C=G+30.*S1/(1+P1)*H(K-1)
Q1=(1.0+2.0*(ALOSS+BLISS)+W(I-1)*W(K)
Q2=(2.0+2.0*(ALP+BLP)+W(I-1)
GO TO 42
40 Q=(W(2)-W(I-1))*60.*S1
Q1=(W(2)-W(I-1))*ALOSS+W(I-1)
Q2=(W(2)-W(I-1))^2*ALP
42 P1=S1
BLISS=ALOSS
LIP=ALP
SUBK=VCY(7.1E-12)
SUBK=VCY(7.1E-12)
SUBK=VCY(1.14E-6)
WRITE(6,35)V(K),E1,E2,S1,SYMBOL,REFL,ALP,SUBK,ALOSS,REFR,EXT1,
*SUBLAP
IF(IPL&.CH.EQ.0) GOTO TO 50
WRITE(9,200) W(K),C,E1,E2,S1,ALP,REFL
WRITE(9,201) W(K),C,REFL,EXT1,ALOSS,SUMM,SUMLAP
*C,SUMSOL

CONTINUE
ALPHA(K)=ALP
SIGMA(K)=S1
LOSS(K)=ALOSS
EPS(K)=E1
EPS2(K)=E2
SUM(K)=SUMM
SUMLOS(K)=SUMSOL
SUMALP(K)=SUMLAP
DATA(K)=REFL
EXT(K)=EXTI

CONTINUE
IF (1PUNCH.EQ.1) WRITE(9,202)
EXT(1)=EXT(2)
SIGMA(1)=SIGMA(2)
LOSS(1)=LOSS(2)
EPS(1)=EPS(2)
SUM(1)=SUM(2)
SUMLOS(1)=SUMLOS(2)
SUMALP(1)=SUMALP(2)
DATA(1)=DATA(2)
EPS2(1)=EPS2(2)
ALPHA(1)=ALPHA(2)
SIGMA(N)=SIGMA(N)
ALPHA(N)=ALPHA(N)
EPS(N)=EPS(N)
SUM(N)=SUM(N)
SUMLOS(N)=SUMLOS(N)
SUMALP(N)=SUMALP(N)
LOSS(N)=LOSS(N)
DATA(:)=DATA(:)
EXT(:)=EXT(:)
EPS2(:)=EPS2(:)
RETURN
SUBROUTINE LINEAR(X,Y,DY,N,S,A,B,C,D)
C
C******************************************************************************
C THIS ROUTINE DOES A LINEAR FIT TO DATA
C
C******************************************************************************
C
C PROGRAM BY KEVIN CUMMINGS
C******************************************************************************
C
DIMENSION X(50),Y(50),DY(50),A(50),B(50),C(50),D(50)
DOUBLE PRECISION X,Y,DY,A,B,C,D
M=N-1
DO 10 I=1,M
   J=I+1
   A(I)=Y(I)
   B(I)=(Y(J)-Y(I))/(X(J)-X(I))
   C(I)=0.
   D(I)=0.
10    CONTINUE
   A(N)=Y(N)
   B(N)=0.
   C(N)=0.
   D(N)=0.
RETURN
SUBROUTINE MAXMIN (X, N1, NPTS, XMIN, XMAX, NMAX)

C**********************************************************************
C THIS ROUTINES FIND THE MAXIMUM AND MINIMUM OF DATA
C**********************************************************************
C
DIMENSION X(NPTS)

XMAX = 0.
XMIN = 1.E10

DO 10 M = N1, NPTS
   IF (X(M) .GT. XMAX) NMAX = M
   XMAX = X(NMAX)
   IF (X(M) .LT. XMIN) XMIN = X(M)
10 CONTINUE

RETURN
SUBROUTINE MIRROR (V,RATIO,NP,VMIR,NMIR,NMTR,IFUN)

C************************************************************************
C THIS ROUTINE INTERPOLATES A VALUE FOR THE DATA IN VMIR AND THEN
C USES THIS TO SCALE RATIO. THE INTERPOLATION IS A LINE BETWEEN
C THE TWO VMIR POINTS WHICH ARE ABOVE AND BELOW THE POINT IN V.
C
C IFUN=0 => RATIO*RMIR
C IFUN=1 => RATIO/RMIR
C************************************************************************
C
DIMENSION V(NP),RATIO(NP),VMIR(NMIR),RMIR(NMIR)

DO 40 K=1,NP
   IF (V(K).LE.VMIR(1)) GO TO 40
      N=1
10   IF (V(K)-VMIR(N)) .GE. 30,30,20
20      N=N+1
   IF (N.GT.NMIR) GO TO 40
   GO TO 10
30   SLOPE=(RMIR(N)-RMIR(N-1))/(VMIR(N)-VMIR(N-1))
   RBACK=RMIR(N-1)+SLOPE*(V(K)-VMIR(N-1))
   IF (IFUN.EQ.0) RATIO(K)=RATIO(K)*RBACK
   IF (IFUN.EQ.1) RATIO(K)=RATIO(K)/RBACK
40   CONTINUE
RETURN
SUBROUTINE N2POW(NP,MP,MLPTS,NU)

C**********************************************************************
C THIS ROUTINE FINDS THE NEXT LARGEST POWDER OF TWO
C**********************************************************************
C
NX=NP
IF(MLPTS .NE. 0) NX=MLPTS
NP=16
NU=4
76 IF (NP .GE. NX) GOTO 77
    MP=MP*2
    NU=NU+1
    GOTO 76
77 CONTINUE
XMP=NP
RETURN
SUBROUTINE SETUP1 (Y, YY, NP, MP2)

C
C*------------------------------------------------------------------*
C THIS ROUTINE SETS UP ONE SIDED DATA FOR FOURIER TRANSFORM
C
C*------------------------------------------------------------------*
C
DIMENSION Y(NP), YY(MP2)

NR = NP + 1
MP = MP2 / 2
MM = MP + 1

DO 75 K = 1, NP
    YY(K) = Y(K)
75 CONTINUE

DO 81 K = NR, MM
    YY(K) = 0.
81 CONTINUE

MP1 = MP - 1

DO 85 K = 1, MP1
    YY(MM + K) = YY(MM - K)
85 CONTINUE

RETURN
SUBROUTINE SETUP2 (Y, YY, NP, MP, KF)

C******************************************************************************************
C THIS ROUTINE SETS UP TWO SIDED DATA FOR FOURIER TRANSFORM
C******************************************************************************************
C
DIMENSION Y(NP), YY(MP)
KFZERO=NP-KF+2
KLZERO=MP-KF+1
NP=KFZERO-1
DO 91 K=1, NP
   YY(K)=Y(K+NP-1)
91 CONTINUE
IF(KFZERO .GT. KLZERO) GO TO 94
DO 93 K=KFZERO, KLZERO
   YY(K)=0.
93 CONTINUE
94 CONTINUE
NP=KLZERO+1
DO 96 K=NP, MP
   YY(K)=Y(K-NP)
96 CONTINUE
RETURN
SUBROUTINE SETUPS (X,Y,NP,S)

C******************************************************************************************************************************************************
C THIS SUBROUTINE PREPARES DATA FOR SMOOTHING.
C SMOOTHING IS DONE WITH CUBIC SPLINE ROUTINE SMOOTH.
C DATA IN SINGLE PRECISION ARRAYS X,Y.
C NP IS NUMBER OF POINTS
C S INDICATES THE AMOUNT OF SMOOTHING DONE.
C IF DELY IN SMOOTH IS THE STANDARD DEVIATION OF THE POINTS Y THEN
C S REPRESENTS THE CHI SQ VALUE OF THE SMOOTHED LINE TO THE DATA.
C******************************************************************************************************************************************************
C
DOUBLE PRECISION XD,YD,DELY,A,B,C,D
DOUBLE PRECISION SD
DIMENSION X(1500),Y(1500)
    DIMENSION XD(1500),YD(1500)
    DIMENSION DELY(1500),A(1500),B(1500),C(1500),D(1500)
1 FORMAT (1X,'CARD AT FREQUENCY=','F12.2,' IS OUT OF PLACE')
XTEST=0.0
DO 101 K=1,NP
    IF (X(K) .LT. XTEST) GOTO 301
    XD(K)=ALOG(X(K))
    YD(K)=Y(K)
    DELY(K) CHOOSE TO SIMULATE THE NOISE
    DELY(K)=0.01*SQRT(Y(K)) + 0.001
    XTEST=X(K)
101 CONTINUE
SD=S
CALL SMOOTH (XD,YD,DELY,NP,SD,A,B,C,D)
DO 201 K=1,NP
    Y(K)=A(K)
201 CONTINUE
RETURN
301 CONTINUE
WRITE (6,1) XTEST
RETURN
SUBROUTINE SMOOTH(X,Y,DY,N,S,A,B,C,D)

C*******************************************************************************
C               SM O O T H ( X , Y , D Y , N , S , A , B , C , D )
C*******************************************************************************
C*               SM O O T H IN G  B Y  S P L I N E  F U N C T I O N S
C*               X( I ) A R E  S T R I C T L Y  I N C R E A S I N G  (O R  D E C R E A S I N G—S E E  C O M M E N T  B E L O W )
C*******************************************************************************

C IMPLICIT REAL*8 ( A-H,O-Z)
DIMENSION X(3000),Y(3000),DY(3000),A(3000),r(3000),C(3000),
*E(3000),
*R(3000),R1(3000),R2(3000),T(3000),T1(3000),U(3000),V(3000)
C
N1=1
C
H=X(2)-X(1)
F=(Y(2)-Y(1))/H
DO 100 I=2,N
C=H
II=X(I+1)-X(I)
E=F
F=(Y(I+1)-Y(I))/II
A(I)=F-E
T(I)=2.0*(C+U)/3.0
T1(I)=U/3.0
R2(I)=DY(I-1)/C
R(I)=DY(I+1)/II
R1(I)=-DY(I)/II-DY(I-1)/II
100 CONTINUE
R(1)=C.0
R1(N)=0.0
R2(N)=0.0
C
DO 200 I=2,N
B(I)=R(I)*R(I)+R1(I)*R1(I)+R2(I)*R2(I)
C(I)=R(I)*R1(I+1)+R1(I)*R2(I+1)
IF (I.NE.N1) D(I)=R(I)*R2(I+2)
200 CONTINUE
D(N+1)=0.0
C
P=0.0
F2=-S
C
NEXT ITERATION!
C
300 L=0.0
U(1)=0.0
DO 400 I=2,N
IF (I.LE.2) GO TO 250
R2(I-2)=C*R(I-2)
E=C*R2(I-2)
R(I-1)=F*H(I-1)
R(I)=1.0/(P*B(I)+T(I)-F*R(I-1)-E)
U(I)=A(I)-R1(I-1)*U(I-1)
IF (I .NE. K) U(I)=U(I)-K*U(I-2)
F=P*C(I)+T1(I)-H*R(I-1)
C = I
D(I)=P
400 CONTINUE
U(N)=0.0
C
DO 500 I=2,NN1
I=NN1+2-I
U(I)=R(I)*U(I)-R1(I)*U(I+1)
IF (I .NE. NN1) U(I)=U(I)-R2(I)*U(I+2)
500 CONTINUE
C
E=0.0
H=0.0
DO 600 I=1,NN1
G=H
H=(U(I+1)-U(I))/(X(I+1)-X(I))
V(I)=(H-G)*BY(I)*BY(I)
E=E+V(I)*(H-G)
600 CONTINUE
V(N)=-H*BY(N)*BY(N)
E=E-V(N)*H
G=F2
F2=E*H
IF (F2 .GE. 0.99999 OR. 0.99999*2 .IF. C) GO TO 800
C
F=0.0
H=(V(2)-V(1))/(X(2)-X(1))
DO 700 I=2,NN1
G=H
H=(V(I+1)-V(I))/(X(I+1)-X(I))
G=H-G1(I-1)*R(I-1)
IF (I .NE. 2) G=G-R2(I-2)*R(I-2)
F=1+G1(I)*G
R(I)=G
700 CONTINUE
P=H-P*F
IF (R .LE. 0.0) GO TO 500
C
C USE NEGATIVE BRANCH OF SQUARE ROOT IF Y(1) ARE STRICTLY DECREASING
C
P=P+(C-F2)/((P+D)*RT(I)/)/U)
GO TO 500
C
FINAL STEP AFTER CONVERGENCE

C

800 DO 900 I=1,N
   A(I)=Y(I)-P*A*(1)
   C(I)=U(I)
900 CONTINUE
   DO 1000 I=1,NH1
   H=X(I+1)-X(I)
   D(I)=(C(I+1)-C(I))/(3.*H)
   B(I)=(A(I+1)-A(I))/H-(H*D(I)+C(I))*H
1000 CONTINUE
RETURN
SUBROUTINE STON(SA, NP, KMAX, SACUT, KFIRST, KLAST)
C
C******************************************************************************
C SUBROUTINE FOR CALCULATING THE FIRST AND LAST POINTS WHICH
C ARE ABOVE THE NOISE OF THE SPECTRUM.
C
C SA IS THE ARRAY OF NP POINTS (SPECTRUM).
C KMAX IS THE ELEMENT NUMBER OF THE LARGEST POINT IN SA.
C KFIRST AND KLAST ARE RETURNED AND ARE THE FIRST AND LAST ELEMENT
C NUMBERS THAT ARE ABOVE SACUT.
C******************************************************************************
C
DIMENSION SA(NP)
KFIRST=1
KLAST=NP
DO 10 K=1,KMAX
JJ=K
IF (SA(J).LT.SACUT) GO TO 20
10 CONTINUE
20 CONTINUE
DO 30 K=JJ,KMAX
IF (SA(K).GT.SACUT) GO TO 40
KFIRST=K
30 CONTINUE
40 CONTINUE
LO 50 K=KMAX,NP
IF (SA(K).GT.SACUT) KLAST=K
50 CONTINUE
RETURN
SUBROUTINE TRANSF(YY,MP,T,NU)

C
C******************************************************************************
C CALL FOURIER TRANSFORM
C******************************************************************************
C
DIMENSION YY(MPT),S(2050),INV(2050)
CALL RBA(F,YY,NU,INV,S,IFERR)
RETURN
This appendix includes plots of the reflectance, conductivity and dielectric function of the samples not shown in chapter VI. $f'$ indicates the volume fraction was determined by weight and "not corrected" implies the surface scattering has not been subtracted from the data.
Figure 135

Reflectance

Frequency (cm$^{-1}$)

f = 0.085
Figure 136

Reflectance

Frequency (cm$^{-1}$)

\( f = 0.172 \)
Figure 137

Reflectance

Frequency (cm$^{-1}$)

\[ f = 0.186 \]
Figure 138

Frequency (cm⁻¹)

Reflectance
Figure 139

Reflectance

Frequency (cm\(^{-1}\))

\[ f = 0.330 \]
Figure 140

Frequency (cm$^{-1}$)

Reflectance

$f = 0.334$
Figure 141

Reflectance

Frequency (cm⁻¹)

\( f = 0.767 \)
$f' = 0.20$
not corrected

Reflectance

Frequency (cm$^{-1}$)

Figure 144
$f' = 0.30$

not corrected

Figure 145
$f' = 0.40$

not corrected

Figure 146
Reflectance

$f' = 0.60$
not corrected

Frequency (cm$^{-1}$)

Figure 147
Reflectance

Frequency (cm$^{-1}$)

$f' = 0.70$
not corrected
Reflectance

\[ f' = 0.80 \]

not corrected

Frequency (cm\(^{-1}\))

Figure 149
Reflectance

$F' = 0.90$
not corrected

Frequency (cm$^{-1}$)

Figure 150
Figure 151

Conductivity (ohm·cm⁻¹)

Frequency (cm⁻¹)

$F = 0.085$
Figure 152

Conductivity (ohm-cm$^{-1}$) vs Frequency (cm$^{-1}$)

$f = 0.172$
Figure 154

Conductivity (ohm-cm)^{-1}

Frequency (cm^{-1})

$\text{f} = 0.218$
Conductivity (ohm-cm$^{-1}$)

Figure 155

$\text{Frequency (cm}^{-1}\text{)}$

$\text{f} = 0.330$
Figure 156

Conductivity (ohm-cm)$^{-1}$

Frequency (cm$^{-1}$)

$f = 0.334$
Figure 157

Conductivity (ohm-cm⁻¹)

Frequency (cm⁻¹)

\( f = 0.767 \)
Figure 158

Conductivity (ohm-cm⁻¹) vs Frequency (cm⁻¹)

- Conductivity ranges from 0 to 10,000 ohm-cm⁻¹.
- Frequency ranges from 0 to 45,000 cm⁻¹.

Anomalous behavior observed at f = 0.808.
Dielectric Function

$\frac{f}{\pi} = 0.085$

Frequency (cm$^{-1}$)

Figure 159
Dielectric Function

Frequency (cm$^{-1}$)

Figure 16

\[ f = 0.172 \]
Figure 161

Dielectric Function

Frequency (cm⁻¹)

\( f = 0.186 \)
Figure 162

Frequency (cm$^{-1}$)

$\nu = 0.218$
Dielectric Function

Frequency (cm$^{-1}$)

Figure 163
Dielectric Function

Frequency (cm$^{-1}$)

$f = 0.334$

Figure 164
Dielectric Function

$\epsilon = 0.767$

Frequency (cm$^{-1}$)

Figure 165
Dielectric Function

Frequency (cm$^{-1}$)

Figure 166
APPENDIX F

OPTICAL PROPERTIES OF CESIUM
TETRACYANOQUINOIDIMETHANIDE. Cs\(\text{T}_{3}\)CNQ3

The following paper is from work that we did from September 1977 to December 1980. At that time I started the work which is contained in this thesis. The paper is given here to give a complete indication of graduate research.
Optical properties of cesium tetracyanoquinodimethanide, $\text{Cs}_2(\text{TCNQ})_3$

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(Received 2 April 1981)

Room-temperature polarized reflectance measurements have been made on cesium tetracyanoquinodimethanide, $\text{Cs}_2(\text{TCNQ})_3$, over the frequency range between the far infrared and the near ultraviolet. The optical properties of the compound were obtained by Kramers-Kronig analysis. These properties are dominated by vibrational features at low frequencies and by electronic excitations at high frequencies. The observed vibrational features include ordinary intramolecular modes and "anomalous" infrared activity of the totally symmetric vibrations. This latter absorption results from the interaction of these vibrations with the unpaired electron on the TCNQ$^-$ ion. Two electronic excitations are observed for the electric field polarized along the TCNQ chains. The excitation higher in frequency is attributed to an intermolecular charge transfer from one TCNQ$^-$ ion to an adjacent ion, while the lower-frequency excitation results from a charge-transfer transition to an adjacent neutral molecule. Estimates for the effective on-site Coulomb repulsion energy $U$ of 1.14 eV, and for the transfer matrix element $t$ of 0.17 eV, are obtained from these data. Experimental values for the electron-molecular-vibration coupling constants are also obtained.

I. INTRODUCTION

This paper describes the results of a study of the optical properties of cesium tetracyanoquinodimethanide, $\text{Cs}_2(\text{TCNQ})_3$. We have measured the room-temperature polarized reflectance of single crystals of $\text{Cs}_2(\text{TCNQ})_3$ over the frequency range between the far infrared and the near ultraviolet. The optical properties have been obtained by Kramers-Kronig analysis of the reflectance.

The electronic properties of radical-ion organic solids, such as $\text{Cs}_2(\text{TCNQ})_3$, are determined by the relative importance of three basic interactions of the unpaired electrons of the ions. These interactions are the overlap of the electronic wave function between sites, the Coulomb repulsive interaction between two electrons on the same or adjacent sites, and the interaction of the electron with phonons (both lattice vibrations and intramolecular modes of the molecule). Optical data can be used to measure the strengths of these interactions.

$\text{Cs}_2(\text{TCNQ})_3$ is a complex TCNQ salt by virtue of its 2:3 stoichiometry. The crystal structure, determined by Fritchie and Arthur, consists of chains of TCNQ molecules and Cs$^+$ ions along the $b$ axis. In the TCNQ chain, the bond lengths indicate that pairs or dimers of TCNQ$^-$ ions are placed between TCNQ$^0$ neutral molecules. The basic formula unit then consists of two ions and one neutral molecule. The [100] and [001] projections of this structure are shown in Fig. 1.

The room-temperature dc conductivity of $\text{Cs}_2(\text{TCNQ})_3$, $\sim 10^{-3} \Omega^{-1}\text{cm}^{-1}$, is intermediate between the highly insulating 1:1 TCNQ salts such as K-TCNQ and the "metallic" compounds such as TTF-TCNQ (where TTF stands for tetraphiafulvalene). The temperature dependence of the con-
ductivity is characteristic of a semiconductor with a full energy gap of 0.72 eV. Magnetic measurements\textsuperscript{6} yield a smaller estimate for the gap of 0.1 eV.

The optical properties of Cs\textsubscript{2}(TCNQ)\textsubscript{3} have been studied several times previously.\textsuperscript{7-17} The first measurements were by Iida,\textsuperscript{7} who made unpolarized measurements above 0.5 eV and interpreted the results in terms of charge-transfer excitations dominated by Coulomb repulsion. Electronic transitions have been studied by a number of workers\textsuperscript{3}-\textsuperscript{13} since Iida. Polarized reflectance measurements to study vibrational modes in Cs\textsubscript{2}(TCNQ)\textsubscript{3} have been made by Belousov et al.,\textsuperscript{14} between 0.05 eV (400 cm\textsuperscript{-1}) and 0.6 eV (5000 cm\textsuperscript{-1}). Other infrared measurements have been made by Kondow and Sakata,\textsuperscript{15} GIRLANDO ET AL.,\textsuperscript{16} and KHURSAN DOVA ET AL.\textsuperscript{17}

Despite this significant amount of work, we have made comprehensive measurements of the optical properties of Cs\textsubscript{2}(TCNQ)\textsubscript{3}. This work was motivated by a number of reasons: First, there has been no work in the far infrared (below 400 cm\textsuperscript{-1}); there has been no comprehensive study using polarized light spanning the vibrational and electronic excitation regions, and many of the previous studies stopped near 0.5 eV where we find an absorption maximum. Second, the structure of Cs\textsubscript{2}(TCNQ)\textsubscript{3}, consisting as it does of linear chains of dimers spaced by neutral molecules, makes this work a companion piece to earlier studies\textsuperscript{18} of D(CH\textsubscript{3})Fe-TCNQ [D(CH\textsubscript{3})Fe stands for decamethylferrocinium; this system contains isolated dimers] and \textsuperscript{19,20}K-TCNQ (a linear chain of interacting dimers). Third, we were interested in comparing the optical properties of Cs\textsubscript{2}(TCNQ)\textsubscript{3} with those of N(CH\textsubscript{3})\textsubscript{3}H-I-TCNQ.\textsuperscript{21} Both compounds have an average charge per TCNQ molecule of 2e/3; in Cs\textsubscript{2}(TCNQ)\textsubscript{3} the molecules are not uniformly spaced along the chain while in N(CH\textsubscript{3})\textsubscript{3}H-I-TCNQ they are uniformly spaced. These structural differences have profound effects on the optical properties.

The next section of the paper describes sample preparation and optical techniques while the third section presents our reflectance data and the results of the Kramers-Kronig analysis. In the final section, we discuss the electronic transitions and the vibrational features that we observe.

II. EXPERIMENTAL TECHNIQUES

The 2:3 Cs\textsubscript{2}(TCNQ)\textsubscript{3} was prepared by the method of Melby et al.\textsuperscript{22} Ultrapure cesium iodide (Alfa) and gradient sublimed 7,7,8,8-tetracyano-p-quinodimethane were mixed in a 1:1 ratio in suitably pure hot acetonitrile.\textsuperscript{22} The hot intense green solution was sealed and placed in a preheated Dewar which slowly equilibrated with ambient temperature. After two weeks the product was collected by filtration and air dried. Large well-formed crystals suitable for optical studies were prepared by this technique.

The room-temperature polarized reflectance of Cs\textsubscript{2}(TCNQ)\textsubscript{3} crystals was measured using two instruments. Between 700 and 30000 cm\textsuperscript{-1} (0.09 - 3.37 eV) we used a vacuum spectrometer built around a Perkin-Elmer model 16U grating monochromator. Figure 2 is a diagram of this spectrometer. The entire spectrometer can be evacuated to pressures below 1 Torr to reduce the absorption by atmospheric water vapor in the infrared region. All surfaces within the vacuum box were covered with 3M Nextel\textsuperscript{18} flat black paint to reduce stray light. Three sources, four gratings, and three detectors were used to cover the infrared, visible, and near ultraviolet regions with moderate resolution, \(\Delta\omega/\omega \sim 10^{-3}\). Long-pass and bandpass filters eliminated unwanted orders of diffraction. A large spherical mirror imaged the exit slit of the monochromator onto a single crystal mounted in the sample holder. A second spherical mirror focused the reflected light onto the detector. The detector was a thermocouple below 4000 cm\textsuperscript{-1} (0.5 eV) with a glow bar source, a PbS photoconductor between 4000 and 15000 cm\textsuperscript{-1} (0.5 - 1.9 eV) with a tungsten lamp source and a photomultiplier above 15000 cm\textsuperscript{-1} with either the tungsten source or a deuterium lamp source. The tungsten source was used up to 27000 cm\textsuperscript{-1} (3.3 eV) and a deuterium lamp was used at higher frequencies. In the middle infrared a wire grid polarizer was utilized while dichroic polarizers were used in the near infrared through ultraviolet regions.

Below 700 cm\textsuperscript{-1} (0.09 eV) a Michelson interferometer, diagrammed in Fig. 3, was used to measure the polarized reflectance of a mosaic of Cs\textsubscript{2}(TCNQ)\textsubscript{3} crystals. The interferometer and its operation have been described previously.\textsuperscript{21} However, an assembly has been added to allow polarized reflection measurements. With four different thicknesses of Mylar for beam splitters, a frequency region from 10 to 700 cm\textsuperscript{-1} (0.002 - 0.09 eV) was examined with a resolution of \(\Delta\omega/\omega \sim 10^{-2}\). A wire grid polarizer was used throughout this region. An accurate absolute value for the reflectance was obtained by comparing the reflectance
FIG. 2. Diagram of grating spectrometer used to cover the 700 – 30,000 cm\(^{-1}\) region.

FIG. 3. Diagram of Michelson interferometer used to cover the 10 – 700 cm\(^{-1}\) region.
from the mosaic with the reflectance of the same mosaic after coating with gold. By taking the ratio of these values an absolute measurement of the reflectance was obtained for the far infrared.

III. EXPERIMENTAL RESULTS

The reflectance of Cs₂(TCNQ)₅ with E ||b and E ||a from the far infrared to the ultraviolet is shown in Fig. 4. Between 4000 and 30 000 cm⁻¹ (0.5—3.7 eV) there are two broad maxima in both polarizations. These maxima are associated with electronic transitions in the material. Figure 5 shows in detail the reflectance from 10 to 3000 cm⁻¹ (0.001—0.04 eV). The sharp features in this region are associated with molecular vibrations. Notice the sharp low-frequency rise in the E ||a component of the reflectance.

Because an extremely large frequency region was covered, a Kramers-Kronig analysis²⁴ of the reflectance should provide reasonably accurate values for the optical constants. In the performance of the analysis conventional extrapolation procedures were used. At very low frequencies the reflectance was assumed constant. Between the highest-frequency data point and 200 000 cm⁻¹ (25 eV) the reflectance was extrapolated as 1/ω² to simulate interband transitions while above 200 000 cm⁻¹ a 1/ω⁴ form, appropriate for free-electron behavior, was used. The computer program determines the phase shift on reflection from the Kramers-Kronig integral. From the reflectance and phase all of the usual optical functions are calculated.

The frequency-dependent conductivity σ₁(ω) is given over the whole frequency region in Fig. 6; the low-frequency details are shown in Fig. 7. The energies of the maxima in σ₁(ω) give the energies of electronic or vibrational transitions in the solid more closely than the absorption coefficient α or the imaginary part of the dielectric function. Figure 6 shows quite clearly that the strengths of the electronic transitions in E ||a are three to four times greater than those in E ||b. The small negative values of σ₁(ω) which occur near the strong structures at low frequencies arise because little apodization was used on the interferogram from the Michelson interferometer.

Figure 8 shows the real part of the dielectric function ε₁(ω) on a logarithmic frequency scale. The dielectric function displays the usual derivative-like structure at frequencies near the conductivity maxima. Extrapolation of the infrared data to zero frequency gives a value of 5.0 ± 0.1 for the static dielectric constant.

IV. DISCUSSION

A. Electronic transitions

In this section we compare our experimental results with theoretical approaches appropriate for
FIG. 6. Frequency-dependent conductivity obtained by Kramers-Kronig analysis of the reflectance for room temperature Cs$_2$(TCNQ)$_3$. The conductivity for $E \parallel a$ is shown as a dotted line while that for $E \parallel b$ is shown as a solid line.

Cs$_2$(TCNQ)$_3$. These theories all stress the importance of the Coulomb interaction for determining optical properties. This interaction is important because an electron transferred to an adjacent molecule has its energy raised by the Coulomb interaction with the electron on that and neighboring molecules. Implicit in these models is the assumption that the electrons are localized on individual molecular sites. Delocalization across many sites to form energy bands would make the Coulomb interaction of the electrons much less important.$^{11,21}$

In a model proposed by Hubbard,$^{25}$ TCNQ charge-transfer salts are assumed to form a one-dimensional localized array of electrons. Because Cs$_2$(TCNQ)$_3$ has two valence electrons for every three molecules the array has two sites occupied by

FIG. 7. Frequency-dependent conductivity at low frequencies.

FIG. 8. Real part of the dielectric function obtained by Kramers-Kronig analysis of the reflectance for room temperature Cs$_2$(TCNQ)$_3$. Note that the figure has a logarithmic frequency scale.
electrons and then one site vacant. This model of 
Cs₂(TCNQ)₃ is strongly supported by the x-ray 
data,¹ which imply that two molecules are negative 
and one is neutral. With this arrangement there 
can be two charge-transfer transitions. The first is 
the transition of an electron to another already oc­
cupied site. We will call this charge-transfer exci­
tation the "dimer" transition because it occurs 
within the dimers of negatively charged molecules. 
The second transition is that of an electron to a 
site which is unoccupied or a "neutral" transition. 
The dimer transition energy is determined by both 
on-site and off-site Coulomb interaction strengths 
while the neutral transition energy involves only 
the off-site terms. Hubbard calculated the on-site 
interaction energy from the disproportionation en­
ergy for the reaction 2TCNQ⁻→TCNQ+ + TCNQ⁻⁻⁻­⁻ while the off-site energies were cal­
culated from the electrostatic interaction of the 
charge distribution on nth-neighbor TCNQ ions 
of the TCNQ chain. The off-site terms include 
only those neighbors within three lattice sites of 
the transition electron under consideration when 
calculating the energies of each configuration. 

By calculating the Coulomb energy associated 
with the final state and subtracting the energy of 
the ground state we can estimate the energy for 
each transition. These energies are given in Table 
I. The values of on-site and off-site Coulomb in­
teractions used were those given by Hubbard²⁵ with 
modification of the "screening by polarization" be­
cause the dielectric constant of Cs₂(TCNQ)₃ is less 
than the material (TTF-TCNQ) Hubbard dis­
cussed. The neutral transition is calculated to have 
an energy of \( E_N = 1400 \text{ cm}^{-1} \) (0.17 eV). However, 
from Fig. 6 and Table I we find experimentally 
\( E_N = 3900 \text{ cm}^{-1} \) (0.48 eV). It appears that Hub­
bard overestimated the value of the third-order 
off-site interaction energy. To reproduce accurate­
ly our experimental data, the value of the third-or­
derm term must be reduced to very near zero. The 
model predicts that the dimer transition should oc­
cur at \( E_{\text{CT}} = 8000 \text{ cm}^{-1} \) (1.0 eV, approximately the value of \( U_{\text{CT}} \); CT here means charge transfer), a 
frequency which is lower than the experimentally 
determined frequency of 9980 cm⁻¹ (1.24 eV). As 
will be shown below, this discrepancy arises from 
the neglect of the transfer integral \( t \) in this model. 

A theory for the dimer interaction has been 
described, in terms of the Hubbard model, by 
Harris and Lange²⁷ and elaborated by Rice.²⁸ This 
theory focuses specifically on the interaction within 
the dimer of the singly occupied \( \pi \) molecular orbital 
of the two TCNQ⁻ ions. The theory used as 
parameters the overlap matrix element or transfer 
integral \( t \) and the on-site Coulomb interaction \( U \). 
The transfer integral represents the overlap of elec­
tronic wave functions within the dimer and the 
Coulomb interaction describes the net cost of hav­
ning both electrons occupy the same molecular orbital. 

When these interactions are considered, the original 
energy level of the monomer splits into four 
levels in the dimer. The ground state is a bonding 
arrangement with one electron on one molecule 
and the other electron, with opposite spin, on the

---

**TABLE I. Electronic excitation energies in Cs₂(TCNQ)₃.**

<table>
<thead>
<tr>
<th>Elect. trans</th>
<th>Rice data³</th>
<th>Hubbard Ref. 28</th>
<th>Hubbard Ref. 25</th>
<th>Tanaka Ref. 12</th>
<th>Previous experimental data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Δₓ</td>
<td>751 b</td>
<td>756</td>
<td></td>
<td>766 c</td>
<td></td>
</tr>
<tr>
<td>( E_N )</td>
<td>3872</td>
<td>1371(4436) f</td>
<td>5800(6000)</td>
<td>5500</td>
<td>3650</td>
</tr>
<tr>
<td>( E_{\text{CT}} )</td>
<td>9977</td>
<td>9970</td>
<td>10800(11000)</td>
<td>10600</td>
<td>11600</td>
</tr>
<tr>
<td>( E_{\text{LE1}} )</td>
<td>16411</td>
<td>17200(17 700)</td>
<td>16500</td>
<td>17000</td>
<td></td>
</tr>
<tr>
<td>( E_{\text{LE2}} )</td>
<td>26348</td>
<td>(30000)</td>
<td>28000</td>
<td>26600</td>
<td></td>
</tr>
</tbody>
</table>

³Data obtained from conductivity, \( \sigma_f(\omega) \) (this work).
⁴Data taken from Ref. 6 (751 cm⁻¹ = 540 K).
⁵Recalculated with third-order interaction equal to zero.
⁶Calculated values are given with corresponding observed values in parentheses.
⁷One-half the value discussed by Ref. 12.
⁸Pressed powder unpolarized spectra from Refs. 7, 13, and 29.
⁹Pressed powder spectra with polarization determined by transmission from Ref. 11.
other molecule. The next level is a triplet state having one electron on each molecule but with parallel spins. This state is excitable magnetically from the ground state with energy

$$\Delta_s = \left(U^2/4 + 4t^2\right)^{1/2} - U/2.$$  (1)

Above the triplet level is a state where two electrons, with opposite spin, are localized on one of the two molecules. This "charge-transfer" state is coupled by the electric dipole operator to the ground state and is at an energy

$$E_{CT} = U/2 + \left(U^2/4 + 4t^2\right)^{1/2}$$  (2)

above the ground state. Finally, the highest level is an antibonding version of the ground state.

The optical charge-transfer excitation, polarized along the $b$ axis joining the two molecules, occurs at $\omega_{CT} = E_{CT}/\hbar$. The dielectric tensor has been derived by Rice et al. and is given by

$$\epsilon(\omega) = \epsilon_r + \frac{4\pi ne^2b^2}{\hbar^2} \times \frac{4t^2/\left(U^2/4 + 4t^2\right)^{1/2}}{\omega_{CT}^2 \left[1 - D(\omega)\right] - \omega^2 - i\omega\gamma}.$$  (3)

In Eq. 3, $\epsilon_r$ includes the contribution of other excitations to the dielectric tensor, $n$ is the density of molecules, $b$ is the intradimer separation, $\gamma$ is a phenomenological linewidth, and $D(\omega)$ is a function which describes the effects arising from the coupling of the unpaired electron to the internal vibrations of the TCNQ molecule. In the region of electronic transitions, however, $D(\omega) < 1$ so we can neglect this function here. The tensorial character comes from

$$(\vec{A} = (1/N) \sum_j^{N} \vec{a}_j \vec{a}_j/|\vec{a}_j|^2).$$

($\vec{a}_j$ is the vector joining the centers of the $j$th dimer and $N$ is the number of dimers). For Cs$_2$(TCNQ)$_3$, $b = 3.22$ Å and the diagonal component of $\vec{A}$ along the $b$ crystallographic axis is $A_{bb} = 0.995$. The charge-transfer band has an oscillator strength which can be obtained by integrating the conductivity $\sigma_1(\omega)$ over the charge-transfer band

$$\int \sigma_1(\omega)d\omega = \frac{\pi ne^2b^2}{\hbar^2} \frac{2t^2}{\left(U^2/4 + 4t^2\right)^{1/2}}.$$  (4)

The oscillator strength then may be rewritten by using a partial conductivity sum rule

$$S(\omega) = N_e \frac{m}{m^*} \frac{2mV_0}{\pi e^2} \int_0^\infty \sigma_1(\omega)d\omega.$$  (5)

In Eq. (5) $m$ is the electronic mass, $m^*$ is the effective mass of the conduction electrons, $V_0$ is the volume per anion, and $N_e = nV_0$. The parameters $t$ and $U$ may be calculated from optical data on the frequency of the charge-transfer band [Eq. (2)] and its oscillator strength [Eqs. (4) and (5)].

The charge-transfer excitation is the second peak in the $E || b$ conductivity at 9980 cm$^{-1}$ (1.24 eV, Fig. 6). Figure 9 shows a partial sum rule $S(\omega)$ for Cs$_2$(TCNQ)$_3$. By subtracting the value of $S'(7500 \text{ cm}^{-1})$ from $S'(7700 \text{ cm}^{-1})$, Fig. 9 gives $(m/m^*) N_e = 0.23$ for the dimer transition. Using these values in the dimer theory we obtain $U = 1.14$ eV (9240 cm$^{-1}$) and $t = 0.17$ eV (1350 cm$^{-1}$). The quantity $(m/m^*) N_e$ can also be calculated from the observed plasmon frequencies, using

$$\omega_p^2 - \omega_{p1}^2 = \frac{4\pi ne^2}{m^*\epsilon_m}.$$  (6)

where $\omega_p$ is the screened plasmon frequency for each transition and $\epsilon_m$ is the high-frequency dielectric constant. Figure 10 displays the electron-energy-loss function and shows that $\omega_{p1} = 6620$ cm$^{-1}$ and that $\omega_{p2} = 11600$ cm$^{-1}$. With $\epsilon_m = 1.3$ from Fig. 8 we calculate $(m/m^*) N_e = 0.22$ in close agreement with the earlier value.

The values for $t$ and $U$ are consistent with previously reported data on similar systems. The agreement between these dimeric values of $U$ and $t$ and those obtained for D(CH$_3$)$_2$Fc-TCNQ ($U = 1.0$ eV and $t = 0.27$ eV) is quite good. Since D(CH$_3$)$_2$Fc-TCNQ contains contain isolated dimers, this agreement lends confidence to our use of this model for the dimers in Cs$_2$(TCNQ)$_3$. In addition, Eq. (1) predicts the activation energy for the magnetic susceptibility. Using the values for $U$ and $t$ above we calculate an activation energy of 543 K. Experimentally Cs$_2$(TCNQ)$_3$ has an activation energy of 540 K (Ref. 6) in good agreement with this estimate.

Table I shows a comparison between experimental data and the theories which are discussed here.

A third model which uses a modified Hubbard Hamiltonian has been described by Tanaka et al. Three interactions are included in this model: the
"dimer" charge transfer, the "neutral" charge transfer, and a "localized excitation" of an electron from a lower orbital in TCNO\(^-\) to an upper energy state. From numeric computations and fitting to their data they find \(E_{\text{CT}} = 10800 \text{ cm}^{-1}\) and \(E_N = 5800 \text{ cm}^{-1}\). They find the transfer integral \(t = 0.27 \text{ eV}\) and estimate \(U = 1.5 \text{ eV}\) for \(\text{Cs}_2(\text{TCNO})_3\). These values are consistently higher when compared to our results of \(t = 0.17 \text{ eV}\) and \(U = 1.14 \text{ eV}\) (see Table I). It is clear that the discrepancy arises because they fit their theory to the absorption coefficient, which tends to peak at higher frequencies than the corresponding structure in the conductivity.

The third transition of an electron excited to a higher orbital or localized excitation was shown to be polarized along the \(a\) axis with an energy \(E_{\text{LEL}} = 17200 \text{ cm}^{-1}\). In Fig. 6 the energy of the first localized excitation appears as the peak in the \(E||a\) conductivity at \(E_{\text{LEL}} = 16400 \text{ cm}^{-1}\) (2.0 eV). A second localized excitation occurs at \(E_{\text{LEL}} = 26350 \text{ cm}^{-1}\) (3.3 eV). Again Tanaka et al.\(^{12}\) have consistently higher values for excitation energies.

To make a final comparison between experiment and theory we note that the one-dimensional Hubbard model has been solved exactly at \(T = 0 \text{ K}\) by Lieb and Wu.\(^{31}\) They find that for \(t >> U\) the electrons delocalize into a single conduction band but for \(t << U\) the electrons remain localized on particular molecules forming a semiconductor in the half-filled-band case. The minimum band gap in this semiconductor is

\[
E_g \approx U - 4t.
\]

By using the values of \(U\) and \(t\) obtained from the dimer transition, we find \(E_g = 0.46 \text{ eV}\). This value is not in very good agreement with the experimental results of Blakemore et al.\(^5\) who obtain \(E_g = 0.72 \text{ eV}\) for \(\text{Cs}_2(\text{TCNO})_3\) using dc conductivity measurements. Interestingly, the gap obtained from dc conductivity falls almost exactly between the two transitions observed in \(E||b\).

According to Tanaka et al.\(^{12}\) somewhat better results can be obtained if the transfer integral is calculated for the neutral transition and then \(t\) is averaged over the nearest neighbors. Using their values in the calculation we obtain \(E_g = 0.90 \text{ eV}\). Only when third-neighbor terms are included in the average of the transfer integral \(t\) does the estimate [Eq. (7)] of the activation energy begin to
predict the experimental value.

If we compare the results from Cs$_2$(TCNQ)$_3$ with another TCNQ system that has $\frac{2}{3}$ of an electron per molecule in its unit cell, N(CH$_3)_3$H-I-TCNQ$^{21,32,33}$ we notice the electronic spectra are quite different. Neither the neutral nor dimer transition occurs in the spectra of N(CH$_3)_3$H-I-TCNQ. Instead, a single low-lying peak is observed, centered at 1600 cm$^{-1}$. In Cs$_2$(TCNQ)$_3$ the Coulomb interactions are strong and therefore the electrons are assumed to be localized, while in N(CH$_3)_3$H-I-TCNQ the electrons are assumed to be uniformly distributed causing it to be a semiconductor with an energy gap of approximately 0.17 eV. Comparison between these two compounds indicates to us that electronic structure of TCNQ compounds is not determined simply by charge transfer and Coulomb interactions but instead is controlled by crystal structure or by other interactions.

### B. Vibrational modes

A series of strong, narrow infrared absorption bands in Cs$_2$(TCNQ)$_3$ is shown in Figs. 5 and 7. As discussed by Rice,$^{28}$ some of these bands appear for a dimer on account of electron-molecular-vibration coupling. In nondimerized TCNQ the totally symmetric ($a_g$) molecular vibration modes, having no dipole moment, are optically inactive. In a dimer, however, the antisymmetric combinations of these $a_g$ modes couple directly to the dimer charge-transfer excitations and therefore drive oscillations in the radical electrons electric dipole moment. These “dimer charge oscillations” give infrared activity to the $a_g$ modes polarized in the direction of the dimer axis. The oscillations are described by $D(\omega)$ in Eq. (3) where

$$D(\omega) = \sum_{\alpha=1}^{G} \lambda_{\alpha} \frac{\omega_{\alpha}^3}{\omega_{\alpha}^2 - \omega^2 - i\omega \gamma_{\alpha}}.$$  

In Eq. (8), $G$ is the number of modes, $\omega_{\alpha}$ is the “bare” frequency of the $\alpha$th $a_g$ mode, $\gamma_{\alpha}$ is the linewidth of the mode, and $\lambda_{\alpha}$ is a dimensionless constant which indicates the strength of the dimer charge-transfer-molecule-vibration coupling:

$$\lambda_{\alpha} = \frac{16\mu^2}{(\hbar\omega_{\alpha})^2(U^2/4 + 4i^2)^{1/2}} \frac{g_{\alpha}^2}{\hbar\omega_{\alpha}},$$

where $g_{\alpha}$ is the $a_g$ electron-molecular-vibration coupling constant for mode $\alpha$. (Typically, $\lambda_{\alpha} \sim 10^{-2}$.) These equations can be used to obtain “experimental” values for the parameters $\omega_{\alpha}$, $g_{\alpha}$, and $\gamma_{\alpha}$. Before a fit can be done, however, the many modes seen in Fig. 7 must be assigned.

When reviewing the papers of previous workers that have assigned vibrational modes to the optical spectra of TCNQ$^-$, one gets a confusing picture because many earlier workers did not assign $a_g$ modes to dimeric forms of TCNQ. The assignment of modes in the case of Cs$_2$(TCNQ)$_3$ is further complicated by the fact that both TCNQ$^0$ and TCNQ$^-$ are present in the spectra.

In Table II, we present an assignment of the observed vibrational modes of Cs$_2$(TCNQ)$_3$. The first three columns give the symmetry species, the vibrational mode (following the notation of Girlando and Pecile$^{34}$), and our observed frequencies. The next column gives theoretical estimates for the frequencies, while the last two columns list observed frequencies in the neutral molecule$^{34}$ and in the radical anion.$^{35}$ A recent calculation of the normal modes of TCNQ$^0$ and TCNQ$^-$ by Khatakale and Devlin$^{36}$ differs only slightly from the frequencies in Table II. Some of the expected frequencies for the vibrations of the neutral molecule and the radical ion are so close that they cannot be separated in our data. In addition, many of the modes associated with the TCNQ$^0$ molecule do not appear in our spectra. None of the $b_{1u}$ neutral molecule vibrations were identified, while low-frequency modes (below $b_{2u}v^{0}_{1u}$ and $b_{1u}v^{0}_{3u}$) were probably too weak to be seen in the reflectance. Those features which have not been seen previously (e.g., $b_{2u}v^{0}_{1u}$, $v^{0}_{5u}$, $v^{0}_{5u}$, and $v^{0}_{6u}$) were assigned on the basis of the calculated frequency and the expected polarization dependence of each symmetry species. The relative strength of each symmetry species in Cs$_2$(TCNQ)$_3$, for all three polarizations is given in Table III. The modes of the ion are twice as strong as those of the neutral molecule. Notice in Fig. 7 that $b_{2u}$ modes only appear in $\tilde{E}\|a$ polarization and $b_{2u}$ modes are only seen for $\tilde{E}\|b$, while $b_{1u}$ modes are seen in both polarizations. The $b_{1u}v^{0}_{5u}$ and $b_{2u}v^{0}_{6u}$ modes are very weak in our spectrum and therefore have the greatest uncertainty. Several weak modes between 700 and 1000 cm$^{-1}$ are not observed because of a poor signal-to-noise ratio in our instrumental overlap region. Most of our remaining assignments follow previous work$^{14,34-38}$ with very little change. The $a_g$ modes appear in both polarizations but, of course, occur only for the TCNQ$^-$. 
### TABLE II. Observed vibrational frequencies in Cs₂(TCNQ)

<table>
<thead>
<tr>
<th>Symmetry species</th>
<th>Vibrational mode</th>
<th>C₅(TCNQ)⁻⁰</th>
<th>Other TCNQ compounds:</th>
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<tr>
<td></td>
<td>Freq.</td>
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<td>Calculation</td>
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<td>vs</td>
</tr>
<tr>
<td></td>
<td>ν₂′</td>
<td>1585</td>
<td>vs</td>
</tr>
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<td>vs</td>
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<tr>
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<tr>
<td></td>
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<td>107</td>
<td>m</td>
</tr>
</tbody>
</table>

a) v \_N \rightarrow \text{could not distinguish between TCNQ}^0 \text{and TCNQ}^{-} \text{modes.}

b) Data from \(\sigma_{(\text{TCNQ})}\) this work.

TCNQ^0 \text{calculations taken from Ref. 34 and TCNQ}^{-} \text{calculations taken from Ref. 35.}

d) Observed frequencies. Line indicates mode was not observed. vs = very strong, s = strong, m = medium, w = weak, and vw = very weak.

### TABLE III. Calculated relative strength of vibrational modes.

| Mode   | \(\hat{E}||a\) | \(\hat{E}||b\) | \(\hat{E}||c\) |
|--------|----------------|----------------|----------------|
| b₁u    | 0.25           | 0.33           | 0.43           |
| b₂u    | 0.60           | 0.62           | 0.80           |
| b₃u    | 0.96           | 0.00           | 0.02           |
| b₄u    | 1.96           | 0.00           | 0.04           |
| b₅u    | 0.96           | 0.50           | 0.48           |
| b₆u    | 0.02           | 1.22           | 0.78           |

After assigning the \(a_{9}\) features in our data, we have fit the dimer charge oscillation of Rice,\(^{38}\) Eqs. (3), (8), and (9), to the data. A nonlinear least-squares fit\(^{39}\) to the \(\hat{E}||b\) conductivity was used to extract the parameters for each \(a_{9}\) mode. Unfortunately, our data between 700 and 1000 cm\(^{-1}\) were not of sufficient quality to observe the \(a_{9}\) modes in this region.

Figure 11 shows the conductivity data and the fit to this data. The parabolic-like background was
simulated by using a complex frequency-dependent dielectric function for the high-frequency background \( \varepsilon_r \). The fitting procedure gave values between 4 and 25 cm\(^{-1}\) for the \( \gamma_\alpha \). The values for the unperturbed frequencies \( \omega_\alpha \) and the electron-molecular-vibration coupling constants \( g_\alpha \) are given in Table IV. Table IV also summarizes other experimental\(^{18,20,30}\) and theoretical\(^{40,41}\) values for these parameters. Notice that the calculated frequency is always higher than the observed frequency in the conductivity (i.e., the effect of the coupling to the electron is to lower the frequency of the mode). The values obtained for \( g_\alpha \) are in general agreement with both theoretical and observed values in a variety of TCNQ systems. However, the values of \( g_4, g_5, \) and \( g_{10} \) considerably exceed the values expected from theory. It is suspected that the large value for \( g_{10} \) along with the large \( \gamma_{10} \) may be caused by a problem with an overlapping structure in the reflectance spectrum. The observed frequencies for the modes are consistent for each material and we note that many of the very strong modes in the \( \mathbf{E} || b \) conductivity arise from the dimer charge oscillations.

In summary, by measuring the optical properties of \( \text{Cs}_2(\text{TCNQ})_3 \), we have examined electronic ener-

![Table IV. Electron-molecular-vibration coupling parameters for \( \text{Cs}_2(\text{TCNQ})_3 \).](https://example.com/table.png)

| Mode | \( \omega_\alpha \) in cm\(^{-1}\) | \( g_\alpha \) in meV | \( \mathbf{E} || b \) (Ref. 19) | Theory (Ref. 36) |
|------|-----------------|-----------------|-----------------|-----------------|
| \( \alpha_4 \) | 2314 | 64 | 2195 | 101 |
| \( \alpha_5 \) | 2225 | 106 | 1955 | 67 |
| \( \alpha_6 \) | 2210 | 81 | 1995 | 67 |
| \( \alpha_7 \) | 2230 | 106 | 1995 | 67 |
| \( \alpha_8 \) | 2230 | 106 | 1995 | 67 |
| \( \alpha_9 \) | 2192 | 73 | 2195 | 43 |
| \( \alpha_{10} \) | 2192 | 73 | 2195 | 43 |

\* Data from this work.

**FIG. 11.** Frequency-dependent conductivity for \( \text{Cs}_2(\text{TCNQ})_3 \) (10 - 3000 cm\(^{-1}\)). The points represent the data for \( \mathbf{E} || b \) and a fit of the theory of electron-molecular-vibration coupling in the dimer to the data is shown as the solid line. The numbers correspond to the assigned \( \omega_\alpha \) modes of the TCNQ\(^{+} \) molecule.
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gies and electron-molecular-vibration coupling in this material. Five interactions have been investigated in this organic crystal: the transfer matrix element ($t$), the on-site Coulomb repulsion ($U$), the off-site or neighboring Coulomb interactions, the interaction energy between charge-transfer and localized excitations, and the electron-phonon coupling constants ($g_a$). From analysis of the dimer charge-transfer excitation we obtain the values $U = 1.4$ eV and $t = 0.17$ eV. If these values are applied to linear-chain TCNQ systems, then the bandwidth would be $W = 4t = 0.7$ eV $< U$. Since $U > 4t$ the Coulomb interactions are strong and the picture of localized electrons used to describe Cs$_2$(TCNQ)$_3$ is valid.

By extending the optical work below 500 cm$^{-1}$ on Cs$_2$(TCNQ)$_3$, we have been able to examine more modes of vibration in the TCNQ$^0$ molecule and TCNQ$^-$ ion. From analysis of the $a_g$ modes, values for the electron-phonon coupling constants were obtained. We have also attempted to clarify some of the confusion which exists in the literature by systematically assigning vibrational modes of TCNQ$^0$ and TCNQ$^-$ in the optical spectra.

Acknowledgment

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