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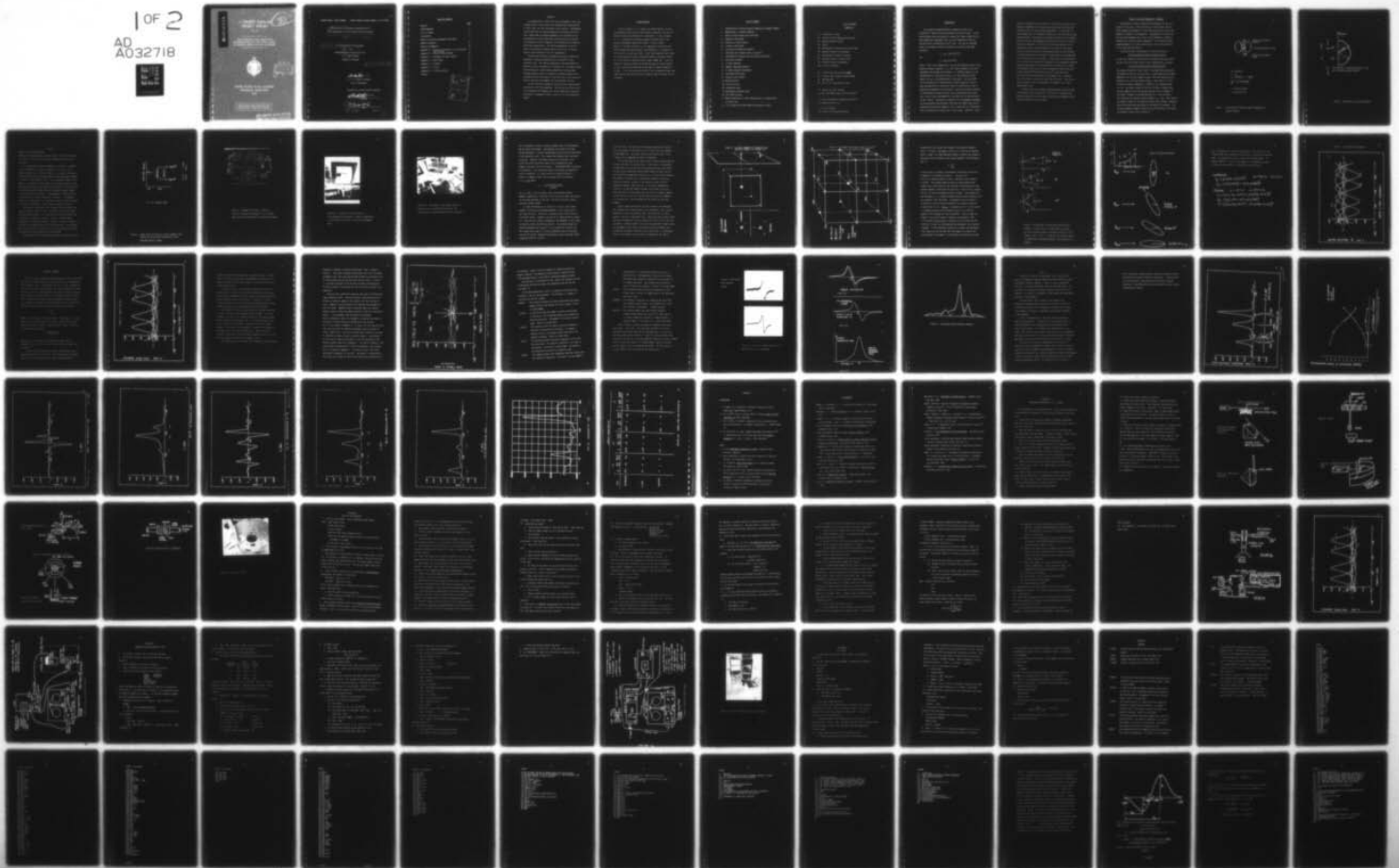
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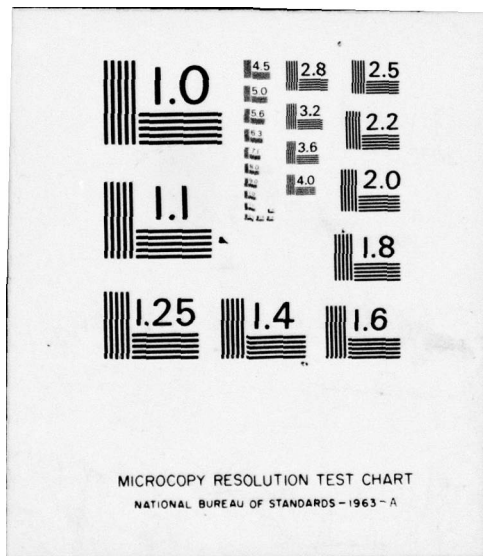
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A TRIDENT SCHOLAR  
PROJECT REPORT

NO. 80

“THE ELECTRON SPIN RESONANCE  
DETERMINATION OF SITE POPULATIONS  
IN ERBIUM DOPED CALCIUM FLUORIDE”



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United States. Naval Academy - Trident Scholar project report, no. 80 (1976)

6 "The Electron Spin Resonance Determination of Site Populations in Erbium Doped Calcium Fluoride"

9 Research report

21 Report on A Trident Scholar Project Report

10 by

Midshipman Danny Hilton Mills, 1976

U. S. Naval Academy

Annapolis, Maryland

14 USNA-TSPR-80

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11 3 June 1976

Date

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## ABSTRACT

The populations of erbium ions in the tetragonal, cubic, and trigonal sites in  $\text{CaF}_2$  crystals were measured for concentrations of .01%, .03%, .1%, and .3% erbium in  $\text{CaF}_2$  crystals. Experimental results show that the relative population of erbium ions in the cubic (quasi-cubic or perhaps aggregate) site increased as the concentration of total erbium ions increased while the relative site population in the tetragonal site decreased with increasing erbium ion concentration. The relative population in the trigonal site increased slightly from the .01% to the .1% concentration, then decreased in the .3% concentration.

Electron spin resonance techniques were used to obtain the absorption resonance characteristics of  $\text{CaF}_2:\text{Er}^{3+}$  in the different sites. The relative populations were determined as a function of total concentration of erbium ions. The doped crystals were maintained at liquid helium temperature (4.2K) and spin resonance spectra taken as a function of azimuthal angle of the DC magnetic field with respect to the [110] axis of the crystal in order to determine the symmetry and thus identify the site.

The data was then recorded for selected lines, digitized and processed in a PDP-8 minicomputer. The data was sent into a file in the Honeywell 635 computer and received additional processing using the APL language in order to arrive at the site population figures.

ACKNOWLEDGMENTS

I wish to thank Dr. C. W. Rector, my Trident Advisor, for his encouragement during several severe attacks of Murphy's Law, for his technical advice and instruction in ESR and APL. I wish to thank Dr. J. J. Fontanella for making my project possible and for his amazing experimental energy and insight. I wish to thank Major D. A. Wright, CAF and Dr. H. M. Neustadt for their help with PDP-8 programs and digital theory, and Professor D. A. Nordling for his help with pictures and slides. To Mr. Norm Stead and Chuck Stump go my many thanks for their invaluable technical assistance, and to Mr. Dick Crebbs for constructing the crystal GYMBAL JIG. I wish to especially thank my parents and friends who kept me in their prayers so that I would have confidence and strength to remain steadfast in my work. I wish to praise Jesus Christ, for His company on many long nights and for the beautiful world of physics that He created for our enjoyment.

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### INTRODUCTION

This project was made possible by questions raised in Dr. Fontanella's<sup>1</sup> research with erbium-doped rare earth crystals. He has found evidence that the dielectric constant for these crystals can be made temperature independent over a certain temperature range for some particular concentration of  $\text{Er}^{3+}$  ions. The real and imaginary parts of the complex dielectric constants are given by the Debye equations:

$$\epsilon' = \epsilon_H'' + A/[T(1+\omega^2\tau^2)]$$

and

$$\epsilon'' = A\omega\tau/[T(1+\omega^2\tau^2)]$$

where  $\epsilon'$  and  $\epsilon''$  are, respectively, the real and imaginary parts of the complex dielectric constant,  $\epsilon_H''$  is the "high" frequency limit and  $A$  represents the strength of the dipole.  $A = Np^2/3\epsilon_0k$  where  $N$  is the concentration of a particular dipole,  $p$  is the particular dipole moment, and  $\epsilon_0$  is the permittivity of free space. The ratio  $Np^2/T$  can be factored out of the dielectric constant equations, and for some concentration of a particular dipole a cancellation of the  $1/T$  temperature dependence can be achieved. Each of the kinds of dipoles in erbium-doped rare earth crystals can be associated with a particular site or local environment for the erbium ion in the rare earth crystal lattice. Electron spin resonance is an independent technique for distinguishing the different sites from one another and also for determining the relative number of ions in each site as a function of total concentration of erbium ions in the crystal. With this infor-

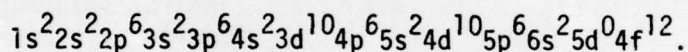
mation Dr. Fontanella believes that it is possible to develop a temperature independent strain gauge or pressure gauge which would be extremely useful in many military applications. In his paper<sup>1</sup> on erbium doped  $\text{CaF}_2$ , Dr. Fontanella alluded to a site that had not been reported before. He observed five different dipoles in his research, but he could find correspondence with only four of the five dipoles previously reported.<sup>2</sup> The fifth in his work was observed at low temperatures and at high concentrations of erbium in the crystal. Since this dipole occurred at high concentrations and the strength increased monotonically with nominal concentration he concluded that this dipole was cluster associated. A paper soon to be published by C.R.A. Catlow<sup>3</sup> gives models and arguments for an aggregation mechanism becoming predominate as the concentration of erbium ions increases. This aggregate site is said to be associated with quasi-cubic site by many researchers.<sup>3,4</sup> My work with  $\text{CaF}_2:\text{Er}^{3+}$  shows that the g splitting value associated with this aggregate site is constant for all rotational orientations about the  $[110]$  axis. This gives a strong suggestion that the aggregate site geometry is at least approximately cubic.

By finding the area of energy absorption peaks associated with the different sites in  $\text{CaF}_2:\text{Er}^{3+}$ , I can give Dr. Fontanella the relative population ratios he needs to explain the temperature compensation mechanism in his crystals.

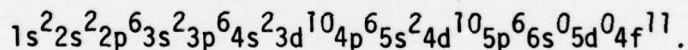
THEORY OF ELECTRON PARAMAGNETIC RESONANCE

The problem of trying to determine the abundance of ions in a crystal is very basic. Once the ions are in the crystal, how can their presence be detected? For the erbium used in my crystals the detection technique is paramagnetism. Paramagnetism is defined for the transition elements and is said to exist whenever a system of charges has a resultant angular momentum.<sup>1</sup> This resultant angular momentum appears in the rare earth group as ions having partially filled inner electron shells.

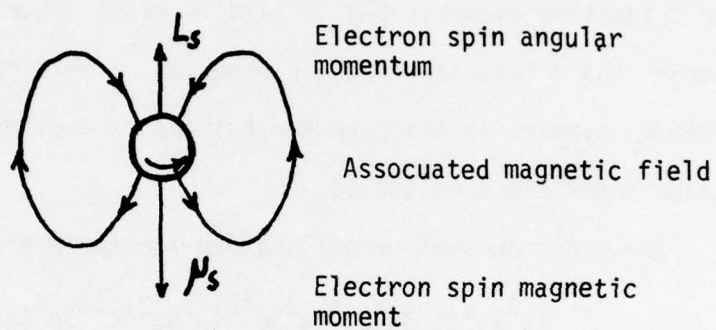
The electron shell configuration for the erbium atom is:



In the ionic condition, two electrons are removed from the 6s shell and one from the 4f shell giving a shell configuration as follows:



The unpaired electron in the 4f shell is shielded from the exterior environment by the full 5s and 5p shell. Associated with the angular momentum is an intrinsic magnetic moment since the electron can be thought of as a spinning negative charge. (See Figure 1). A free electron has angular momentum  $L_s = \hbar\sqrt{3/4}$  for spin quantum number  $m_s = \pm \frac{1}{2}$ . An external magnetic field will produce a torque on the magnetic moment causing the angular momentum vector to precess at the Larmor<sup>2</sup> frequency ( $2\pi \cdot 2.8026$  MHz/Gauss for a free electron). This quantizes the resultant angular moment  $L_{s,2} = m_s \hbar$ . (See Figure 2) The magnetic moment of the unpaired electron thus provides a handle by which we can grab onto the erbium ion and detect its presence. The resultant magnetic moment<sup>3</sup> resolved along the direction of the external magnetic field B can be written as:



For electrons:

$$s = 1/2$$

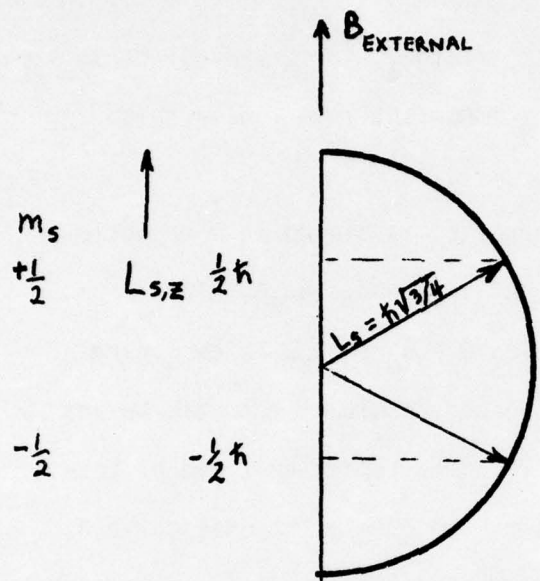
$$L_s = \sqrt{s(s+1)} \hbar = \sqrt{3/4} \hbar$$

$$\frac{\mu_s}{L_s} = 2(1.001159615) \frac{e}{2m}$$

$e$  = electron charge

$m$  = electron mass

Figure 1. Visualization of Electron Angular Momentum and Magnetic Moment



The electron in an external magnetic field has a resultant magnetic moment.

Figure 2. Quantization of Angular Momentum

$$\mu = g\mu_B m_s$$

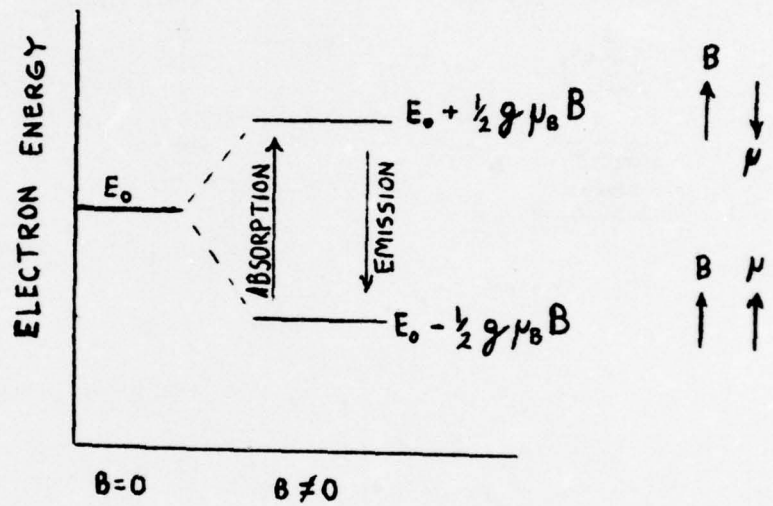
where  $\mu_B$  is the Bohr magnetron

where  $g$  is the spectroscopic splitting factor. For a free electron  $g = 2.0023$ . This factor will be very important later on in this discussion.

If an unpaired electron with energy  $E_0$  is placed in a magnetic field it experiences a change in energy  $\Delta E = -\mu B = g\mu_B B$ . The energy level has split into two levels,  $E = E_0 \pm g\mu_B B$ . See Figure 3. The electron has the least energy when the resultant magnetic moment is parallel to the magnetic field. If our alternating field of frequency  $\nu$  is applied at right angles to the external magnetic field, the electron may undergo an energy level transition. This means that the electron absorbed energy,  $h\nu$ , and the magnetic moment flipped to the anti-parallel direction. This phenomena is called electron spin resonance or electron paramagnetic resonance. The resonance condition is given by  $\Delta E = h\nu = g\mu_B B$  and the energy is made available in the form of microwaves. Figure 4 shows a typical ESR set up.

The klystron is the source of microwaves and the DC magnet provides the external magnetic field. The cavity contains the sample with the magnetic moment. It is one arm of a microwave bridge used for detection of magnetic resonance. Energy is absorbed when a paramagnetic ion undergoes magnetic resonance. The loss of energy is detected as a leakage current in the crystal detector. This leakage must be constant until a resonance occurs or false energy absorption information will be processed by the ESR equipment.

The opposite arm from the klystron contains the reference cavity.



$$\Delta E = -\mu B = m_s g \mu_B B = \pm g \mu_B B$$

Figure 3. Energy level splitting in a static magnetic field showing the two possible orientations of the resultant magnetic moment.

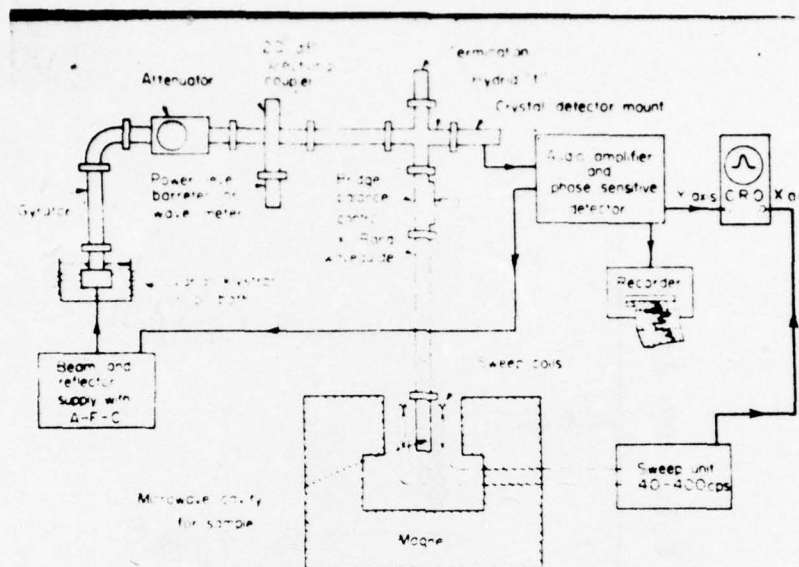


FIG. 3. Block diagram of X band EPR spectrometer.

Figure 4. Diagram of ESR System. Note the klystron, microwave bridge(hybrid "T"), DC magnet sweep coils that produce the first derivative output.

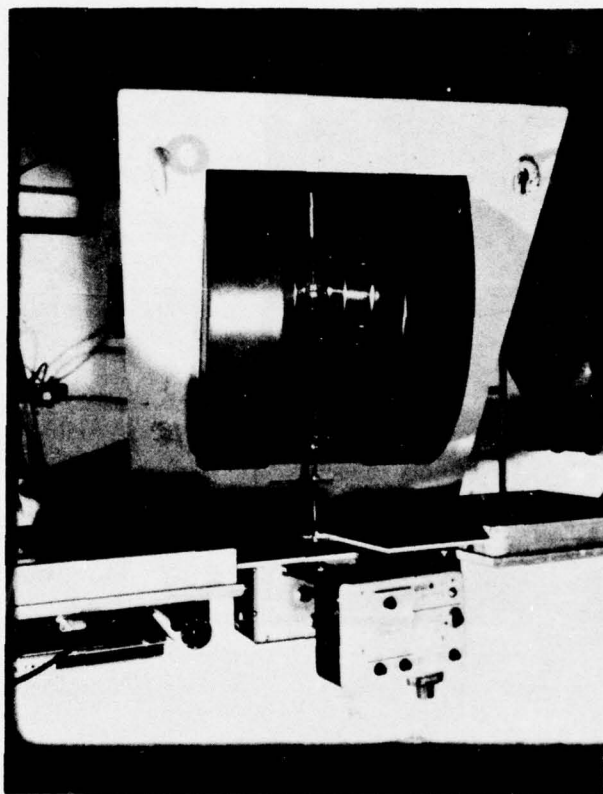


Figure 4a. DC magnet and K-band klystron in room temperature configuration. Note: all experiments in this report used X-band at liquid helium temperatures.

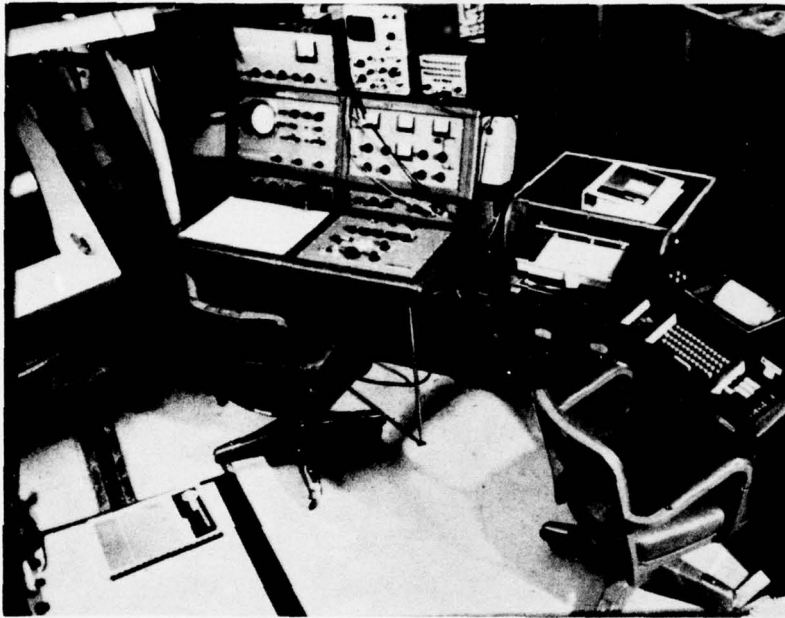


Figure 4b. ESR console in the middle, magnet on the left, strip recorder to the right of the console, and a computer terminal for data reduction.

This is necessary in order to ensure standing waves in the waveguide and to balance the bridge. (See Appendix B for details on using the ESR equipment.) The ESR instrumentation takes the first derivative of the absorption curve. This locates the resonance point much more accurately. However if the Phase Tuning on the klystron is not correct the first derivative output will be asymmetrical with respect to the base line of the signal. (See Appendix E\* for discussion of distortion.) This distortion shows up later when the absorption curve is recovered. If a free ion with an unpaired electron is placed in a magnetic field, the ion energy levels are given by  $E = E_0 \pm g\mu_B B$  where

$$g = 1 + \frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)},$$

and L, S, and J, are the orbital, spin, and resultant angular momenta, respectively. The extra frills on g are to take into account all the other electrons in the ion. The ion can be said to have a resultant magnetic moment.

If, now, the erbium ion is placed in a crystal, the g-factor becomes a little more environment-dependent. The crystals used in this study are  $\text{CaF}_2$ . Calcium is a divalent cation, while erbium is a trivalent cation. Suppose a calcium ion is replaced with an erbium ion. There must be a charge compensating ion somewhere in the crystal to keep the crystal electrically neutral. The dominant charge compensating mechanism for  $\text{CaF}_2:\text{Er}^{3+}$  is an interstitial fluorine ion. The crystals were grown in a fluorine atmosphere and are very pure. Thus the  $\text{O}^{2-}$  and  $\text{OH}^-$  compensation mentioned in Heist and Fong<sup>4</sup> (1970)

\* SEE APL PROGRAM "DISTORT"

is not a factor. The position of the charge compensating fluorine ion, with respect to the erbium ion, will affect the local geometry of the erbium ion. This means that the g-splitting factor is now a tensor, and is dependent on spatial orientation.

In  $\text{CaF}_2$  the fluorine ions form a cubic lattice structure and the calcium ions form a face-center cubic. Each calcium is surrounded by eight fluorine ions and are in alternating fluorine cube centers. In other words alternating fluorine cube centers are empty and can be filled with a compensating fluorine ion. If the fluorine occupies the center of fluorine ions in the nearest neighbor site along a  $[100]$  axis from the erbium ion, the erbium ion sees 4-fold or tetragonal symmetry. (See Figure 5). If the charge compensating fluorine is in the next-nearest neighbor site along a  $[111]$  axis from the erbium ion, the erbium ions see 3-fold or trigonal symmetry. If the fluorine is very far from the erbium ion the local symmetry of the erbium ion is not distorted and the erbium ion sees cubic symmetry.

Figure 6 shows the possible fluorine locations for tetragonal and trigonal sites although there are six tetragonal sites, they are degenerate in pairs along  $[001]$ ,  $[010]$ , and  $[100]$  axes, so there appears to be only 3 equivalent sites. There are eight trigonal sites, but they are degenerate in pairs along  $[111]$ ,  $[\bar{1}\bar{1}\bar{1}]$ ,  $[1\bar{1}\bar{1}]$ , and  $[\bar{1}\bar{1}1]$  directions, so there appears to be only four equivalent trigonal sites. The tetragonal sites can be distinguished from the trigonal sites by choosing the proper rotational axis of the crystal. As mentioned earlier, the g-factor is now a tensor and depends on the spatial

Figure 5. Four-fold symmetry of tetragonal site.  
Three-fold symmetry of trigonal site.

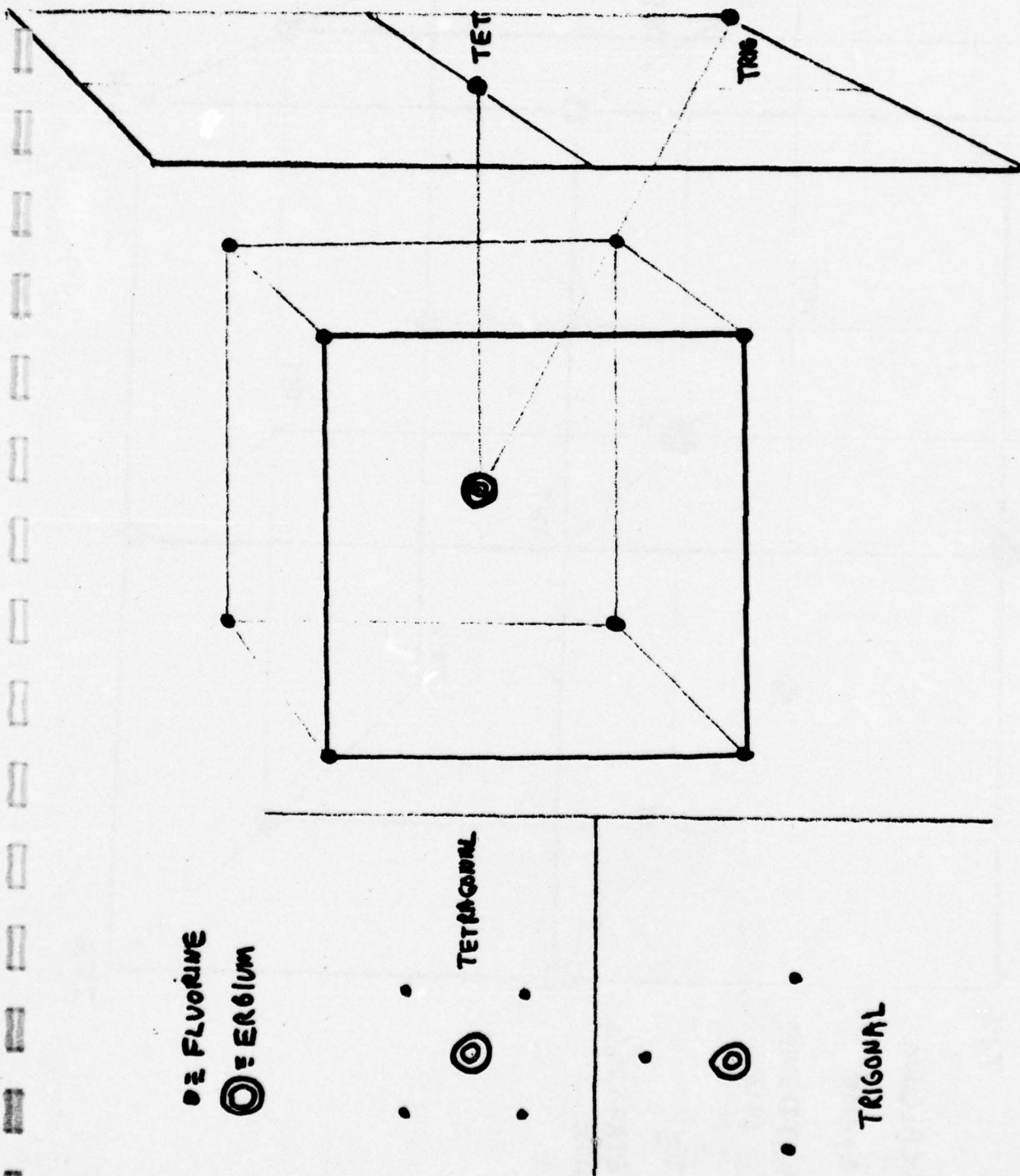
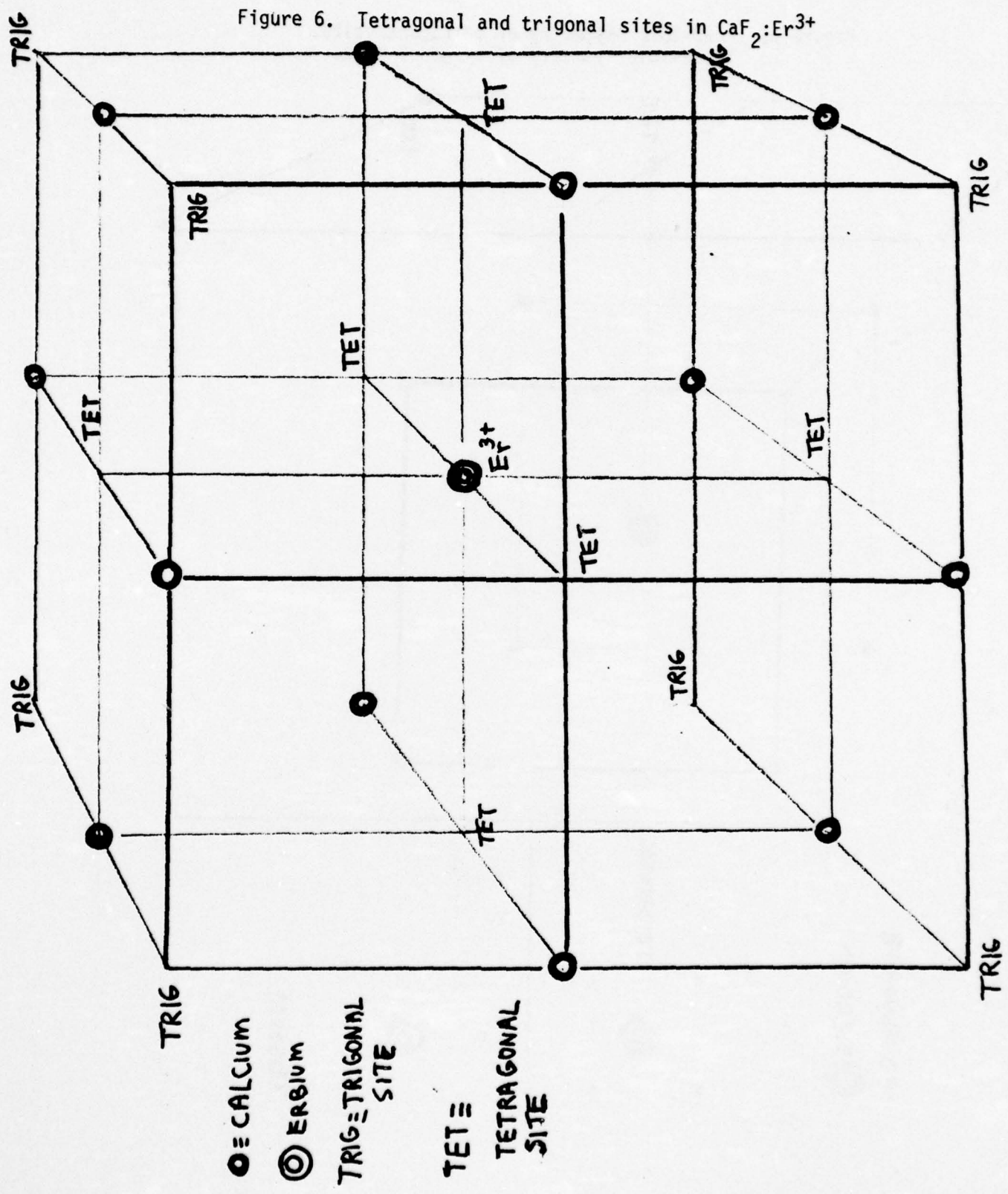


Figure 6. Tetragonal and trigonal sites in  $\text{CaF}_2:\text{Er}^{3+}$



orientation of the crystal with respect to the external magnetic field. In Figure 7 the general case of  $g$  as a function of rotation angle is shown. For some rotational angles,  $g$  defines the change of the energy level splitting as the external magnetic field increases, that is

$$g = \frac{\Delta E}{\mu_B B}$$

As the crystal is rotated in the magnetic field about a given axis,  $g$  changes as illustrated in Figure 7. The set of all  $g$ 's for all rotations about all axes is defined as the splitting ellipsoid. The distance from the center of the ellipsoid (the erbium ion) to the surface of the ellipsoid in the direction of the external magnetic field gives the value of  $g$ . Note that as  $g$  changes the  $\Delta E = h\nu$  from the microwaves remains constant. The frequency of the microwaves,  $\nu$ , is constant therefore giving constant energy  $h\nu$  for any resonance that take place. The magnetic field (in Gauss) is varied over a certain range and whenever the resonance condition is satisfied,  $\Delta E = h\nu = g\mu_B B_{\text{ext}}$ , a resonance occurs. As the crystal is rotated,  $g$  changes and the resonance occurs at a different magnetic field strength for that orientation. Figure 8 shows the change in  $g$  as the ellipsoid is rotated in the magnetic field. C. W. Rector<sup>5</sup> analyzed several rotational axis and found that the [110] axis is best for distinguishing the tetragonal sites from the trigonals. In the rotational spectrum of  $g$  values, two tetragonal sites show up as one line and the third appear in a second line. Three trigonal lines appear in the spectrum, two behaving the same

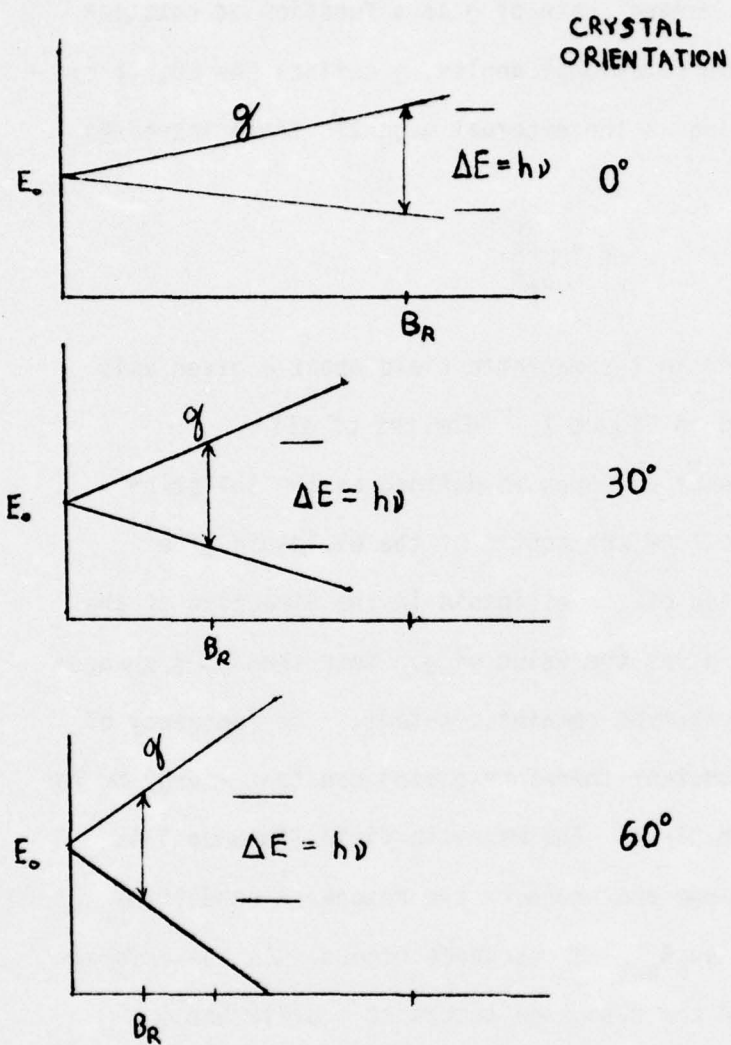


Figure 7. Relationship of Energy Level Splitting and g-factor. As the crystal is rotated about a symmetry axis in an external magnetic field the g-splitting factor changes. Note: Since  $\nu$  is constant, the resonance energy is constant but the resonant magnetic field strength,  $B_R$ , changes.

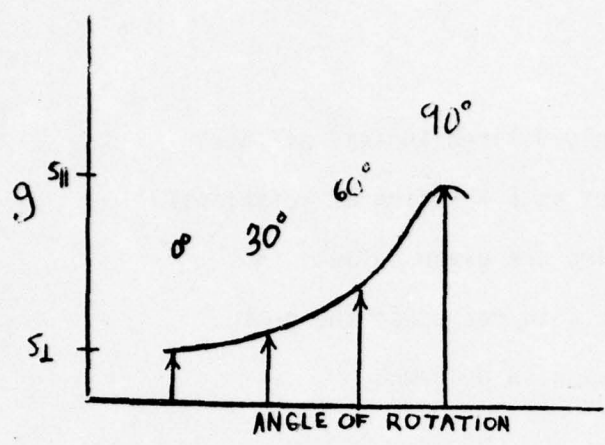
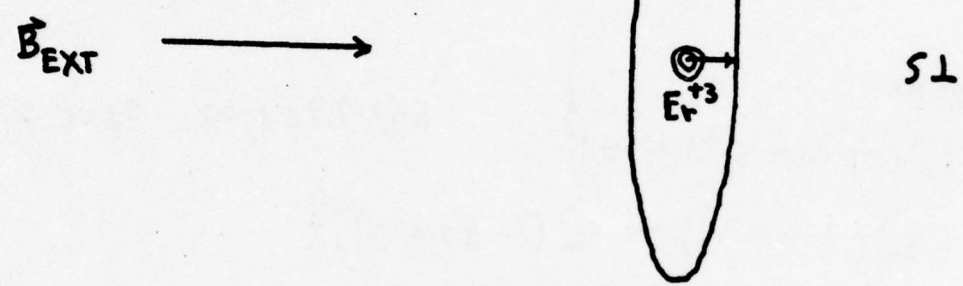


Figure 8. Splitting Ellipsoid



FLUORIDE



way, thus appearing as one line, giving only 3 lines instead of four. Figure 9 shows the g spectrum for the sites as a function of rotational angle. The equations for the g of each line are given below. A program "ESRLOT" is given in the Appendix E to reproduce the g-map. A listing of the values at 5° intervals may also be found.

## TETRAGONAL

$$S_z = (S_{||}^2 \cos^2 \theta + S_{\perp}^2 \sin^2 \theta)^{\frac{1}{2}} \quad S_{||} = 7.78 \pm .02 \quad S_{\perp} = 6.25 \pm .01$$

$$S_{x,y} = (S_{||}^2 (\frac{1}{2} \sin^2 \theta) + S_{\perp}^2 (1 - \frac{1}{2} \sin^2 \theta))^{\frac{1}{2}}$$

## TRIGONAL

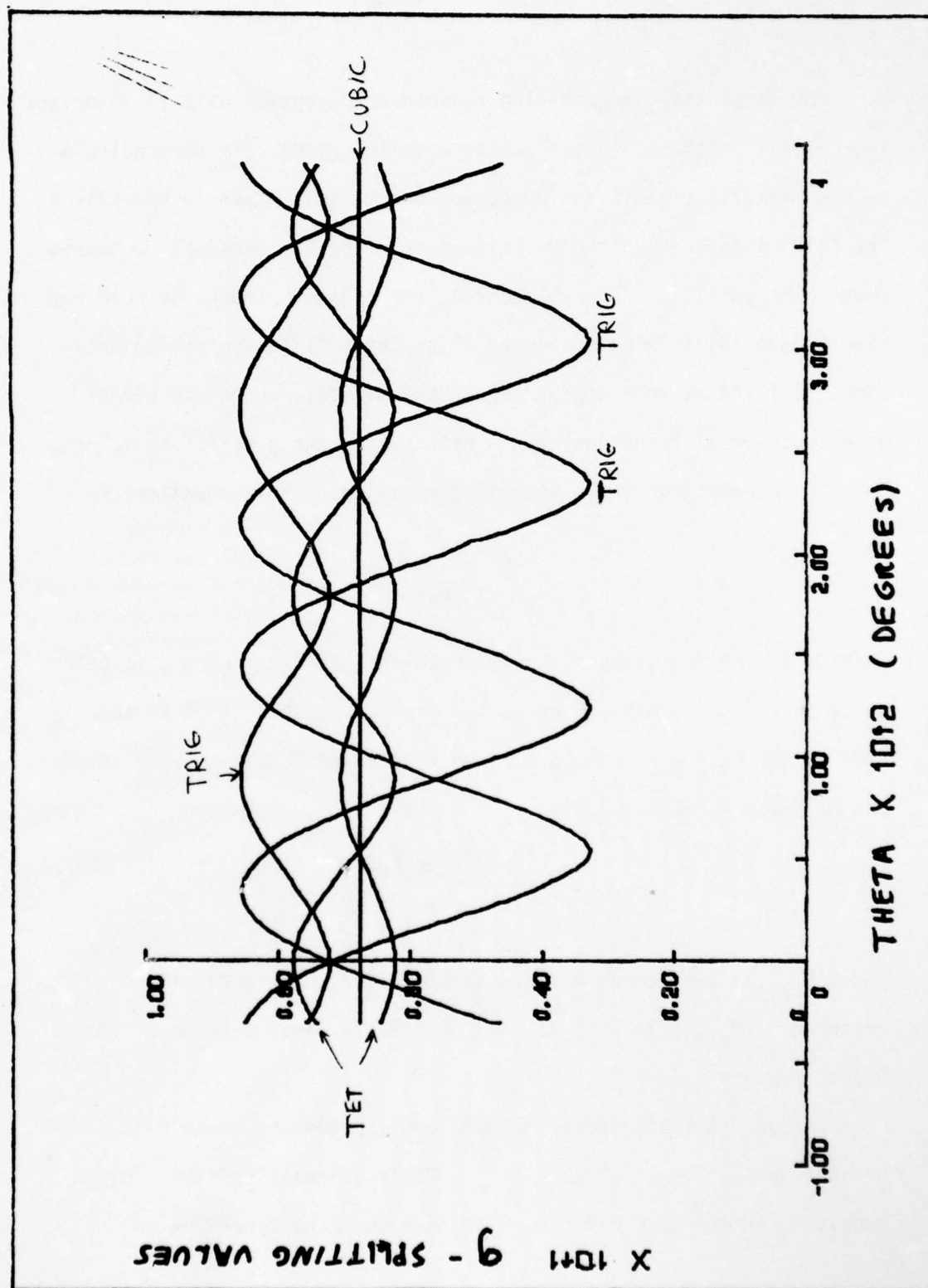
$$S_{||} = 3.29 \pm .01 \quad S_{\perp} = 8.55 \pm .02$$

$$S_1 = (S_{||}^2 \cos^2(\theta - 54.75^\circ) + S_{\perp}^2 \sin^2(\theta - 54.75^\circ))^{\frac{1}{2}}$$

$$S_{2,\bar{4}} = (\frac{1}{3} S_{||}^2 \cos^2 \theta + S_{\perp}^2 (1 - \frac{1}{3} \cos^2 \theta))^{\frac{1}{2}}$$

$$S_3 = (S_{||}^2 \cos^2(\theta + 54.75^\circ) + S_{\perp}^2 \sin^2(\theta + 54.75^\circ))^{\frac{1}{2}}$$

Figure 9. g-Splitting Value Spectrum



### METHOD OF RESEARCH

The first step in gathering resonance absorption data is to orient the crystal in the microwave cavity with the [110] axis perpendicular to the magnetic field. The procedure for this is given in Appendix A. The [110] axis becomes the rotational axis for the external DC magnet. Once the crystal is properly mounted, the magnetic resonance road map (See Figure 10) is used to locate  $0^\circ$  or the [001] azimuthal orientation. I found it more useful to map the magnetic resonance points as a function of rotational angle rather than the g splitting values. The map is made from the g splitting equation by this equation:

$$B = \frac{h\nu}{g\mu_B},$$

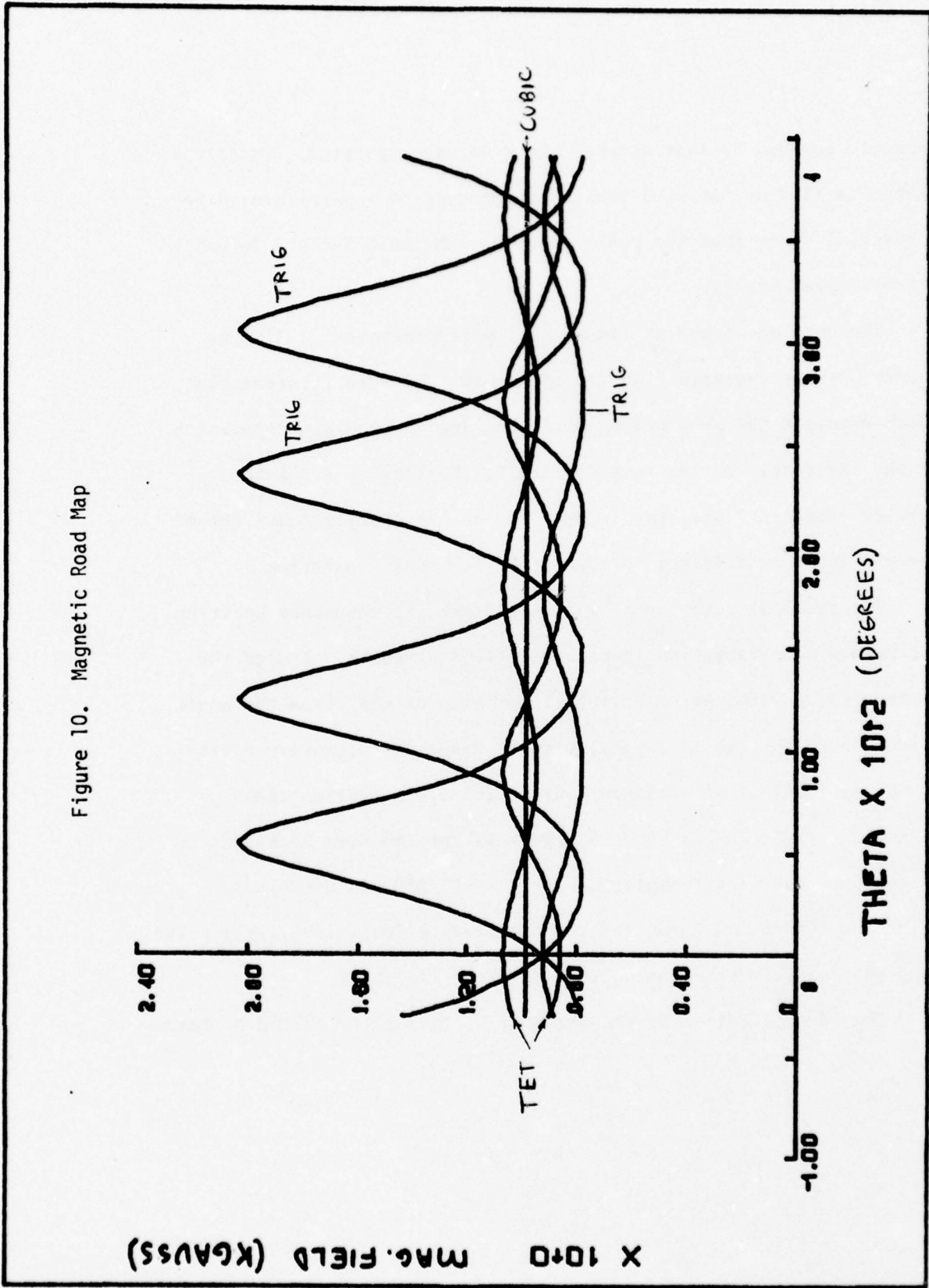
where  $\nu$  is the frequency of the microwaves. The frequency  $\nu$  is determined by using a small amount (a few grains) of DPPH taped to the side of the cavity. DPPH has a fixed g value of  $2.0036 \pm .0003$  and  $\nu$  can be found by this formula:

$$\nu = \frac{(2.0036)\mu_B B_{\text{ext}}}{h}$$

where  $B_{\text{ext}}$  is the magnetic field strength for which DPPH will resonant. ( $B_{\text{ext}} \approx 3.29$  to  $3.5$  KG) Figure 10 gives a graph of the B spectrum.

I found that the tetragonal and cubic resonance peaks have a greater separation at  $0^\circ$  (or  $180^\circ$ ). Other orientations that looked promising on the road map proved to have too many hyperfine or

Figure 10. Magnetic Road Map



harmonic resonances that crowded the resonance spectrum. Ideally I wanted to find an isolated peak corresponding to a particular site. However, I found that the peaks overlap. The best I could do was to minimize peak overlap.

The data was taken at liquid helium temperatures ( $4.2^{\circ}\text{K}$ ) to reduce lattice vibrations and to reduce the spin-orbit interaction, which broadens the absorption curves, making an accurate separation of the individual curves very difficult. Working at  $4.2^{\circ}\text{K}$  the lattice vibrations are "frozen out" and the absorption peaks become sharper and more distinct, producing better peak separation.

The trigonal site can be isolated since its resonance spectrum has such a wide variation in magnetic field strength. I used the resonance ( $-1.74\text{KG}$ ) at an azimuthal rotation of  $+39^{\circ}$  from the angle which I used for the tetragonal sites. Since the microwave cavity is not cylindrical it presents a different cross-section to the magnetic field and as the the magnet is rotated from  $0^{\circ}$  magnet to  $60^{\circ}$  magnet, the signal amplitude decreases. DPPH is used as a reference absorption curve for the two orientations since its g value does not change with rotation in a magnetic field.

The identification of the sites at  $0^{\circ}$  (hereafter called  $\theta^{\circ}$ -theory

and, when in reference to magnet orientation,  $\theta^\circ$ -mag) is shown in Figure 11. The larger tetragonal peak accounts for 2/3 of the total tetragonal sites, while the smaller peak accounts for the other third. For the trigonal spectrum the two lines that vary from  $g = 8.55$  to  $g = 3.29$  each represent 1/4 of the total trigonal site population. The third trigonal line accounts for 2/4 of the total trigonal site population.

With the sites identified I began the real work of getting areas under absorption curves. The basic problem I encountered here was getting a consistent symmetric line shape in the first derivative curve. Appendix B gives the details for handling the equipment for best line shape. Appendix E has a discussion about the software method I used to correct for phase distortion in the first derivative output. I also proposed a few variations on the method. After the resonance signal is as symmetric as possible the signal is recorded on a Hewlett Packard instrumentation tape recorder. This is also covered in Appendix B. As soon as all the recordings are done, they are taken to a PDP-8E minicomputer which has analog to digital capabilities. The analog voltage signal recorded on the tape is converted to numbers stored in the PDP-8 memory. The procedure for this and for sending the numbers to the DTSS (Dartmouth Time Sharing System) system are in Appendix C. One item of interest is the low pass moving average digital filter incorporated in the software. This is discussed in Appendix G. The result of this filter gives outstanding "smoothness" to the data. The program is constructed so that either the filtered or non-filtered data may be displayed on an

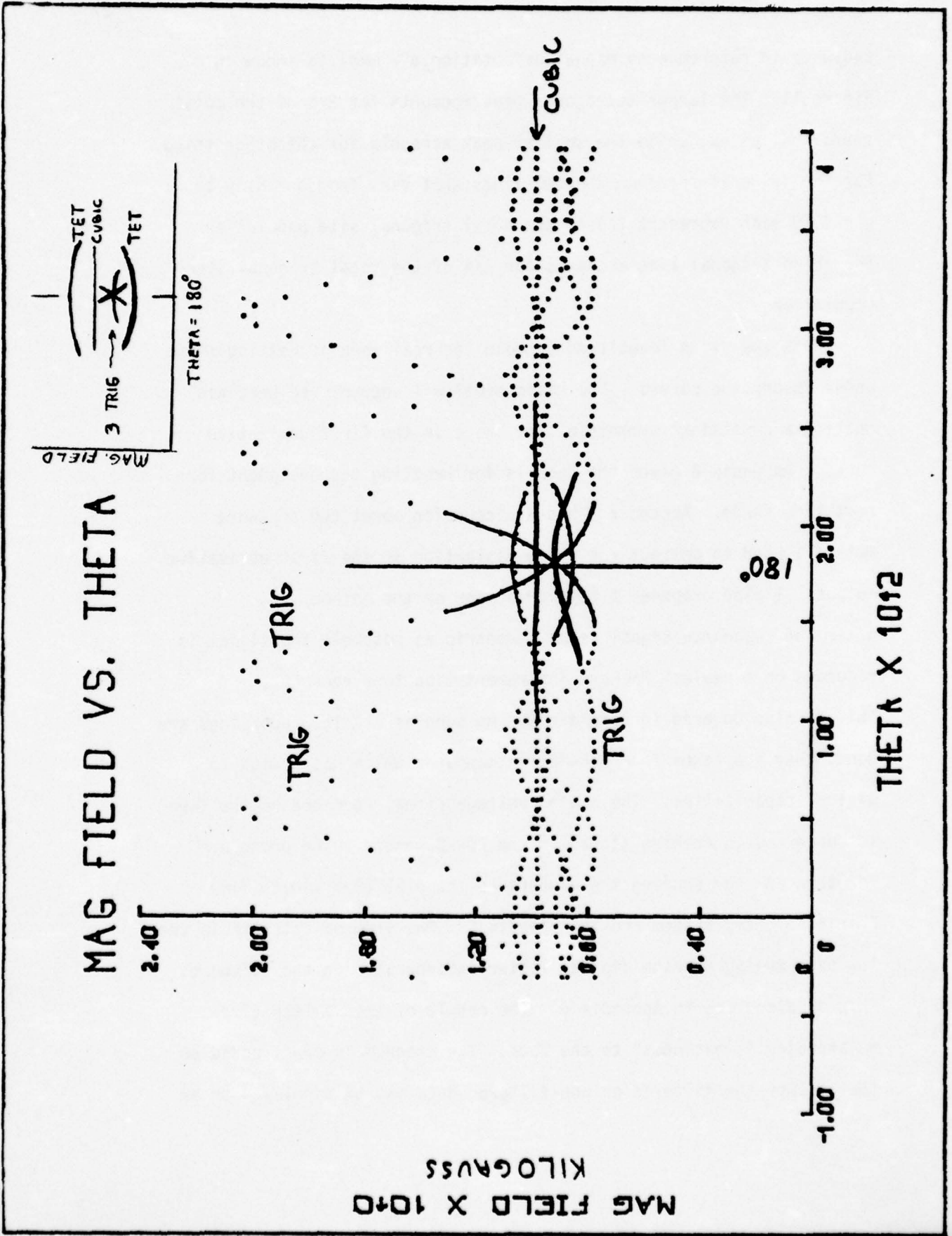


Figure 11. 0° or 180° [001] Azimuthal Orientation

oscilloscope. Figure 12 gives an example of a DPPH curve with and without filtering. The operator has the option of controlling the filter parameter which is the width of the moving summation window.

Once the data is transferred to DTSS, several APL programs are used to manipulate the data to recover the absorption curve and get the area under it.

By following Appendices A thru E a researcher can duplicate the procedure I used for the experiment. The following is a summary of the action of each APL program.

- RAWCOR: This program eliminates the PDP-8 modulo 4096 wrap-around, removes DC bias, and corrects for initial potato. Result is called CORDAT.
- CUTPLOT: Is used to cut down the number of points to be plotted. In this way a file of 4096 data points may be reduced to 200 plotting points. See Appendix D for use of plotted graph. Result is called CPOUT.
- DISTORT: This program corrects for phase distortion produced by imbalance in phase tuning on klystron. It assumes a Gaussian error in the leakage current that detects the magnetic resonance. Result is called CORD.
- INTTEG: This program performs indefinite integration on the first derivative data. The range of integration is an input to the program. The result is called ICURV. The output is the absorption curve with an integration ramp.
- ABSCOR: This program corrects the integration ramp that results from the indefinite integration. The result is called CORDATA.

- FIT: This program fits a particular absorption curve to a Gaussian curve. The boundaries of the curve are inputs. Amplitude A and exponential coefficient B are outputs; ST is standard deviation. The mid-point of the Gaussian curve is found by the program. The result is called CURFIT.
- INTSIM: This program performs the definite integration on the fitted curve to arrive at a number equal to the area under the fitted curve.
- APLTOBAS: This program is necessary for converting APL data files into standard graphic format. Use CUTPLOT while in APL; exit from APL; run APLTOBAS (a BASIC program).
- ESR PLOT: This program outputs the g-splitting or magnetic resonance point spectra for  $\text{CaF}_2:\text{Er}^{3+}$  in table form or in a form suitable for plotting. (a BASIC program). It requires "Split" as an output file. (from  $-30$  to  $390^\circ$ )

Figure 14 shows a pictorial procedure for recovering the absorption curves. Figure 14a. shows the phase distortion of a first derivative curve (dark line) and its corrected shape. This is done with the program called "DISTORT." Figure 14b. shows the DPPH first derivative line and 14c. shows the indefinite integration results (INTTEG). Figure 15 shows the results of a complex erbium spectrum and shows how the program "FIT" will separate the curves. All that remains is to use "INTSIM" to find the area of the fitted curves.

Figure 12. Unfiltered  
DPPH resonance  
signal.

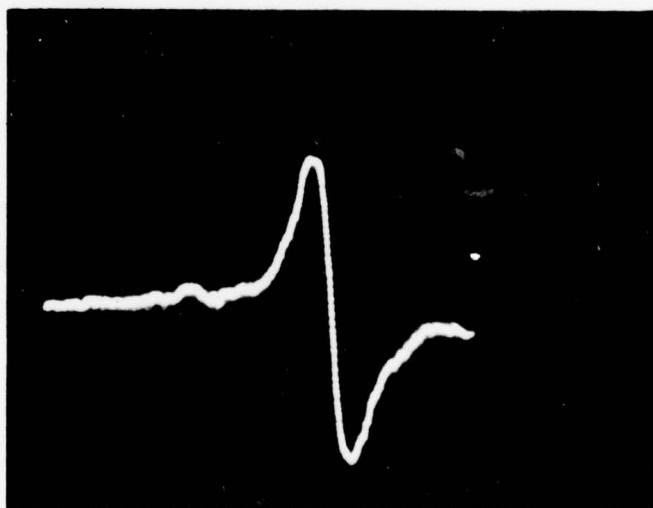
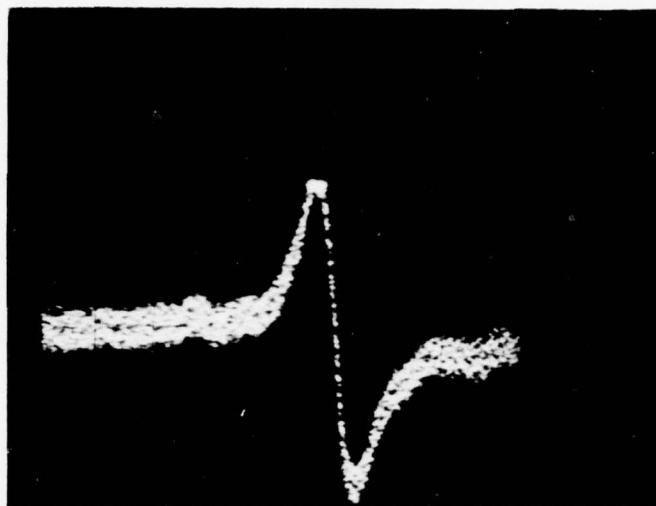
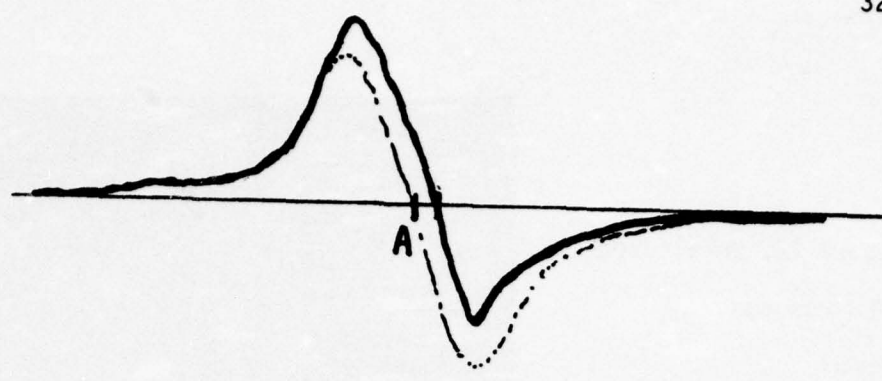


Figure 13. results of digital filter on 17 Hz  
beat frequency in ESR equipment.



### PHASE DISTORTION

Figure 14a.

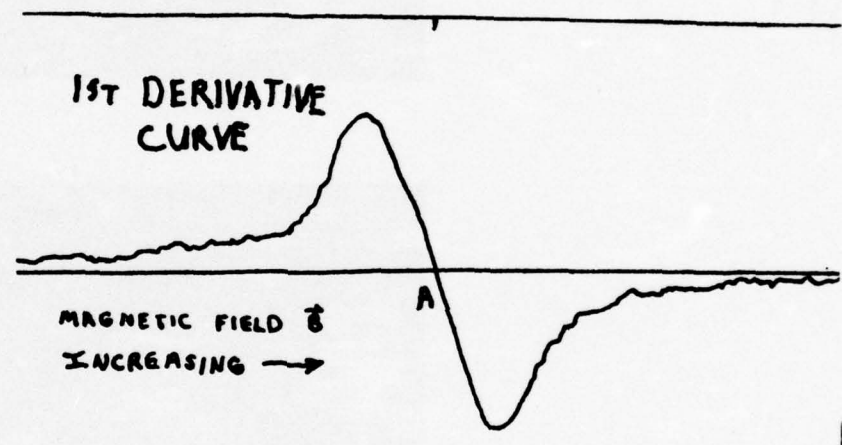


Figure 14b.

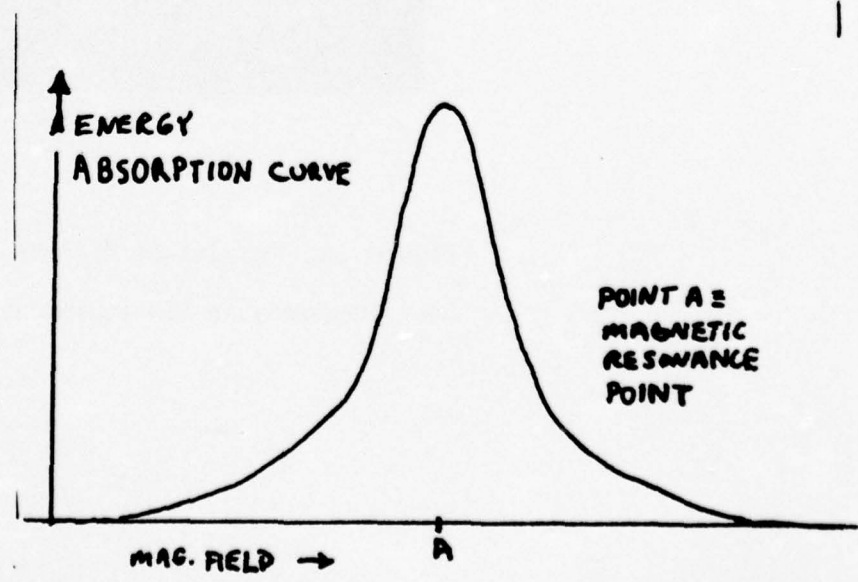


Figure 14c.

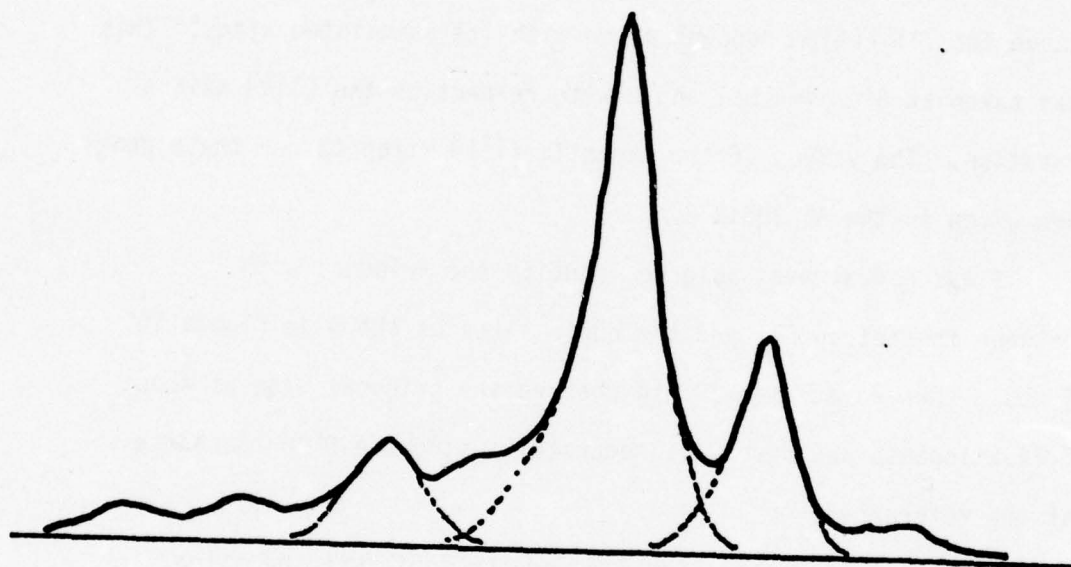


Figure 15. Overlapping Erbium resonance spectrum.

## RESULTS

I was able to identify the tetragonal, cubic, and trigonal sites in the magnetic resonance spectrum of erbium doped  $\text{CaF}_2$  using the magnetic resonance read map. Figure 16 shows an absorption curve for .1% erbium concentration with its associated sites. This was taken at  $0^\circ$  azimuthal angle with respect to the  $[110]$  axis of rotation. The values of the magnetic field strength for these peaks are given in the Appendix G.

I was not always able to identify the trigonal site between the tetragonal and the cubic sites as shown in Figure 16. I would then rotate to  $+39^\circ$  to observe the trigonal site at about 1.74 kilogauss and record it separately using the DPPH resonance as the reference.

In the .3% concentration I found the cubic site becoming dominant in absorption. I noted that in the rotational study of that concentration, the g-splitting value associated with the cubic did not change. As I stated in the introduction to this paper, this cubic site has recently been thought to be an aggregate or cluster of erbium ions and the associated interstitial fluorines. My studies show that the cluster must be at least cubic in nature.

My results on the relative populations of the sites as a function of total concentration of erbium ions is shown in Figure 17. The cubic becomes dominant as the concentration of erbium increases. Perhaps the tetragonals are crowding each other and becoming aggregates. Figures 18 through 23 shows some first derivative curves and their associated absorption curves. In Figure 23, the .01% erbium, I

had a little extra to do in order to recover the absorption curve that would be suitable for definite integration. I took the data for the .01% before I realized the serious effects of phase distortion. Figure 24 gives the relative percent figures for each concentration of erbium.

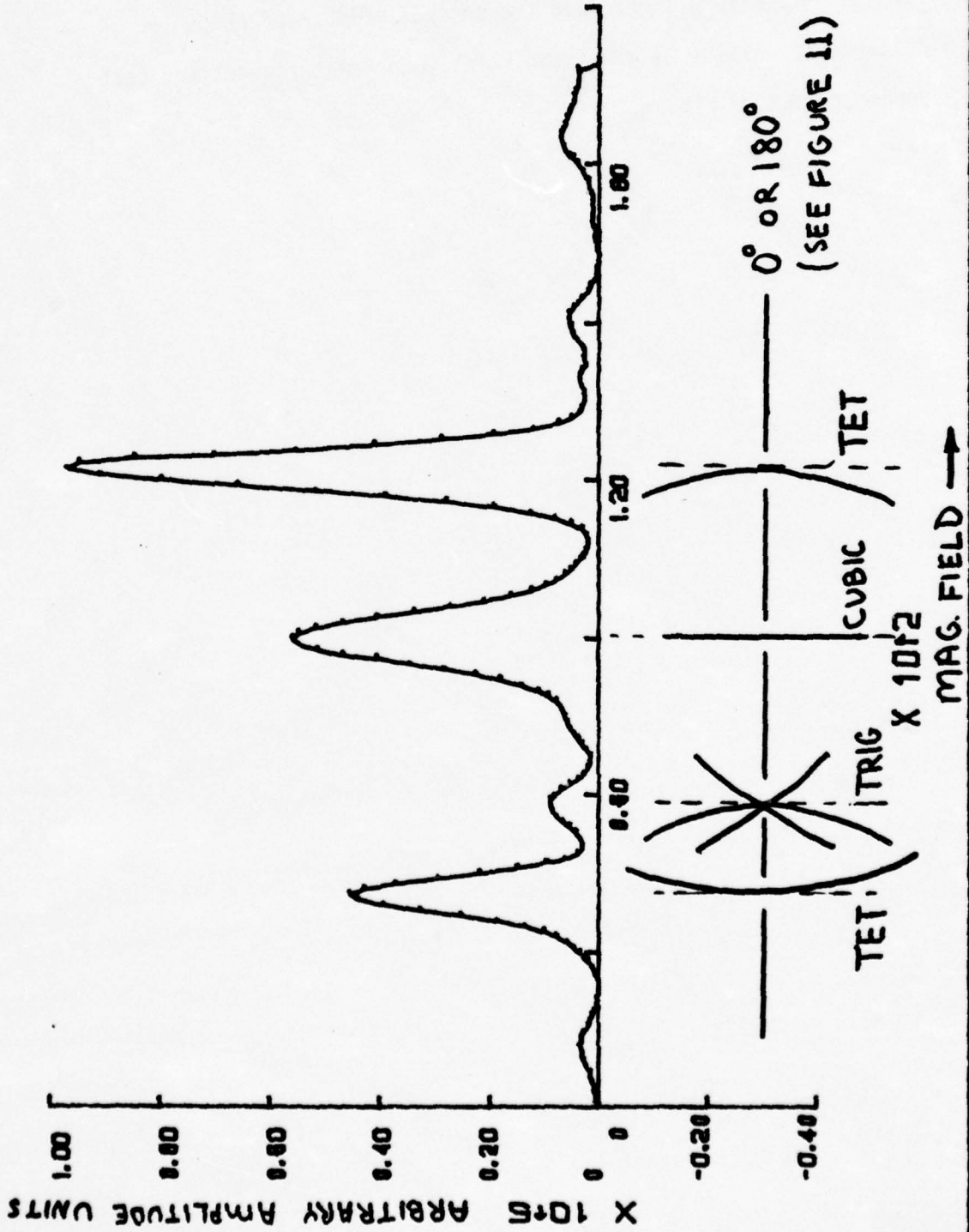


Figure 16. Site identification.

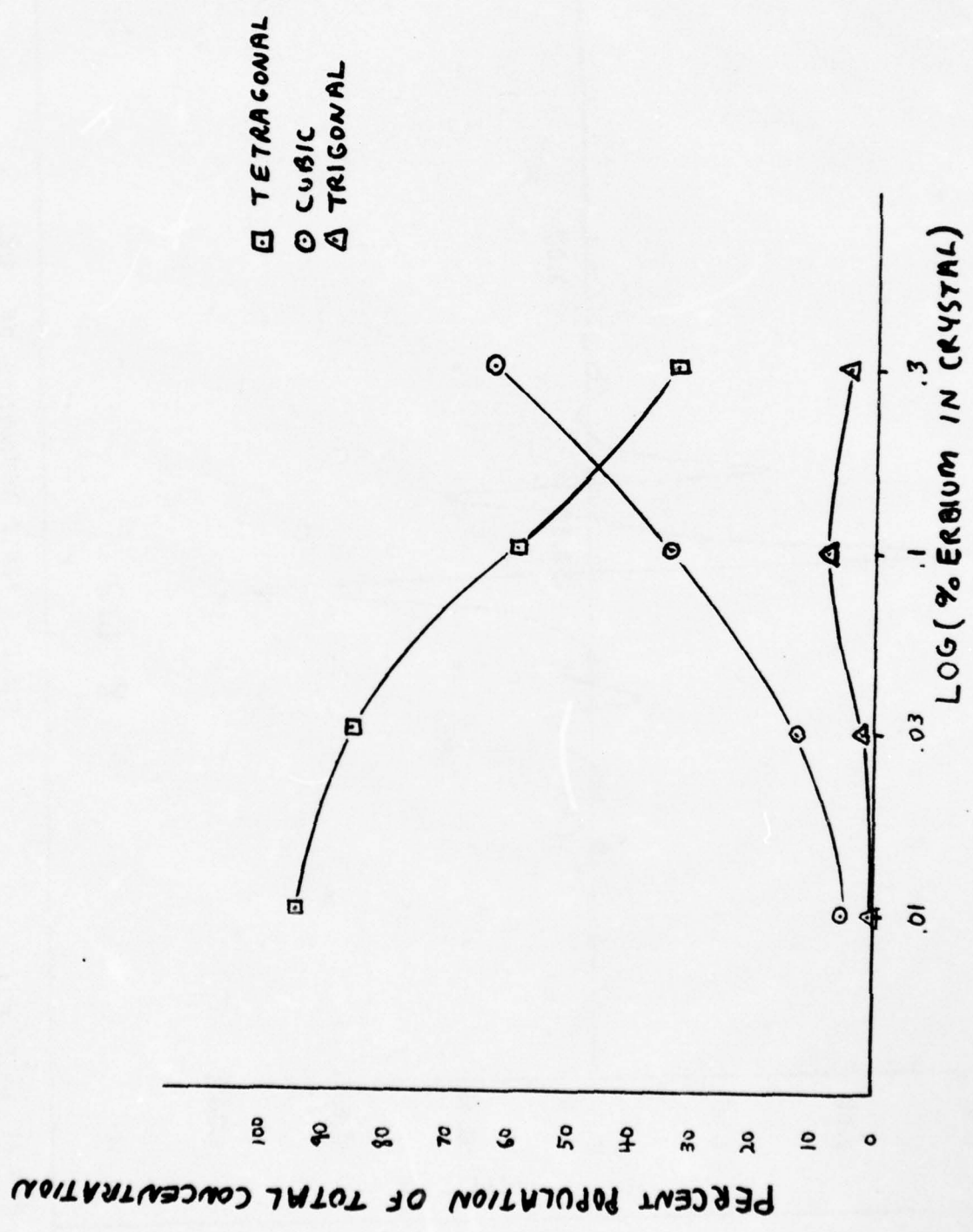
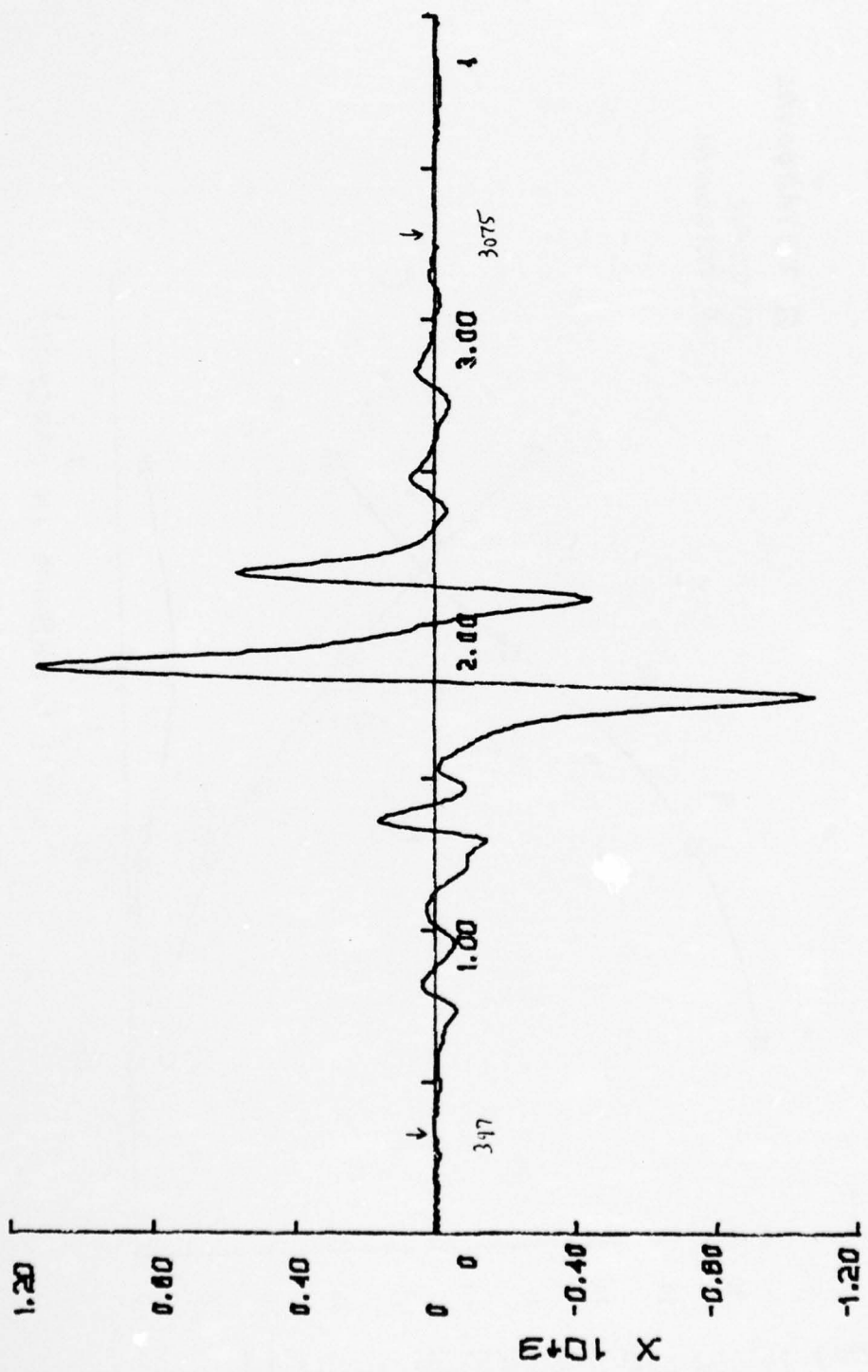


Figure 17. Percent Population of Total concentration vs. Concentration of Erbium ions.



X 10<sup>12</sup>

400 p/s  
3968 p/s

FIG 18. FIRST DERIVATIVE OF .390

TIME 227 pos 12 p/20

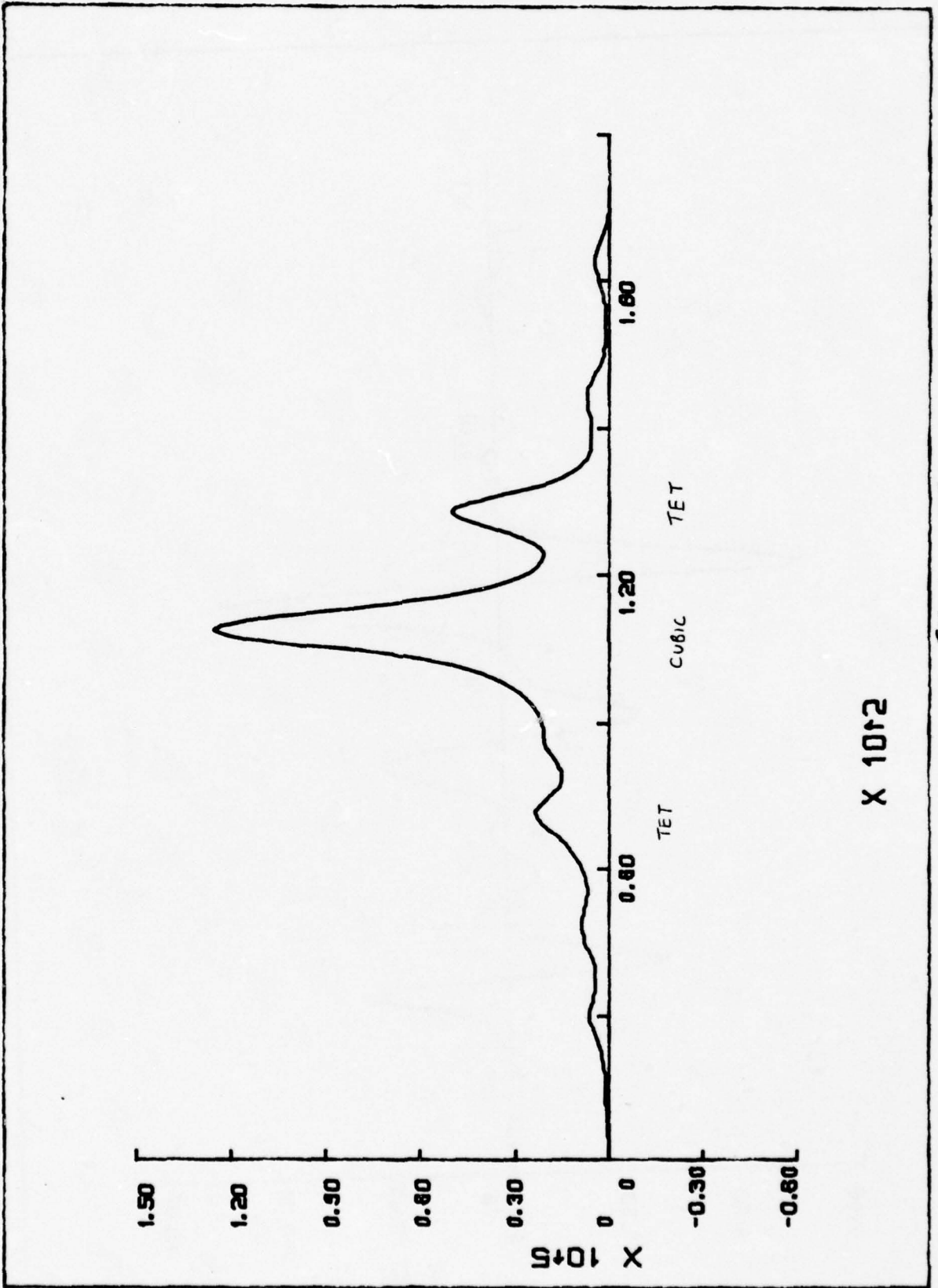
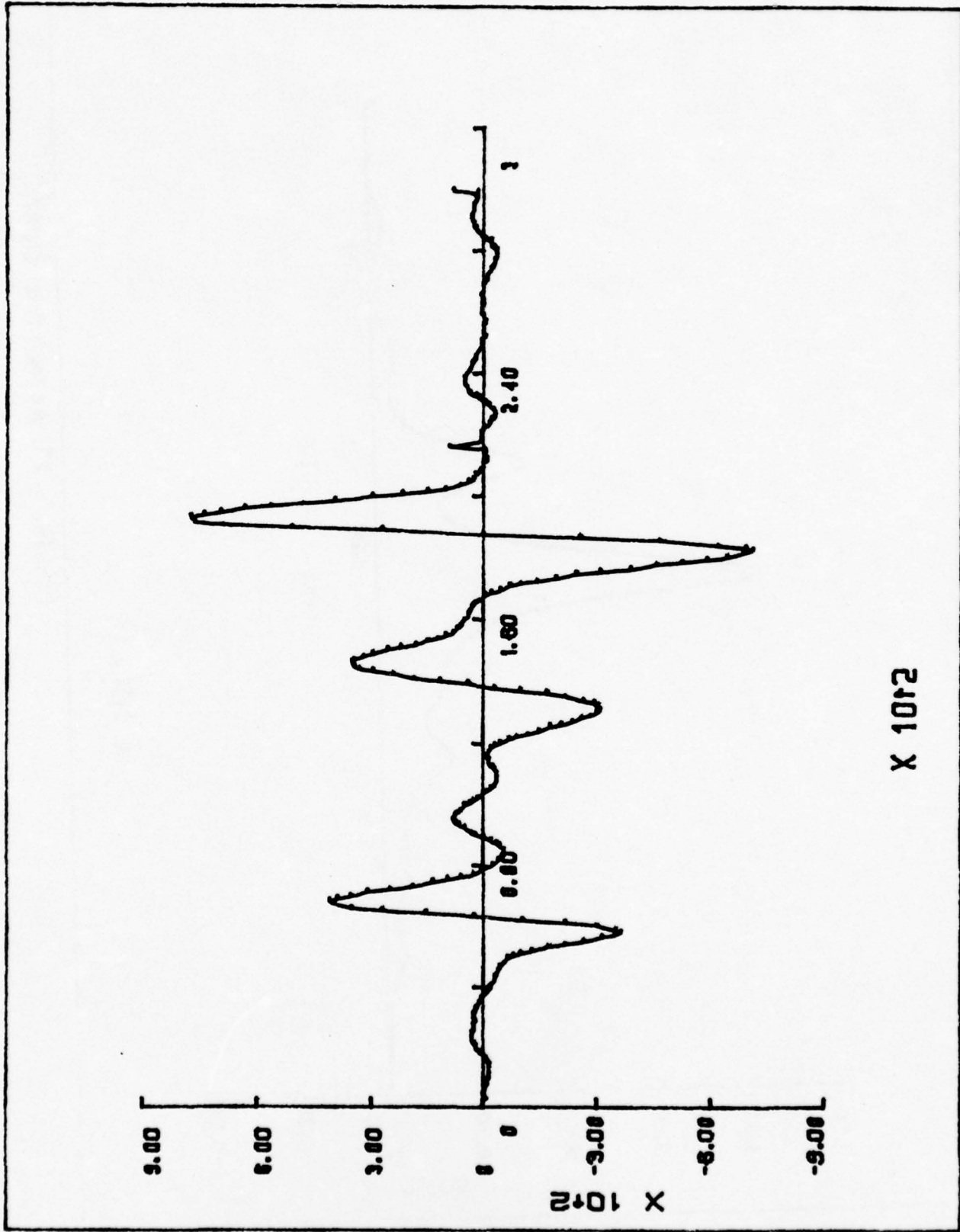


FIG. 19. .3% ABSORPTION CURVE

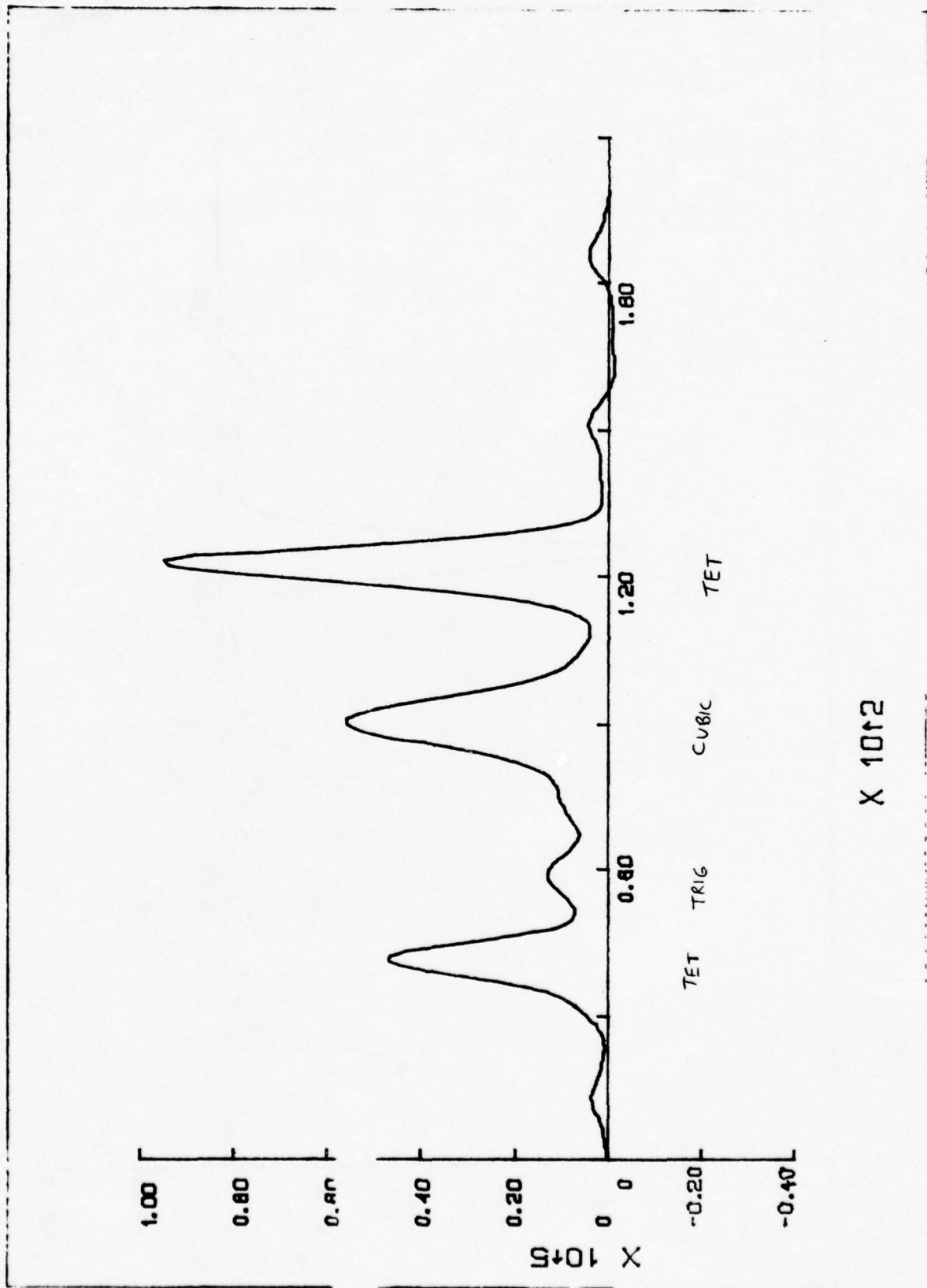


X 10<sup>2</sup>

FIG. 20 FIRST DERIVATIVE OF .17<sub>0</sub>

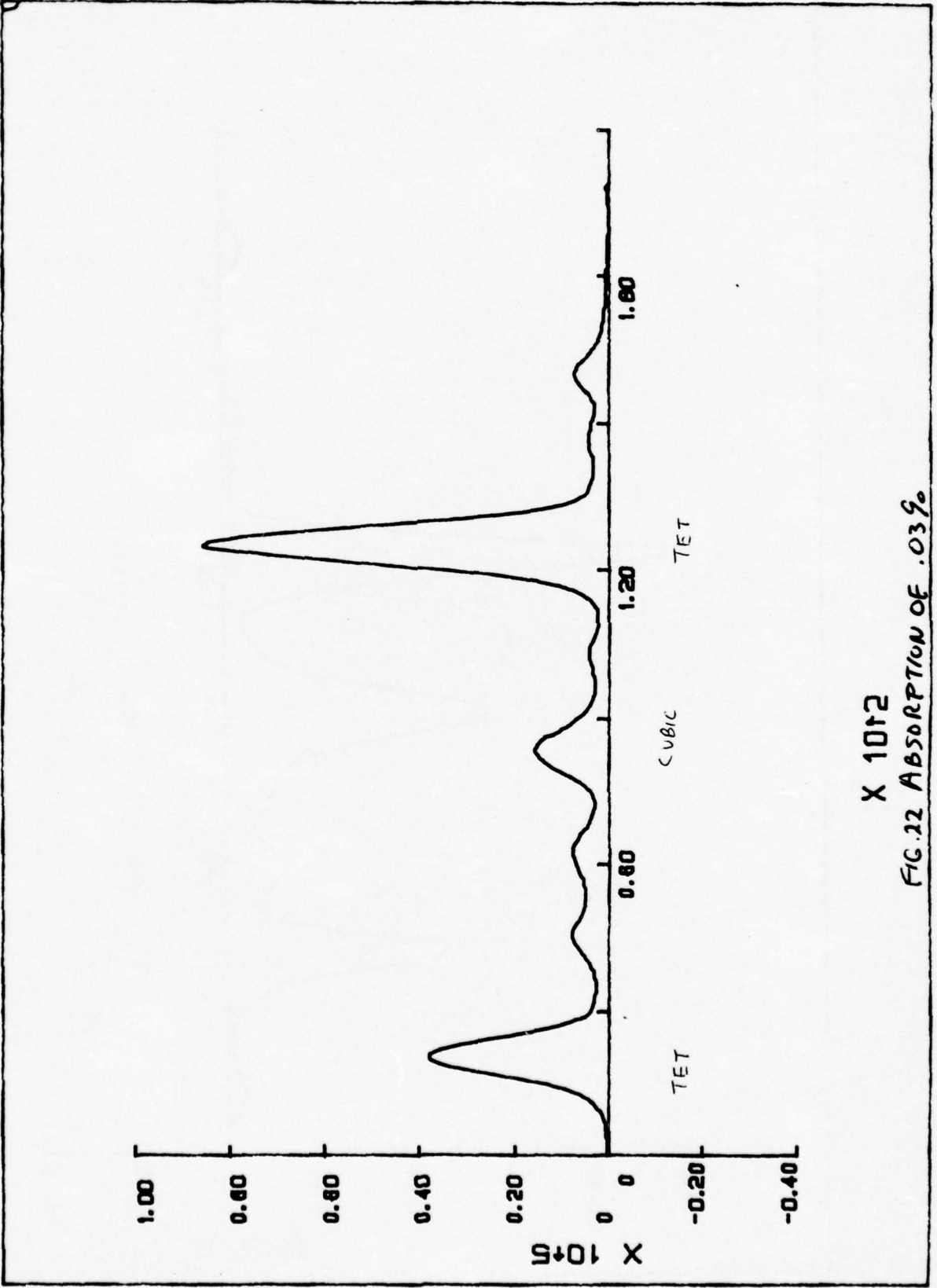
40  
 57201  
 SA.F.2. EPT3 .17<sub>0</sub> -60.10MS

APR 22 1953 842 'A'



X 10<sup>5</sup>

FIG. 21 ABSORPTION CURVE OF .170



X 10<sup>5</sup>  
FIG. 12 ABSORPTION OF .03%

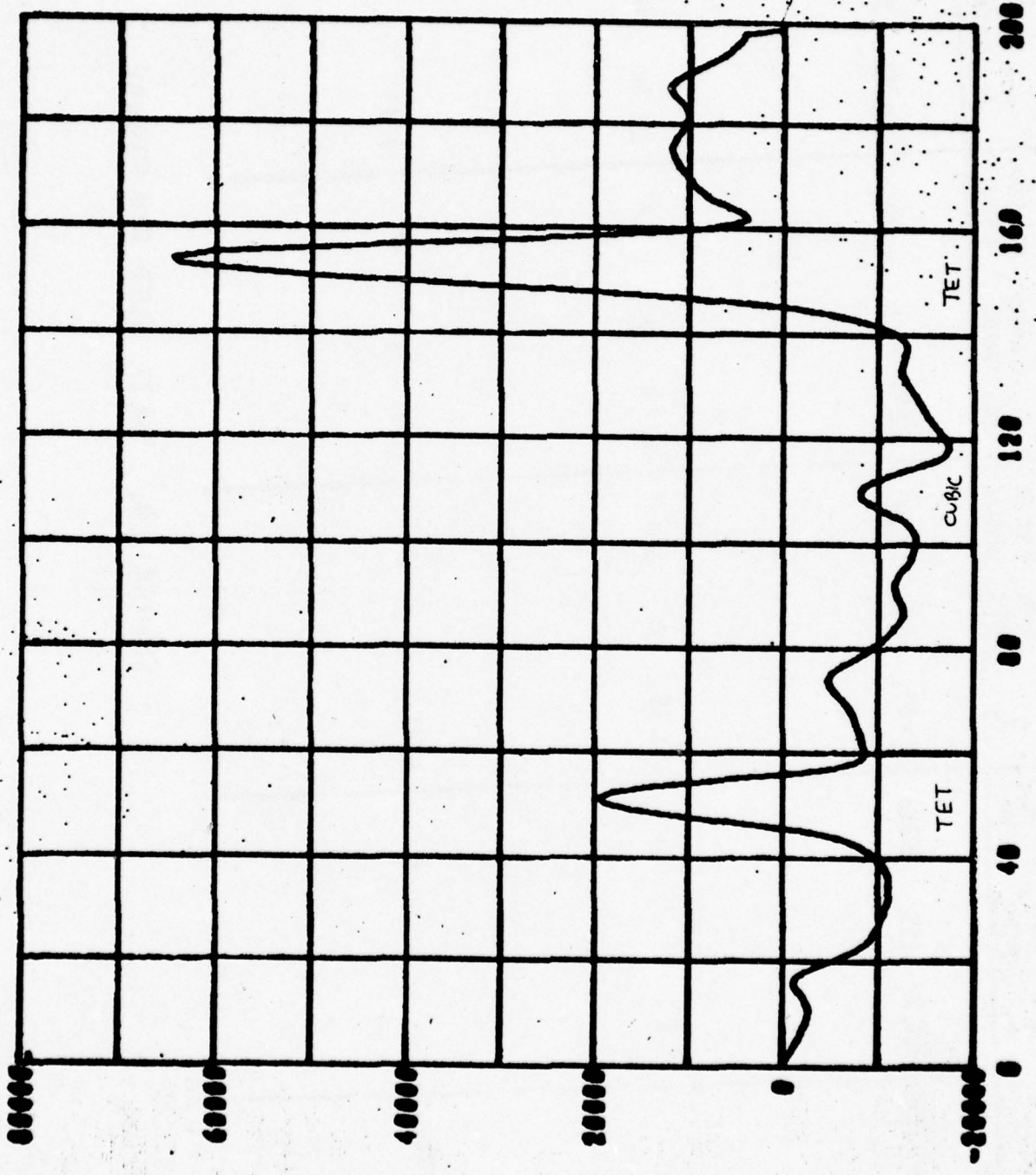


FIG 23. ABSORPTION OF .01%



## FOOTNOTES

## INTRODUCTION

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2. A.D. Franklin and J.M. Crissman and K.F. Young, J. Phys. C: Solid State Phys. 8, 1975, 1244-1266.
3. C.R.A. Catlow, "The Defect Properties of Anion Excess Alkaline Earth Fluorides-Part I: Low Defect Concentration," (Unpublished), p.1
4. R.H. Heist and F.K. Fong, "Maxwell-Boltzmann Distribution of  $\text{M}^{3+}$ -F Interstitial Pairs in Fluorite Type Lattices"; Physical Review B, Vol. 1 Num. 7, 1970, p. 2970, 2975-2976.

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2. Varian Associates, "V-4502 Principles of Operation" (Technical Pub Num. 87-114-300 C864), p.2-2.
3. J.S. Blakemore, Solid State Physics, (W.B. Saunders Company, Philadelphia, 1974), p.456.
4. R.H. Heist, and F.K. Fong, "Maxwell-Boltzmann Distribution of  $\text{M}^{3+}$ -F Interstitial Pairs in Fluorite Type Lattices"; Physical Review B, Vol. 1, Num.7, 1970, p 2971-2972.
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APPENDIX A  
PROCEDURE FOR MOUNTING A F.C.C. CRYSTAL

1. Orient GYMBAL JIG for perpendicularity. Make sure the crystal end of the mounting rod maintains a fixed location in space for any rotation.
2. Orient laser to shine across diameter of Spencer Spectrometer Table at a height just above mounting platform (Silica Glass) lying on the table (Figure A1).
3. Make sure table is level by using a prism to reflect the beam  $360^\circ$  about table onto chart paper. If beam hits paper at equal distance from bottom of paper, through  $360^\circ$ ; then table is level.
4. Wash all gear with acetone and rinse with methyl alcohol.
5. For F.C.C. crystals cleavage planes are  $[111]$  planes two  $[111]$  planes intersect in  $[110]$  line. Therefore you must get two good cleavage planes to intersect forming a  $[110]$  axis (Figure A2).
6. Use full strength duco cement and glue the mounting rod to the crystal as close to the  $[110]$  axis as you can (Figure A3).
7. Insert rod into teflon swivel (white and adjust length to be just above the silica glass. Put rubber cement on outer surface of swivel (Figure A4).
8. Orient crystal so that laser beam is reflected to same height above table for both faces. To compare one face to another, move laser thru small angle. Rotate table and thus crystal to see if crystal reflection height is constant (Figure A5).
9. Prepare dilute duco with 40% acetone added.

10. Align silica glass as shown in Figure A7.
11. Apply dilute duco to NDN used surfaces. Continue to monitor reflections until glue is dry. The reflections should not move for proper alignment of [110] axis  $\arctan(Y/X) < 3^\circ$  (Figure A6).
12. When dry (an hour at least) wrap a layer of rubber cement around crystal and top of silica glass. This holds crystal in place at liquid helium temperatures in case the duco becomes brittle and breaks its bond.
13. When dry (30 minutes) orient crystal in bottom of microwave cavity as in Figure A7. Thus,  $0^\circ$  location on road map will nearly be  $0^\circ$  magnetic when you start looking for axial orientation of crystal. See road map Appendix B. Put small amounts of rubber cement on sides of silica glass but not under it (Figure A8). Allow 30 minutes to dry.
14. For reference a sample of DPPH should be placed in the cavity. Open the DPPH bottle and insert an extended paper clip all the way to the bottom of the bottle. Some DPPH will adhere to the wire, and this is a sufficient amount of DPPH to use. Rub off some of the DPPH onto a piece of tape and cut tape away from rest of tape. Attach tape to wall of cavity.
15. Attach cavity to wave guide as in Figure A9. You are now ready to go to Appendix B.

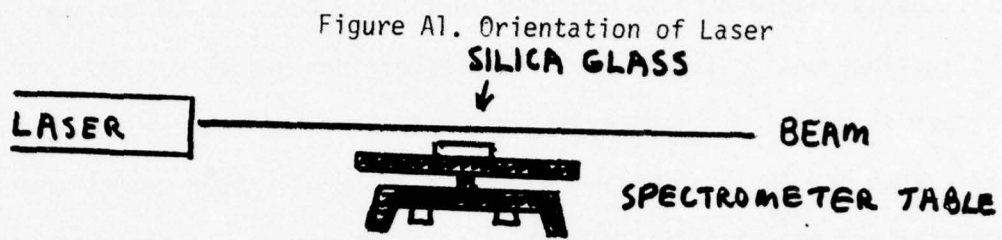


Figure A2. Cleavage of  
[111] Planes and the  
[110] Axis

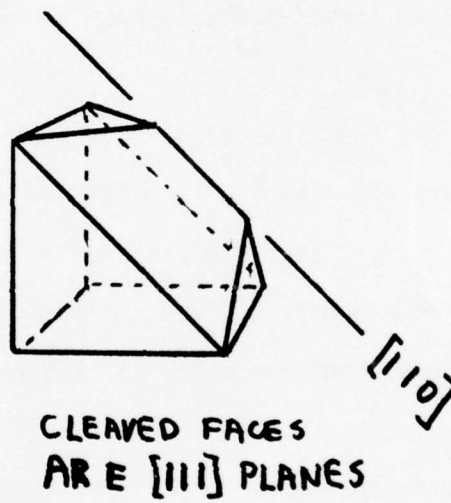
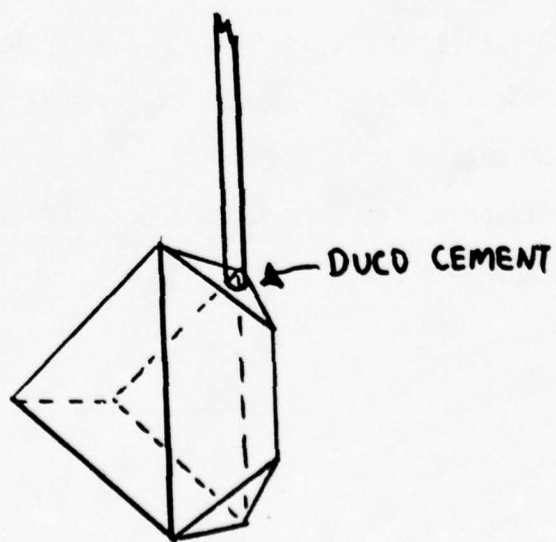


Figure A3. Mounting Rod  
and Crystal



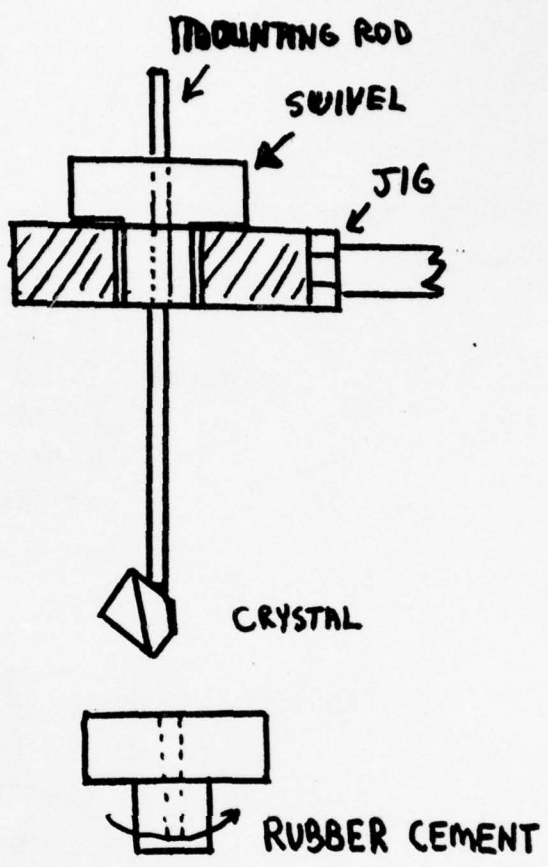


Figure A4. Swivel

Figure A5. Orientation of Crystal with Jig and Laser.

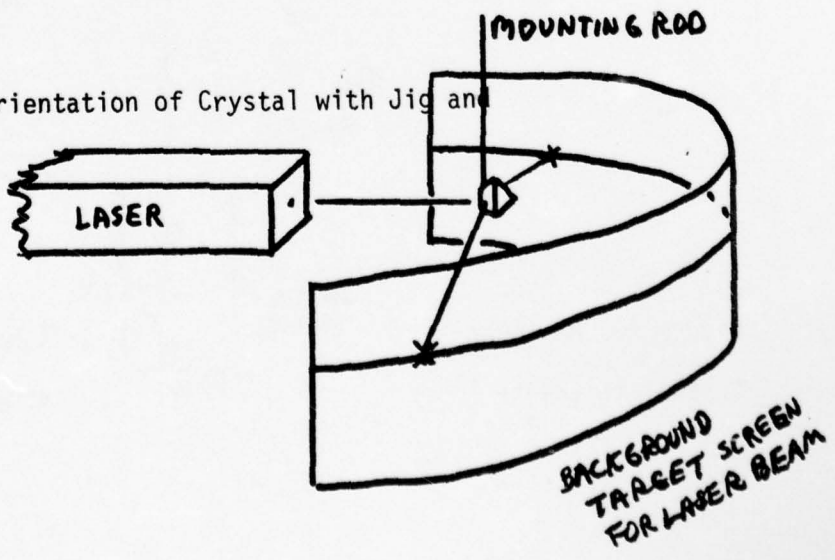


Figure A6. Mounting Crystal to Silica glass.

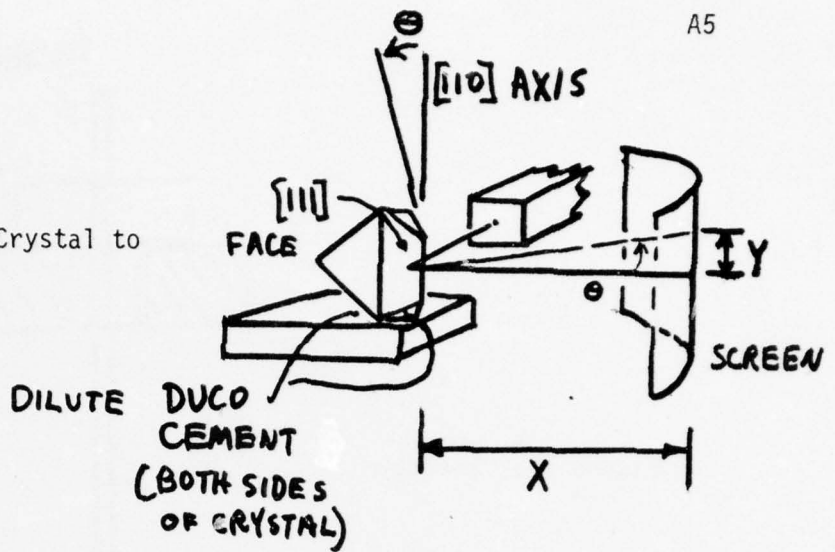


Figure A7. Orientation of Crystal in Cavity

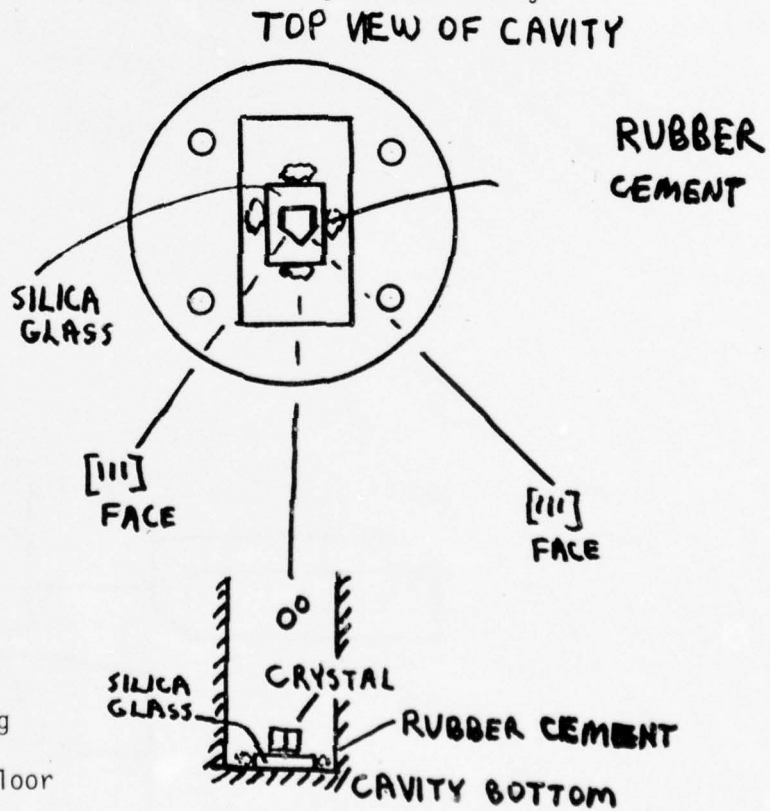


Figure A8. Attaching Crystal to Cavity Floor

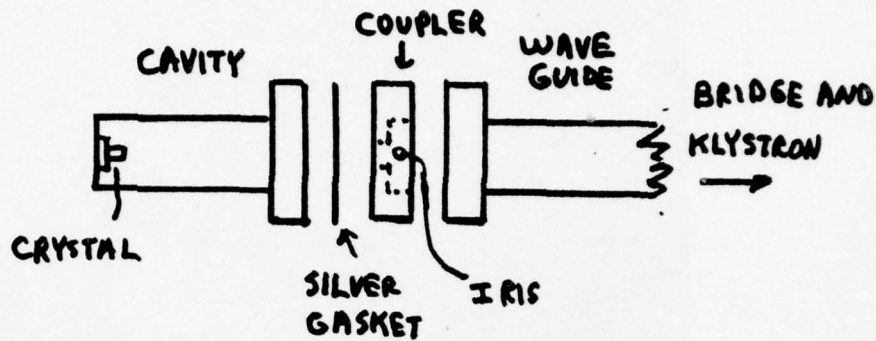


Figure A9. Attaching Cavity to Waveguide

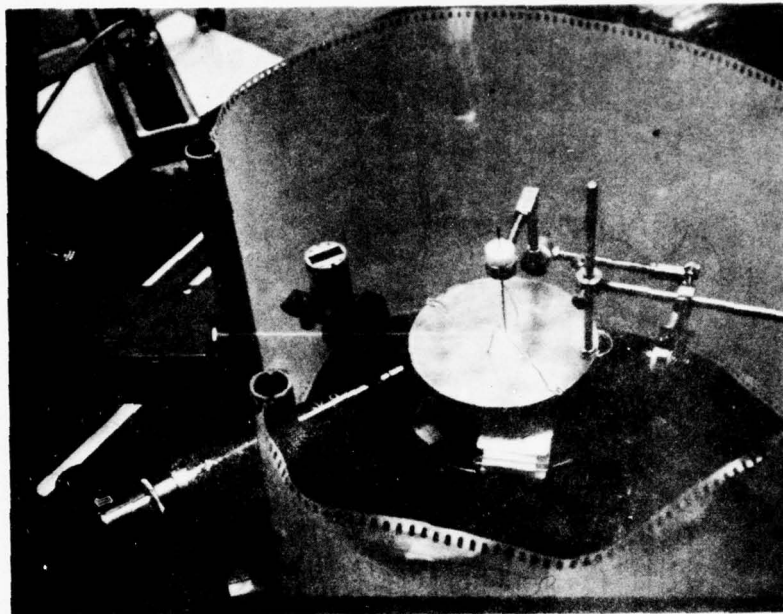


Figure A10. Picture of Assembly

## SET-UP OF ESR EQUIPMENT

1. Turn on cooling water - next to NMR magnet power supply.

NOTE: 90psi before filter.

80 psi after filter

20 psi on magnet

water flow into large cylindrical drain

water flow into small cylindrical drain for your particular

KLYSTRON (X or KBAND)

(For my work I used X band.)

2. Turn on power to Westinghouse "Main A" box in corner on left side of magnet bench (up is on).
3. Make sure fan in "Feldial Mark II" panel in varian consol is rotating. You can hear it vibrating if it is working. Failure of this fan causes "Potato" an uncontrollable drift of voltage output to strip recorder pen to the left or right. (The fan cools power transistors in the circuitry.)
4. Follow starting instructions in varian manual V-4502 Operating Instructions PUB number 87-114-200 D368.  
High Power: Page 3-5 to 3-27  
Low Power: Page 3-29 to 3-56  
Since I used low power with a reference cavity all my comments will apply to low power only.
  - a. Start on page 3-31 read precautions.
  - b. Initial setup ends on page 3-34. Let system warm up at least 3 hours and up to 12 hours.
5. While system is warming up refer to Procedures for Handling Liquid Helium PUB Number 87-250-031 A865. Page 14-19 "Pre Cooling Procedure" and page 1-1 to 1-7 for various precautions and interesting facts

about liquid helium. It is recommended that gloves and safety mask be used while working with liquid nitrogen and helium.

6. Open wooden cabinet containing waveguide and cryostats.
7. Carefully lower waveguide and cavity (See Appendix A) into helium cryostat.
8. Carefully lower helium cryostat into nitrogen cryostat. Be sure that styrofoam insulator is in place around liquid helium cryostat.
9. Make sure that the helium cryostat is not touching the nitrogen cryostat by observing that the helium cryostat is hanging free in the nitrogen cryostat.
10. Slide the cryostat and waveguide assembly on to rails above magnet and center the cavity between the pole faces and helmholtz coils.
11. About every 10-12 runs re-establish the vacuum in the helium cryostat. Then leak a small amount of nitrogen gas into the vacuum. See page 14-15 in Procedures for Handling Liquid Helium .
12. Connect the flexible waveguide and H-bend section between klystron and cryostat. Be sure screws are tight.
13. Before starting liquid nitrogen transfer start a 5 lb/sec flow of helium gas into helium valve on top of the microwaveguide. This flushes out atmospheric air and moisture which would condense and form ice. (This would draw microwave power and give false resonance information.) Be sure to open the other helium valve and put a rubber stopper in the remaining hole on top of the waveguide section.
14. Transfer liquid nitrogen to the top of the nitrogen cryostat.
15. Go back to V-4502 Op. Instructions page 3-35 and continue thru page 3-37. This sets up the dip in the power mode of the klystron on

the scope. (Use signal level = 1600)

16. Liquid helium transfer:

- a. Place pressurizing tube on liquid helium dewar. (See Figure B1)
- b. Take out rubber stopper on top of waveguide section.
- c. Put on gloves.
- d. Take transfer tube and insert it into cryostat and liquid helium dewar. (See Figure B2)
- e. Stop helium gas flow and connect helium gas to pressurizing tube.
- f. Start 5 lb/sec flow of helium gas.
- g. Watch scope for movement of dip as cold He gas enters the cavity. It will shrink, increasing the frequency, and dip will move off to the right.
- h. As liquid helium enters the cavity the dip will move very quickly to the left. This is because of the change of dielectric constant from gas to liquid in the cavity.
- i. When liquid helium level is one inch below the level of the liquid nitrogen stop helium gas flow.
- j. Disconnect rubber tube between helium dewar and helium gas tank. This allows excess helium gas pressure to leak off.
- k. Put on gloves.
- l. Remove transfer tube and replace it on the wall mount.
- m. Put in rubber stopper and close helium valves on top of waveguide.

17. Start again in V-4502 Op. Instructions page 3-37 (8) and continue thru page 3-41. Be sure to go to page 2 after you finish page 3-41.

This talks about adjusting the crystal detector.

18. Set up for recording resonance signal on strip recorder. Continue

with page 3-42 to 3-50. I used generally:

- Sig Lev 630
- Swp Frq 400
- Ref Pha 3.8 (RED)
- Leakage 250 $\mu$ A
- Response 1
- Sig Lev from 2 to 630

19. To adjust reference phase:

- a. Find DPPH resonance (3.34-3.30 KG).
- b. Set range to 250.
- c. Move percent of range dial until recorder is driven to a maximum swing. Adjust reference phase until maximum is achieved.

20. You are now ready to find axial orientation of crystal. To familiarize yourself with the magnetic resonance look at Figure B3. This is the road map. For another copy of the road map, See Appendix E under ESRPLOT. In Appendix A I told you how to get the 0° or 180° orientation near the 0° magnet orientation. The procedure for getting the 0° theoretical is as follows:

- a. Set up Fieldial panel:
  - Time  $\equiv$  1 min
  - Dial  $\equiv$  (Field set-KG) 1000
  - Range  $\equiv$  1.0 KG
  - Triangular Sweep
- b. Start at 0° magnet and take a one minute sweep through 1 KG.
- c. Rotate 5° and repeat until you have gone thru  $\pm 60^\circ$ . This will give you an excellent view of the resonance spectra.
- d. Look for similarities in resonance patterns on each side of 0° magnet. Note on road map that spectrum is identical on either side of 0° theoretical and a crossing occurs at approximately  $\pm 55^\circ$ . From

the symmetry of resonance spectra you should be able to get within 2.5° of true 0° theoretical. The whole idea is to find 0° theoretical because this angle has the best separation of the different site absorption curves.

21. You are now ready to worry about symmetry of the first derivative curve.

a. Read page 5-11 to 5-14 in EPR Operational Techniques PUB Number 87-114-402 C864 and page 2 to 3 in V4502 Operating Instructions.

b. Using the following settings you can eliminate many of the problems:

(1) On the klystron: attenuation 4.0

cryostat isolator 2.0

(2) On the varian console: time 10 minutes

response 1.0

sweep field 630

Reference phase should not be changed from step 18.c. These settings will correct saturation, too fast scan rate, and give correct modulation for line shape.

22. You are now ready to try to make a particular first derivative curve symmetric.

23. a. For  $C_aF_2$  doped with erbium the main cubic and tetragonal resonances occur within 500 to 1500 gauss. Set magnet for 0° theoretical.

b. Set TIME at 10 minutes.

c. Set RANGE at 1 KG.

d. Set FIELD SET dials at 1.000 KG.

- e. Set POR DIAL (PERCENT OF RANGE DIAL) at -45 this should be a region of magnetic field in which there are no major resonances.
- f. Center the strip recorder pin on the chart paper.
- g. Move the POR DIAL to +45. If the pen does not return to center you have a major "Potato" problem.
- h. Monitor AFC "Cat's Eye" on varian console scope. Probably the AFC will be shifted to the extreme left or right.
- i. If pen shifted to the left you have up potato; to the right is down potato. Down potato has an AFC shifted to the left. Up potato has an AFC shifted to the right.
- j. Move the PHASE TUNING on the klystron either left or right to move the AFC back towards a symmetrical display.
- k. To increase PHASE TUNING you must rotate the dial to a setting much greater than the value you want, then rotate it back to the desired value. Same for decreasing it an extreme rotation past the desired value. Then a return to the desired value. This is done to momentarily confuse the AFC and make a change possible.
- l. After any change to the PHASE TUNING the AFC ERROR must be corrected and LEAKAGE CURRENT (Controlled by the SLIDE-SCREW TUNER MICROMETER on right side of klystron) must be maintained at  $250\mu\text{A}$  when not in resonance. NOTE: Leakage current increases with a clockwise rotation of the slide-screw tuner and decreases with counter-clockwise rotation.
- m. Go to e. until pen shift is gone.
- n. Find a major peak in the resonance spectra and set the POR DIAL for 5% less than that peak's resonance value. Using the TIME =

10 MIN and RANGE = 1KG, punch INCREASE and sweep through to the resonance. Now if one half of first derivative curve is shorter than the other, you must correct the phase tuning according to the following rules:

To shift symmetry right -- increase phase tuning.

To shift symmetry left -- decrease phase tuning.

The method of change is outlined in k.

o. Go to n. until you are satisfied with symmetry. NOTE: You can never get all of the phase distortion out but the more symmetric the better. The program "distort" will take out the rest of the distortion.

- p. (1) Now set up tape recorder as shown in Figure B4.  
 (2) Recorder switch on EPR consol must be turned to PDP-8 position.  
 (3) Signal level and the external amplifier must be adjusted so as not to saturate the external amplifier (741 chip  $\pm 9$  volts output range).

NOTE: External amplifier has 3 positions:

X25

X50

X500.

The signal has to go thru one of these. There is a switch on the bottom that when rotated counter-clockwise divides the input by 10.

Signal amplification then is summarized as follows:

$$(\text{SIG LEV}) \times \begin{pmatrix} 25 \\ 50 \\ 500 \end{pmatrix} \times \begin{pmatrix} 1 \\ 1 \\ 10 \end{pmatrix}$$

- (4) When you are certain that you are not saturating an amplifier, put TAPE RECORDER MONITOR on RECORD, channel #1. Set POR DIAL to  $\pm 45$  and zero the meter using balance control on EPR consol.
  - (5) Make a trial run through entire spectra observing signal on scope and TAPE RECORDER MONITOR to make sure you are recording what you want to record.
  - (6) Monitor the control level on channel #4 to see if input level gives 95% for high and 0% for low level. This level controls the PDP-8 analog to digital converter by telling it when to take data.
  - (7) Make sure channel #2 is on and internally set for. Flutter compensation. (Front panel comes open) This compensates the other three channels for flutter.
  - (8) Turn off strip recorder.
  - (9) Put POR DIAL on -50 in control level high area.
  - (10) Punch record on tape recorder.
  - (11) Punch increase on consol.
24. After recording a spectrum go back to step n. of 23. and see if the symmetry has shifted. It is quite fragile and may be unsatisfactory now. Keep working.
25. Record DPPH at approximately 3.32 KG using steps 23 e. thru 24.
26. After recording tet and cubic sites and DPPH rotate  $+39^\circ$  on mag and set FIELD-SET dials to 1740.
27. Find an appropriate amplification and identify trigonal resonance. Use above procedure to get symmetry. Record trigonal and

DDPH resonance.

28. Go to Appendix C for transfer of analog data, to digital data,  
and to DTSS.

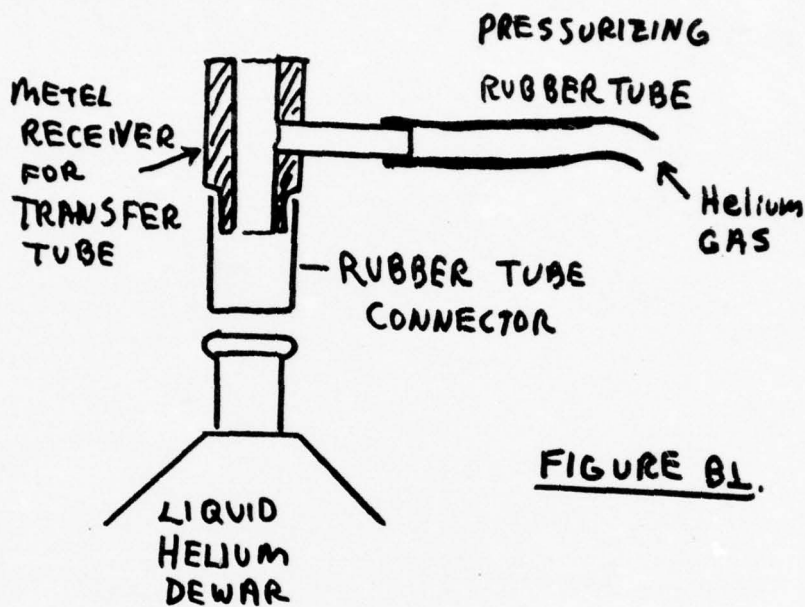


FIGURE B1.

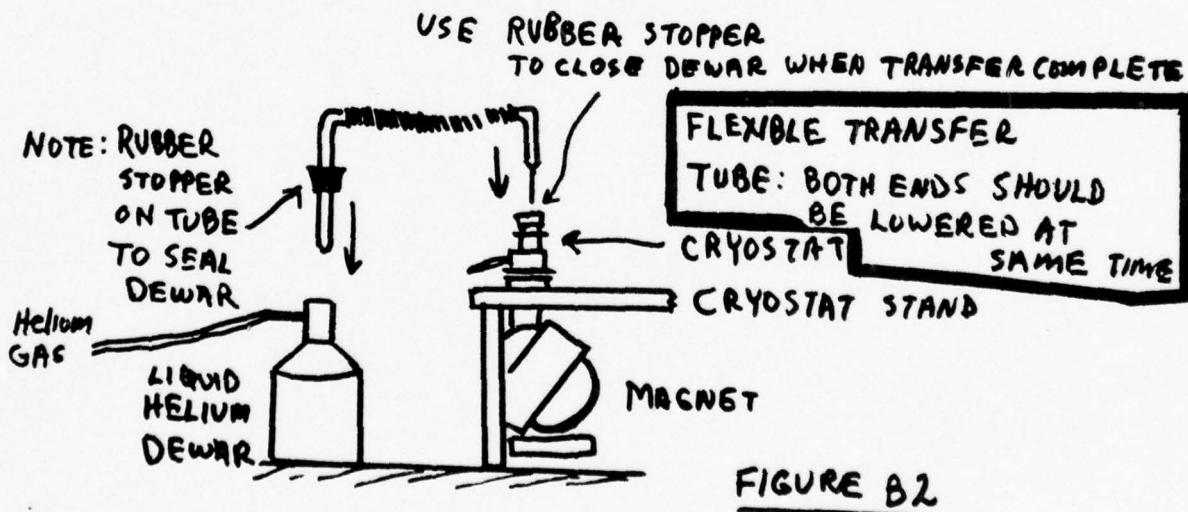
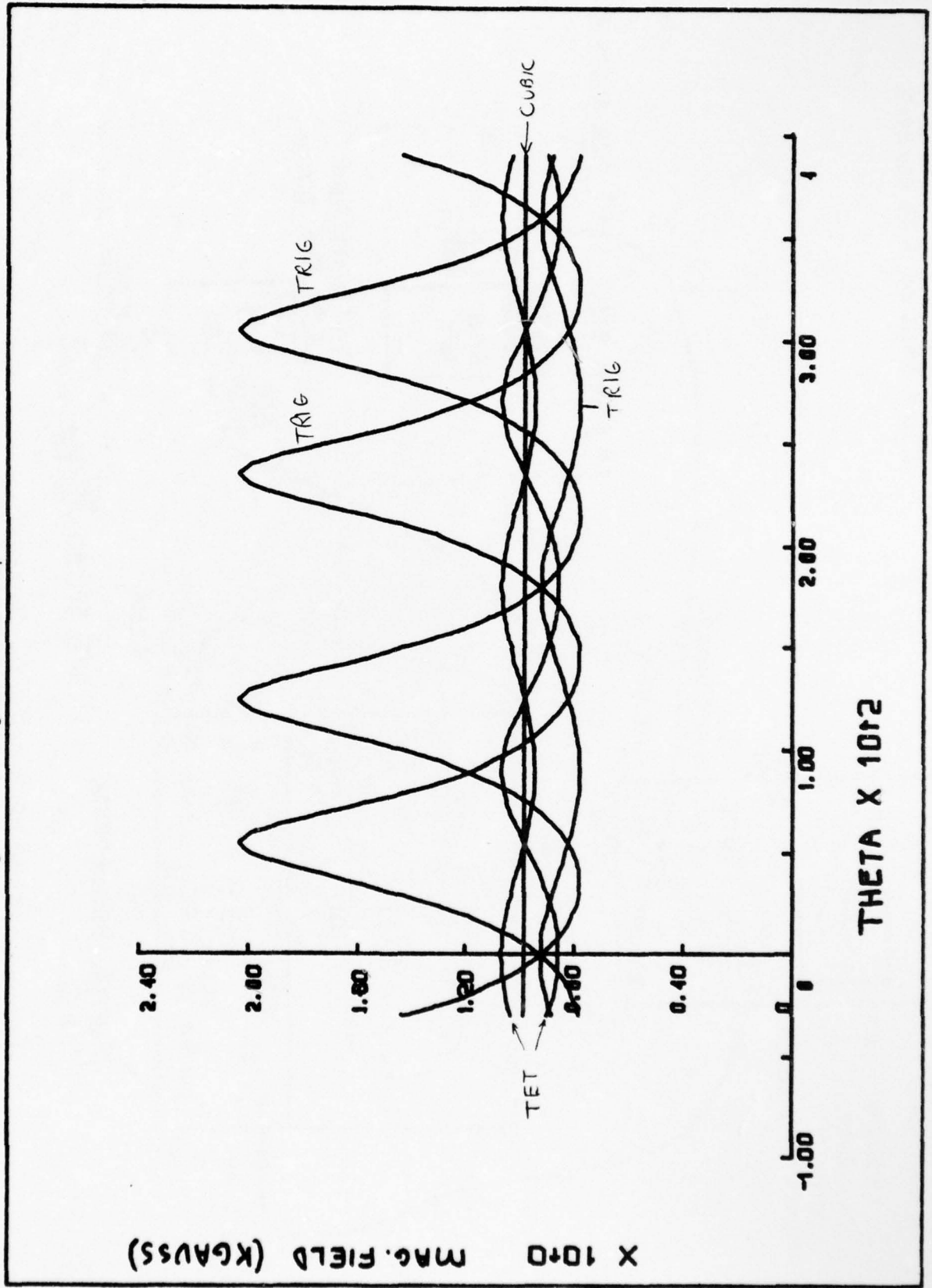


FIGURE B2

Figure B3. Magnetic road map



MAG. FIELD (KGAUSS) X 10+0

THETA X 10+2

MAKE SURE 10V SUPPLY FOR 741 AMPLIFIER IS ON. LOCATED INSIDE BACK OF ESR CONSOLE.

B12

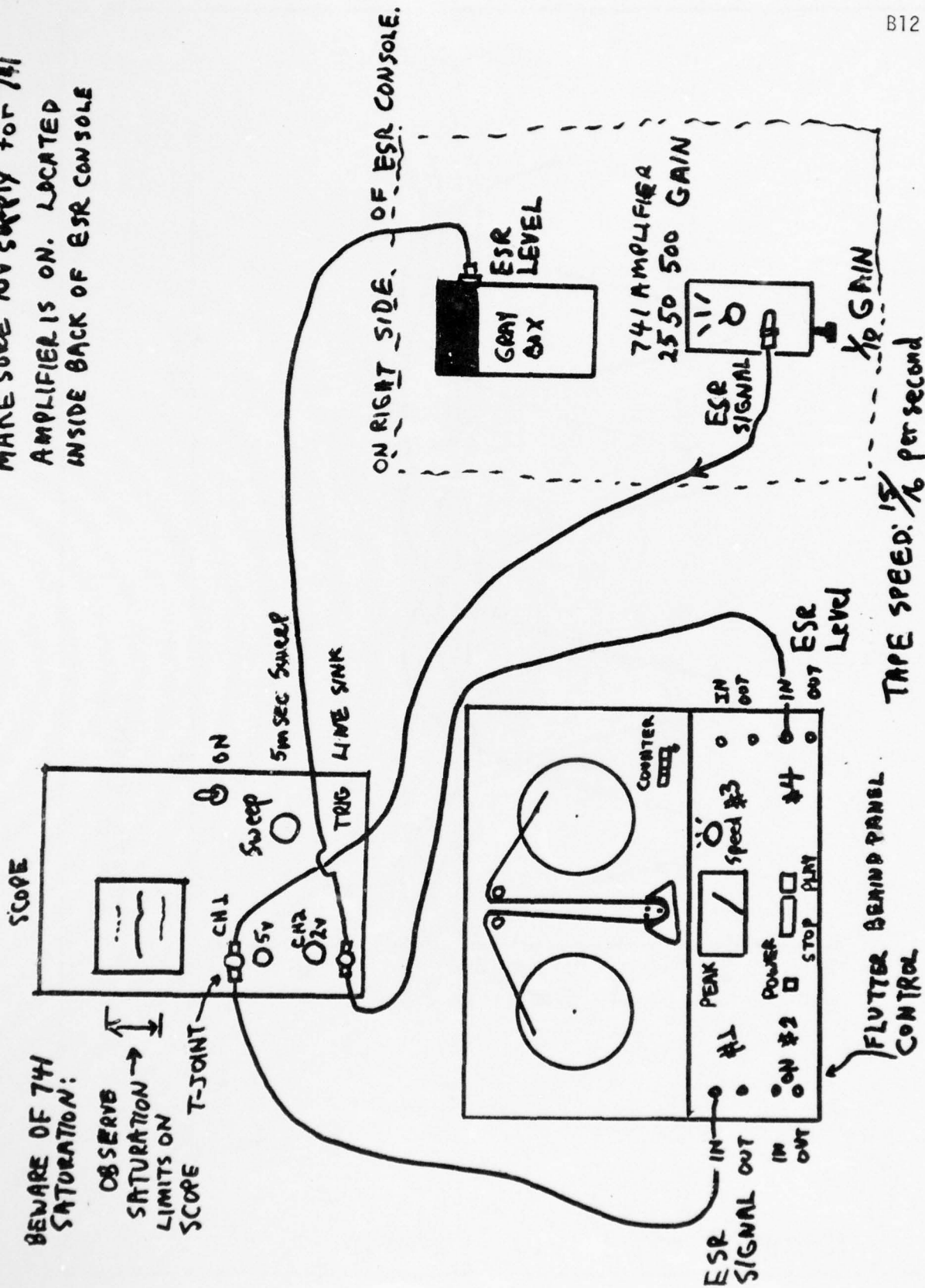


Figure B4. Hook-up for Recording ESR Signal

## APPENDIX C

## PROCEDURE FOR DATA TRANSFER TO DTSS

1. Go to Room E-6, PDP-8 room, on Michelson lab deck.
2. Set up tape recorder, oscilloscope, and PDP-8 as shown in Figure C1.
3. Refer to REDIFAX #1 to turn on machine #1.
4. Refer to REDIFAX #2 to connect to DTSS time sharing.
5. You must have these programs in your catalog:

```

DIGACQ      DUB(EMPTY)
CORGOS      PUB(EMPTY)
UNPACK
INTO DUB
MY_LIST (EMPTY)
MY_BIN (EMPTY)

```

DIGACQ and CORGOS are used on the PDP-8 so they must be assembled in PDP-8 binary. To do this refer to REDIFAX #5. The assembled versions of DIGACQ and CORGOS can be saved. I called them DIGACQB and CORGOB.

Note: PDP-8 programs use octal numbers.

6. DIGACQB must be sent to PDP-8 memory. Refer to REDIFAX #4.

EXAMPLE

- a. Type: OLD DIGACQB/NPA/PUN/PAR\0
- b. Wait for a bell and carriage return. Signifying that transfer is complete.
  - 0 ≡ Zero.
  - ≡ Back Slash ≡ Capital L
- c. Type: CTRL SHIFT 0 (Letter O). You are now in "ODT." Refer to REDIFAX #4.

d. Type: 200/ Should get: 7604 This is the instruction line #200 in DIGACQB. If not go to a. and start again.

7. Setting switch register for Date Sampling Rate.

a. One number from the  $M555_8$  column must be placed on the switch register.

Run Time Minutes	Sec	$M555_{10}$ (Base 10)	$M555_8$ (Octal)
1	60	146.48	222
2.5	150	366.21	556
5	300	732.4	1334
10	600	1464.84	2670

Formula for  $M555_{10} \equiv (\text{Run time (sec)} \times 10^4)/4096$ .  $10^4/\text{sec}$  is the frequency of clock in PDP-8 program. 4096 data words of storage.  $M555_{10}$  must be converted to octal  $M555_8$ . The procedure for this is as follows:

- $(M555_{10}/8^L) = X$  where L is largest power of 8 for which  $M555_{10} > 8^L$ .
- Record the Integer part of X.
- And multiply the decimal part of X by 8.
- Go to b. until you have enough places of the octal number.

EXAMPLE:  $146.48_{10} \Rightarrow 222_8$

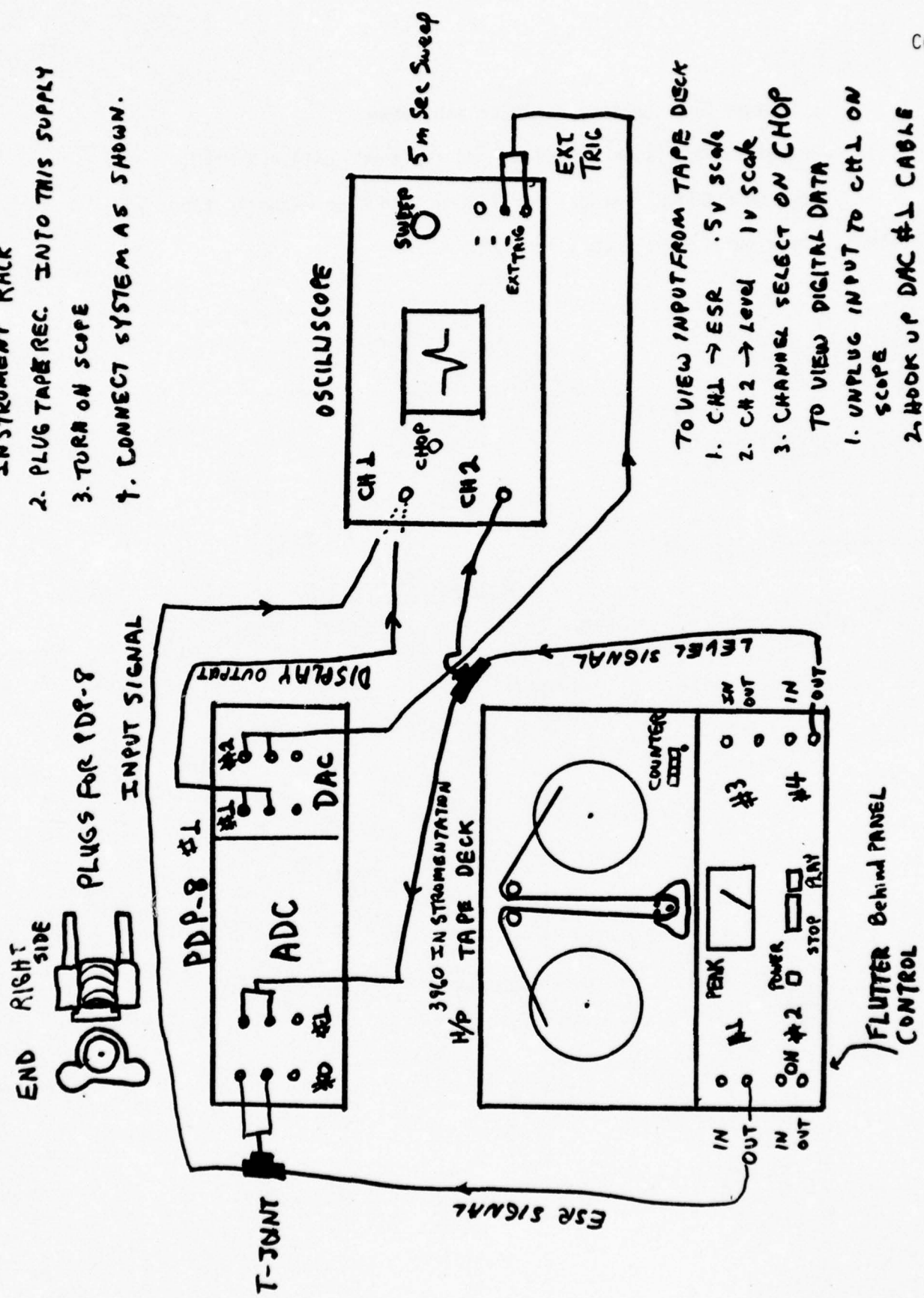
- $(146.48_{10}/8^2) = 2.28875$  Record 2
- $(2.28875-2)(8) = 2.31$  Record 22
- $(.31)(8) = 2.48$  Record 222
- $(.48)(8) = 3.84$  Record 222.3
- Round to nearest lower value = 222.

8. Run PDP-8 Program.
  - a. Type: 200G.
  - b. Switch register lights should read 0207  
(000 010 000 111)
  - c. On tape recorder put "MONITOR" on "REPRODUCE 4."
  - d. Push play (forward) button.
  - e. When meter level goes to high level raise switch register 0 to upper position. (NOTE: Scope trace from Channel #2 should be high also.) See 257 blinking.
  - f. When level falls (indicating that PDP-8 should take data) Sw. Reg. lights should read 241. You can monitor data on scope ch #1.
  - g. Wait until 377 (blinking) comes on, indicating all data taken, level is high and program is in display mode. (000 011 111 111)
  - h. Detach cable from scope ch #1 and connect D/A channel #1 to scope channel #1 and see data display.
    - i. Push Sw. Reg. 0 down to see unfiltered data.
    - j. If data is not filtered satisfactorily:
      - (1) Halt program.
      - (2) Set 7000 on Sw. Reg. (111 000 000 000).
      - (3) Punch ADDR LOAD, EXT ADDR LOAD, CLEAR, CONT. Type: 150/  
Should get: 0017.
      - (4) Type: NEW OCTAL NUMBER. (See REDIFAX #3)
      - (5) Type: 320G
      - (6) Observe with Sw. Reg. 0 = NP. Go to (1) if not satisfied.
    - k. If satisfied halt program and put 4000 on Sw. Reg.
    - l. Punch ADDR LOAD, EXT ADDR LOAD, CLEAR, CONT.

9. Sending filtered data to DTSS (See REDIFAX #11).
  - a. Type: /OLD CORGOB/NPA/PUN/PAR\0
  - b. Wait for bell and carriage return from computer.
  - c. Type: /UNS.RESULT./DIR
  - d. Receive: SPEAK!
  - e. Type: CTRL SHIFT 0 (Letter 0)
  - f. Receive: CARRIAGE RETURN
  - g. Type: 2700/
  - h. Receive: 0000
  - i. Type: 0003 for filtered data or 0002 for non-filtered data
  - j. Type: LINE FEED
  - k. Receive: 2701/0000
  - l. Type: 0000 STARTING LOCATION OF DATA
  - m. Type: LINE FEED
  - n. Receive: 2702/0000
  - o. Type: 7777 END LOCATION OF DATA
  - p. Type: CARRIAGE RETURN
  - q. Type: 2600G
  - r. Wait until you get "READY" (Could be as long as 5 minutes)
  - s. Type: STR RAN 12 (Carriage Return)
  - t. Receive: READY NEW FILE IS .RESULT.
  - u. Type: /SAV/OLD UNPACK/RUN/OLD INTO DUB/RUN See example printout (Figure C2)
10. You are now ready to:
  - a. Put DUB on DTSS system mag tape for storage.
  - b. Start number crunch to get absorption curve.

- c. Start over because computer went down.
- 11. Output of DUB is an APL file, in the form DATA = N 3.R0.
- 12. See "BACKGROUND" manual for instructions for magnetic tape; you must check out a tape from Ward Hall.

1. TURN ON POWER IN BACK OF PDP-8 INSTRUMENT RACK
2. PLUG TAPE REC. INTO THIS SUPPLY
3. TURN ON SCOPE
4. CONNECT SYSTEM AS SHOWN.



- TO VIEW INPUT FROM TAPE DECK
1. CH1 → ESR .5V scale
  2. CH2 → LEVEL 1V scale
  3. CHANNEL SELECT ON CHOP
- TO VIEW DIGITAL DATA
1. UNPLUG INPUT TO CH1 ON SCOPE
  2. HOOK UP DAC #1 CABLE TO CH1 ON SCOPE

FIGURE C1

Figure C1. Hook-up for Data Transfer



Figure C2. Set-up of PDP-8, Scope, and Tape Recorder

APPENDIX D  
DATA CRUNCH

1. I assume that APL data file "DATA = N8.R0" is in BASIC FILE CALLED DUB.
2. Run XAPL (After each system command or completion of program A "?" will be given.
3. )Read DUB.
4. .RODATA  
Receive: N 8
5. )Read APLLIB\*\*\*:RAWCOR  
RAWCOR DATA  
Receive: NEW NAME CORDAT
6. Check first and last numbers in OCRDAT=0  
Ex: 1 ↑ CORDAT (char ret)  
          0  
      "1 ↑ CORDAT (char ret)  
          0  
  
If not look at data and go to 5.
7. At this point you can )REA APLLIB\*\*\*:CUT PLOT and look at data or continue with 3. NOTE: Result of CUTPLOT is CPOUT. This must be written into a basic file by )WR1 FILE NAME; CPOUT. It may be advisable to )SCR FILE NAME first.
8. You probably need to write CORDATA into a file and )EXIT. If your work space in APL is small, you may be near the limit if you have 4000 PDP-8 data numbers in DUB. Then "RUN XAPL" and read CORDATA back into work space.
9. Correct phase distortion in first derivative data.
  - a. CUTPLOT must be used to plot 200 of N data points using

procedure 7. Each distorted first derivative curve must be corrected individually. The scale of "X" axis plot will be 0 to 200. There are  $N/200$  real data points associated with each point on the plot. Pick out the limits of your distorted first derivative curve and input these as limits of "DISTORT" program. Refer to Appendix E for the program description.  $LIMITS = (L_1)(N)/200 \quad (L_2)(N)/200$  where  $L_1, L_2$  are X coordinates from plot.

- b. )REA DISTORT
- c. DISTORT CORDATA
- d. Receive: CORD See Step 10
- e. CORDATA = CORD
- f. Repeat c. thru e. until all individual distortions are gone.

10. To make sure distort worked, see if  $.CE/CORD = .AB.FL/CORD$ .

11. Perform indefinite integration of first derivative curve to get absorption curve.

```
)READ APLLIB***:INTTEG
```

```
INTTEG CORD
```

```
Receive: I CURV
```

12. You may need to write ICURV into a file and exit, run XAPL, read ICURV back into work space.

13. Correct for integration ramp in absorption curve.

```
)REA APLLIB***:ABSCOR
```

```
ABSCOR ICURV
```

```
Receive: CORDATA
```

14. Read 7. In order to fit a particular absorption curve, it will be necessary to plot the entire absorption spectra and to select a

suitable segment of the absorption spectrum. Follow the procedure for determining segment limits as outlined in step 9. Follow step 7. to plot CORDATA.

15. Scratch file containing ICURV. Write CORDATA into file that used to contain ICURV.

```
)REA FIT  
FIT CORDATA
```

This will return the Gaussian parameters, amplitude, exponent coefficient, and standard deviation. Data is now in CURFIT.

16. CURFIT is a true Gaussian distribution. The interval of X components is the integer 1 so no special double precision program for integration need be run.

```
17. )REA APLLIB***:INTSIM  
INTSIM CURFIT  
OUTPUT = AREA
```

18. This completes crunch except for amplification factors used in original data.

$$\frac{\text{Area}}{\text{Amplification Factor}} = \text{True Area.}$$

19. Continue with next data batch at step 1. or write paper for publication and receive Ph.D.

## APPENDIX E

## PROGRAMS

- DIGACQ: A PDP-8 program to convert the analog ESR signal into digital numbers.
- CORGOS: Sends data from PDP-8 to DTSS. See Redifax #11.
- UNPACK: Changes coded data into a random access file.
- INTODUB: Changes a random access file into an APL file.
- 
- RAWCOR: This program eliminates the PDP-8 modulo 4096 wrap-around, removes DC bias, and corrects for initial potato. Result is called CORDAT.
- CUTPLOT: Is used to cut down the number of points to be plotted. In this way a file of 4096 data points may be reduced to 200 plotting points. See Appendix D for use of plotted graph. Result is called CPOUT.
- DISTORT: This program corrects for phase distortion produced by imbalance in phase tuning on klystron. It assumes a Gaussian error in the leakage current that detects the magnetic resonance. Result is called CORD.
- INTTEG: This program performs indefinite integration on the first derivative data. The range of integration is an input to the program. The result is called ICURV. The output is the absorption curve with an integration ramp.
- ABSCOR: This program corrects the integration ramp that results from the indefinite integration. The result is called CORDATA.

- FIT: This program fits a particular absorption curve to a Gaussian curve. The boundaries of the curve are inputs. Amplitude A and exponential coefficient B are outputs; ST is standard deviation. The mid-point of the Gaussian curve is found by the program. The result is called CURFIT.
- INTSIM: This program performs the definite integration on the fitted curve to arrive at a number equal to the area under the fitted curve.
- APLTOBAS: This program is necessary for converting APL data files into standard graphic format. Use CUTPLOT while in APL; exit from APL; run APLTOBAS (a BASIC program).
- ESR PLOT: This program outputs the g-splitting or magnetic resonance point spectra for  $\text{CaF}_2:\text{Er}^{3+}$  in table form or in a form suitable for plotting. (a BASIC program). It requires "Split" as an output file. (from  $-30$  to  $390^\circ$ )

## DIGACQ

100 \*106  
110 LOOK, 0  
120 DCA TEMP1  
130 TAD K3001  
140 ADSC  
150 ADCV  
160 JMS I SAMPI  
170 TAD M2000  
180 SMA CLA  
190 JMP LAST1  
200 CLA  
210 TAD K3000  
220 ADSC  
230 ADCV  
240 CLA  
250 TAD TEMP1  
260 JMP I LOOK  
270 LAST1, CLA  
271 TAD ONE  
272 TAD STIND  
273 DCA STIND  
280 LS,CLA  
290 TAD I K101  
300 DCA I STIND  
310 ISZ STIND  
320 JMP LS  
330 JMP I DISPI  
340 K3001, 2001  
350 M2000, -2000  
360 K3000, 2000  
370 M555, -222  
380 K5400, 5400  
390 STIND, 0  
400 MATAL, 0  
410 SIG,4000  
420 L, 17  
430 K100, 100  
440 JTAL, 0  
450 TEMP, 0  
460 0  
470 TEMP1, 0  
480 K101, 0101  
490 SAMPI, SAMP  
500 DISPI, 320  
501 ONE, -1  
510 \*200  
520 LAS  
530 CIA  
540 DCA M555  
550 LAS

-2-

DIGACO (continued)

560 SMA CLA  
570 JMP .-2  
580 TAD K3001  
590 ADSC  
600 ADCV  
610 JMS SAMP  
620 TAD M2000  
630 SPA CLA  
640 JMP .-3  
650 JMS SAMP  
660 TAD M2000  
670 SMA CLA  
680 JMP .-3  
690 CLA  
700 DCA STIND  
710 TAD K3000  
720 ADSC  
730 ADCV  
740 STA  
750 CLZE  
760 CLA  
770 TAD M555  
780 CLAB  
790 CLA  
800 TAD K5400  
810 CLOE  
820 CLA  
830 6221 / CDF2  
840 LOOP1, CLSK  
850 JMP .-1  
860 CLSA  
870 JMS SAMP  
880 JMS LOOK  
890 DCA I STIND  
900 ISZ STIND  
910 JMP LOOP1  
920 JMP LAST1  
930 SAMP, 0  
940 ADSF  
950 JMP .-1  
960 ADRB  
970 ADCV  
980 JMP I SAMP  
990 \*270  
1000 DISP, LAS  
1010 SMA  
1020 JMP .+3  
1030 6231  
1040 JMP .+2  
1050 6221

-3-

## DIGACQ (continued)

1060 CLA  
1070 TAD K3000  
1080 6552  
1090 CLA  
1100 6552  
1110 DCA STIND  
1120 LOOP2, TAD I STIND  
1130 6551  
1140 CLA  
1150 ISZ STIND  
1160 JMP LOOP2  
1170 ISZ STIND  
1180 JMP , -1  
1190 JMP DISP  
1200 \*320  
1210 SWAB  
1220 TAD K100  
1230 DCA MATAL  
1240 UPTHAR, TAD MATAL  
1250 DCA STIND  
1260 TAD L  
1270 CIA  
1280 DCA JTAL  
1290 CAM  
1300 DST  
1310 TEMP  
1320 LOOP3, 6221  
1330 TAD I STIND  
1340 6201  
1350 TAD SIG  
1360 MQL  
1370 DAD  
1380 TEMP  
1390 DST  
1400 TEMP  
1410 CLA  
1420 ISZ STIND  
1430 ISZ JTAL  
1440 JMP LOOP3  
1450 CAM  
1460 DAD  
1470 TEMP  
1480 DVI  
1490 L  
1500 ACL  
1510 TAD SIG  
1520 6231  
1530 DCA I MATAL  
1540 6201  
1550 ISZ MATAL

05/14/76

DIGACQ (continued)

1560 TAD MATAL  
1570 TAD K100  
1580 SZA CLA  
1590 JMP UPTHAR  
1600 JMP DISP  
1610 \$

-1-

## CORGOS

100 \*2600  
110 CLA  
111 TAD K7600  
112 AND POINT  
113 DCA POINT  
114 TAD K7600  
115 AND TALLY  
116 TAD K177  
117 DCA TALLY  
120 TAD FELD  
130 CLL RTL  
140 RAL  
150 TAD KCDF  
160 DCA +1  
170 CDF  
180 CLA  
190 6224 / RIF  
200 DCA FELD  
210 LOOP, CLA  
220 TAD I POINT  
230 7012 / RTR  
240 7012 / RTR  
250 AND K377  
260 JMS SEND  
270 CLA  
280 TAD I POINT  
290 AND K17  
300 CLL RTL  
310 RTL  
320 DCA TEMP  
330 ISZ POINT  
340 TAD I POINT  
350 AND K7400  
360 CLL RTL  
370 RTL  
380 RAL  
390 TAD TEMP  
400 JMS SEND  
410 CLA  
420 TAD I POINT  
430 AND K377  
440 JMS SEND  
450 ISZ POINT  
455 NOP  
460 CLA  
470 TAD TALLY  
480 CMA  
490 TAD POINT  
500 SZA  
510 JMP LOOP

05/14/76

20:31:40

## CORGOS (continued)

520 TAD FELD  
530 TAD KCDF  
540 DCA .+1  
550 CDF  
553 JMP I K4000  
554 SEND, 0  
555 6311 / TSF3  
556 JMP .-1  
557 6316 / TLS3  
558 CLA  
560 JMP I SEND  
562 \*2700  
564 FELD, 0  
566 POINT, 0  
568 TALLY, 0  
870 TEMP, 0  
880 M8, -10  
890 K377, 377  
910 K7400, 7400  
920 K17, 17  
930 K4000, 4000  
960 KCDF, CDF  
963 K7600, 7600  
966 K177, 177  
970 \$

-1-

## UNPACK

```
90' THIS PROGRAM UNPACKS THE RANDOM ACCESS FILE THAT CONTAINS
91' THE DATA FROM THE PDP-8 AND RECONSTRUCTS IT INTO MEANINGFUL DATA
92' SEE MASS TRANSFER OF DATA IN REDIFAX
100 LET I=0
110 DIM A(4096),S(13)
120 FILE #1: ".RESULT:"
125 FILE #2: "PUB"
130 FOR J = 1 TO LOF(#1)
140 READ #1 : S$
150 CHANGE S$ TO S
160 FOR K= 0 TO 3
170 LET I=I+1
180 LET A(I)=16*S(3*K+1)+INT(S(3*K+2)/16)
190 LET I=I+1
200 LET A(I)=256*MOD(S(3*K+2),16)+S(3*K+3)
210 NEXT K
220 NEXT J
230 SCRATCH #2
240 FOR J= 1 TO I
250 WRITE #2: A(J)
260 NEXT J
270 END
```

-1-

## INTODUB

```
70' THIS PROGRAM PUTS 496 ROWS OF 8 NUMBER DATA INTO FILE
71' DUB. SEE TEXT FOR DETAILS
72' TO GET RID OF AVERAGING DEADSPACE WE LOSE THE FIRST 8 ROWS
73' AND THE LAST 8 ROWS OF PDP-8 DATA
100 FILE #1: "PUB"
110 FILE #2: "DUB"
120 SCRATCH #2
121 FOR I = 1 TO 64
122 READ #1: Q
123 NEXT I
125 PRINT #2: "DATA =";INT(LOF(#1)/8)-16;"8.RO"
130 FOR N = 1 TO LOF(#1)/8-16
140 READ #1:X
150 READ #1:Y
151 READ #1:Z
152 READ #1:A
153 READ #1:B
154 READ #1:C
155 READ #1:D
156 READ #1:E
160 PRINT #2:X;Y;Z:A;B;C;D;E
170 NEXT N
175 PRINT #2:
180 PRINT "DATA IN DUB"
190 END
```

-1-

RAWCOR

```
$ RAWCOR D
[1] .CM ELIMINATES PDP-8 FIELD WRAP-AROUND, REMOVES DC BIAS,
[2] .CM AND CORRECTS FOR INITIAL POTATO;
[3] ''
[4] CORDAT=,D
[5] D=0
[6] CORDAT=CORDAT+4095#-2048;LECORDAT
[7] CORDAT=CORDAT-1^CORDAT
[8] X=1^CORDAT
[9] Y="1^CORDAT
[10] CORDAT=CORDAT+("1+,IO,ROCORDAT)#(X-Y)%("1+,ROCORDAT)
[11] '''CORDAT'' IS CORRECTED RAW DATA MATRIX.'
[12] ''
[13] 'DIMENSIONS OF CORDAT ARE';,ROCORDAT
$K
```

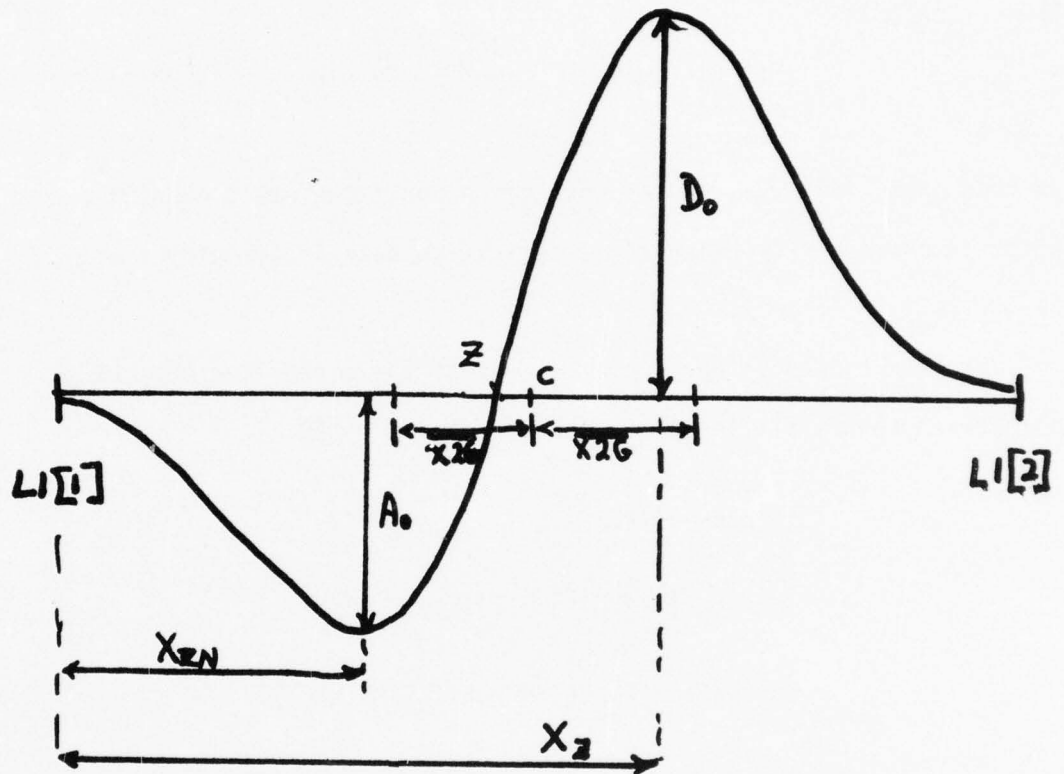
```
$ CUTPLOT;BIG;N;NP;NN
[ 1] .CM NILADIC OPR WHICH SELECTS AN INPUTTED NUMBER OF
[ 2] .CM EQUALLY SPACED VALUES FROM INPUTTED DATA; USED
[ 3] .CM TO CUT DOWN THE NUMBER OF POINTS TO BE PLOTTED.
[ 4] .CM OUTPUT IS AN N BY 2 MATRIX, THE FIRST COLUMN
[ 5] .CM BEING THE INTEGERS FROM 0 TO N-1.
[ 6] ''
[ 7] 'INPUT DATA VECTOR.'
[ 8] BIG=,@
[ 9] ''
[10] N=,ROBIG
[11] 'INPUT NUMBER OF POINTS DESIRED.'
[12] NP="1+@
[13] NN=.FL(0;5+N%NP)
[14] IF 4088<NP#NN THEN NN=NN-1
[15] CPOUT=(NP,NN).ROBIG
[16] CPOUT=CPOUT[;1],"1^BIG
[17] NP=1+NP
[18] CPOUT=.TR(2,NP).RO(("1+.IONP).CPOUT)
[19] ''
[20] 'PLOT MATRIX IS CALLED ''CPOUT'';'
[21] NP;' VALUES OUT OF';,ROBIG;' ARE USED.'
[22] ''
$K
?
```

-1-

## DISTORT

```
$ DISTORT DAT
[1] 'THIS PROGRAM CORRECTS FOR PHASE DISTORTION'
[2] 'INPUT DER CURVE LIMITS'
[3] L1=@
[4] DAT=, DAT
[5] CDAT=DAT["1+L1[1]+; IO(1+--/L1)]
[6] DO=, CE/CDAT
[7] AO=, FL/CDAT
[8] XZ="1+L1[1]+CDAT; IODO
[9] XZN="1+L1[1]+CDAT; IOAO
[10] X2G=0; 5#(XZ-XZN)
[11] C=, CE((XZ+XZN)#0.5)
[12] B1=0; 5%(X2G*2)
[13] J=(0; 5#-DO+AO)#*(B1#(X2G)*2)
[14] CORD=J#*(-B1#((-C)+; IO(.RODAT))*2)
[15] CORD=CORD+DAT
[16] 'DATA IN CORD'
$K
```

"DISTORT" Inputs the entire resonance spectra and then asks for the "X" limits between which you want to apply the leakage current distortion correction. The first derivative distortion is assumed to be caused by improper phase balance between phase tuning on the klystron and the energy absorption detection circuits (from crystal detector to the leakage current meter on the ESR console). During a run through a magnetic absorption range the leakage current must not drift from  $250\mu\text{A}$  (an arbitrary constant for convenience). However, during a resonance, the leakage current must increase then decrease as the microwave detection bridge in the klystron becomes unbalanced indicating that some energy has been absorbed as a resonance point was passed. Since I am assuming a Gaussian absorption curve, I also assume that the leakage current distortion is an Gaussian curve. The effect of this program is to simulate the Gaussian leakage current distortion and subtract this from the first derivative data. See Figure E1 and E2. The following picture shows where the parameters for distort come from this picture. Note that  $|A_0| < |D_0|$ . See Appendix B for the procedure that would have corrected this.



$\overline{X2G} \equiv$  position for non-distorted distribution first derivative peaks.

General form:

$$y = A \text{ EXP}[-B(x-C)^2]$$

$$y' = -2BA(x-C)\text{EXP}[-B(x-C)^2]$$

$$y'' = 4B^2A(x-C)^2\text{EXP}[-B(x-C)^2] + (-2BA)\text{EXP}[-B(x-C)^2]$$

At  $x-C = \overline{X2G}$

$$y''(\overline{X2G}) = 0 = 4B^2A(\overline{X2G})^2\text{EXP}[-B(\overline{X2G})^2] + (-2BA)\text{EXP}[-B(\overline{X2G})^2]$$

$$4B^2A(\overline{X2G})^2\text{EXP}[-B(\overline{X2G})^2] = 2BA \text{ EXP}[-B(\overline{X2G})^2]$$

Factor out  $2BA \text{ EXP}[-B(\overline{X2G})^2]$  from both sides

$$2B(\overline{X2G})^2 = 1$$

$$B = \frac{1}{(2)(\overline{X2G})^2}$$

The amplitude F of the leakage current Gaussian distortion curve is proportional to

$$(|A_0| - |D_0|)/2 \cdot \frac{|A_0| - |D_0|}{2} \propto F$$

In this case,  $|A_0| < |D_0|$ , the correction amplitude would be negative which is correct to bring first derivative back to symmetry i.e.,  $|A_0| = |D_0|$ .

It is not obvious but the amplitude of the correction must be normalized to the fitting parameter B. At  $x-C = \overline{x2G}$

$$F \text{ EXP}[-B(\overline{x2G})^2] = (|A_0| - |D_0|)/2$$

$$F = \text{EXP}[B(\overline{x2G})^2] \cdot (|A_0| - |D_0|)/2$$

$$\therefore \text{Correction Function} = F \text{ EXP}[-B(x-C)^2]$$

-1-

## INTTEG

```

$   INTTEG;D;BND;S;H;N;NEXT
[1] .CM NILADIC OPER TO DO AN "INDEFINITE" INTEGRATION OF A
[2] .CM VECTOR OF Y-VALUES FOR EQUALLY SPACED X-VALUES.
[3] .CM FOR MAX NUMBER OF DATA POINTS (SAY 4024), MAY USE
[4] .CM OVER 50 SECS RUN TIME. AFTER INTEGRATION BEST TO
[5] .CM WRITE WHAT YOU NEED INTO FILES, EXIT, AND THEN
[6] .CM 'RUN APL' AGAIN, STARTING FRESH ON RUN TIME;
[7] ''
[8] 'INPUT VECTOR OF VALUES TO BE INTEGRATED.'
[9] D=,@
[10] ''
[11] 'INPUT RANGE OF INTEGRATION AS A TWO-COMPONENT VECTOR.'
[12] 'THEN WAIT PATIENTLY.'
[13] BND=@
[14] DD=D["1+BND[1]+.IO1+--/BND]
[15] S=;RODD
[16] ICURV=S,ROO
[17] H=0.5#(--/BND)%("1+S)
[18] ICURV[1]=H#DD[1]
[19] ICURV[2]=H#+/2^DD
[20] N=2
[21] NEXT:N=N+1
[22] ICURV[N]=ICURV[N-1]+H#(DD[N-1]+DD[N])
[23] .GO(N<S)/NEXT
[24] ''
[25] 'LIMITS OF INTEGRATION: FROM';BND[1];' TO';BND[2];';'
[26] 'X-INCREMENT IS';2#H
[27] 'OUTPUT INTEGRATED Y(X) IS CALLED ''ICURV'';'
[28] ''
$K

```

AD-A032 718

NAVAL ACADEMY ANNAPOLIS MD  
THE ELECTRON SPIN RESONANCE DETERMINATION OF SITE POPULATIONS I--ETC(U)  
JUN 76 D H MILLS  
USNA-TSPR-80

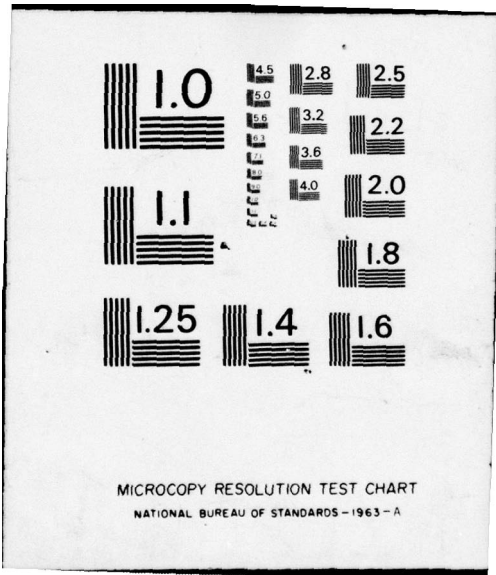
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2 OF 2  
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MICROCOPY RESOLUTION TEST CHART  
NATIONAL BUREAU OF STANDARDS-1963-A

-1-

ABSCOR

```
$ ABSCOR OD
[1] .CM MONADIC OPR WHICH CORRECTS DATA FOR BASELINE SLOPE.
[2] OD=.OD
[3] CORDATA=OD+("1+.IO.ROOD)#((1^OD)-("1^OD))%("1+.ROOD)
[4] CORDATA=-CORDATA
[5] 'NEW VECTOR CALLED ''CORDATA''.'
[6] ''
$K
```

-1-

FIT

```

$ FIT DAT
[1] .CM THIS PROGRAM FITS AN ESR ABSORPTION CURVE TO A GAUSSIAN
[2] .CM CURVE. THE LIMITS BOUNDING THE CURVE ARE INPUTS.
[3] .CM THE AMPLITUDE AND THE EXPONENTIAL COEFFICIENT ARE
[4] .CM OUTPUTS. THE STANDARD DEVIATION OF THE DATA FROM THE
[5] .CM GAUSSIAN IS GIVEN.
[6] 'INPUT PEAK LIMITS L1 L2'
[7] L1=@
[8] CDL1=DAT["1+L1[1]+.IO+--/L1]
[9] YMAX=.CE/CDL1
[10] XMAX="1+L1[1]+CDL1.IOYMAX
[11] FD1=(CDL1>0.5#.CE/CDL1)/CDL1
[12] G1=DAT["1+L1[1]+.IO(XMAX-L1[1])]
[13] FD2=(G1<0.5#.CE/CDL1)
[14] NPTSG1=FD2.IOO
[15] STARTPT=("1+L1[1]+NPTSG1)
[16] N=:ROFD1
[17] X=STARTPT+"1+.ION
[18] S=+/(X-XMAX)*2
[19] Q=+/.LGFD1
[20] R=+/(.LGFD1)#((X-XMAX)*2)
[21] P=+/(X-XMAX)*4
[22] M=2 2:RO(N,(-S),S,(-P))
[23] V=Q,R
[24] DATFIT=M SIMEQ V
[25] X="1+L1[1]+.IO.ROCDL1
[26] DATFIT[1]=*DATFIT[1]
[27] CURFIT=DATFIT[1]#*-DATFIT[2]#(X-XMAX)*2
[28] ST=(((+/(CURFIT-CDL1)*2)%("1+.ROCDL1))*0.5)
[29] 'AMPLITUDE =' ;DATFIT[1];' B =' ;DATFIT[2]
[30] 'STANDARD DEVIATION =' ;ST
[31] 'DATA IN CURFIT'
$K
$ SOLN=CF SIMEQ C;JDEX;DEL;M
[1] .CM THIS DYADIC OPERATOR OBTAINS THE SOLUTION (VECTOR VC)
[2] .CM OF A SET OF LINEAR SIMULTANEOUS EQUATIONS --
[3] .CM THE DETERMINANT OF ITS COEFFICIENTS (CF) IS THE
[4] .CM PREOPERAND AND THE VECTOR OF CONSTANT TERMS (C)
[5] .CM IS THE POSTOPERAND.
[6] VC=C;JDEX=0;DEL=DET CF;
[7] NEXTJ:M=CF
[8] M[;JDEX=JDEX+1]=C
[9] VC[JDEX]=(DET M)%DEL
[10] .GO(JDEX<.ROC)/NEXTJ
[11] SOLN=VC
$K
$ Z=DET MM;K
[1] MM[K,1;]=MM[1,K=K.IO.CE/K=:ABMM[;1];]
[2] Z=(1.E"9<.ABMM[1;1])#MM[1;1]#"1*K.NE1
[3] .GOO#.IO;OR/(1.EQ.ROMM),0.EQZ
[4] Z=Z#DET 1 1.DAMM-MM[;1].SO.#MM[1;]#MM[1;1]
$K

```

"FIT." Inputs the entire magnetic absorption resonance spectrum. You can then specify the X coordinate limits which contain the absorption curve to be fitted to a Gaussian curve. It then finds all the points in the set greater than half the height of the peak. The amplitude (A) and exponential coefficient (B) are found. The midpoint of the curve is taken as the average X coordinate distance between the negative and positive first derivative peaks. Therefore M is known from data. The following is the derivation for A and B.

Gaussian Curve Fit:

$$y = A \text{ EXP}[-B(x-m)^2]$$

M  $\equiv$  Midpoint of the Gaussian curve; found from data

$$\ln y = \ln A + (-B)(x-m)^2$$

$$F = C + (-B)(x-m)^2$$

Di  $\equiv$  ith Data Point

Least Squares Sum:

$$\sum (F - \ln Di)^2 = S(C, B)$$

Let

$$Z = \ln Di$$

$$\frac{\partial S}{\partial C} = 2 \sum (F - Z) \frac{\partial F}{\partial C} = 0$$

$$\frac{\partial S}{\partial B} = 2 \sum (F - Z) \frac{\partial F}{\partial B} = 0$$

$$\frac{\partial F}{\partial C} = 1; \quad \frac{\partial F}{\partial B} = -(x-m)^2$$

$$\frac{1}{2} \frac{\partial S}{\partial C} = \Sigma [C - B(x-m)^2 - Z] = 0$$

$$-\frac{1}{2} \frac{\partial S}{\partial B} = \Sigma [C - B(x-m)^2 - Z] [x-m]^2 = 0$$

$$\Sigma C - B \Sigma (x-m)^2 - \Sigma Z = 0$$

$$C \Sigma (x-m)^2 - B \Sigma (x-m)^4 - \Sigma Z (x-m)^2 = 0$$

Let

$$\Sigma (x-m)^2 = S$$

$$\Sigma (Z) (x-m)^2 = R$$

$$\Sigma (x-m)^4 = P$$

$$\Sigma C = C \Sigma 1 = CN$$

$$CN - BS - Z = 0$$

$$CS - BP - R = 0$$

$$\begin{bmatrix} N - S \\ S - P \end{bmatrix} \begin{bmatrix} C \\ B \end{bmatrix} = \begin{bmatrix} Z \\ R \end{bmatrix} \Rightarrow \begin{bmatrix} C \\ B \end{bmatrix} = \begin{bmatrix} N - S \\ S - P \end{bmatrix}^{-1} \begin{bmatrix} Z \\ R \end{bmatrix}$$

$$A = \text{EXP}(C) = \text{EXP}(\ln A)$$

Therefore A and B are found.

-1-

## INTSIM

```

$   INTSIM DAT
[.5] .CM THIS PROGRAM PERFORMS DEFINITE INTEGRATION
[.6] .CM ON INPUT DATA FILE USING SIMPSON'S
[.7] .CM RULE.  THE PROGRAM FINDS AN EVEN NUMBER
[.8] .CM OF SEGEMENTS BY DROPPING THE LAST DATA POINT
[1]  S=6
[1.1] DATA=DAT
[2]  X=.IO2
[5]  .GO((.RODAT) .NE 2#.FL((.RODAT))%2)/NEXT
[6]  DATA="1;DADAT
[7]  NEXT:N=.FL("0.5+.RODATA)
[9]  I=((("1+.RODATA)%(3#N))#+/(1,((N-1).RO4 2),1)#DATA
[10] 'THE COMPUTED VALUE OF THE INTEGRAL IS:'
[11] S SIGNIF I
$K
$   SIG=S SIGNIF B;A;C;M;N
[1]  N=1+"2#B<0
[2]  A=N#(B+B.EQ0)
[3]  C=.FL10.LG,A
[4]  M=(10.LG,A)-C
[5]  SIG=(.ROA).RO( ;FL(0.5+10*M+S-1))#10*1+C-S
[6]  SIG=N#(SIG-B;EQ0)
$K

```

-1-

## APLTBAS

```
100' THIS PROGRAM CHANGES ANY SET OF [N 2,RO] APL DATA MATRICES
110' IN A GIVEN FILE INTO STANDARD GRAPHIC FORMAT;
120' WRITTEN BY DANNY MILLS '76 (MAR 1976).
130 DIM V(100)
140 PRINT "APL DATA FILE NAME";
150 LINPUT X$
160 FILE #1: X$
170 FILE #2: ""
180 LINPUT #1: Y$
190 LINPUT #1:Y$
200 IF Y$ <> " " THEN 230
210 PRINT #2: "1E37,1E37"
220 GO TO 410
230 CHANGE Y$ TO V
240 FOR K1 = 1 TO V(0)
250 IF V(K1) <> 34 THEN 270
260 LET V(K1) = 45
270 NEXT K1
280 FOR K1 = 1 TO V(0)
285 IF V(K1)=45 THEN 310
290 IF V(K1) = 32 THEN 310
300 GO TO 320
310 NEXT K1
320 FOR L1 = K1 TO V(0)
330 IF V(L1) = 32 THEN 345
335 IF V(L1)<> 45 THEN 360
336 CHANGE V TO V$
337 LET Y$ = SEG$(V$,1,L1-1)
338 LET Z$ = SEG$(V$,L1,LEN(V$))
339 LET V$= Y$&CHR$(44)&CHR$(32)&Z$
340 CHANGE V$ TO V
341 GO TO 370
345 LET V(L1)=44
350 GO TO 370
360 NEXT L1
370 CHANGE V TO Y$
380 PRINT #2: Y$
390 IF END #1 THEN 430
400 GO TO 190
410 IF END #1 THEN 430
420 GO TO 180
430 RESET #2
440 SCRATCH #1
450 FOR I = 1 TO 7000
460 LINPUT #2: R$
470 PRINT #1: R$
480 IF END #2 THEN 500
490 NEXT I
500 PRINT "CHANGED TO STANDARD GRAPHIC FORMAT"
520 END
```

-1-

## ESR PLOT

```
100 LET H = .7147788*9.348
105 LET Q = 1
110 FILE #1: "SPLIT"
116 SCRATCH #1
120 LET S1 = 6.25
130 LET S2 = 7.78
140 LET T1 = 8.55
150 LET T2 = 3.29
160 LET P = 3.14159/180
165 PRINT " TABLE OR GRAPH";
166 INPUT X$
167 IF X$="GRAPH" THEN 170
168 IF X$="TABLE" THEN 500
169 GO TO 165
170 PRINT "B OR G";
171 INPUT Y$
172 IF Y$="B" THEN 179
173 LET H = 1
174 LET Q=-1
179 FOR T=-30 TO 390 STEP 5
180 LET S3 = SQR((S2*COS(P*T))^2+(S1*SIN(P*T))^2)
190 PRINT #1: T;",";H/S3^Q
200 NEXT T
210 PRINT #1: "1E37,1E37"
220 FOR T = -30 TO 390 STEP 5
230 LET S4 = SQR(S2^2*.5*(SIN(P*T))^2 + S1^2*(1-.5*(SIN(P*T))^2))
240 PRINT #1: T;",";H/S4^Q
250 NEXT T
260 PRINT #1: "1E37,1E37"
270 FOR T = -30 TO 390 STEP 5
280 LET B = (T-54.75)*P
290 LET S5 = SQR((T2*COS(B))^2 + (T1*SIN(B))^2)
300 PRINT #1: T;",";H/S5^Q
310 NEXT T
320 PRINT #1: "1E37,1E37"
330 FOR T = -30 TO 390 STEP 5
340 LET C = (T+54.75)*P
350 LET S6 = SQR((T2*COS(C))^2 + (T1*SIN(C))^2)
360 PRINT #1: T;",";H/S6^Q
370 NEXT T
380 PRINT #1: "1E37,1E37"
390 FOR T = -30 TO 390 STEP 5
400 LET C = (T+54.75)*P
410 LET S7 = SQR(1/3*(T2*COS(P*T))^2 + T1^2*(1-1/3*(COS(P*T))^2))
420 PRINT #1: T;",";H/S7^Q
430 NEXT T
440 PRINT #1: "1E37,1E37"
450 FOR T = -30 TO 390 STEP 5
460 LET S8 = 6.78
470 PRINT #1: T;",";H/S8^Q
```

-2-

ESRPLOT (continued)

```
480 NEXT T
490 PRINT #1: "1E37,1E37"
499 GO TO 700
500 PRINT "B OR G";
501 INPUT Y$
502 IF Y$="B" THEN 510
503 LET H = 1
504 LET Q=-1
510 CONTINUE
511 PRINT #1: " T   TET1   TET2   TRIG1   TRIG2   TRIG3   CUBIC"
512 FOR T= -30 TO 390 STEP 5
521 LET S3 = SQR((S2*COS(P*T))^2+(S1*SIN(P*T))^2)
531 LET S4 = SQR(S2^2*.5*(SIN(P*T))^2 + S1^2*(1-.5*(SIN(P*T))^2))
541 LET B = (T-54.75)*P
542 LET S5 = SQR((T2*COS(B))^2 + (T1*SIN(B))^2)
551 LET C = (T+54.75)*P
552 LET S6 = SQR((T2*COS(C))^2 + (T1*SIN(C))^2)
562 LET S7 = SQR(1/3*(T2*COS(P*T))^2 + T1^2*(1-1/3*(COS(P*T))^2))
581 LET S8 = 6.78
582 LET S3=INT((H/S3)^Q*10000+.5)/10000
584 LET S4=INT((H/S4)^Q*10000+.5)/10000
585 LET S5=INT((H/S5)^Q*10000+.5)/10000
586 LET S6=INT((H/S6)^Q*10000+.5)/10000
587 LET S7=INT((H/S7)^Q*10000+.5)/10000
588 LET S8=INT((H/S8)^Q*10000+.5)/10000
599 PRINT #1: T;S3;S4;S5;S6;S7;S8
600 NEXT T
700 END
```

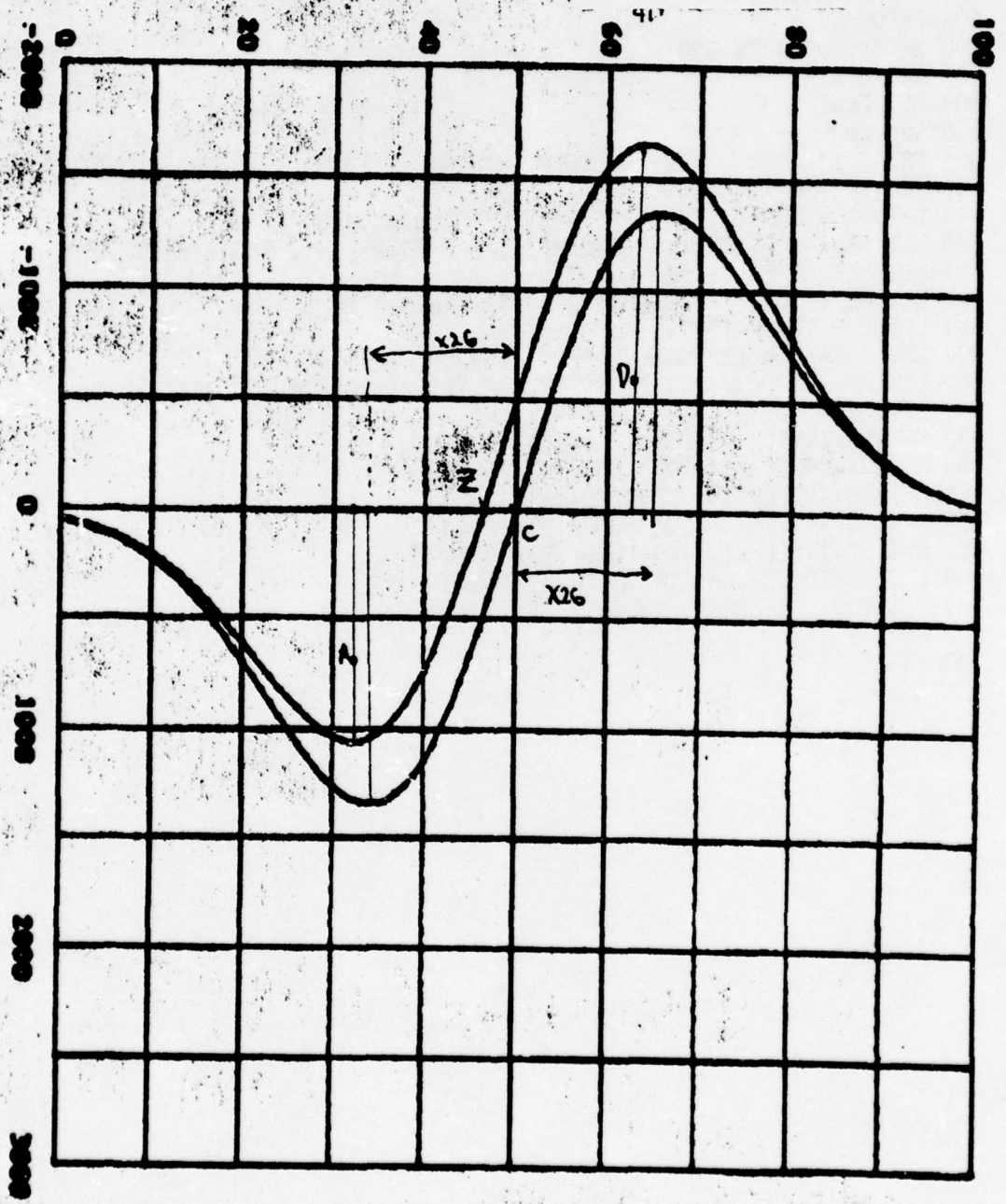


Figure E1. Shows the simulated Gaussian Error in the Leakage Current of the Microwave Bridge: Distorted First Derivative Curve. FIG E1

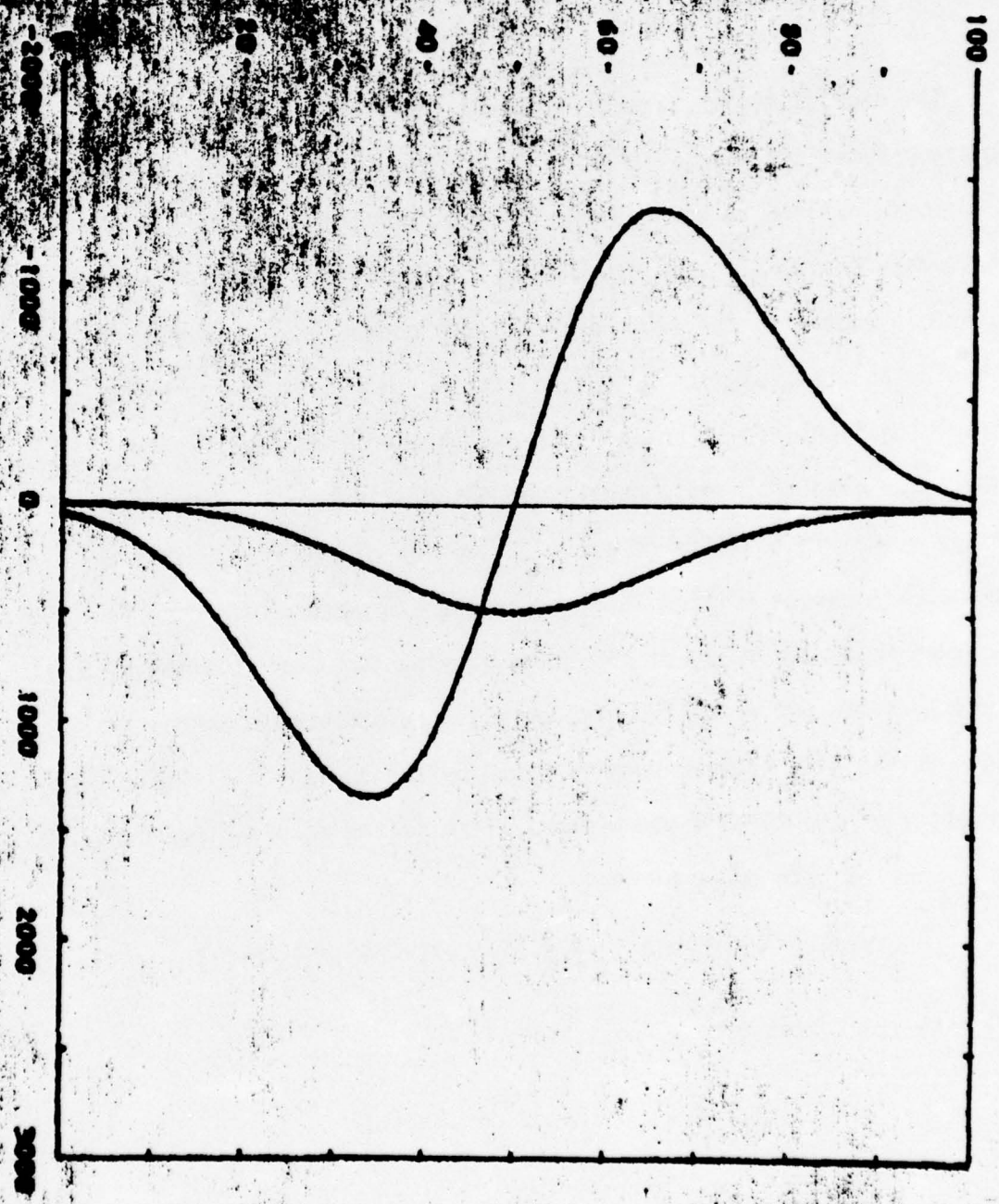


Figure E2. Undistorted First derivative curve, and error function used to obtain Figure E1. **FIG E2**

APPENDIX G  
 DERIVATION OF TRANSFER FUNCTION  
 OF DIGITAL MOVING AVERAGE FILTER

The digital moving average filter is basically a moving window memory  $L$  locations wide. It sums the contents of the first  $L$  memory locations in field 2, divides by  $L$ , and stores this number in the  $L$ th memory location in field 3 of the PDP-8 memory. The window then moves one number to the right and runs the contents of memory locations 2 thru  $L+1$ , divides by  $L$ , and stores the result in the  $L+1$ th memory location. This continues through the entire memory. The idea is to make the window contain an integral number of wavelengths of the signal to be filtered out. The action of the filter in the time domain can be written in terms of the  $K$ th memory location. Each location holds the value of some time varying function at time  $(K)(S)$  where  $K$  is the number of the sample (e.g. the 5th sample taken:  $K=5$ ) and  $S$  is the time between samples taken by the analog to digital converter on the PDP-8 minicomputer. ( $1/S$  is the sampling frequency.) For  $L$  samples [ $K$ th to  $(K-L+1)$ th].

$$Y(K) = \frac{1}{L} [X(K) + X(K-1) + X(K-2) + \dots + X(K-L+2) + X(K-L+1)]$$

Now take the Z-transform of both sides

$$\begin{aligned} Y(z) &= \frac{1}{L} [X(z)Z^0 + X(z)Z^{-1} + \dots + X(z)Z^{-L+1}] \\ &= \frac{X(z)}{L} (1 + Z^{-1} + Z^{-2} + \dots + Z^{-L+1}) \end{aligned}$$

The transfer function  $\equiv Y(z)/X(z) = H(z)$

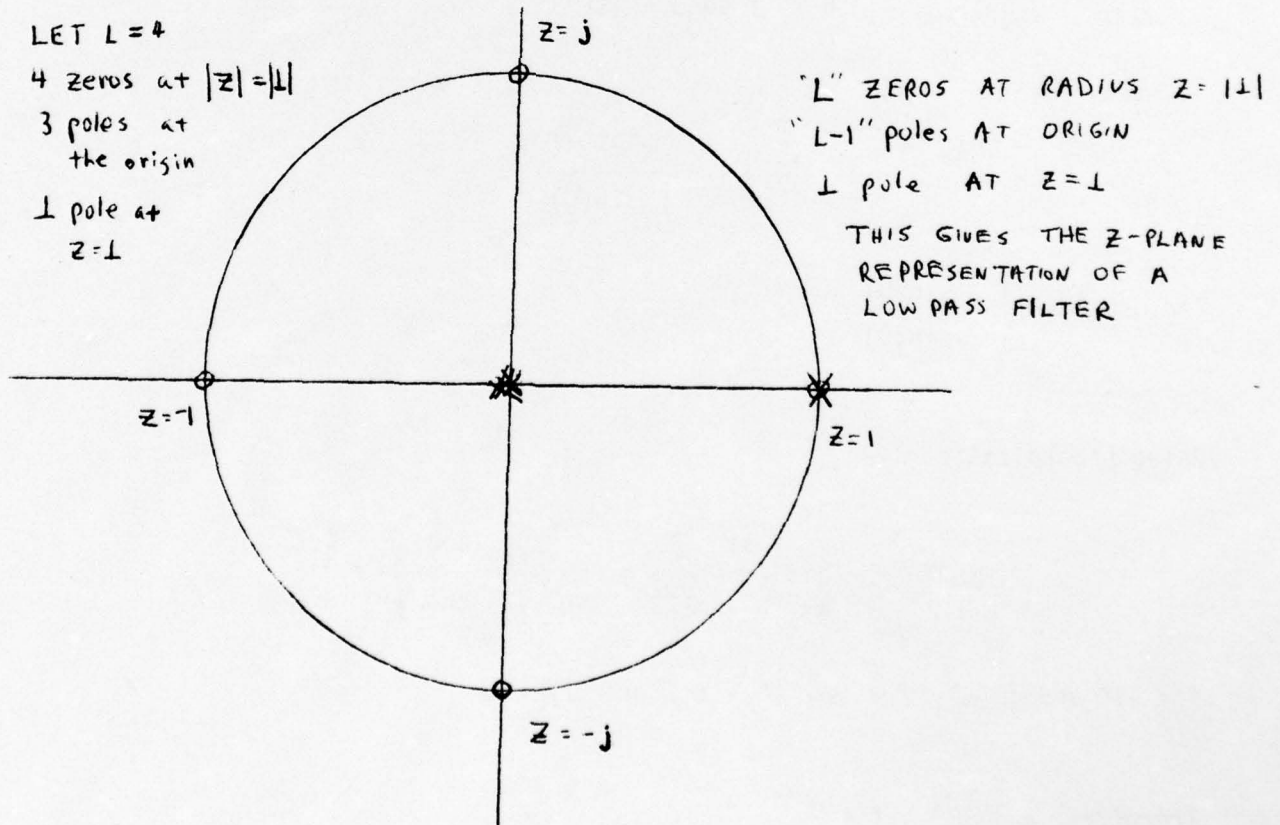
$$H(z) = \frac{1}{L}(1+z^{-1}+z^{-2}+\dots+z^{-L+1})$$

Using the identity

$$\sum_{K=0}^{K=L-1} z^{-K} = \frac{1-z^{-L}}{1-z^{-1}}$$

$$H(z) = \frac{1}{L} \frac{1-z^{-L}}{1-z^{-1}} = \frac{z}{Lz^L} \frac{z^L-1}{z-1} = \frac{1}{Lz^{L-1}} \frac{z^L-1}{z-1}$$

This is visualized in the Z domain as follows:



NOTE:  $L = 15_{10}$  IN THIS EXPERIMENT

Let  $Z = e^{j\omega}$

$$H(j\omega) = \frac{1}{L} \frac{e^{j\omega L}}{[e^{j\omega(L-1)}][e^{j\omega}-1]} = \frac{e^{\frac{j\omega L}{2}} [e^{\frac{j\omega L}{2}} - e^{-\frac{j\omega L}{2}}]}{L [e^{j\omega(L-0.5)}] [e^{\frac{j\omega}{2}} - e^{-\frac{j\omega}{2}}]}$$

$$|H(\omega)| = \frac{|1| |e^{\frac{j\omega L}{2}} - e^{-\frac{j\omega L}{2}}|}{L |1| |e^{\frac{j\omega}{2}} - e^{-\frac{j\omega}{2}}|}$$

Using Euler's identities

$$e^{j\omega} = \cos\omega + j\sin\omega$$

$$e^{-j\omega} = \cos\omega - j\sin\omega$$

$$|H(\omega)| = \frac{\sin(\frac{L\omega}{2})}{L \sin(\frac{\omega}{2})}$$

$$\text{For } \omega=0 \quad |H(0)| = \frac{\sin(0)}{\sin(0)}$$

Using L'Hospital's rule

$$|H(\omega)|_{\omega=0} = \lim_{\omega \rightarrow 0} \frac{\sin \frac{L\omega}{2}}{L \sin(\frac{\omega}{2})} = \lim_{\omega \rightarrow 0} \frac{L/2 \cos \frac{L\omega}{2}}{L/2 \cos \frac{\omega}{2}} = 1$$

$$\text{For } \omega \neq 0 \text{ and } |H(\omega)| = 0 \quad \sin \frac{L\omega}{2} = 0 \quad \text{or} \quad \frac{L\omega}{2} = n\pi$$

$$\text{Therefore } \omega = \frac{2n\pi}{L} \quad f = \frac{n}{L}$$

$$\omega = \frac{2\pi}{L}, \frac{4\pi}{L}, \frac{6\pi}{L}, \dots, \pi, \text{the Nyquist frequency.}$$

For an unstable condition (pole in denominator)

$$\sin \frac{\omega}{2} = 0 \text{ or } \frac{\omega}{2} = n\pi \text{ therefore } \omega = 2n\pi ,$$

but at  $\omega = 2n\pi$  the numerator equals

$$\sin \frac{2n\pi L}{2} = \sin n\pi L = 0$$

for all integers  $n$  and  $L$ . As stated before

$$\frac{\sin(0)}{\sin(0)} = 1.$$

There are no unstable frequencies for the filter. The frequency that is filtered out is given by

$$\omega = \frac{2n\pi}{L} \quad 2\pi f = \omega \quad f = \frac{n}{L}$$

I chose  $L = 15$  (17 in octal) so that any data periodic over 15 samples is filtered out. The sampling time was

$$\frac{10 \times 60}{4096} = .146$$

seconds or a frequency of 6.8/sec.

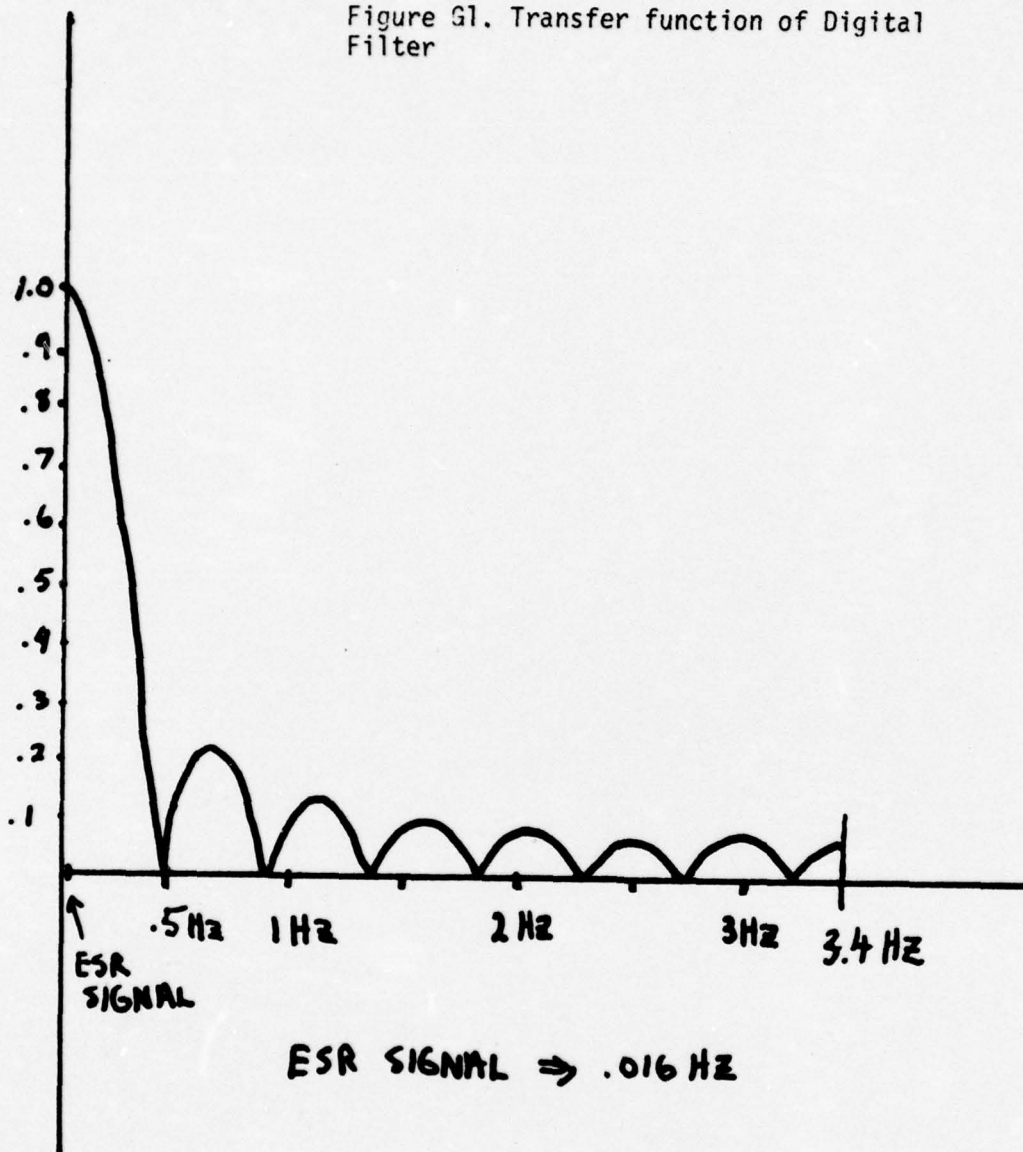
The Nyquist frequency is then 3.4 Hz. A typical resonance of a large peak takes 30 seconds with the range set at 1000 Gauss and sweep time set for 10 minutes. This gives a frequency of .033 Hz =  $f$  and  $\omega = 2\pi f = .066\pi$ .

$$\omega = \frac{\pi f}{f_{\text{Nyquist}}} = \frac{\pi(.033)}{3.4}$$

$$H(.066\pi) = \frac{\sin 15 \frac{\omega}{2}}{15 \sin \frac{\omega}{2}} = .9747$$

So there is a slight attenuation in the signal. See Figure G1 for a graph of frequency response.

Figure G1. Transfer function of Digital Filter



APPENDIX H

TABLES OF B AND G

ROAD MAP VALUES

## SPLITTING VALUES

-1-

SPLIT

AS A FUNCTION OF "T"  
ANGLE OF ROTATION

T	TET1	TET2	TRIG1	TRIG2	TRIG3	CUBIC
-30	7.4271	6.4611	8.5195	4.6626	7.585	6.78
-25	7.5296	6.4015	8.4339	5.1146	7.4867	6.78
-20	7.6169	6.3496	8.2942	5.573	7.4008	6.78
-15	7.687	6.3073	8.102	6.024	7.3303	6.78
-10	7.7383	6.2758	7.8594	6.4569	7.278	6.78
-5	7.7695	6.2565	7.5695	6.8631	7.2457	6.78
0	7.78	6.25	7.2359	7.2359	7.2348	6.78
5	7.7695	6.2565	6.8631	7.5695	7.2457	6.78
10	7.7383	6.2758	6.4569	7.8594	7.278	6.78
15	7.687	6.3073	6.024	8.102	7.3303	6.78
20	7.6169	6.3496	5.573	8.2942	7.4008	6.78
25	7.5296	6.4015	5.1146	8.4339	7.4867	6.78
30	7.4271	6.4611	4.6626	8.5195	7.585	6.78
35	7.3121	6.5264	4.235	8.5499	7.6924	6.78
40	7.1874	6.5952	3.855	8.525	7.8051	6.78
45	7.0566	6.6655	3.5511	8.4449	7.9198	6.78
50	6.9233	6.735	3.3543	8.3106	8.0328	6.78
55	6.7915	6.8018	3.2902	8.1235	8.1408	6.78
60	6.6655	6.8638	3.3683	7.8859	8.2409	6.78
65	6.5495	6.9194	3.5772	7.6005	8.3303	6.78
70	6.4478	6.9671	3.8901	7.2711	8.4068	6.78
75	6.364	7.0055	4.2761	6.902	8.4683	6.78
80	6.3016	7.0336	4.707	6.4989	8.5133	6.78
85	6.263	7.0508	5.1604	6.0683	8.5408	6.78
90	6.25	7.0566	5.6186	5.6186	8.55	6.78
95	6.263	7.0508	6.0683	5.1604	8.5408	6.78
100	6.3016	7.0336	6.4988	4.7071	8.5133	6.78
105	6.364	7.0055	6.902	4.2761	8.4683	6.78
110	6.4478	6.9671	7.2711	3.8901	8.4068	6.78
115	6.5495	6.9194	7.6005	3.5772	8.3304	6.78
120	6.6655	6.8638	7.8858	3.3683	8.2409	6.78
125	6.7915	6.8018	8.1235	3.2902	8.1408	6.78
130	6.9233	6.735	8.3106	3.3543	8.0328	6.78
135	7.0566	6.6655	8.4449	3.5511	7.9198	6.78
140	7.1874	6.5952	8.525	3.855	7.8052	6.78
145	7.3121	6.5264	8.5499	4.235	7.6924	6.78
150	7.4271	6.4611	8.5195	4.6626	7.585	6.78
155	7.5296	6.4015	8.4339	5.1146	7.4867	6.78
160	7.6169	6.3496	8.2942	5.573	7.4008	6.78
165	7.687	6.3073	8.102	6.024	7.3303	6.78
170	7.7383	6.2758	7.8594	6.4569	7.278	6.78
175	7.7695	6.2565	7.5695	6.8631	7.2457	6.78
180	7.78	6.25	7.2359	7.2359	7.2348	6.78
185	7.7695	6.2565	6.8632	7.5695	7.2457	6.78
190	7.7383	6.2758	6.4569	7.8594	7.278	6.78
195	7.687	6.3073	6.024	8.1019	7.3303	6.78
200	7.6169	6.3496	5.573	8.2942	7.4008	6.78
205	7.5296	6.4015	5.1146	8.4339	7.4867	6.78
210	7.4271	6.4611	4.6626	8.5194	7.585	6.78

-2-

## SPLIT (continued)

215	7.3121	6.5264	4.235	8.5499	7.6924	6.78
220	7.1874	6.5952	3.855	8.525	7.8051	6.78
225	7.0566	6.6655	3.5511	8.4449	7.9198	6.78
230	6.9233	6.735	3.3543	8.3106	8.0328	6.78
235	6.7915	6.8018	3.2902	8.1235	8.1408	6.78
240	6.6655	6.8638	3.3683	7.8859	8.2409	6.78
245	6.5495	6.9194	3.5772	7.6005	8.3303	6.78
250	6.4478	6.9671	3.8901	7.2711	8.4068	6.78
255	6.364	7.0055	4.2761	6.902	8.4683	6.78
260	6.3016	7.0336	4.707	6.4989	8.5133	6.78
265	6.263	7.0508	5.1604	6.0683	8.5408	6.78
270	6.25	7.0566	5.6186	5.6186	8.55	6.78
275	6.263	7.0508	6.0682	5.1604	8.5408	6.78
280	6.3016	7.0336	6.4988	4.7071	8.5133	6.78
285	6.364	7.0055	6.902	4.2761	8.4683	6.78
290	6.4477	6.9671	7.2711	3.8901	8.4068	6.78
295	6.5495	6.9194	7.6005	3.5772	8.3304	6.78
300	6.6655	6.8638	7.8858	3.3683	8.2409	6.78
305	6.7915	6.8018	8.1235	3.2902	8.1408	6.78
310	6.9233	6.7351	8.3106	3.3543	8.0328	6.78
315	7.0566	6.6655	8.4449	3.5511	7.9198	6.78
320	7.1874	6.5952	8.525	3.855	7.8052	6.78
325	7.3121	6.5264	8.5499	4.235	7.6924	6.78
330	7.4271	6.4611	8.5195	4.6626	7.5851	6.78
335	7.5296	6.4015	8.4339	5.1146	7.4867	6.78
340	7.6169	6.3496	8.2942	5.573	7.4008	6.78
345	7.687	6.3073	8.102	6.024	7.3303	6.78
350	7.7383	6.2758	7.8594	6.4569	7.278	6.78
355	7.7695	6.2565	7.5695	6.8631	7.2457	6.78
360	7.78	6.25	7.2359	7.2358	7.2348	6.78
365	7.7695	6.2565	6.8632	7.5695	7.2457	6.78
370	7.7383	6.2758	6.4569	7.8594	7.278	6.78
375	7.687	6.3073	6.024	8.1019	7.3303	6.78
380	7.6169	6.3496	5.573	8.2942	7.4008	6.78
385	7.5296	6.4015	5.1146	8.4339	7.4867	6.78
390	7.4271	6.4611	4.6626	8.5194	7.585	6.78

## TABLE OF MAGNETIC RESONANCE VALUES

-1-

SPLIT AS A FUNCTION OF "T"  
ROTATION ANGLE (GIVEN IN KGAUSS)

T	TET1	TET2	TRIG1	TRIG2	TRIG3	CUBIC
-30	0.8996	1.0342	0.7843	1.433	0.8809	0.9855
-25	0.8874	1.0438	0.7923	1.3064	0.8925	0.9855
-20	0.8772	1.0523	0.8056	1.199	0.9028	0.9855
-15	0.8692	1.0594	0.8247	1.1092	0.9115	0.9855
-10	0.8635	1.0647	0.8502	1.0348	0.9181	0.9855
-5	0.86	1.068	0.8827	0.9736	0.9222	0.9855
0	0.8588	1.0691	0.9234	0.9234	0.9236	0.9855
5	0.86	1.068	0.9736	0.8827	0.9222	0.9855
10	0.8635	1.0647	1.0348	0.8502	0.9181	0.9855
15	0.8692	1.0594	1.1092	0.8247	0.9115	0.9855
20	0.8772	1.0523	1.199	0.8056	0.9028	0.9855
25	0.8874	1.0438	1.3064	0.7923	0.8925	0.9855
30	0.8996	1.0342	1.433	0.7843	0.8809	0.9855
35	0.9138	1.0238	1.5777	0.7815	0.8686	0.9855
40	0.9296	1.0131	1.7333	0.7838	0.8561	0.9855
45	0.9469	1.0024	1.8816	0.7912	0.8437	0.9855
50	0.9651	0.9921	1.992	0.804	0.8318	0.9855
55	0.9838	0.9824	2.0308	0.8225	0.8208	0.9855
60	1.0024	0.9735	1.9837	0.8473	0.8108	0.9855
65	1.0202	0.9657	1.8679	0.8791	0.8021	0.9855
70	1.0363	0.959	1.7176	0.9189	0.7948	0.9855
75	1.0499	0.9538	1.5626	0.9681	0.789	0.9855
80	1.0603	0.95	1.4195	1.0281	0.7849	0.9855
85	1.0669	0.9477	1.2948	1.1011	0.7823	0.9855
90	1.0691	0.9469	1.1892	1.1892	0.7815	0.9855
95	1.0669	0.9477	1.1011	1.2948	0.7823	0.9855
100	1.0603	0.95	1.0281	1.4195	0.7849	0.9855
105	1.0499	0.9538	0.9681	1.5626	0.789	0.9855
110	1.0363	0.959	0.919	1.7176	0.7948	0.9855
115	1.0202	0.9657	0.8791	1.8679	0.8021	0.9855
120	1.0024	0.9735	0.8473	1.9837	0.8108	0.9855
125	0.9838	0.9824	0.8225	2.0308	0.8208	0.9855
130	0.9651	0.9921	0.804	1.992	0.8318	0.9855
135	0.9469	1.0024	0.7912	1.8816	0.8437	0.9855
140	0.9296	1.0131	0.7838	1.7333	0.8561	0.9855
145	0.9138	1.0238	0.7815	1.5777	0.8686	0.9855
150	0.8996	1.0342	0.7843	1.4331	0.8809	0.9855
155	0.8874	1.0438	0.7923	1.3064	0.8925	0.9855
160	0.8772	1.0523	0.8056	1.199	0.9028	0.9855
165	0.8692	1.0594	0.8247	1.1092	0.9115	0.9855
170	0.8635	1.0647	0.8502	1.0348	0.9181	0.9855
175	0.86	1.068	0.8827	0.9736	0.9222	0.9855
180	0.8588	1.0691	0.9234	0.9234	0.9236	0.9855
185	0.86	1.068	0.9736	0.8827	0.9222	0.9855
190	0.8635	1.0647	1.0348	0.8502	0.9181	0.9855
195	0.8692	1.0594	1.1092	0.8247	0.9115	0.9855
200	0.8772	1.0523	1.199	0.8056	0.9028	0.9855
205	0.8874	1.0438	1.3064	0.7923	0.8925	0.9855
210	0.8996	1.0342	1.433	0.7843	0.8809	0.9855

-2-

## SPLIT (continued)

215	0.9138	1.0238	1.5777	0.7815	0.8686	0.9855
220	0.9296	1.0131	1.7333	0.7838	0.8561	0.9855
225	0.9469	1.0024	1.8816	0.7912	0.8437	0.9855
230	0.9651	0.9921	1.992	0.804	0.8318	0.9855
235	0.9838	0.9824	2.0308	0.8225	0.8208	0.9855
240	1.0024	0.9735	1.9837	0.8473	0.8108	0.9855
245	1.0202	0.9657	1.8679	0.8791	0.8021	0.9855
250	1.0363	0.959	1.7176	0.9189	0.7948	0.9855
255	1.0499	0.9538	1.5626	0.9681	0.789	0.9855
260	1.0603	0.95	1.4195	1.0281	0.7849	0.9855
265	1.0669	0.9477	1.2948	1.1011	0.7823	0.9855
270	1.0691	0.9469	1.1892	1.1892	0.7815	0.9855
275	1.0669	0.9477	1.1011	1.2948	0.7823	0.9855
280	1.0603	0.95	1.0281	1.4195	0.7849	0.9855
285	1.0499	0.9538	0.9681	1.5626	0.789	0.9855
290	1.0363	0.959	0.919	1.7176	0.7948	0.9855
295	1.0202	0.9657	0.8791	1.8679	0.8021	0.9855
300	1.0024	0.9735	0.8473	1.9837	0.8108	0.9855
305	0.9838	0.9824	0.8225	2.0308	0.8208	0.9855
310	0.9651	0.9921	0.804	1.992	0.8318	0.9855
315	0.9469	1.0024	0.7912	1.8816	0.8437	0.9855
320	0.9296	1.0131	0.7838	1.7333	0.8561	0.9855
325	0.9138	1.0238	0.7815	1.5777	0.8686	0.9855
330	0.8996	1.0342	0.7843	1.4331	0.8809	0.9855
335	0.8874	1.0438	0.7922	1.3064	0.8925	0.9855
340	0.8772	1.0523	0.8056	1.199	0.9028	0.9855
345	0.8692	1.0594	0.8247	1.1092	0.9115	0.9855
350	0.8635	1.0647	0.8502	1.0348	0.9181	0.9855
355	0.86	1.068	0.8827	0.9736	0.9222	0.9855
360	0.8588	1.0691	0.9234	0.9234	0.9236	0.9855
365	0.86	1.068	0.9736	0.8827	0.9222	0.9855
370	0.8635	1.0647	1.0348	0.8502	0.9181	0.9855
375	0.8692	1.0594	1.1092	0.8247	0.9115	0.9855
380	0.8772	1.0523	1.1989	0.8056	0.9028	0.9855
385	0.8874	1.0438	1.3064	0.7923	0.8925	0.9855
390	0.8996	1.0342	1.433	0.7843	0.8809	0.9855

redifax i

REDIFAX  
A REFERENCE MANUAL  
FOR THE  
PDP-8 MINICOMPUTER

(Included as a convenience to the reader/operator)

Compiled & Edited by:

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INDEX TO REDIFAX SHEETS

<u>#</u>	<u>Subject</u>
1	Turn On/Off : Start/Stop Program
2	Connecting to Time Share
3	ODT
4	8 SHARE
5	8 MAP
6	Restoring System
7	Crash Recovery
8	Binary Loader
9	RIM Loader
10	Configuration
11	Mass Data Transfers to Time Share

TURNING MACHINE ON & OFF: STARTING & STOPPING A PROGRAM

The Key (on a chain) switch controls the power.  
Turn to mid position only for normal use.  
Turn to left for off.

- To start a program running:

Turn machine on.  
Set starting address on switch register.  
Press LOAD ADDR.  
Press CLEAR, CONTINUE.

Usual starting address are:

0200 - Working program	} See REDIFAX #4&3
4000 - 8SHARE	
7000 - ODT	

- To stop a program simply press HALT. A halted program may be restarted from beginning as above or allowed to continue from where it was by pressing CONTINUE.
- To cause a program to go one instruction at a time keep HALT switch down and press CONTINUE repeatedly.
- Be sure to restore the system before shutting down. (See REDIFAX 6 ).

---

For more details on starting programs (e.g. starting a program in a different field) see 'Small Computer Handbook'.

CONNECTING TO TIME SHARE SYSTEM

- Machine I

Turn on 'Jefferson Box' and punch in A, D, F, G, H, J, & K. (Pressing M clears any former key in).

Turn on Beehive Terminal (push button) and press Half Duplex Button. The Beehive is optional but provides a useful monitor.

Dial up TSS using left hand modem and usual procedure (Dial 8 only).

If 8SHARE is not already running, start it (See REDIFAX 4).

Communication with TSS should be evidenced by sign-on message.

- Machine II

Turn on the machine and start 8SHARE (REDIFAX 1&2).

Dial up TSS using right hand modem and usual procedure (Dial 8 only).

Communications should be evidenced by sign-on message.

- Both Machines - Pressing TALK-CLEAR on related modem will disconnect.

Connection remains intact even if machines are not in 8SHARE and communication may be resumed by simply starting 8SHARE. Of course, if no activity occurs over a long period TSS will disconnect. Restart as above.

ØDT HIGHLIGHTS

- To start ØDT see REDIFAX 1. Start location is 7000. Normally resident in field0.
- To Open Register ABCD : type ABCD/ , where ABCD is the octal address. ØDT responds with the octal contents.
- To Modify an Open Register : type the desired new octal value followed by a carriage return or line feed.
- To Close an Open Register without Modification : type carriage return or line feed.
- To Open Next Register in Sequence : type line-feed. This will also close the previously opened register (with or without modification). ØDT responds with octal address/octal contents of next register.
- To start a program at octal location WXYZ, type WXYZG. ØDT gives a line-feed/carriage return and passes control to stated location.
- To place a breakpoint at octal location WXYZ type WXYZB. ØDT responds with a line-feed/carriage return and retains control. When you start your program running the instruction at WXYZ will be replaced by a trap which will return control to ØDT when program control reads WXYZ (instruction at WXYZ has not been executed).
- To continue running from a breakpoint, type OC. ØDT responds with line-feed/carriage return, executes the original instruction at the breakpoint, and transfers control back to the program.
- To remove a breakpoint, type OB.
- To transfer control from ØDT to 8SHARE, type CØNTROL-SHIFT-Ø (all at once).
- To transfer control from 8SHARE to ØDT, type CONTROL-SHIFT-L (all at once).

For complete details on ØDT see Chapter 5, pp 68-83, of Introduction To Programming and EE Dept document '8SHARE' which details local modifications to ØDT.

NOTE: "0" represents zero.  
"Ø" represents the alphabetic character O.

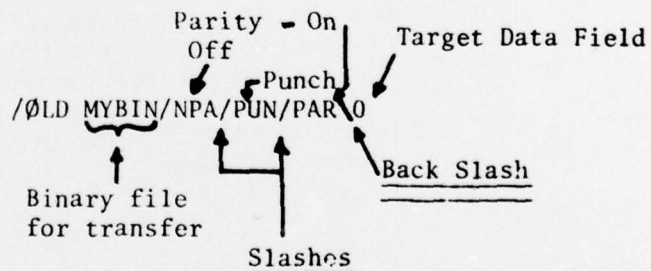
8SHARE HIGHLIGHTS

- To start 8SHARE and connect to TSS see REDIFAX 1 & 2. Starting location is 4000. (Will operate in field0 only).
- To dialogue with TSS :Start 8SHARE and connect to TSS. Interaction from keyboard is almost the same as if you were using any other ASR33/TTY in the yard.

Exceptions:

- (a) Bells from TSS don't ring and in general TSS control characters are ignored.
- (b) Lower case text from TSS prints out garbage.
- (c) Back slash (upper case L) and back arrow (Upper case Ø) are reserved: be very careful to avoid these unless you intend a binary data transfer - see below.
- (d) Only about one page may be listed without restarting, because of speed differentials and limited buffering.
- (e) The only way to stop transmission from TSS is by typing S : the other break mechanisms available at most yard terminals don't work with 8SHARE.
- (f) CONTROL-SHIFT-Ø passes control to ØDT.

- To transfer a binary program from TSS, follow this example: (Assuming dialogue with TSS is already in effect).



8SHARE will respond with a CR/LF after the Target Data Field is typed and the keyboard will go dead until the transfer of the binary file is complete. (The bells that ring just before the keyboard reactivates may be ignored).

- To transfer a binary file to TSS, see 8SHARE document.

For full details on 8SHARE see the EE Dept Document '8SHARE'.

8MAP HIGHLIGHTS

- To assemble a program using 8MAP you must have (on your TSS account):

- (a) A source file of the mnemonic form instructions you wish to have assembled.
- (b) A saved file which will receive the assembly listing.
- (c) A saved file which will receive the binary program.

Basically 8MAP takes the source file, checks its consistency, and produces:

- (a) a statement of errors found.
- (b) a resultant binary program in a form that may be loaded into the PDP-8.
- (c) an assembly listing of the binary program which shows the source code, and the way it has been assembled (i.e. location and value of each instruction).

- To use 8MAP type, RUN 8MAP.

It will respond with:

SOURCE;LISTING;BINARY;ERROR;SYMTAB--

At this point you are expected to supply at least three pieces of information, i.e., the file names for your source file, listing file, & binary file, in that order. Usually your current file will be the source file - indicate this by a ; and then type the name of your listing and binary file separated by a ; and followed by a CR. (Ignore the ERROR and SYMTAB files).

8MAP then takes over, prints any error messages and builds the listing & binary files, and returns control to you with the same file current. Previous contents of files specified for listing and binary are lost.

Full details on 8MAP may be obtained by typing /OLD PDP8LIB\*\*\*:D0CB/LIS. (Be prepared for a 6 or 7 page print-out).

Illustrative Example:

To create a 'do nothing' program.

```

      Opening Required Files, if not already available.
      |
      v
/NEW DUNOTE/SAV/NEW MYLIS/SAV/NEW MYBIN/SAV/BRI
*OLD DUNOTE
*100 *200
110 JMP . } Building Source Program
120 $
/REP/RUN 8MAP ← Calling 8MAP
SOURCE;LISTING;BINARY;ERROR;SYMTAB--;MYLIS;MYBIN
NORMAL TERMINATION ← Current File implied for SOURCE
    
```

\* - Underscore signify material typed by TSS

RESTORING THE SYSTEM SOFTWARE:

(See also Crash Recovery - REDIFAX #7)

**MACHINE I:** The operating system for Machine I is on a tape cassette labelled MASTER SYSTEMTAPE. Locate and mount this cassette on either drive, if not already mounted. Basic steps are:

- Press Rewind (unlabelled black button beside drive)
- Set 4540 on switch register (SR)
- Press ADDR LOAD
- Set SR to 0000
- Press EXT D ADDR LOAD
- Set SR to 0100 if cassette on drive B, otherwise leave SR at 0000.
- Press CLEAR/CONTINUE.

Tape should read in and stop with 4600 showing on top set of lights - if not see REDIFAX #7. Any user programs previously resident will be lost.

**MACHINE II:** The operating system is on a full-folded paper tape labelled MASTER SYSTEM TAPE-MACHINE II. Locate and mount this tape in the high speed reader with leader over the read sensors. (Leader has only the outside hole punched).

The basic steps are:

- Set 7777 on SR.
- Press ADDR LOAD.
- Set SR to 0010.
- Press EXT D ADDR LOAD.
- Press CLEAR/CONTINUE.

Full details on the use of the Cassette Handler are contained in the EE Department document "DUMpload".

CRASH RECOVERY PROCEDURES:

Various crash status' may occur depending on the machine and the extent of the problem. The basic idea is that if the loader necessary for recovery to the next higher level is intact, then there is no need to go further down the recovery procedure.

- MACHINE I:

Status DI: Simple loss of system but with DUMpload intact. Follow procedure given in REDIFAX #6.

Status CI: Loss of system including DUMpload, but with BIN LOADER intact. Locate the binary tape DUMpload and read in with procedure given in REDIFAX #8. Machine will then be in state DI.

Status BI: Loss of system including DUMpload and BIN LOADER, but with RIM LOADER intact. Locate the tape BINARY LOADER and read in with the procedure given in REDIFAX #9. Machine will then be in status CI.

Status AI: Total crash: Key in RIM LOADER as described in REDIFAX #9. Machine will then be in status BI.

- MACHINE II:

Status CII: Loss of system but BIN LOADER intact in Field I. Follow procedure given in REDIFAX #6.

Status BII: System and Field I BIN LOADER lost. Locate and read in the tape BINARY LOADER as per REDIFAX #9. Machine will then be in state CII.

Status AII: Total crash. Key in RIM LOADER as described in REDIFAX #9. Machine will then be in status BII.

USING THE BINARY LOADER:

Lo-Speed - (This description applies to all cases except the read-in of Machine II's system tape for which REDIFAX #6 applies).

- Place the binary tape in the low speed reader with leader (Only outside hole punched) on the read holes.
- Press START on reader.
- Set SR to 0000 and press EXTD ADDR LOAD.
- Set SR to 7777 and press ADDR LOAD.
- Press CLEAR & CONTINUE.

Paper Tape should read in, and halt in the trailer.

Hi-Speed - (Machine II only)

- Press binary tape in hi-speed reader with leader over the read holes.
- Set SR to 0010 and press EXTD ADDR LOAD.
- Set SR to 7777 and press ADDR LOAD.
- Set SR to 3777.
- Press CLEAR & CONTINUE.

Paper Tape should read in and halt in the trailer.

Note: For full details on use of binary loader see 'Introduction to Programming'.

ENTERING AND USING THE RIM LOADER:

The RIM LOADER is the 'last line of defense' in the sense that it is a very simple program which we can key in to read in a special format tape for a more powerful program (BIN LOADER).

Reading in the BIN LOADER tape with RIM:

- Locate the tape BINARY LOADER and mount on the low speed reader with leader (only outside hole punched) over the read holes.
- Set SR to 0000 for Machine I or 0011 for Machine II.
- Press EXT D ADDR LOAD.
- Set SR to 7756 and press LOAD ADDR.
- Set the low speed reader to START.
- Press CLEAR & CONTINUE

Tape should read in but does not come to a stop on its own.

Entering RIM LOADER:

Should the misfortune of a total system crash befall you:

- Set SR to 0000 for Machine I or 0011 for Machine II and press EXT D ADDR LOAD.
- Set SR to 7756 and press ADDR LOAD.
- Locate the plaque on the machine face labelled RIM LOADER and enter the octal code shown in the LOW column as follows:
  - (a) Set SR to given octal code.
  - (b) Lift DEPOSIT switch.
  - (c) Repeat at (c) until all code is entered.
  - (d) Check code by setting SR to 7756 and pressing LOAD ADDR.
  - (e) Set rotary switch to MD.
  - (f) Press EXAMINE; lower lights will display code in location one before location displayed on upper lights.
  - (g) Repeat (f) until all instructions are checked.
  - (h) If a discrepancy is found it is recommended that you start afresh.
  - (i) Read in the BINARY LOADER as detailed above.

<u>Feature</u>	<u>Machine I</u>	<u>Machine II</u>
Basic PDP8E	Yes	(N/A)
Extended Memory Unit	Yes	(DC 2X)
Memory Fields	4Fields: (0,1,2,3)	(DC 2X)
Real Time Clock (Lab Option)	Yes	(DC 13)
Analog/Digital Converter	2 Channels: (0,1)	(DC 53)
Digital/Analog Converters	2 Channels (1,2) (DC 55)	(DC 55,56)
ASR33 & KL8-EA Port (110 Baud)	Yes	(DC 03 & 04)
KL8-EC Port to TSS (300 Baud)	Yes	(DC 05 & 06)
High Speed Paper Tape	No	(DC 01 & 02)
Cassette System	Yes	(DC 70)
Extended Arithmetic Unit	Yes	(N/A)
Digital Buffered I/O	Yes	(DC 50)

**EE424 REDIFAX #10**  
**Machine configurations**  
**as of Jan 76**

\*Note: A/D converters are of different type in the two machines and are not completely software compatible.

Details of all devices contained in 'Small Computer Handbook'.

"DC" Device Code.

Yes  
 Yes  
 2Fields: (0,1)  
 Yes  
 \*16 Channels:  
 only 6 wired out (0 to 5)

12 Channels  
 only 6 wired out

(To be installed)

17 December 1975

REDIFAX #11

From: Major D. A. Wright  
To: All users of EE Dept Minicomputers

Subj: Mass data transfers to time share

1. A new system program is now available which facilitates large data transfers to TSS. This new program "CØRGØ" has two advantages over transfers using 8 SHARE. First, it moves data 33% faster; second, the resultant data file can be easily converted to a form amenable to processing under BASIC, by means of a subsidiary program "UNPACK." (These programs are available under the mini-lab's account number E02100 and are both saved public.)

2. Prior to moving data CØRGØ must be brought down to the PDP8 by 8 SHARE, (i.e./OLD\*E02100:CØRGØ/NPA/PUN/PAR 0). When ready to move the data a target file named "PUB" must be opened and readied, (i.e./OLD PUB/SCR/DIR). Time share will respond with (3) SPEAK! and wait for the data transfer to begin.

3. The parameters of the data transfer must be conveyed to CØRGØ as follows: Go to ØDT, (i.e., press CONTROL-SHIFT Ø) and enter the field, start location and end location for the data transfer in locations 2700-2702 respectively. The actual data transfer is then initiated by passing control to 2600: (i.e., 2600G), and proceeds at the rate of 20 PDP-8 words/second.

4. When the data transfer is complete CØRGØ will pass control to 8 SHARE (recognizable by a carriage return) and after a 10 second time-out, time share will respond "READY." Don't touch the keyboard during time-out, as anything typed will be appended to the transfer.

5. The resultant file (.RESULT.) should be converted to Random Access Numeric format by the following steps:

STR RAN 12  
/SAV/ØLD UNPACK/RUN.

Upon completion the file PUB will contain one entry for each word of core transferred and will be unsigned (i.e., 4000 thru 7777 octal will show up as 2048 thru 4095). If signed numbers are desired, the sign can be easily restored in any program which processes the file.

6. If you want to preserve the data long-term, be sure to get it into another file, else the next usage of PUB will destroy it.

7. Note that CØRGØ only passes full pages of core, regardless of the start and end locations. That is, the transfer starts at the first location of the page containing the start address and ends on the last location of the page containing the end address.

**UNCLASSIFIED**

Security Classification

**DOCUMENT CONTROL DATA - R & D**

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author)		2a. REPORT SECURITY CLASSIFICATION	
U.S. Naval Academy, Annapolis.		<b>UNCLASSIFIED</b>	
2b. GROUP			
3. REPORT TITLE			
The electron spin resonance determination of site populations in erbium doped calcium fluoride.			
4. DESCRIPTIVE NOTES (Type of report and inclusive dates)			
Research report.			
5. AUTHOR(S) (First name, middle initial, last name)			
Danny Hilton Mills.			
6. REPORT DATE		7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
3 June 1976.		127	20
8a. CONTRACT OR GRANT NO.		9a. ORIGINATOR'S REPORT NUMBER(S)	
b. PROJECT NO.		U.S. Naval Academy, Annapolis - Trident Scholar project report, no. 80 (1976)	
c.		9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)	
d.			
10. DISTRIBUTION STATEMENT			
This document has been approved for public release ; its distribution is UNLIMITED.			
11. SUPPLEMENTARY NOTES		12. SPONSORING MILITARY ACTIVITY	
		U.S. Naval Academy, Annapolis.	
13. ABSTRACT			
<p>The populations of erbium ions in the tetragonal, cubic, and trigonal sites in CaF<sub>2</sub> crystals were measured for concentrations of .01 o/o, .03 o/o, .1 o/o, and .3 o/o erbium in CaF<sub>2</sub> crystals.</p> <p>Experimental results show that the relative population of erbium ions in the cubic (quasi-cubic or perhaps aggregate) site increased as the concentration of total erbium ions increased while the relative site population in the tetragonal site decreased with increasing erbium ion concentration. The relative population in the trigonal site increased slightly from the .01 o/o to the .1 o/o concentration, then decreased in the .3 o/o concentration.</p> <p>Electron spin resonance techniques were used to obtain the absorption resonance characteristics of CaF<sub>2</sub>:ER<sup>(3+)</sup> in the different sites. The relative populations were determined as a function of total concentration of erbium ions. The doped crystals were maintained at liquid helium temperature (4.2K) and spin resonance spectra taken as a function of azimuthal angle of the DC magnetic field with respect to the [110] axis of the crystal in order to determine the symmetry and thus identify the site.</p> <p>The data was then recorded for selected lines, digitized and processed in a PDP-8 minicomputer. The data was sent into a file in the Honeywell 635 computer and received additional processing using the APL language in order to arrive at the site population figures.</p> <p>The data and all informations gained included in the paper.</p>			