# FOURIER SPECTROSCOPY

IN THE FAR INFRARED

#### by

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PHYSICS

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#### ABSTRACT

An infrared Fourier spectrophotometer has been set up in the solid state labaratory of the University of British Columbia.

A cryostat has been built and adapted to the spectrometer.

A computer program to analyze the data and plot the spectrum has been written.

As a demonstration of the system's capability, the transmission spectrum from 40 cm<sup>-1</sup> to 330 cm<sup>-1</sup> of boron doped silicon was obtained for the sample at liquid helium temperature. This spectrum was compared to earlier work done by Colbow in the region 240 cm<sup>-1</sup> to 330 cm<sup>-1</sup>.

A spectrum of boron and indium doped silicon was investigated in the hope of finding B<sup>-</sup> and In<sup>+</sup> ionized centres. These were not found at the impurity concentrations and temperatures used.

A transmission spectrum of intrinsic silicon at liquid helium temperature was obtained for the region  $40 \text{ cm}^{-1}$  to 330 cm<sup>-1</sup>.

A comparison of the above spectra suggests that the low energy tail of the boron doped and boron and indium doped samples is due to a frequency dependant value of reflectivity as is seen from the spectrum for intrinsic silicon.

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# SECTION I

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#### INTRODUCTION

## 1. Spectroscopy in the Far Infrared

The infrared region of the electromagnetic spectrum is subdivided into the near (500 cm<sup>-1</sup> to 12,500 cm<sup>-1</sup>), mid (200 cm<sup>-1</sup> to 500 cm<sup>-1</sup>) and far (10 cm<sup>-1</sup> to 200 cm<sup>-1</sup>) infrared regions.

Photographic methods, whereby the spectrum is spacially dispersed and the effect on a photographic film is studied, is prohibited in most of the infrared spectrum. The reason for this is the lack of a photographic film or other similar device which is sensitive to wavelengths longer than 1 micron.

For optical studies in the infrared, there are several spectographic means available. These are the conventional prism and grating spectrometers and also interferometric spectrometers, such as those employing a Fabry-Perot or a Michelson interferometer.

2. Advantages and Disadvantages of a Michelson Interferometer

In the infrared spectral region, the conventional spectrometer generally employs a grating rather than a prism, since a significantly greater flux and resolving power may be obtained. In the far infrared, the lack of materials with high dispersive powers dictates the use of gratings as the dispersive element.

A disadvantage associated with gratings is the presence of other overlapping orders of diffraction. The optical filtering required to eliminate these also reduces the intensity of useful radiation. This becomes a decided disadvantage in the energy limited far infrared.

In the infrared spectral region, detector noise is usually very much greater than any other source of noise. This type of noise is of a random nature and is essentially independent of the signal level.

For the same resolving power, the amount of radiation admitted by the slit of a grating spectrometer is much less than for a Michelson, Fabry-Perot, or lamellar grating spectrometer. In the infrared spectral region, we can increase the overall S/N (signal to noise) ratio by using one of the above interferometric spectrometers, since the detector noise does not increase appreciable when the amount of radiation falling on the detector is increased. This is known as the Jacquinot advantage.

If N spectral elements are observed in a time interval T, then the grating or Fabry-Perot spectrometer samples each element for a time, t = T/N. When a Michelson interferometer is employed, the full time of observation is afforded each spectral element. For random noise, such as that which is characteristic of infrared detectors, this means an increased S/N ratio by a factor of  $\sqrt{N}$ . This advantage was first pointed out by Fellgett<sup>1</sup> and is now referred to as Fellgett's advantage.

In order to double the resolution of the Michelson interferometer, we must double the maximum displacement of the moveable mirror. If we wish to retain the same S/N ratio, then the time required to sample the spectrum must be twice

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as long. To double the resolution using a grating spectrometer, both entrance and exit slit widths must be halved. The flux of radiation available to the detector is then  $\frac{1}{4}$ of the original value. For a detector signal which is time integrated, the pure signal varies proportional to the time and any random noise signal varies proportional to the square root of the time. To retain the same S/N ratio would then require a time 16 times greater than the original spectrum.

For high resolution or for obtaining a spectrum over a large range of frequencies where the intensity is low, the Michelson interferometer is of particular use. It does have the drawback that it requires the use of a computer to do the Fourier transforms. When computing facilities are available, the Michelson interferometer is a particularly good instrument to cover the far and mid infrared regions.

3. Other Interferometric Spectrometers

Closely related in principle to the Michelson interferometer is the interferometric modulator<sup>2</sup>, which employs a lamellar grating with a variable depth. Because of mechanical difficulties, this type of interferometer is generally used in the long wavelength regions.

The SISAM<sup>3</sup> (Spectrometre Interferential à Selection par l'Amplitude de Modulation) is essentially a Michelson interferometer in which the mirrors are replaced by gratings. These gratings are inclined at equal angles to the radiation incident from the beam splitter. This method scans selectively through the spectrum and does not, therefore, possess the Fellgett advantage.

4. History and Use of the Michelson Interferometer in the Infrared

The Michelson interferometer was first developed and used by Michelson around the turn of the century. The work carried out by Michelson was in the visible region of the electromagnetic spectrum.

The first application of the Michelson interferometer to infrared spectroscopy was by Rubens and Wood in 1911.

A further brief history of the use of the Michelson interferometer for spectroscopic studies in the infrared spectral region is given by Jacquinot<sup>3</sup>.

The developmental work on the Michelson interferometer as applied to infrared spectroscopy was carried out at four major centres: National Physics Laboratory, Teddington, Middlesex, U. K.; Johns Hopkins University, Baltimore, Maryland, U.S.A.; Université de Paris, Paris, France; and C.N.R.S. (Centre National de la Recherche Scientifique), Bellevue, France.

This type of instrument is used for research in a wide variety of chemical and physical studies in the infrared. Some of the types of studies where it is employed are: lattice vibrations, magnetic resonance, superconductivity, astronomy, optical constants, electronic effects in semiconductors, meteorology, molecular spectroscopy, and the study of plasmas.

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## SECTION II

## THEORY OF THE MICHELSON INTERFEROMETER

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1. The Interferogram Function

Consider a monochromatic plane wave normally incident upon an ideal Michelson interferomenter, operating in a vacuum.



Figure 1. Michelson Interferometer

When the two mirrors are equidistant from the beam splitter, there is no phase difference between the two beams upon recombining. This position of mirror M2 is designated as the zero path difference (x = 0) and all path differences, which are twice the mirror displacement from zero path difference, are measured with respect to this origin.

If:

- t = the transmission coefficient of the beam
   splitter
- r = the reflection coefficient of the beam splitter
- R = the reflection coefficient of mirrors M1 and M2

then, upon recombining, the electric vector is of the form:  $|\vec{E}| = (rtRE_o)(cos(wt-2\pi ka) + cos(wt-2\pi k(a+x)))$  $= (rtRE_o)Re(exp(i(wt-2\pi ka))(exp(-i2\pi kx) + 1))$  (1) Let us consider a plane polarized monochromatic plane wave for which  $|\vec{E}| = |\vec{H}|$  and  $\vec{E} \perp \vec{H}$ .

The intensity of an electromagnetic wave is given by the time average of the Poynting vector,  $\overrightarrow{S}$ . We therefore have:

 $I = \langle S \rangle_{t} = (c/8\pi) (\vec{E}x\vec{H}^{*}) = (c/4\pi) (rtRE_{o})^{2} (1 + cos(2\pi kx))$ (2)

We now consider an unpolarized plane wave which will have different coefficients of reflection and transmission for the sigma and pi polarizations at the beam splitter. The reflection coefficients for the mirrors M1 and M2 are the same for each polarization since the wave is normally incident.

Allowing also the wave to be heterochromatic with a spectral distribution of intensities which is not constant, then E will vary with frequency. In general, the product (rtR) may also be frequency dependent. We therefore write:

$$(c/4\pi)(rtRE_{o})_{\pi}^{2} + (c/4\pi)(rtRE_{o})_{\sigma}^{2} = I(k)$$
(3)
We then have, for any path difference x:

We then have, for any path difference x:

$$I(x) = \int_{0}^{\infty} I(k)(1 + \cos(2\pi kx))dk = \int_{0}^{\infty} I(k)dk + \int_{0}^{\infty} I(k)\cos(2\pi kx)dk$$

$$For \ x = 0, we have:$$

$$I(0) = 2\int_{0}^{\infty} I(k)dk$$
(5)

and for  $x = \infty$  we have:

$$I(\sim) = \int I(k) dk$$
 (6)

Equation 6 is derived from equation 4 when the cosine term goes to zero. This follows, since for very large values of x, cos  $2\pi kx$  is a very rapidly varying function of k and the average value of  $I(k)\cos 2\pi kx$  over any cycle will be zero.

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From equations 4 and 6, we have:  $I(x) = I(-) + \int_{0}^{\infty} I(k) \cos(2\pi kx) dk$ (7) From equations 5 and 6:

$$I(\boldsymbol{\omega}) = \frac{1}{2}I(0) \tag{8}$$

We may define a function:

$$F(x) = I(x) - \frac{1}{2}I(0) = I(x) - I(\infty) = \int_{0}^{\infty} I(k)\cos(2\pi kx) dk$$
(9)

In applying the interferometer to spectroscopy, filters are applied, so that I(k) = 0 for  $k \ge K$ , where K is the maximum wave number of interest. We therefore have:

$$F(x) = \int_{0}^{K} I(k) \cos(2\pi kx) dk$$
(10)

In practice, the ideal and perfectly aligned interferometer is not realized. As a consequence, there is an additional phase difference,  $\mathscr{O}(k)$ , introduced. Therefore:

$$F(x) = \int_{\kappa} I(k)\cos(2\pi kx - \phi) dk$$

$$= \int_{\kappa} I(k)\cos\phi\cos(2\pi kx) dk + \int_{\kappa} I(k)\sin\phi\sin(2\pi kx) dk$$
(11)

### 2. Fourier Transforms

The exponential Fourier transform is defined by:

$$g(k) = \int_{\infty}^{\infty} f(x) \exp(i2\pi kx) dx$$
(12)

$$= \int_{\infty} f(x) \cos(2\pi kx) dx + i \int_{\infty} f(x) \sin(2\pi kx) dx$$
 (12a)

The inverse transform is given by:

$$f(x) = \int_{\infty}^{\infty} g(k) \exp(-i2\pi kx) dk$$
(13)  
=  $\int_{\infty}^{\infty} g(k) \cos(2\pi kx) dk - i \int_{\infty}^{\infty} g(k) \sin(2\pi kx) dk$ (13a)

If f(x) is an even function, that is f(-x) = f(x),

then from 12a we have that:

$$(k) = \int_{\infty}^{\infty} f(x)\cos(2\pi kx) dx = 2 \int_{0}^{\infty} f(x)\cos(2\pi kx) dx$$
(14)

This is referred to as the Fourier cosine transform.

Likewise, is f(x) is an odd function of x, that is,

f(-x) = -f(x), then:

$$g(k) = i \int_{\infty} \tilde{f}(x) \sin(2\pi l \alpha) dx = 2i \int_{\Omega} \tilde{f}(x) \sin(2\pi l \alpha) dx$$
(15)

This is called the Fourier sine transform with a multiplying factor of 1.

We may write equation 12a as: g(k) = c(k) + i s(k), where c and s refer to the cosine and sine transforms respectively.

Tables of calculated Fourier transforms may be found in Cambell and Foster<sup>4</sup> or Bateman<sup>5</sup>.

3. Calculating the Spectrum

If we consider F(x) as the function f(x) in a Fourier transform, then from equation 11:

$$c(k_{1}) = \int_{\infty}^{\kappa} F(x)\cos(2\pi k_{1}x) dx$$

$$= \int_{0}^{\kappa} I(k)\cos\phi \{\int_{\infty}^{\infty} c \tilde{o} s(2\pi k_{1}x)\cos(2\pi kx) dx\} dk$$

$$+ \int_{0}^{\kappa} I(k)\sin\phi \{\int_{\infty}^{\infty} c \tilde{o} s(2\pi k_{1}x)\sin(2\pi kx) dx\} dk$$
(16)

$$\int_{-\infty}^{\infty} \cos(2\pi k_{1}x) \cos(2\pi k_{2}x) dx$$
  
=  $\frac{1}{2} \int_{-\infty}^{\infty} (\exp(i2\pi (k + k_{1})x) + \exp(i2\pi (k - k_{1})x))$   
=  $\frac{1}{2} (\delta(k + k_{1}) + \delta(k - k_{1}))$  (17)

where  $\delta$  is the Dirac delta function, and is defined by:

Wo oloo

$$\delta(k + L) = \int_{\infty}^{\infty} \exp(i2\pi(k + L)x) dx$$
(18)

$$\int_{\infty} \cos(2\pi k_1 x) \sin(2\pi k_2) dx = 0$$
(19)

since the integrand is an odd function of x.

Therefore:  

$$c(k_{1}) = \frac{1}{2} \int_{0}^{1} I(k) \cos \phi \left\{ \delta(k + k_{1}) + \delta(k - k_{1}) \right\} dk$$

$$= \frac{I(k_{1})}{2} \cos \phi$$
(20)

since I(k) = 0 for  $k \ge K$  and we also have  $k = \frac{1}{\lambda} \ge 0$ .

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Similarly:

$$S(k_1) = (I(k_1)/2) \sin \phi$$
 (21)  
Thus:

$$\left|g(k_{1})\right| = (c^{2}(k_{1}) + s^{2}(k_{1}))^{\frac{1}{2}} = \frac{1}{2}I(k_{1})(\sin^{2}\phi + \cos^{2}\phi)^{\frac{1}{2}}$$
(22)

and then:

$$I(k_{1}) = 2 |g(k_{1})| = 2(c^{2}(k_{1}) + s^{2}(k_{1}))^{\frac{1}{2}}$$
(23)

If we are only interested in relative intensities, we may drop the factor of 2 and write:

$$I(k_{1}) = (c^{2}(k_{1}) + s^{2}(k_{1}))^{\frac{1}{2}}$$
(2<sup>*L*</sup>)

If the interferogram function, F(x), is symmetric about x = 0, that is,  $\mathscr{O}(k) = 0$ , then:

$$S(k) = 0$$
 and  $I(k) = C(k)$  (25)

In this case, it would only be necessary to record I(x)on one side of the zero path difference. In the case when  $\emptyset(k) \neq 0$ , it would also be possible to obtain all the necessary information by recording one side only, if we knew the exact position of the zero phase difference.

## 4. Finite Integration Limits

In practice, the interferogram is obtained over a limited range of path differences. The range of the integration limits then becomes  $\pm X$ , rather than  $\pm \infty$ , where  $\pm X$  is the maximum positive and negative path difference.

To examine the effect of the finite integration limits, we consider the case of a monochromatic plane wave of wave number  $k_1$  in an ideal interferometer.

From equation 9, therefore:  $F(x) = I(k_1)\cos(2\pi k_1 x)$ 

(26)

The Fourier transform of F(x) over the finite range

of x may be written as:

T(x) = 0

= 1

$$\int_{\infty}^{\mathbf{I}(\mathbf{k}_{1})\cos(2\pi\mathbf{k}_{1}\mathbf{x})\exp(i2\pi\mathbf{k}\mathbf{x})\mathbf{T}(\mathbf{x})d\mathbf{x}}$$

where:

 $\begin{array}{l} |\mathbf{x}| > \mathbf{X} \\ |\mathbf{x}| \leq \mathbf{X} \end{array}$ 

(27)

We now make recourse to the convolution theorem, which may be stated as follows:

The Fourier transform of the product of two functions, f(x) and g(x) is the convolution of their transforms F(y)and G(y), where the convolution is defined by:

$$F \star G = \int_{X} G(t)F(y - t)dt$$
The Fourier transform of T(x) is:  

$$\int_{X} T(x)\exp(i2\pi kx)dx = \int_{X} \exp(i2\pi kx)dx$$

$$= \int_{X} (\cos(2\pi kx) + i\sin(2\pi kx))dx = \left(\frac{\sin(2\pi kx)}{2\pi k} - \frac{i\cos(2\pi kx)}{2\pi k}\right) \Big|_{-X}^{X}$$

$$= \frac{2\sin(2\pi kx)}{2\pi k}$$
(29)

The Fourier transform of F(x) is:

$$\int I(k_{1})\cos(2\pi k_{1}x)\exp(i2\pi k_{x})dx$$

$$= \frac{1}{2} \int I(k_{1})(\exp(i2\pi k_{1}x) + \exp(-i2\pi k_{1}x))\exp(i2\pi k_{x})dx$$

$$= \frac{1}{2} \int I(k_{1})(\exp(i2\pi (k + k_{1})x) + \exp(i2\pi (k - k_{1})x))dx$$

$$= \frac{1}{2} I(k_{1})(\delta(k + k_{1}) + \delta(k - k_{1}))$$
(30)

The convolution of the transforms is then:  $\int_{0}^{\infty} \left( \frac{1}{2} \left( \frac{1}{2} \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \left( \frac{1}{2} \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \right) \left( \frac{1}{2} \left( \frac{1}{2} \left( \frac{1}{2} \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \right) \left( \frac{1}{2} \left( \frac{1}{2} \left( \frac{1}{2} \right) \left( \frac{1}{2} \left( \frac{1}{2} \right) \right) \left( \frac{1}{2} \left( \frac{1}{2} \left( \frac{1}{2} \left( \frac{1}{2} \right) \right) \left( \frac{1}{2} \left( \frac{$ 

$$\int_{\infty}^{2} \left( \frac{\sin(2\pi t X)}{2\pi t} \right) \left( \frac{1(k)}{2} \frac{1}{2} \left( \delta(k + k) - t \right) + \delta(k - k) - t \right) dt$$

$$= I(k_1) X \frac{\sin(2\pi (k + k)) X}{2\pi (k + k) X} + \frac{\sin(2\pi (k - k)) X}{2\pi (k - k) X}$$
(31)
The maximum value of the function  $\frac{1 \sin \theta}{2\pi (k - k)}$  is unity

and occurs when  $\Theta = 0$ . If  $\Theta = 2 \pi (k - k_1) X$ , then the

**~**⊥∨**~** 

maximum occurs at  $k = k_1$ .

If we now consider the contribution to the spectrum from the term  $\Theta = 2\pi(k_1 + k)X$ , we find that its maximum value occurs for  $k = -k_1$ . This is not a physically realizable situation since  $k = \frac{i}{\lambda} \ge 0$ . We may see a small contribution from values of  $k \ge 0$ , but these will be negligible for  $k_1$ greater than 10 cm<sup>-1</sup>. We see this by considering the maximum value of  $\frac{\sin 2\pi(k_1 + k)X}{2\pi(k + k_1)X} \le \frac{1}{2\pi(k + k_1)X}$ , for positive values of k. For  $k = k_1 = 10$  cm<sup>-1</sup>, we have a maximum value for this term of  $\frac{1}{40\pi X}$ . Even for an extremely small value of X, such as 1 cm, we still only have  $\frac{1}{4\pi}$  which is small in comparison to unity, the contribution of the other term. The effect of this term becomes even less important as k and/or  $k_1$  increases.

The monochromatic line is thus spread out and its frequency spectrum is modulated by  $\frac{\sin \Theta}{\Theta}$ , where  $\Theta = 2\pi (k - k_1)X$ .

This function is referred to as the spectral window. The form of this function is shown by curve a in Figure 2.



curve a  

$$n = 1$$

$$e = 2\pi (\ell - \ell) \chi$$
curve b  

$$n = 2$$

$$e = \pi (\ell - \ell) \chi$$

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#### 5. Apodization

The form of the spectral window may be modified by using a different truncating function,  $T^{1}(x)$ . This amounts to multiplying F(x) by another function before multiplying by T(x), that is:  $\int_{exp(i2\pi kx)(F(x)G(x))T(x)dx} = \int_{exp(i2\pi kx)F(x)T^{1}(x)dx} (22)$ 

where  $T^{1}(x) = G(x)T(x) = G(x)$   $|x| \le X$ = 0 |x| > X

This process is called apodization and its use can result in the reduction of the height of the side lobes, at the cost of a reduction in resolution.

A common apodization function is given by:

$$\Gamma^{1}(x) = 0 |x| \ge X$$
  
=  $1 - \frac{|x|}{X} x \le X$  (33)

(32)

The spectral window is given by  $F(k) \times T^{\perp}(k)$ .

The Fourier transform of  $T^{1}(x)$  is:  $\int_{X} (1 - ix) \exp(i2\pi ix) dx = 2 \frac{\sin(2\pi ix)}{2\pi ix} - \frac{1}{X} \int_{X} \cos(2\pi ix) dx$   $= 2 \frac{\sin(2\pi ix)}{2\pi ix} - \frac{2}{X} \left( \frac{x \sin(2\pi ix)}{2\pi ix} + \frac{\cos(2\pi ix)}{(2\pi ix)^{2}} \right) \Big|_{0}^{X}$ 

$$= 2(\frac{1 - \cos(2\pi kX)}{(2\pi k)^{2}X}) = \frac{4X \sin^{2}(2\pi kX)}{(2\pi k)^{2}X^{2}} = X \left(\frac{\sin(\pi kX)}{\pi kX}\right)^{2}$$
(34)

If F(x) is as before, then:  $F(k) \star T^{1}(k) = \int_{-\infty}^{\infty} \frac{\left(\sin(\pi kX)\right)^{2}}{(\pi kX)^{2}} \left(\frac{I(k_{1})}{2} \left(\delta(k + k_{1} - t) + \delta(k - k_{1} - t)\right) dt$   $\approx \frac{I(k_{1})X}{2} \left(\frac{\sin(\pi(k - k_{1})X)}{(\pi k - k_{1})X}\right)^{2}$ (35)

where the term  $\left(\frac{\sin\Theta}{\Theta}\right)^2$  for  $\Theta = \pi (k + k_1)X$  is negligible as before.

The form of this spectral window is shown by curve

#### b of Figure 2.

Gebbie and Twiss<sup>6</sup> have shown that this has the effect of reducing the side bands to approximately 5% of the height of the main peak, as compared to 15% for the original spectral window.

It will be noted that, for the apodization function given above, the height of the main peak is reduced by a factor of 2. If the sample spectrum is to be ratioed with a reference spectrum, then the intensities obtained are not affected, other than a broadening of the bands. The integrated intensity over a band should remain the same.

6. Maximum Path Difference Limitations on Resolution

The resolution of an optical instrument is its ability to dinstinguish between two spectral lines which are close together. The minimum separation of two lines of equal intensity which can be distinguished is called the resolution.

The most common method of calculating the theoretical resolution of an instrument is to consider two monochromatic lines. For curves a and b of Figure 2, Jacquinot<sup>3</sup> defines the resolution as the distance between the first two zeros. For the unapodized case (curve a), the resolution is the 1/2X. For the apodized case (curve b), the resolution is given by 1/X.

Martin<sup>7</sup> points out that this is somewhat naive, since in practice we never deal with pure monochromatic spectral lines, but a distribution of frequencies about a central peak value. Martin chooses a Gaussian distribution  $e^{-b(k_1-k)^2}$  for which the interferogram would be  $B e^{-\pi^2 x^2/b} \cos_2 \pi k_i x_j$ , where b and B are constants.

We now consider two such peaks, of equal intensity and of half-width w, which are separated by w. We find that the sum of the intensities is a doublet (Figure 3), which suffers a dip of approximately 7.3% at the mid-point between the two peaks.

Figure 3. Resolution for a Gaussian Distribution

The half-width is given by  $w = (2.77/b)^{\frac{1}{2}}$ . We see that the envelope of the interferogram will be reduced to  $e^{-\pi^2/2.77} = .028$  when x = 1/w and decreases rapidly as x increases. If we obtain the interferogram up to x = 1/w, the calculated spectrum is essentially the same as the true spectrum, since the contribution, to the transform, from x = 1/w to  $\infty$  is negligible. Martin quotes a value of 5% for the dip under this condition, which is still sufficient for the two peaks to be distinguished.

The value obtained for the resolution using the above condition is given by:

 $w = 1/\chi$ 

(36)

In the case where the apodization function discussed earlier is used, the resolution is given by  $\sqrt{2}/X$ .<sup>8</sup>

If we are looking at broad band spectra, for which the width of the spectral line is much larger than the resolution, we see from the above that we do not have the problem of side lobes in the transformed spectra. In this case, there is then no need to apodize.

7. Admission Angle and Resolving Power

Until now, we have only considered a plane wave which is normally incident upon the interferometer. We now consider the effect of a plane wave incident at an angle  $\Theta$ .

The optical arrangement being considered is shown in Figure 4.



Figure 4. Michelson Interferometer

For the purpose of calculating the path differences between rays 1 and 2, the optical system may be considered as shown in Figure 5.

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x = 2d;  $b \cos \Theta = d$ ;  $b \sin \Theta = a/2$ ;  $a \sin \Theta = c$ Figure 5. Equivalent Ray Diagram for the Interferometer

The path difference between rays 1 and 2 is given

$$p.d. = 2b - c = 2b - asine = 2b - 2bsin^{2}e$$
$$= 2(d/cose)(1 - sin^{2}e) = 2dcose$$
(37)

For a monochromatic plane wave incident at angle  $\Theta$  we then have:

$$F(x) = I(k_1) \cos(2\pi k_1 x \cos \theta)$$

by:

The Fourier transform of F(x) is given by:

$$g(k) = \int_{-\infty}^{\infty} F(x)T(x)\exp(i2\pi kx)dx$$

$$= G(k) + t(k) \text{ where } G(k) \text{ and } t(k) \text{ are the Fourier}$$
(38)

transforms of F(x) and T(x) respectively.

Now:  

$$G(k) = \int_{\infty} \widetilde{I(k_1)} \cos(2\pi k_1 \cos \Theta x) dx$$

$$= \underbrace{I(k_1)}_{2} \int_{\infty} (\exp(i2\pi k_1 \cos \Theta x) + \exp(-i2\pi k_1 \cos \Theta x)) \exp(i2\pi kx) dx$$

$$= \underbrace{I(k_1)}_{2} (\delta(k + k_1 \cos \Theta) + \delta(k - k_1 \cos \Theta))$$
(39)

For a uniformly radiating disc of solid angle  $\mathcal{L}$ , the contribution from various angles of incidence between  $\Theta$  and  $\Theta + d\Theta$  is proportional to the corresponding

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solid angle  $d \mathcal{L} = 2\pi \sin \Theta d\Theta = -2\pi d(\cos \Theta)$ .

We now consider a source such as described above, when used with the Michelson interferometer. Then:

 $cose = cose_{m}$   $G(k) = AI(k_{1}) \int (\delta(k + k_{1} cose) + \delta(k - k_{1} cose)) d(cose)$   $= A I(k_{1}) \text{ if } k = \pm k_{1} cose$ for some cose' such that  $0 \le cose \le cose' \le 1$ 

(40)

= 0 otherwise

where A = constant $\Theta_m$  corresponds to the total solid angle  $\Lambda$ 

As before, we will neglect k < 0.

G(k) is then a step function, having a constant, non-zero value for  $k_1 \cos \Theta_m \le k \le k_1$ , and zero otherwise.

Neglecting the effect of finite integration limits and considering only small values of  $\Theta$ , we now consider the resolution of two frequencies with wave numbers  $k_1$  and  $k_2$ . G(k) is shown in Figure 6, for two elements which are easily resolved.



Figure 6. Angular resolution

To be resolved,  $k_2 \cos \bigoplus_m$  must be greater than k1. For calculation purposes, we may assume that they are just resolved when  $k_2 \cos \bigoplus_m = k_1$ . Then:

 $\Delta k = k_2 - k_1 = k_1 (1/\cos \theta_m - 1) = k_1 (1 - \cos \theta_m)$ 

The resolving power is defined  $as^{m}R = k/\Delta k$ , where k is the average value of the wave numbers of the two frequencies just resolved. Thus:

$$k = \frac{k_1 + k_2}{2} = \frac{k_1}{2} \frac{(1 + \cos \Theta_m)}{\cos \Theta_m} \text{ and}$$
$$R = \frac{1 + \cos \Theta_m}{2(1 - \cos \Theta_m)} \simeq \frac{1}{1 - \cos \Theta_m} \text{ for small } \Theta_m.$$

Now:

Therefore, we have the result which Jacquinot  $^{2}$ 

gives, that is:

 $R \int = 2TT$ 

(42)

## 8. Resolution

There are two factors which govern the resolution, namely the maximum path difference and the admission angle. The true resolution will be less than the sum of these resolutions calculated independently of each other and greater than either of them individually. The admission angle is chosen such that the resolution calculated for the maximum wave number of interest is less than the resolution determined by the maximum path difference. The resolution is then within a factor of 2 as calculated using the maximum path difference.

If we consider a monochromatic source with an admission angle which allows a maximum angle of incidence onto the interferometer of  $\Theta_m$ , then:

 $F(x) \sim \int_{k_1 \cos \theta_m} \cos(2\pi kx) dk = \frac{1}{2\pi x} (\sin(2\pi k_1 x) - \sin(2\pi k_1 \cos \theta_m x))$ 

$$= \frac{1}{\pi x} \left\{ \cos\left(\frac{2\pi k_{1}x}{2} + \frac{2\pi k_{1}\cos\theta}{2}\right) \sin\left(\frac{2\pi k_{1}x}{2} - \frac{2\pi k_{1}\cos\theta}{2}x\right) \right\}$$

$$\approx \left\{ 1/(\pi x) \right\} \left\{ \cos\left(2\pi k_{1}x\right) \sin\left(\frac{\pi k_{1}x\theta^{2}}{2}\right) \right\}$$
(43)
for  $\Theta_{m}$  small.

Since the arguement of the cosine term is larger than the arguement of the sine term, we have a cosine variation which has an envelope of  $\frac{1}{11 \text{ x}} \sin \frac{\pi \text{ k}_1 \text{ x} \Theta_m^2}{2}$ This envelope tends to zero as x tends to  $\frac{2}{\text{k}_1 \Theta_m^2}$ . Since we have  $R = \frac{k}{\Delta \text{ k}} = \text{kX}$  and  $\Lambda = 2\pi(1 - \cos \Theta_m) \approx \pi \Theta_m^2$  then  $R \Omega = \text{kX} \pi \Theta_m^2 = 2\pi$  and  $X = 2/(\text{k}\Theta^2)$ 

We see that for a given wave number, the resolution as defined by 1/X is limited by the choice of the admission angle.

The theoretical resolution is not always realized in practice. When the fluctuations in F(x) become comparable to the noise, then it is useless to sample the interferogram beyond this value.

For high resolution, the admission angle must be reduced, hence reducing the amount of radiation available. In the case of strong absorption or reflection, the S/Nratio may be such that it dictates that the sampling of the interferogram be terminated. It is then the S/Nratio which limits the resolution attainable.

9. False Energies

In order to be able to calculate the intensity at the maximum frequency of interest, we must sample at least twice per cycle. In the spacial variation, this means:

 $(2\pi kx' - 2\pi kx) = \Pi$ ; that is, 24x = 1/K (44) where  $\Delta x$  is the spacial sampling interval and K is the

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maximum frequency of interest.

The effect of digitization is that the integrals must be approximated by sums, that is:

$$\begin{aligned} (k_{i}) &= \sqrt{F(x)}\cos(2\pi k_{i}x)dx \approx \frac{1}{2}(F(0) + F(\Delta x)\cos(2\pi k_{i}\Delta x))\Delta x \\ &+ \frac{1}{2}(F(\Delta x)\cos(2\pi k_{i}\Delta x) + F(2\Delta x)\cos(2\pi k_{i}2\Delta x))\Delta x + \cdots \\ &+ \frac{1}{2}(F((N-1)\Delta x)\cos(2\pi k_{i}(N-1)\Delta x) + F(N\Delta x)\cos(2\pi k_{i}N\Delta x))\Delta x \\ &+ \frac{1}{2}(F(0) + F(-\Delta x)\cos(2\pi k_{i}\Delta x))\Delta x + \cdots \\ &+ \frac{1}{2}(F(-(N-1)\Delta x)\cos(2\pi k_{i}(N-1)\Delta x) + F(-N\Delta x)\cos(2\pi k_{i}N\Delta x)\Delta x \end{aligned}$$

$$= \Delta x \left( F(0) + \left( \frac{F(N\Delta x) + F(-N\Delta x) \right) \cos(2\pi k_{1} N\Delta x)}{2} + \sum_{m=1}^{N-1} \left( \frac{F(m\Delta x) + F(-m\Delta x)}{2} \right) \sin(2\pi k_{1} M\Delta x) \right)$$

$$(45)$$

and similarly:

$$s(k_{i}) = \Delta x \left\{ \frac{(F(N\Delta x) - F(-N\Delta x))sin(2\pi k_{i}N\Delta x)}{2} + \sum_{m=1}^{N-1} \frac{(F(m\Delta x) - F(-m\Delta x))sin(2\pi k_{i}m\Delta x)}{2} \right\}$$

$$+ N\Delta x = \pm X.$$

$$(4.6)$$

where

Because of the finite sampling interval and consequent approximation of the integrals by sums, there are "false energies" introduced at ki due to radiation with frequencies greater than K and equal to  $2nK - k_1$  and  $2(n - 1) K - k_1$ where  $n \ge 1$  and is integral.

This may be seen from the following:

(47)  $2\pi(2nK - k_i)m\Delta x = 2\pi mn - 2\pi k_im\Delta x$ since  $K = \frac{1}{2}(\frac{1}{2}x)$ .

#### Therefore:

 $\cos(2\pi(2nK - k_i)max)I(2nK - k_i)$  $= I(2nK - k_i)(\cos(2\pi mn) + \cos(2\pi k_i m \Delta x))$ =  $I(2nK-k_i)(1 + \cos(2\pi k_i max))$  $=I(2nK - k_i) + I(2nK - k_i)\cos(2\pi k_i m \Delta x)$ 

(48)

Thus, upon Fourier analysis, this radiation of higher frequencies becomes indistinguishable from that of  $k_1$  and these terms will contribute to the calculated values of  $c(k_1)$  and  $s(k_1)$ .

In order to eliminate these false energies, it is necessary to reduce I(k) to zero for  $k \ge K$ .

# SECTION III.

#### INSTRUMENTATION OF THE SPECTROMETER

1. The Spectrometer

The spectrometer used for the work in this thesis is a FS-720 Fourier spectrophotometer, employing a stepping motor drive. The unit is manufactured by Beckman RIIC Limited. A ray diagram for the instrument, taken from the instruction manual, is given in Figure 7.

In order to eliminate water vapour absorption of the infrared radiation, the spectrometer is held under a vacuum during the course of an experiment. The vacuum is produced using a Precision Scientific model 150 pump, rated at 150 litres/minute free air displacement. This produces an ultimate vacuum of approximately 10 microns after one hour of pumping. A cold trap is incorporated into the pumping line to prevent back streaming of oil vapour from the pump, since it is extremely important that oil, which absorbs very strongly, does not collect on the optical components of the spectrometer.

A vacuum connection has been installed on one side of the source module, to which a pirani gauge is normally attached. This connection serves also to employ a mass spectrometer leak detector.

The electronics of the spectrometer are operated from a regulated power supply (Stabiline 1E 5101).

2. Source



FIGURE 7: RAY DIAGRAM FOR R.I.I.C. MODULAR FOURIER SPECTROPHOTOMETER FS-720

Work in the infrared is limited by the availability of sources of sufficient intensity. There are two types of sources commonly available, namely grey hot bodies, for which the emissivity is a constant less than unity, and mercury arcs.

Grey hot bodies are best used for wave numbers greater than 100 cm<sup>-1</sup>. Shown in Figure  $8^9$  is a comparison of the performance of a mercury arc lamp (working pressure of 3 atmospheres) and a globar (operated at  $1200^{\circ}$ K). The lamp used was the same type as is employed in the FS-720, a Phillips' HPK, 125 W lamp.

The high pressure of the mercury vapour in the lamp broadens the discrete emission lines and a broad band spectra is obtained. The intensity of the emitted radiation is pressure dependent, increasing with pressure.

The envelope of the lamp is of fused quartz, which absorbs the infrared radiation of the arc above 200 cm<sup>-1</sup>. The main source of infra radiation above 200 cm<sup>-1</sup> is then due to the hot envelope itself. The surface of the envelope is "dimpled" to reduce interference effects.

Cooling of the lamp is provided by a water cooled lamp housing. The lamp is protected against overheating by a thermostat which cuts off the lamp power supply if the temperature of the lamp base exceeds  $65 - 75^{\circ}$ C.

> 449 449 8 6 9 7 8 6 7 8 8 7 7 7 7

Figure 8. Comparison of a Mercury Lamp to a Globar

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# 3. Beam Splitter

The interchangeable beam splitters are made from mylar (polyethylene terephalate) and are of thicknesses 6, 12, 25, 50 and 100 microns.

The transmitted radiation through the interferometer depends on the product of squares of the transmission and reflection coefficients, t and r respectively, of the beam splitter. If no absorption occurs, then  $|r|^2 + |t|^2 = 1$ and the maximum of the product  $|r|^2|t|^2$  occurs when  $|r|^2 = |t|^2 = 0.5$  and  $|rt|^2$  is then 0.25. This product may be very much less depending on the polarization, as is shown in Appendix A. This is a serious drawback and is one of the main reasons why the lamellar grating interferometer is superior in the very far infrared region of very low intensity radiation.

Figure 9, taken from the instruction manual, shows the relative beam splitter efficiencies, neglecting absorption. The diagram is erroneous in that the correct condition for a maximum is  $Bd = (N - \frac{1}{2})\Pi$ ,  $(N=1, 2, 3 \dots)$ that is,  $k = \frac{(N - \frac{1}{2})}{2nd(1 - 1/2n^2)^{\frac{1}{2}}}$  as is shown in Appendix A (In the Appendix,  $k = 2\frac{\pi}{2}$ , here  $k = \frac{1}{2}$ ). Likewise, the condition for a minimum is  $k = \frac{N}{2nd(1 - 1/2n^2)^{\frac{1}{2}}}$ . For n = 1.6,  $(1 - 1/2n^2)^{\frac{1}{2}} = .9$ . The correct locations of the maxima and minima are then shifted to  $1/(.9)^2 = 1.23$  times

the values shown in Figure 9.

In regions of low efficiency, the S/N ratio decreases and the beam splitter size must therefore be chosen for the

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FIGURE 9: RELATIVE BEAM SPLITTER EFFICIENCIES

appropriate spectral range. A number of separate spectra may be needed to cover the spectral region, of interest, especially in the lower energy end of the spectrum.

Since the radiation is not normally incident upon the beam splitter, the sigma and pi coefficients of reflection and transmission are different, resulting in the beam being strongly polarized. A calculation of this polarization is given in Appendix A.

4. Admission Angle and Resolving Power

The collimating mirror for the source is an f:1.7 surface alumnized off-axis paraboloid. The focal length is given by f = (f number) (linear diameter of entrance pupil).

For the FS-70:

 $f \simeq (1.7)(3 \ge 2.54) \simeq 13.0 \text{ cm}$ 

From equation 42, the theoretical resolving power is given by:

$$R = \frac{2\pi}{\sqrt{2}} \approx \frac{2\pi}{\pi} \left(\frac{2f}{d}\right)^2 = 8 \left(\frac{f}{d}\right)^2$$
(50)

(49)

where:

\_\_\_\_ = the solid angle subtended by the source at the centre of the collimating mirror

f = the focal length of the collimating mirror

d = the linear diameter of the source.

The source aperture of the FS-720 is variable in steps of 3, 5 and 10 mm diameter. We therefore have theoretical resolving powers of  $1.48 \times 10^4$ ,  $5.4 \times 10^3$  and  $1.35 \times 10^3$  respectively for the above apertures.

In order to maintain these theoretical resolving

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powers, we require the admission angle of the detector to be as large as or larger than the largest solid angle subtended by the source, since the effective admission angle, that is, that through which radiation from the interferometer enters the detector, is the same as the angle subtended by the source.

#### 5. Drive

The position of the moveable mirror is controlled by a stepping motor. The mirror may be moved either to the left or right of zero path differences in steps of 5, 10, 20, 40 and 80 microns path difference. From equation 44, this would allow maximum calculateable wave numbers of 1000, 500, 250, 125, and 62.5 cm<sup>-1</sup> respectively for the above stepping intervals.

The maximum path difference is  $X = \pm 5$  cm from which the maximum obtainable resolution as defined by equation 36 is  $.2 \text{ cm}^{-1}$ .

The gating times or time periods between samples are 0.53, 1.07, 2.13, 4.27, 8.53, 17.06 and 34.13 seconds.

6. Detector

The detector employed in the FS-720 is a Golay, fitted with a 3 mm diameter diamond window and is manufactured by Unicam Instruments Limited.

The Golay cell is a pneumatic chamber, sealed at one end by a radiation absorbing film and at the other by a mirror membrane. The cell contains xenon gas which, when warmed by the absorbing film, expands and causes a distortion of the flexible mirror membrane. The distortion of the mirror is converted into an electrical signal by means of an optical system which reflects light off the mirror surface onto a photomultiplier. The amount of light incident on the photomultiplier depends on the distortion of the mirror membrane. The operating point of the detector is chosen such that the signal of the photomultiplier bears a linear relationship to the mirror displacement.

Light from the source is chopped at 15 HZ by a rotating blade. This produces a corresponding oscillation in the mirror membrane and hence in the electrical signal from the photomultiplier. The radiation signal received from the rotating blade of the chopper becomes the zero reference signal when the output signal of the detector is demodulated and amplified. The ambient radiation does not then appear in the amplified signal.

The pneumatic chamber has a small leak connecting it with a ballasting chamber on the far side of the mirror membrane. The time required for the two chambers to reach equilibrium pressure is of the order of several seconds and therefore has little effect on the signal due to the chopped radiation from the source. The response of the cell is shown in Figure 10, taken from the Golay instruction manual.

The leak between the two chambers prevents slow changes in the ambient temperature from affecting the signal.

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Figure 10. Response of the Golay Detector

A comprehensive description of a Golay detector is given by  $Hadni^2$ .

The root mean square equivalent noise input at any frequency and in a certain bandwidth is defined as the r.m.s. signal at the same frequency which would equal the r.m.s. noise in the same bandwidth. For the detector used in the FS-720, the quoted value of the R.M.S.E.N.I. is  $4 \times 10^{-11}$  watts at 15Hz in a bandwidth of 0.1 Hz.

The sensitivity in this system is defined as the ratio: <u>R.M.S. volts (15 Hz) Output</u> R.M.S. watts (15 Hz) radiation Input

This has an approximate value of 2 x  $10^5$  volts/watt for the detector employed with the FS-720.

The absorbing membrane in the detector employed is quoted as having a constant response for all wavelengths in the range 1 to 1000 microns.

The diamond window of the detector transmits approximately 50 - 60% of the incident radiation in the range  $10 - 1000 \text{ cm}^{-1}$ .

Below 40 cm<sup>-1</sup>, Perry, Geik and Young<sup>8</sup> note that the S/N ratio for a Golay detector rapidly decreases and it then becomes advantageous to use a detector which has a greater

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# detectivity.

In the very far infrared, there are only three other detectors which are used appreciably, all of which require operation at low temperatures. These are the carbon bolometer, germanium bolometer and indium antiminide photodetector. A comparison of the response of the above detectors is given in the paper mentioned above.

### 7. Electronics

The voltage signal produced by the Golay detector bears a linear relationship to the radiation intensity incident upon the detector. This relationship is given by the sensitivity.

The voltage signal is amplified, demodulated, integrated and filtered before being fed into an analogue to digital converter. A full description of the above system is given in the instruction manual.

# 8. Filtering

As previously discussed, filtering is necessary to eliminate "false energies". Filtering is also required to prevent unwanted short wavelength radiation from overloading the detector to the extent that the low intensity far infrared radiation may not be measureable because the dynamic range of the analogue to digital converter is not sufficient for the detection of this weak signal against the background of high intensity short wavelength radiation (see Section IV). Black polyethylene acts as an optical filter, strongly attenuating frequencies of wave number greater than 500 cm<sup>-1</sup>. The condensing lens of the detecting system is made of black polyethylene and thus serves as a filter as well as a lens.

Other optical filters, supplied by Beckman Instruments, with different cut-off frequencies, are used. Transmission curves for these are shown in Figure 11.

Electronic filtering is employed in the amplifying circuitry. The value of the time constant in the RC filter is appropriately chosen to filter out the unwanted high frequencies, as well as the residual ripple of the demodulated 15 Hz frequency due to chopping.

If the highest frequency of interest has a wave number K and we sample at least twice per cycle for this maximum frequency, then we require a time,  $2\Delta t$ , to sample one complete cycle. The time required for each sample is  $\Delta t$ .

Therefore:

$$w_{max} = 2\pi f = 2\pi / (2\Delta t) = \pi / (\Delta t)$$
 (51)

In order that frequencies of interest are not appreciable attenuated and that the unwanted high frequencies are strongly attenuated, we require that:

 $\tau_{w_{\text{max}}} \simeq 1$  (52)

that is, the 3db point.

Therefore:

$$L \simeq \frac{\Delta T}{\pi}$$
(7)  
The FS-720 has time constants of 0.5.1.2 & 8 and

1 2 2 1



# 16 seconds.

#### SECTION IV

# DYNAMIC RANGE

Since the Fourier transform is a linear operation, we may regard the interferogram as a noise interferogram plus a signal interferogram, that is:

 $F(x) = F(x)_N + F(x)_S$  for noise of a random nature. In order to observe the signal interferogram, we require that:

$$\frac{F(x)_{S}}{F(x)_{N}} > \frac{N}{S} \qquad \text{that is: } S/N > \frac{F(x)_{N}}{F(x)_{S}}$$

The dynamic range, or distinguishable signal levels, of the analogue to digital converter must be greater than  $\frac{F(x)_N}{F(x)_S}$  in order to fully utilize the signal. The FS-720 has a 12 bit binary A/D converter and can therefore distinguish 1 bit in 4,096.

A large portion of the d.c. interferogram signal,  $I(\infty)$ , may be subtracted before being fed to the A/D converter, by adjusting the "zero offset" voltage. The entire range of the A/D converter may then be filled with the varying portion of the signal, F(x).

 $Mertz^{10}$  has shown that:

$$\frac{\overline{s}}{(\overline{n_{I}^{2}})^{\prime _{2}}} = \sqrt{\frac{\Delta \nu_{n}}{\Delta \nu_{s}}} \frac{\underline{1}_{o}}{\sqrt{\overline{n_{I}^{*}}}\sqrt{N'}}$$

where:

**S** = the average spectral intensity

$$\sqrt{n_1^2}$$
 = the r.m.s. noise per unit abscissa of the interferogram

$$\sqrt{n_s^2}$$
 = the r.m.s. noise per unit abscissa of the spectrum

 $\Delta V_{s}$  = the spectral bandwidth

 $\Delta \nu_n =$  the noise bandwidth -

 $I_{o}$  = the amplitude of the peak to peak envelope of the central fringes of the interferogram

N = the number of resolved elements in the spectrum.

The ratio  $\overline{s}/\overline{n_s}$  may be improved by decreasing  $4\nu_s$  by filtering and by decreasing  $n_I$  using longer integrating times.

If the spectrum consists of a background and a very narrow line, then the dynamic range and S/N ratio must be greater than the ratio of the area under the background spectral curve to the area under the line curve in order that the narrow feature can be distinguished.

# SECTION V

### ADAPTATIONS FOR LOW TEMPERATURE WORK

A cryostat was constructed which may be attached to the spectrometer sample chamber, after removing the top cover plate of the chamber.

A stand with an adjustable height setting was built in order to support the cryostat, such that it did not place any weight on the spectrometer.

The cryostat consists of an outer brass shell, containing two dewars. Both dewars are suspended from the top of the outer shell by stainless steel tubing, in order to reduce heat flow into the inner part of the cryostat.

The outermost dewar is a brass jacket containing liquid nitrogen, A 1 5/8" O.D. copper tube extends downward from the bottom of this container and surrounds the tail of the inner dewar, thus acting as a radiation shield. At the lower end of the shield are two diametrically opposite 7/8" diameter holes, which allow the radiation from the interferometer to pass to the sample and then out again to the detector.

The inner dewar is a one litre stainless steel can. A thin 1" diameter stainless steel tube extends downward from the bottom of the can and is sealed at the lower end by a copper plug, which is threaded to accept a copper sample holder, shown in Figure 12. An indium pad is placed between the plug and sample holder to provide a good thermal contact.

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Figure 12. Sample Holder.

The stainless steel tube also extends approximately 2/3 of the way up into the inner dewar. This facilitates easy conversion to a variable temperature cryostat. (Reference: R. W. MacPherson<sup>11</sup>).

In order to prevent heat leaks due to conduction and convection, the space between the various components of the cryostat must be evacuated. Since the spectrometer pumping system could not produce a sufficiently low pressure for the cryostat to operate effectively, it was necessary to isolate the two systems. A diffusion pump was used to pump the cryostat to a lower pressure than the spectrometer. The isolation of the system was initially accomplished by means of two  $\frac{1}{4}$ " thick soft polyethylene windows with a cryostat tailpiece. This was found to be unsatisfactory due to strong signal absorption, especially at high energies. Finally, the spectrometer "purge kit" unit was used. This unit is the same as the standard sample cell module except that it has a vacuum tight  $\frac{1}{4}$ " thick hard polyethylene window, covering the entrance aperture.

The spectral distribution for the spectrometer using the purge kit and a 25 G (6 micron) beam splitter is shown in Figure 13.

A holder for the optical filters was made, which fits on the cryostat tailpiece.

The arrangement of the helium return and vacuum system pumping lines is shown in Figure 14.



FIGURE 1.3: SPECTRAL INTENSITY DISTRIBUTION

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# SECTION VI

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# THEORY OF IONIZED CENTRES IN DOUBLE DOPED SILICON

If a group III atom replaces a silicon atom in a perfect lattice, a hole state is produced. This hole state is loosely bound to the impurity site. The hole in the ground state of the impurity atom may be excited by electromagnetic radiation. These excitations can therefore be investigated by means of absorption spectra.

Boron doped silicon has been studied by Colbow<sup>12</sup>. Shown in Figure 15 are the normal ground state energy levels for the individual impurities. Besides the ground state, there are excited hole states which are bound and lie between the ground state and the valence band.



Figure 15. Ground States of Singly-Doped Silicon

It is believed that, when silicon is doped with both boron and indium, ionized impurity atoms could be formed. This is illustrated in Figure 16.



Figure 16. Possible Ground States of Doubly-Doped Silicon

The B<sup>-</sup> ion resembles a H<sup>-</sup> like ion, for which only the ground state exists. The In<sup>+</sup> also resembles a H<sup>-</sup> like ion, only with the charges of the nucleus and electron reversed. We assume, then, that no excited hole states exist when the impurity centres are ionized.

In order to calculate the electronic energy of the  $B^-$  ion in the lattice, we assume that the ratio of this energy to the binding energy of the boron atom in the lattice is the same as the ratio of the binding energy of the free  $H^-$  ion to the binding energy of the Hydrogen atom, that is:

$$\frac{E_{B}}{E_{B}} = \frac{E_{H}}{E_{H}} \qquad \text{Therefore:} \quad E_{B} = E_{B} \left(\frac{E_{H}}{E_{H}}\right)$$

We then have, for the binding energy of the B-

$$E_{B}$$
 = (.045)  $\left(\frac{.75}{13.6}\right)$  ev = 2.48 x 10<sup>-3</sup> ev  $\approx 7.4 \text{ cm}^{-1}$ 

ion:

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In a similar manner:

$$E_{In^+} = (.155) \left(\frac{.75}{13.6}\right) ev = 8.55 \times 10^{-3} ev$$
  
 $\simeq 69 cm^{-1}$ 

The B<sup>-</sup> impurity is optically inactive; however, the In<sup>+</sup> ion is optically active. Therefore, in order to determine whether the ionization does occur, we look for continuous optical absorption for frequencies with wave numbers greater than 70 cm<sup>-1</sup>. This energy is well below the energy of excitations of the ground state of boron and indium and should therefore be distinguishable from them.

#### SECTION VII

-45-

# EXPERIMENTAL PROCEDURE AND RESULTS

1. Sample Preparation and Mounting

All samples were polished using 600 mesh abrasive on astomet cloth.

Before obtaining a spectrum, the samples were ultrasonically degreased in toluene and then in ethyl alcohol.

To ensure a good thermal contact with the sample holder, a small amount of vacuum grease mixed with powdered silver was placed between the sample and the holder. The grease was used on one end of the sample only, to avoid introducing strains across it when the grease froze.

The front plate of the sample holder was fastened down just sufficiently to hold the sample against the back face of the sample holder (see Figure 12).

A small amount of vacuum grease mixed with powdered silver was also placed on the threads of the copper plug, at the bottom of the 1" diameter stainless steel tube, to ensure a good thermal contact between it and the sample holder.

2. Temperature of the Sample

After the helium boils off in the 1" diameter stainless steel tube to which the sample holder is attached, the sample may be warmed slightly by the incident radiation.

From the spectra obtained, it is seen that there is no dependance of the absorption on  $\lambda^2$  and it is therefore assumed that the temperature of the samples was sufficiently low that free carrier absorption did not have any appreciable effect on the spectra.

3. Results

Shown in Figure 17 is the absorption spectrum of boron-doped silicon at liquid helium temperature. The boron impurity concentration is approximately  $1.3 \times 10^{16}$  atoms/cm<sup>3</sup>. The thickness of the sample is 1.02 mm.

From Colbow<sup>12</sup>, the ratio of the transmission of the reference to the sample spectrum is:

Ratio = 
$$1/T = \frac{1 - R^2 \exp(-2 \propto d)}{(1-R)^2 \exp(-\infty d)}$$

where R is the reflection coefficient of the sample and  $\propto$ the absorption coefficient. The reference used here is the spectrum obtained with no sample in the beam, all other conditions being the same as for a sample spectrum.

Since R is fairly constant (see below), the peaks were due to absorption effects.

We observed peaks 1 through 4 at the same frequencies as did  $Colbow^{12}$ .

An absorption spectrum of silicon doubly doped with boron (N<sub>B</sub> = 2.6 x  $10^{16}$  atoms/cm<sup>3</sup>) and indium (N<sub>I</sub> = 1.8 x  $10^{17}$  atoms/cm<sup>3</sup>), was obtained at liquid helium temperature. for a sample 1.67 mm thick. This spectrum is shown in Figure 18.

The spectrum may be seen to be basically the same as that of the boron-doped silicon, except that the absorption lines are broadened due to impurity concentration effects.

Shown in Figure 19 is the spectrum of a 2.04 mm thick sample of intrinsic silicon at liquid helium temperature.



FIGURE 17: BORON DOPED SILICON

.



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FIGURE 18: DOUBLE DOPED SILICON



RATIO

-64-

There is an oxygen impurity concentration of  $5 \times 10^{17}$  to  $10^{18}$  atoms/cm<sup>3</sup>. These impurities do not affect the spectrum in the region observed here.

For this spectrum we have:

Ratio =  $1/T = \frac{1 + R}{1 - R}$ , since  $\propto = 0$ 

For a constant value of the reflectivity, 1/T does not vary with wave number. As is seen in the spectrum obtained, 1/T varies with wave number. It is thought, therefore, that the reflectivity may be frequency dependent.

Comparing the three spectra described above, we are led to suspect that the low energy tail below 240 cm<sup>-1</sup> in the spectra of the doped silicon samples was due to the reflection characteristic of silicon.

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# SECTION VIII CONCLUSIONS

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Using the FS-720 Michelson interferometer, we were able to obtain the absorption peaks observed by Colbow in boron-doped silicon for the spectral region 240 cm<sup>-1</sup> to 330 cm<sup>-1</sup>. We were also able to extend the spectral region down to 40 cm<sup>-1</sup>.

We were unable to observe any absorption edge which would be indicative of the existence of ionized B<sup>-</sup> and In<sup>+</sup> centres, at the impurity concentrations and temperatures with which we were working.

Comparing the spectrum of the intrinsic silicon with that of the impurity doped silicon samples, we were led to suspect that the low energy tail of the doped silicon spectra was due to a frequency dpdendence of the reflection coefficient of silicon. In order to confirm this, reflectivity measurements should be made using a special reflectance attachment, available from the manufacturer of the spectrometer.

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# APPENDIX A

# POLARIZATION

Consider a non-absorbing film of refractive index  $n_f$  with radiation incident at an angle  $\Theta$  as shown below:



From Snell's law:

 $n_1 \sin \theta = n_f \sin \gamma = n_2 \sin \phi$ 

Stone<sup>13</sup> shows that for both the pi and sigma

polarizations:

$$E_{i} + E_{r} = E_{+} + E_{-} \qquad Y_{1}(E_{i} - E_{r}) = Y_{f}(E_{+} - E_{-})$$

$$E_{+}e^{i\beta d} + E_{-}e^{-i\beta d} = E_{t} \qquad Y_{f}(E_{+}e^{i\beta d} - E_{-}e^{-i\beta d}) = Y_{2}E_{t} \qquad (2)$$

(1)

where the E's are electric vectors associated with the corresponding wave vector of the diagram.

$$\beta = n_{f} k_{o} \cos \gamma$$
 (3)

and:

$$Y_{1}\pi = \frac{n}{\cos \theta} \qquad Y_{f}\pi = \frac{n}{\cos \psi} \qquad Y_{2}\pi = \frac{n}{\cos \phi}$$
$$Y_{1}\sigma = n_{1}\cos \theta \qquad Y_{f}\sigma = n_{f}\cos \psi \qquad Y_{2}\sigma = n_{2}\cos \phi \qquad (4)$$

Stone further shows that  $E_+$  and  $E_-$  may be eliminated in equations 2 to give:

$$E_{i} + E_{r} = (\cos\beta d - iY_{sin\beta} d)E_{t}$$
(5)

$$X_1(E_i - E_r) = (-iY_f \sin\beta d + Y_2 \cos\beta d)E_t$$
(6)

If  $\theta = TV/4$ ,  $n_1 = n_2 = 1$  and  $n_f = 1.6$ , then:

$$\sin \theta = \sin \phi = \cos \theta = \cos \phi = 1/\sqrt{2}$$
(7)

and: 
$$\cos \gamma = (1 - \sin^2 \gamma)^{\frac{1}{2}} = (1 - \frac{1}{1.6\sqrt{2}})^{\frac{1}{2}} \approx .9$$
 (8)

For the pi component, we then have:

$$Y_1 = \sqrt{2}'$$
  $Y_2 = \sqrt{2}'$   $Y_f = 1.6/.9 = 1.78$  (9)

Adding equations 5 and 6 and using equations 7, 8

and 9, we have:

$$2E_{i} = (2\cos\beta d - i(\sqrt{2} + \frac{1.78}{\sqrt{27}})\sin\beta d)E_{t}$$

$$E_{i} = (\cos \beta d - i(1.025) \sin \beta d) E_{t}$$

and therefore:

or:

$$|t_{\pi}|^{2} = \left|\frac{E_{t}}{E_{t}}\right|_{\pi}^{2} = \frac{1}{\cos\beta d + (1.025)^{2} \sin\beta d}$$

$$= \frac{1}{1 + .05 \sin \beta d}$$
(11)

(10)

For the sigma component, we have:

$$Y_1 = 1/\sqrt{2}$$
  $Y_2 = 1/\sqrt{2}$   $Y_f = (1.6)(.9) = 1.44$  (12)

Adding equations 5 and 6 as before, we have:

$$2 E_{i} = (2\cos\beta d - i(\sqrt{2}(1.44) + \frac{1}{\sqrt{2}(1.44)})\sin\beta d)E_{t}$$
(13)

Therefore:

$$\left| t_{\sigma} \right|^{2} = \left| \frac{E}{E_{i}} \right|_{\sigma}^{2} = \frac{1}{\cos^{2}\beta d + (1.26)^{2} \sin\beta d}$$
$$= \frac{.05 \sin^{2}\beta d}{(1 + 0.5 \sin^{2}\beta d)^{2} - (14)}$$

$$\frac{(1+.05\sin^2\beta d)^2}{|r|^2} + |t|^2 - 1$$

For a non-absorbing film,  $|\mathbf{r}|^2 + |\mathbf{t}|^2 = 1$ Therefore:

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$$|\mathbf{rt}|^{2} = |\mathbf{t}|^{2}(1 - |\mathbf{t}|^{2})$$
(15)

For the pi polarization, we have:

$$||rt||^2 = \frac{1}{(1 + .05 \sin \beta d)} \left( \frac{.05 \sin^2 \beta d}{(1 + .05 \sin^2 \beta d)} \right)$$

$$= \frac{.05 \sin^2 \beta d}{(1 + .05 \sin^2 \beta d)^2}$$
(16)

)

The maximum of the expression occurs when  $\sin\beta d = 1$ , that is:

$$\beta d = \pi (n + \frac{1}{2})$$
  $n = 0, 1, 2, 3, ...$  (17)

By a similar analysis, the same condition for a maximum of  $|rt|^2$  applies to the sigma polarization.

For the sigma polarization:

$$|^{2} = \frac{1}{(1 + .58\sin^{2}\beta d)} \left( \frac{.58\sin^{2}\beta d}{1 + .58\sin^{2}\beta d} \right)$$
$$= \frac{.58\sin^{2}\beta d}{(1 + .58\sin^{2}\beta d)^{2}} - (18)$$

If unpolarized radiation is incident upon the interferometer, the percentage polarization in the sigma direction after the two beams recombine is given by:

$$\frac{|\mathbf{rt}|_{\sigma}^{2} - |\mathbf{rt}|_{\sigma}^{2}}{|\mathbf{rt}|_{\sigma}^{2} + |\mathbf{rt}|_{\pi}^{2}} \times 100\%$$
(19)

In order to obtain some idea of the degree of polarization, we consider an example where the value of  $|rt|^2$  for both sigma and pi polarization is a maximum. In this instance we have:

$$|\mathbf{rt}|^{2} = \frac{.05}{(1+.05)^{2}} = \frac{.05}{1.10} = .045$$
$$|\mathbf{rt}|^{2} = \frac{.58}{(1+.58)^{2}} = \frac{.58}{2.50} = .232$$

and the percentage polarization is:

### APPENDIX B

# COMPUTER PROGRAM

The computer program to process the data is written for an IBM model 360/67 computer and an off-line calcomp plotter.

The program contains four subprograms:

(a) FTTAPE: This program converts the binary output to digital form. When the paper tape output is converted to magnetic tape, a value of 256 is placed between the conversion of individual tapes and a value of 512 at the end of the last tape converted.

The code used on the paper tape is 12 bit binary and requires three frames for each output value. This is shown below:  $3 \cdot 2 \cdot 1 = 0$ 

		•	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	3rd frame
		parity channel		2nd frame
l <sup>st</sup>	frame	index $\longrightarrow 0$ 0 0	ÕoÕ Õ Õ	1st frame
			ero channel .	

The parity channel is punched in such a manner that each frame is of odd parity; should a frame be of even parity, the PTAPE routine returns a negative valued integer rather than a positive one.

The zero channel is punched whenever a frame is completely empty of data. This serves as a check that the actual value is zero, rather than that a malfunction of the equipment has occurred.

The conversion to magnetic tape reads each frame separately and is strictly binary. (b) CASJU6: This program arranges the data for RHARM (see below), calls RHARM and computes the intensity and wave number values from the output of RHARM. In the case where spectra are ratioed, the subroutine checks that the reference spectrum has as many or more useable input points as the sample spectrum.

- الر -

(c) RHARM: This is an IBM scientific subroutine which finds the Fourier coefficients of one-dimensional real data. It requires  $2(2)^n$  input values and returns  $2^n + 2$  output values, where n is an integer.

(d) WBPLOT: Provides for the plotting of the transformed data.

There are three modes of operation of the program:

Mode 1: Each interferogram is transformed and the output is plotted as intensity vs. wave number. For each spectrum, the cards required to obtain the transform are: 1. Title

Comp - which may be any additional information
 Mode, NFT, NAPOD, MOVE, LPAGE, XMAX, XMIN
 DINIT, DFINAL, DZERO, DELX

Mode 2: The sample and reference interferograms are transformed. The ratio of the reference to the sample transmission is calculated and plotted as a function of wave number. The program requires that the reference interferogram be transformed with as many or more points either side of zero path difference as is used for the sample.

The cards 1 - 4 used for Mode 1 are used, where card 4 contains values for the sample interferogram. These are followed by card 5 which is the same as card 4 except that it contains the data for the reference run.

Mode 3: This is the same as Mode 2 except that a number of different sample spectra may be ratioed against the same reference spectra.

The cards used are 1 - 5 as for Mode 2, followed by 1 - 4 for each subsequent sample spectrum.

Calculations under Mode 1, 2 or 3 may be made in one complete run, provided the reference spectrum is always preceded by a sample spectrum when running under Mode 2 or 3. Subsequent sample spectrum are ratioed against the last reference spectrum when running under Mode 3.

In the program, the scale on the wave number axis is read in as LPAGE. In order to be compatible with the calcomp routines, it must be 1, 2, 4, 5, 8 or one of these times any integer power of 10.

A flow diagram for the main program and the CASJU6 subroutine are included to aid in understanding the operation of the program.

-59-







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		and a second
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1-	Ċ	**************************************
. 2	ř.	*****0E PATH DIFFERENCE ONTOUT OF EAR INFRARED INTERFEROMETER
2	C C	*****CAMPLE INTEREPOOD AM INTENCITIES COLA(I)
2		WWWWYDEEEDENCE INTEDEEDOODAN INTENCTITES DEI (/I)wwwww
-4		AAAAAAKEFEKENDE INTEKFERUGRAM INTENSITIES KSIO(ITAAAAAA
· >	L L	*****SAMPLE PATH DIFFERENCES SX(I)*****
6	C	*****SAMPLE CALCULATED INTENSITIES SINT(I) *****
7.	C	*****REFERENCE CALCULATED INTENSITIES RINT(I) *****
8.1	C	****REFERENCE PATH DIFFERENCES RX(I) *****
.9	C	****RATIO = RINT/SINT ****
10	C	*****INTERFEROGRAM FUNCTION SS16(I)-INF OR RS16(I)-INF=F(I) ***
11		DIMENSION SS16(9000), RS16(9000), F(9000), SX(9000), RX(9000), SINT(4
12	······································	13) • RATIO (4503) • RINT (4503)
13		COMMON COMP(20), TITLE(20), MODE, LTTS, NMODE3, NAPOD, NABOR T, RESOL.
14		1NONH, DELY, I DAGE, YDAGE, NG, MOVE, YMAY, YMIN
15	a da an	INCHOULDED CARD DADED SNDATA DNDATA
12		DEAL AND ONCE DINE (C) INF
10	e de la companya de l	REAL NU(8195), IPINF(6), INF
17		
18	- · ·	PAPER=6
19	C	*****SE1 ITIS=1 TO ACCEPT SAMPLE DATA ****
20	C	SET NMODE3 = 0 TO INITIALISE MODE = 3 RUNS.SET NABORT=1 ********
21		ITIS=1
22		NMODE3=0
23		NABORT=1
24	, ·	NG=0
25		XPAGE=0.0
26	C	****READ TITLE TO PRINTED OUTPUT AND PLOT****
27	23	READ(5,200) TITLE
28	200	FORMAT(20A4)
29	C	*****READ IN SAMPLE AND REFERENCE COMPOUNDS*****
30		READ (5.200) COMP
31	, c	**************************************
22	Č.	**************************************
22		WWWWWWODE-2 F T FIRST INTEREEROCOAM TO NULAND CINT
22		**************************************
24	C	ANAMAFT SECUND INTREFERUGRAM TU NU AND RINT
35	<u> </u>	*****CALCULATE RATIO=RINT/SINT. PRINT AND PLOT NU AND RATIO
36	C	*****MUDE=3, AS MODE=2, BUT THE THIRD AND FOURTH ETC INTERFEROGE
31	C ·	*****WITH MODE=3 ARE ALL SINT AND ARE RATIOED AGAINST THE
38	C	****MOST RECENT RINT TO GIVE RATIO****
39	С	*****NAPOD=1 APODISE INTERFEROGRAM. NAPOD=2 DO NOT APODISE******
40	С	*****MOVE=1 IS MOIRE DRIVE,MOVE=2 IS STEP DRIVE
41	C	*****LPAGE=SCALE REQUIRED FOR WAVE/CM AXIS ON GRAPH
42	C	*****XMAX IS MAXIMUM FREQUENCY TO BE PLOTTED
43	С	*****XMAX-XMIN SHOULD BE AN INTEGRAL MULTIPLE OF LPAGE
44	С	*****XMIN IS THE LOWEST EREQUENCY TO BE PLOTTED.
45	, <b>.</b>	READ (5.201) MODE .NET .NAPOD . MOVE .L PAGE .XMAX .XMIN
46	201	FORMAT(514.2F10.3)
47	24	WRITE/DADED 2121TIE
$\frac{\tau}{10}$	<u> </u>	
48	<b>^</b>	
49	L, L	******KEAU INTERFERUGRAM INTENSITIES *****
50		GO TO (1,2),ITIS
51	1	CALL FTTAPE(IPINF, SS16, M, LAST)
52		SNDATA=M-9
53		IF(SS16(M-8).EQ.5555.0)GO TO 6

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		-64-
ч 4.1	· · · ·	
54	3	
55		WRITE (PAPER, 203)NC
56	203	ENRMAT(1H0, 19000 SS16 VALUES READ AND 5555 NOT EDUNDI, 14-1GRAPHS
50 57	200	1 DIOTTEDI)
57 50	, ·	
50		
60		$\frac{1}{1} = \frac{1}{1} = \frac{1}$
61	204	EDRMAT()HO. ISAMPLE SIGNALSI. IG. I DOINTS DEAD. EIDST VALUE ISI.
62	204	167.0.1 LAST VALUE ISI.E7.0)
63		GO TO 7
64	2	CALL FTTAPE (IPINE RS16 Malast)
65	<i>ب</i>	RNDATA = M - 9
55		$\frac{1}{1} \frac{1}{1} \frac{1}$
67	8	
5 R		WRITE (PADER 205)NC
60 60	205	ENRMAT (1HO, FONO R SIG VALHES DEAD AND 5555 NOT EDHNOL TATICDADES
70	200	- IDENTIFICATION FOR AND STO VALUES READ AND STOP FOUND (14) CRAFES
71	100	
75	·	
12	1 1	STUP UUUZ NDITE/DADED 2061 DNDATA DS16/11 DS16/DNDATA)
15	204	EDDMAT/140 DEEEDENCE STONALS 1 TO 1 DOINTS DEAD STORT VALUE IT
14	200	FURMAININU, REFERENCE SIGNALS, 10, PUINIS READ, FIRST VALUE IS
1) - 77	· · ·	177009 LAST VALUE 15'97700)
10	L C	****** 7500 DATH DISCOUNCE DOWN DEADING IN MM, FINAL DRUM READING IN MM
11	<u>.</u> L	WWWW ZERU PATH DIFFERENCE URUM READING IN MM, AND THE SAMPLING
10	ຸບ 7	αναστητέκναι τη μισκύνου στάστα Deadle 2021 Dinite Deinal Diedo Dein
19	207	REAU();2077 DINIT ;DFINAL;UZERU;UELX
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04 DE	70	
RA		
87 87		WDITE(DADED OI)
28	91	ENRMAT(1HO. 1 MOTRE DRIVE WAS USED 1)
30		CO TO 97
50		UDITE (DADED 502)
2.1	592	ENRATION STED DRIVE WAS USED IN
32	с С	xxxxxSURTRACT DATH DIFFEDENCE FOR FIDST & DEADINCS USED FOR INF
າ <u>ຼີ</u>		DINIT=DINIT=DELX/250.0
7 <u>,</u>	Ċ,	*****CALCHLATE THE PATH DIEFERENCES IN CM *****
25	•	GO TO (12.13). ITIS
75		
<b>7</b> 7		SX(I) = ((DINIT-D7ERO)/5, 0) - (DELX/10000, 0) = (I-1)
38	14	
29	···· • · ····	$DIAST = (5.0 \times SX(SNDATA)) + D7 FRO$
ົ້າດ		
11	•	WDITE (DADED 200)SY(1) SY(SNDATA) DDIEE
$\frac{12}{12}$	208	EDDMAT(1HO ISAMDLE DATH DIEEEDENCES EIDST ONE ISL EQ / ICM EIL
)2	200	- I ONE IST, FR. 4. TOM. FINAL DOLM DEADING ODCEDVED_CALCHLATED ICL ET
)4		- CONCLES FLOOTF CHALLUNCH READING UDSERVED-CALCULATED IS' FF - 2.1MM. ()
ንጥ ነፍ		CO TO 16
)6	12	DO 15 I = 1 RNDATA
יי דו	С <b>Т</b>	DY/I)-//DINIT_D7ED0)/E 0)_/DELY/10000 0)%/T_1)
<u>э</u> г,	· • · · · ·	NAVII-((DINI)=D/CKU//2+0/=(DELA/10000+0)*(1=1)
••		
•		
		<b>-65-</b>
------------------	------------------	--
:	•	
,		
78	15	CONTINUE
)9		DLAST=(5.0*RX(RNDATA))+DZERO
10		DDIFF=DFINAL-DLAST
ι1		WRITE(PAPER, 209)RX(1), RX(RNDATA), DDIFF
12	209	FORMAT (1HO. REFERENCE PATH DIFFERENCES, FIRST ONE IS
2		1 EINAL ONE IS! E8.4. CM. EINAL DRUM READING OBSERVED-CALCULATED
  - <u>/_</u>		
15	r .	AXXXXCALCHLATE THE INTENSITY FUNCTION FILL-COLALINE OD
12	C ·	$\frac{1}{1} + \frac{1}{1} + \frac{1}$
l, f	16	$INF = (IPINF(1) + IPINF(2) + IPINF(3) + IPINF(4) + IPINF(5) + IPINF(6)) / 6 \cdot 0$
L 8 _		WRITE(PAPER, 210) INF
19	210	FORMAT(1HO, 'INTENSITY AT PLUS INFINITY IS', F10.4)
20-		GO TO(17,18), ITIS
21	17	DO 19 $I=1$ , SNDATA
22		F(I) = SS16(I) - INF
>3	19	CONTINUE
>4	<b>•</b> • • • •	GO TO 101
- ' ) 5	10	DO 2O I - 1 PNDATA
10	20	F(1) = KSIO(1) = INF
27.	20	
28	C	***** READY IU F.I. F(I) WI IH SX(I) OR RX(I)
29	101	GO 10(105,106),111S
30	105	CALL CASJU6(F,SX,SNDATA,SINT,NU,&107,&412)
31	106	CALL CASJU6(F,RX,RNDATA,RINT,NU,&107,&412)
32	107	CONTINUE
33	С	****F. TRANSFORM COMPLETED
34	•	GO TO (30,50,92),MODE
35	с	*****PRINT AND PLOT SS16(1) SX(I), NU(I), SINT(I) READ LAST AND
36	÷ Č	*****RETURN OR EXIT *****
37	30	GD TD(44.134).NET
<del>.</del>		1000000000000000000000000000000000000
20	401	ΝΟΛΤΛ-ΡΝΟΛΤΛ
5.0	401	$\mathbf{C}\mathbf{O} = \mathbf{T}\mathbf{O} = 22$
+U .		
+1	400	
+2	L	*****PAGE HEADINGS, AND SELLI TO GEL PAST FIRST IF *****
+3	33	1= NDA1A+1
44	42	WRITE (PAPER, 212) TITLE
÷5	212	FORMAT(1H1,20A4)
+6.		WRITE (PAPER, 213) COMP
+7	213	FORMAT(1H0,20A4)
¥8		GO TO (408,414),NABORT
ŧ9	414	WRITE(PAPER, 231)
50	231	FORMAT (1HO, 'DATA COULD NOT BE RATIOED, SAMPLE RESULTS PRINTED F:
51		1T. REFERENCE RESULTS FOLLOW!)
52	40.8	WRITE (PAPER.214)
12	··· 214	FORMAT(1HO.8Y.I STONAL AT YILSY IDATH DIEEEDENCE Y CMILSY.
56	<u> </u>	11WAVE/CMI.SV.IINTENCITV AT NHIII
24 15	r	I WAVE/UPI (DA) INTENSITE AT NU') 
>> 	<u>ι</u>	***** LINES YER PAGE COUNTER TO ZERO *****
20 20	•	
) ( . ~	• •	IF(I=NUA IA=1)34;30;30
28	36	LALL PLUIND
59		WRITE(PAPER, 258)NG
50		STOP 222
51	35	DO 34 I=1,NDATA

• •		
• .	· .	
.:		
62		IF(I=NUNU) 38,38,40
63	38	GO TO ( 74,403),ITIS
64	74	WRITE(PAPER, 215)SS16(I), SX(I), NU(I), SINT(I)
65	<del>.</del>	GO TO 41
66	403	WRITE (PAPER,215)RS16(I),RX(I),NU(I),RINT(I)
67	•	GO TO 41
68	215	FORMAT(1H ,9X,F9.4,11X,F8.4,11X,F7.2,7X,E12.5)
69	40	GO TO (406,407),ITIS
70	406	WRITE(PAPER, 217) SS16(I), SX(I)
71	· · ·	GO TO 41
72	407	WRITE(PAPER,217) RS16(I),RX(I)
73	217	FORMAT(1H ,9X,F9.4,11X,F8.4)
74	41	NPC=NPC+1
75	· ·	IF(52-NPC)34,42,34
76	34	CONTINUE
77 -	134	CONTINUE
78	, C	*****CALL PLOTTING ROUTINE, NU IS X AXIS, SINT OR RINT IS Y AXIS
79		GO TO (409,410),ITIS
80	409	CALL WBPLOT(NU,SINT,NONU)
81		NG=NG+1
82	·	WRITE (PAPER, 218)
83	218	FORMAT(1H0, 'SINT PLOTTED')
84	•	GO TO 411
85	. 410	CALL WBPLOT (NU, RINT, NONU)
86		NG=NG+1
87		WRITE (PAPER, 230)
88	230	FURMAI (IHO, 'RINI PLUITED')
89	411	GU + U = (412, 413), NABUR + U = 140T - 0000 + TE - 400E - 0000
90	L C	*****CHECK FUR FURTHER RUNS. LAST=8888 IF MURE RUNS
91	<u> </u>	***** 99991F NU MURE RUNS. *****
92 02	412	IIIS=1 IE (IAST=00001 23.73.22
95	413	IT (LAS) - 20940920
95	- 1 J	NABORT=1
96		GO TO 106
97	C	***** MODE=2 IE SAMPLE DATA PROCESSED OD BACK AND PROCESS
98	C	***** REFERENCE DATA WITH ITIS=2 THEN CALCULATE RATIO
99	č	***** AND PRINT AND PLOT RESULTS *****
00	50	GO TO (51,52),ITIS
01	51	ITIS=2
02		GO TO 24
03	52	DO 53 I=1,NONU
<u>J</u> 4		IF(RINI(1))54,54,55
05	54	WRITE(PAPER,220) NU(I),RINT(I)
26	220	FORMAT(1HO, LATI, E7 2, LWAVE/CM DINT-1, E12 5, LTS NECATIVE OD 75001

	412	1113-1
•	2	IF (LAST-9999) 23,43,23
	413	ITIS=2
		NABORT=1
		GO TO 106
	C	***** MODE=2 IF SAMPLE DATA PROCESSED GO BACK AND PROCESS
	C	***** REFERENCE DATA WITH ITIS=2 THEN CALCULATE RATIO
•	C	**** AND PRINT AND PLOT RESULTS *****
	50	GO TO (51,52),ITIS
	51	ITIS=2
		GO TO 24
·.	52	DO 53 I=1,NONU
	······································	IF(RINI(1))54,54,55
	54	WRITE(PAPER,220) NU(I),RINT(I)

06	220	FURMAI(1HO, 'AI', F7.2, WAVE/CM RINT=', E12.5, 'IS NEGATIVE OR ZERD
07		RATIO(I)=0.0
0.8		GO TO 53
09	55	IF(SINT(I))56,56,57
10	56	WRITE(PAPER, 221)NU(I), SINT(I)
11	221	FORMAT(1H0, 'AT', F7.2, 'WAVE/CM SINT=', E12.5, 'IS NEGATIVE OR ZERO
12		RATIO(I) = 0.0
13		GO TO 53
14	57	RATIO(I)=RINT(I)/SINT(I)
15 👘	53	CONTINUE

. ·			-67-
16	<u></u> `.		WRITE (PAPER, 222) SNDATA, RNDATA, NONU
17.		222	FORMAT(1H0, 'SNDATA=', I4, ' RNDATA=', I4, ' NONU=', I4)
18	· · ·	C	*****SS16,SX,RS16,RX,NU,SINT,RINT,RATIO CALCULATED AND READY FOR
19		C	*****PRINTING AND PLOTTING WHERE NEEDED *****
20		540	GO TO(63,533)NFT
21	· ·	63	NDATA = MAXO(SNDATA,RNDATA,NONU)
22		<u>.</u>	*****PAGE HEADINGS AND SET I TO GET PAST FIRST IF *****
23	•.		I=NDATA+1
24	1997 - 1997 -	88	WRITE(PAPER, 212)TITLE
25			WRITE(PAPER,213)COMP
26	•		WRITE(PAPER, 223)
27		223	FORMAT(1H0,4X, 'SS16(X)',6X, 'SX/CM',5X, 'RS16(X)',6X, 'RX/CM',
28			17X, WAVE/CM, 5X, SINT(NU), 6X, RINT(NU), 7X, RATIO(NU))
29		.С. н	***** LINES PER PAGE COUNTER TO ZERO *****
30		· · ·	NPC=0
31	• • *		IF(1-NDA A-1)64,65,66
32.		66	CTOD 222
> > > > > > > >		66	$\frac{510P}{6A} = \frac{1}{1} \frac{10ATA}{1}$
34		20	$\frac{1}{1} = \frac{1}{1} = \frac{1}$
36		60	IF(1 - SNDATA)70.70.84
37	· · ·;	70	IF(I - RNDATA)71.71.87
38		71	WRITE (PAPER $\cdot$ 224) SS16(T) $\cdot$ SX(T) $\cdot$ RS16(T) $\cdot$ RX(T) $\cdot$ NU(T) $\cdot$ SINT(T) $\cdot$
39			$1  \text{RINT(I)} \in \text{RATIO(I)}$
-07	·	274	$\frac{1}{1} = \frac{1}{1} = \frac{1}$
+1			1E12.5,3X,F8.4)
+2	· ·		GO TO 80
13		68	IF(I - SNDATA)73,73,83
+4		73	IF(I - RNDATA)77,77,78
+5		77	WRITE(PAPER,224)SS16(I),SX(I),RS16(I),RX(I)
16			GO TO 80
⊦7	•	·78	WRITE(PAPER,224)SS16(I),SX(I)
⊦8	•		GO TO 80
⊦9		83	WRITE(PAPER, 228)RS16(I), RX(I)
<b>;</b> 0	•	228	FORMAT(1H ,26X,F9.4,3X,F8.4)
1		<u></u>	GO TO 80
2	•	87	WRITE(PAPER, 227)SS16(I), SX(I), NU(I), SINT(I), RINT(I), RATIO(I)
13		22.7	FORMAT(1H, 3X, F9.4, 3X, F8.4, 28X, F8.2, 3X, E12.5, 3X, E12.5, 3X, F8.4)
→4 . 	• • • • • •		
15		84 95	$\frac{1}{1} = \frac{1}{1} = \frac{1}$
.7		22E	$\frac{1}{1} = \frac{1}{1} = \frac{1}$
- 1		225	-1000000000000000000000000000000000000
9		86	WRITE(PAPER.226)NU(I).SINT(I).RINT(I).RATIO(I)
۰Ó		226	FORMAT(1H -51X - F8 - 2 - 3X - F12 - 5 - 3X - F12 - 5 - 3X - F8 - 4)
Ĩ		80	NPC=NPC+1
2			IF (52-NPC)64,88,64
3		64	CONTINUE
4	······································	533	CONTINUE
5		С	**** CALL PLOTTING ROUTINE TO PLOT NU(I) AS Y AXIS
•6		C	***** AGAINST RATIO(I) AS X AXIS *****
7			CALL WBPLOT(NU,RATIO,NONU)
8			NG=NG+1
9	•		WRITE(PAPER, 229)
		· · · · · · · · · · · · · · · · · · ·	
•. *			

70       229       FORMATTIERD, WATID VS NU PLOTTED')         71       GO TO (412,412,415), MODE         72       415       MMODE3+MODE3+1         73       GO TO 42       C         74       C       ##### REFERFNCE DATA.       FN MODE3=1 DR MODE3=1 DR MODE GO THROUGH MODE=2 ###         76       92       TFINMIDE3-T193;52;52       FORMATTIEND; WATEGE DATA.       FN MODE3=1 DR MODE3=1         76       GO TO 24       GO TO 24       MINDE3-T193;52;52       FORMATTIEND; WATEGE DATA.       FN MODE3=1 DR MODE3=1         78       MINDE3-MODE3+1       TTIS=2       GO TO 24       FORMATTIEND; WATEGE DATA.       FN MODE3=1         79       GO TO 24       TITINIC, CASUBAL       FORMATTIEND; WATEGE DATA.       FN MODE3=1         71       TTIS=2       GO TO 24       FORMATTIEND; WATEGE DATA.       FN MODE3=1         71       TTIS=2       GO TO 24       FORMATTIEND; WATEGE DATA.       FN MODE3=1         72       FARMATTIEND; WATEGE DATA.       FN MODE3=1       FN MARKER DATA.       AND TO         73       STOP 990       END       FN MARKESULTS OF RHARM, AND TO       FN MARKESULTS OF RHARM, AND TO         73       STOP 990       END       FN MARKESULTS OF RHARM, AND TO       FN MARKESULTS OF RHARM, AND TO         74			
223         FURMATTINO, TRATIDIVS NU PLOITED')           GD TO (402,412,415), MODE           24         MMCDE3=MMODE3+1           37         GD TO 12           38         GD TO 12           39         MCDE3=1193,723,232           30         TEIRMODE3-1193,723,232           31         TISE           32         Call Part Part Part Part Part Part Part Part			
229       FORMATTIHO, TRAID VS NU PLOTTED*)         71       GO TO (412,412,415), MODE         73       CO TO 412         74       CO TO 412         75       C ****** MODE=3 IF MHODE3=0, SET IT TO 1 AND GO BACK FOR         75       C ****** REFERENCE DATA. IF NMODE3=1 DR MORE GO TMRDUGH MODE=2 ****         76       92         77       THOMOE3-1193,52,52         78       MHODE3-SHONDC3+1         78       TTS=2         79       MHODE3-HODG3+1         78       TTS=2         79       GO TO 24         80       43         73       STOP 99         74       END         75       C ******SUBCUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO         76       ******SUBREDUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO         76       *******SUBREDUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO         76       ************************************			
10       229       FURMATTIHO, YKATIO'VS NU PLOTTEP')       4.15         11       GO TO (412,412,415,180)       GO TO 142         12       415       MNODE3=MNODE3+1         13       GO TO 142       415         14       C       #**** MODE3 IF NHODE3=0, SET IT TO 1 AND GO BACK FOR         14       C       #**** MODE3-1 IF NHODE3=0, SET IT TO 1 AND GO BACK FOR         15       GO TO 24       50         16       Y       FURMUE3=1793,52,52         17       3       NHODE3=MNODE3+1         18       TIT15=2       GO TO 24         90       43       CALL PLOTMD         18       HAITE (FAPER,258)NG       2258         22       Z58       FURMATTIHO,14, 'GKAPH(S) PLOTTED')         33       STOP 999       EMD         46       C       ###X## KANE MUGER OF DITTE         47       C ##### ESANE MUGER OF DITTS       ###ANSFORMED WITH         56       C ###### ESANE MUGER OF DITTS       ###ANSFORMED WITH         57       SUBRUTINE CASJUG(F,FX,NUM,FINT(81,93),F(9000),FX(9000),INV(2048)       11         51       INTEGER PAPER       SUBRUTINE CASJUG(F,FX,NUM,FINT(81,93),F(9000),FX(9000),INV(2048)         52       NMMOD CASJUG(7),TITLE(20),HODE,TITS,MMODE3,NAPOD,MABOR	÷ .	an a	
<pre>71 G0 T0 (412,412,415),M0DE 72 415 NMODE3=INNODE3+1 73 G0 T0 412 74 C ***** M0DE+3 IF NMODE3=0, SET IT T0 1 AND G0 BACK FOR 75 C ***** M0DE+3 IF NMODE3=1 DR MORE G0 THROUGH M0DE+2 *** 76 92 IF HTMUDE+T19752-52 77 93 NMODE3+NMODE3+1 78 ITIS=2 79 G0 T0 24 79 G0 T0 24 70 C ALL PLOTND 70 WRITE(PAPER,258)NG 71 WRITE(PAPER,258)NG 72 C ******SUBROUTINE T0 ARRANGE DATA FOR RHARM,CALLRHARM, AND T0 73 STOP 99 74 END 75 C *****SUBROUTINE T0 ARRANGE DATA FOR RHARM,CALLRHARM, AND T0 76 ***** SUBROUTINE T0 ARRANGE DATA FOR RHARM,CALLRHARM, AND T0 76 ******SUBROUTINE T0 ARRANGE DATA FOR RHARM,CALLRHARM, AND T0 77 ******SUBROUTINE T0 ARRANGE DATA FOR RHARM,CALLRHARM, AND T0 78 ******SUBROUTINE T0 ARRANGE DATA FOR RHARM,CALLRHARM, AND T0 78 ******SUBROUTINE T0 ARRANGE DATA FOR RHARM,CALLRHARM, AND T0 79 *******SUBROUTINE CASUAL SUBLE AND REFERENCE DATA ARE TRANSFORMED NITH 79 SUBROUTINE CASUALG(F,FX,NUM,FITN,TNU,**,**) 70 DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048) 71 INFEGE PAPER 74 COMMON COMP(20),TITLE(20),M0DE,TTIS,NMODE3,NAPOD,NABORT,RESUL, 75 INONU,DELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN 76 MPAPER 77 NP+0 78 NP+0 79 NM=0 70 D0 4 T=1,NUM 71 IF(FX(1))5,6,7 72 NPAPEN+1 73 G0 T0 4 74 CONTINUE 74 CONTINUE 75 NN=NN+1 76 C ***** FOR SPECTRA T0 BE RATIOED AGAINST EARLIER SPECTRA SET 79 C ***** THINGS UP S0 THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN 71 NPC5 72 *NN=N+1 73 NFS=2*N HEAC ***** 73 NFS=2*NHAP2+NZ 73 NFS=2*NHAP2+NZ 73 NFS=2*NHAP2+NZ 73 NFS=2*NHAP2+NZ 73 NFS=2*NHAP2+NZ 73 NFS=2*NHAP2+NZ 73 NFS=2*NHAP2+NZ 74 WRITE (PAPER,201) MODE,NMODE3 70 IF(NP-NM)71,72,72 73 NFS=2*NHAP2+NZ 73 NFS=2*NHAP2+NZ 73 NFS=2*NHAP2+NZ 73 NFS=2*NHAP2+NZ 73 NFS=2*NHAP2+NZ 73 NFS=2*NHAP2+NZ 74 WRITE (PAPER,201) MODE,NMODE3 75 C *FX+2*NZ 75 NFS=2*NHAP2+NZ 75 NFS=2*N</pre>	70	229	FURMATTINO, RATIO VS NU PLOTTED")
22       415       NMODE3=IMMODE3+I         3       GO TO 412       ****** MODE3=IF NMODE3=0, SET IT TO 1 AND GO BACK FOR         74       C       ****** MODE3+I         75       C       ****** MODE3+I         76       IFTENDUG5+ITY3;52;52       NMODE3+I         78       NMODE3=NMODE3+I       ITTS=2         79       SO TO 24       GO TO 24         80       43       CALL PLOTNO         81       ITIS=2       FORMATICHD;14, GRAPHIS) PLOTTED*I         73       STOP 999       END         74       C       *****SUBRDUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO         75       C       *****SUBRDUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO         76       C       *****SUBRDUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO         77       C       ******EURSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED NITH         78       SUBROUTINE CASUG(F,FX:NUM,FINT,NU,**)       D         79       DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048)       1         74       COMMON COMP(20),TITLE(20),MODE,TTIS,NMODE3,NAPOD,NABORT,RESOL,         74       COMMON COMP(20),TITLE(20),MODE,TTIS,NMODE3,NAPOD,NABORT,RESOL,         75       NP=0       NP=0         76 <td< td=""><td>71</td><td></td><td>GO TO (412,412,415),MODE</td></td<>	71		GO TO (412,412,415),MODE
3         GO 10 412           4         ****** MDDE=3         IF NMODE3=1 OR NORE GO THROUGH MODE2           75         C         ****** REFERENCE DATA. IF NMODE3=1 OR MORE GO THROUGH MODE2           75         C         *****           76         C         *****           77         O         O         O           77         O         O         O         C           77         O         O         O         24           78         INTDE3=         MODE3=1         Ints=2           79         C         C         *****           79         CALL PLOTND         WRITE(PAPER,258)NG           82         SIDP 99         MADE3         SIDP 99           54         END         SIDP 99           55         SIDP 99         MADE3         C           76         C         *****         SUBROUTINE TO ARRANGE DATA FOR RHARM.CALLRHARM. AND TO           76         C         ****         SUBROUTINE TO ARRANGE DATA FOR RHARM.CALLRHARM. AND TO           77         C         ****         SUBROUTINE TO ARRANGE DATA FOR RHARM.CALLRHARM. AND TO           77         SUBROUTINE CASJUG(F,FX,NUH,FINT,KU,***)         D         D	72	415	NMODE3=NMODE3+1
<pre>/4 C ##### MDUE3 IF NMODE3=0, SET IT ID I AND GO BACK FOR *#### REFERENCE DATA. IF NMODE3=1 OR MORE GO THROUGH MODE=2 *** 79 VMODE3=NNODE3+1 78 ITIS=2 79 GO TO 24 79 GO TO 24 79 WARTEF(PAPER,258)NC 70 GO TO 24 70 STOP 99 70 WARTEF(PAPER,258)NC 70 C *****CALCULATE INT(NU) AND NU FROM RESULTS OF RHARM, AND TO 70 ##### ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED NITH 71 C ****** ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED NITH 72 C ****** ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED NITH 73 C ****** ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED NITH 74 END 75 C ****** ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED NITH 75 C ****** ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED NITH 76 C ****** ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED NITH 76 C ****** ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED NITH 76 C ****** ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED NITH 76 C ****** ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED NITH 76 DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048) 76 DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048) 77 NPONUCOMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPDD,NABORT,RESOL, 78 NNDNU,DEX,LPAGE,YPAGE,NG,MOVE,XMAX,XMIN 79 NNDU,DEX,LPAGE,YPAGE,NG,MOVE,XMAX,XMIN 70 DA TET,NUM 71 IF(F(KI1))5.6,7 72 S NM=NM+1 73 GO TO 4 74 CONTINUE 74 CONTINUE 75 OD 74 CONTINUE 75 OD 74 CONTINUE 76 TATA THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN 77 NPOS-2*MP+M2 76 C ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN 78 NROSS-2*MP+M2 79 C ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN 79 NROSS-2*MP+M2 70 IF(RMSS-MES)774,41,41 71 NROSS-2*MP+M2 73 NROSS-2*MP+M2 74 WRITE (PAPER,201) MODE,NMODE3 74 WRITE (PAPER,201) MODE,NMODE3 75 CO TO 73 75 OT 74 76 FORMAT(1H0, 'INSUFFICIENT POINTS TAKEN, MODE=',14,' NMODE3=',14 77 NROSS-2*MP+M2 75 CO TO 74 75 OF 74 WRITE (PAPER,201) MODE,NMODE3 75 CO TO 74 75 OF 74 WRITE (PAPER,201) MODE,NMODE3 75 CO TO 74 75 OF 74 WRITE (PAPER,20</pre>	73	~	GO TO 412
C       ##### REFERENCE DATA. IF NMUDE=I DR MORE GD IHROUGH MDDE=2 *##         75       92       IF(TMUDE=3-1)#352,52         77       93       NMODE3=NMODE3+1         78       ITIS=2         79       GD TO 24         79       GD TO 24         79       GD TO 24         79       GD TO 24         79       STOP 999         81       WRITE(PAPER,258)NG         70       STOP 999         84       END         70       C         71       NETTO P99         72       ******SUBROUTINE TO ARRANGE DATA FOR RHARM,CALLRHARM, AND TO         73       STOP 999         84       END         74       END         75       ******ENSURE THAT SAMPUE AND REFERENCE DATA ARE TRANSFORMED WITH         76       C#******ENSURE THAT SAMPUE AND NEFRERENCE DATA ARE TRANSFORMED WITH         76       DIMENSION FTOATA(16388),FINT(8193),F(9000),FX(9000),INV(2048)         77       NPEO         78       REAL NU(8195)         79       INTEGER PAPER         70       MPEO         71       IF(FX(1))5,6,7         72       NM=NM-1         73       GO TO 4      <	14	C	***** MUDE=3 IF NMODE3=0, SET IT TO 1 AND GO BACK FOR
10       92       IF NUMBERS 1795,22         17       93       NMODES = NUMDES 11         18       ITIS=2         19       GO TO 24         20       43       CALL PLOTND         94       END         258       FURMATTIHO,14, 'GRAPH(S) PLOTTED')         33       STOP 999         44       END         258       FURMATTIHO,14, 'GRAPH(S) PLOTTED')         34       CALL PLOTND         94       END         258       FURMATTIHO,14, 'GRAPH(S) PLOTTED')         35       STOP 999         46       Camaxa Subrowski Standard S	15 77	<i>ل</i>	****** REFERENCE DATA. IF NMUDE3=1 OR MORE GO THROUGH MODE=2 ***
78       ITTIS=2         79       GO TO 24         70       GO TO 24         71       WRITE(PAPER,258)NG         72       SUBROUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO         73       STOP 999         74       END         75       C *****SUBROUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, ALSO TO         76       CUMMON TINE CAS JUG(F,FX,NUM,FINTN,U,**)         76       SUBROUTINE CAS JUG(F,FX,NUM,FINTN,U,**)         77       SUBROUTINE CAS JUG(F,FX,NUM,FINTN,U,**)         78       SUBROUTINE CAS JUG(F,FX,NUM,FINTN,U,**)         79       NPE         70       NPERE         71       INFEGE PAPER         72       COMMON COMP(20), TITLE(20), MODE, TITS, NMODE3, NAPOD,NABGRT,RESUL,         79       NP=0         70       NPERE         71       NPERE         72       NM=0         73       GO TO 4         74       COMMON COMP(20), TITLE(20), MODE AGAINST EARLIER SPECTRA SET	10 77	92	
GO         TO         24           GO         43         CALL PLOTND           WRITE (PAPER,258)NG         XILPLOTND           STOP 999         STOP 999           STOP 999         Stop 999           C         ******CALCULATE INT(NU) AND NU FROM RESULTS OF RHARM, ALSO TO           C         ******CALCULATE INT(NU) AND NU FROM RESULTS OF RHARM, ALSO TO           C         *******CALCULATE INT(NU) AND NU FROM RESULTS OF RHARM, ALSO TO           C         *******CALCULATE INT(NU) AND RUFERENCE DATA ARE TRANSFORMED WITH           B0         C*******CALCULATE INT(NU) AND RUFERENCE DATA ARE TRANSFORMED WITH           B1         ********           B2         SUBROUTINE CASJUG(F,FX,NUM,FINT,NU,**)           D0         DIMENSION FDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048)           P1         1,5 (2048)           P1         1,5 (2048)           P2         REAL NU(8195)           NNNO,DELX,LPAGE,XPAGE,NGY,MOVE,XMXX,XMIN           PAPER         PAPER           P3         NDNU,DELX,LPAGE,XPAGE,NGY,MOVE,XMXX,XMIN           PAPER=6         NP=0           P3         NM=0           D0         D0           D0         4           P4(FX(1))5,6+7           P2         NM	11. 78		
43       CALL PLOTND         NRITE (PAPER, 258)NG         82       258         82       FORMATITHO,14, 'GRAPH(S) PLOTTED')         83       STOP 999         84       END         85       C       *****SUBROUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO         86       C       *****CALCULATE INT(NU) AND NU FROM RESULTS OF RHARM, ALSO TO         87       C       *****ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED WITH         88       C       *****ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED WITH         89       SUBROUTINE CAS JUG (F, FX, NUM, FLINT, NU, **)         90       DIMENSION FTDATA(16388), FINT(8193), F(9000), FX(9000), INV(2048)         91       1, S(2048)         92       REAL NU (8195)         93       INTECER PAPER         94       COMMON COMP(20), TITE(20), MODE, ITTS, NMODE3, NAPOD, NABORT, RESOL,         95       INGNU, DELX, LPAGE, XPAGE, NG, MOVE, XMAX, XMIN         96       NP=0         97       NP=0         98       NZ=0         99       NM=0         90       DU 4 1=1, NUM         91       IF(FX(1))5,647         92       SUBRONCIONE SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         9	79		GO TO 24
WRITE(PAPER,258)NG         2258       FORMAT(TH0;14, 'GRAPH(S) PLOTTED')         33       STOP 999         84       END         85       C       *****SUBROUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO         86       C       *****CALCULATE INT(NU) AND NU FROM RESULTS OF RHARM, ALSO TO         87       C       *****CALCULATE INT(NU) AND NU FROM RESULTS OF RHARM, ALSO TO         88       C       *****CALCULATE INT(NU) AND NU FROM RESULTS OF RHARM, ALSO TO         89       SUBROUTINE CASJUG(F,FX,NUM,FINT,NU,**)         90       DIMENSION FTDATA(1638B),FINT(8193),F(9000),FX(9000),INV(2048)         91       1,S(2048)         92       REAL NU(8195)         93       INTECER PAPER         94       COMMON COMP(20),TITLE(20), MODE,TTIS,NMODE3,NAPOD,NABORT,RESOL,         95       INOULDELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN         96       N2=0         97       NP=0         98       N2=0         99       NM=0         90       DIMENSH         91       IF(FX(1))5,6,7         92       S         93       GO TO 4         94       GO TO 4         95       GO TO 4         96       CANENCH	80	43	
22       258       FORMAT(IH0,14,'GRAPH(S) PLOTTED')         33       STOP 999         4       END         35       C       *****SUBROUTINE TO ARRANGE DATA FOR RHARM,CALLRHARM, AND TO         36       C       *****SUBROUTINE TO ARRANGE DATA FOR RHARM,CALLRHARM, AND TO         37       C       *****SUBROUTINE TO ARRANGE DATA FOR RHARM,CALLRHARM, AND TO         38       SUBROUTINE CASJUG(F,FX,NUM,FIINT,NU,**)         39       SUBROUTINE CASJUG(F,FX,NUM,FIINT,NU,**)         30       DIMENSION FTDATA(I6388),FINT(8193),F(9000),FX(9000),INV(2048)         31       1,S(2048)         32       REAL NU(8195)         33       INTEGER PAPER         34       COMMON COMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPOD,NABORT,RESOL,         36       NPAC         37       NPAC         38       N2=0         39       NP=0         30       D0 4         31       IF(FX(1))5,6,7         32       S         34       CONTINUE         35       MORUMAL         36       OT 4         36       GO TO 4         37       GO TO 4         38       CONTINUE         39       NP=0 <td>31</td> <td></td> <td>WRITE(PAPER • 258)NG</td>	31		WRITE(PAPER • 258)NG
33       STOP 999         84       END         85       C       *****SUBROUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO         86       C       *****SUBROUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, ALSO TO         87       C       *****CALCULATE INT(NU) AND NU FROM RESULTS OF RHARM, ALSO TO         88       C       *****CALCULATE INT(NU) AND NU FROM RESULTS OF RHARM, ALSO TO         89       SUBROUTINE CASJUG(F,FX,NUM,FINT,NU,***)         89       SUBROUTINE CASJUG(F,FX,NUM,FINT,NU,***)         90       DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048)         91       1,S(2048)         92       REAL NU(8195)         93       INTEGER PAPER         94       COMMON COMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPOO,NABORT,RESOL,         95       INOMU,DELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN         96       N2=0         97       NP=0         98       N2=0         90       DUM FRIEND         91       IF(FK(1))5,6,7         92       NM=0         93       GO TO 4         94       6         95       NM=NM+1         96       N2=NZ         97       N=0         98       N2=NZ	82		FORMAT(IHO, 14, 'GRAPH(S) PLOTTED')
84       END         35       C       *****SUBROUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO         86       C       *****CALCULATE INTINU) AND NU FROM RESULTS OF RHARM. ALSO TO         87       C       *****CALCULATE INTINU) AND NU FROM RESULTS OF RHARM. ALSO TO         87       SUBROUTINE CASJUG(F,FX,NUM,FINT,NU,**)         89       SUBROUTINE CASJUG(F,FX,NUM,FINT,NU,**)         90       DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048)         91       1,S(2048)         92       REAL NU(8195)         93       INTEGER PAPER         94       COMMON COMP(20),TITLE(20),MODE,ITIS,NMMODE3,NAPOD,NABORT,RESOL,         95       INONU,DELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN         96       PAPER=6         97       NP=0         98       NZ=0         99       NM=0         90       DU 4 I=1,NUM         91       IF(FX(1))5,6,7         92       GO TO 4         93       GO TO 4         94       CONTINUE         95       GO TO 4         96       N=0         97       NP=NP+1         97       C         98       NZ=0         99       SUB FOR SPECTRA TO BE	B3		STOP 999
35       C       *****SUBROUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO         86       C       *****CALCULATE INT(NU) AND NU FROM RESULTS OF RHARM, ALSO TO         37       C       ******THE SAME THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED WITH         88       C       ******         89       SUBROUTINE CASJUG(F,FX,NUM,FINT,NU,*,*)         90       DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048)         91       1,S(2048)         92       REAL NU(8195)         93       INTEGER PAPER         94       COMMON COMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPOD,NABORT,RESOL,         95       INDINU,DELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN         96       PAPER=6         97       NP=0         98       N2=0         90       D0         91       IF(FX(1))5,6,7         92       NM=NM+1         93       GO TO 4         94       ACONTINUE         95       GO TO 4         96       NP=NP+1         97       ACONTINUE         98       C         99       N=N=N+1         91       GO TO 4         92       GO TO 4         93       GO TO 4	84	•	END
86       C       *****CALCULATE INTINU) AND NU FROM RESULTS OF RHARM. ALSO TO         37       C       ***** ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED WITH         88       C       ******THE SAME NUMBER OF POINTS, *****         89       SUBROUTINE CASJUG(F,FX,NUM,FINT,NU,*,*)         90       DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048)         91       1,S(2048)         92       REAL NU(8195)         93       INTEGER PAPER         94       COMMON COMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPOD,NABORT,RESOL,         95       INDNU,DELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN         96       PAPER=6         97       NP=0         98       NZ=0         99       NM=0         10       IF(FX(1))5,6,7         25       NM=NH+1         23       GO TO 4         24       6       NZ=NZ=N1         25       GO TO 4         26       TO NPENPT1         27       4       CONTINUE         28       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         29       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         29       C       ****** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET </td <td>35</td> <td>С</td> <td>*****SUBROUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO</td>	35	С	*****SUBROUTINE TO ARRANGE DATA FOR RHARM, CALLRHARM, AND TO
37       C       ***** ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED WITH         88       C       *****THE SAME NUMBER OF POINTS. *****         89       SUBROUTINE CASJUG(F,FX,NUM,FINT,NU,*,*)         90       DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048)         91       1,S(2048)         92       REAL NU(8195)         93       INTEGER PAPER         94       COMMON COMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPOD,NABORT,RESOL,         95       INNOU,DELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN         96       PAPER=6         97       NPER=6         97       NPEN=0         98       NZ=0         99       NM=NM+1         91       IF(fX(1))5,6,7         92       S         93       OD 4         94       CONTINUE         95       NM=NM+1         96       OD 4         97       N=N=N+1         93       GO TO 4         94       6         97       NP=NP+1         97       4         98       NZ=0         99       N=N=N+1         90       GO TO 4         916       TPENP+1	86	С	*****CALCULATE INT(NU) AND NU FROM RESULTS OF RHARM. ALSO TO
68       C       *****THE SAME NUMBER OF POINTS, *****         89       SUBROUTINE CASJUG(F,FX,NUM,FINT,NU,*,*)         90       DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048)         91       1,S(2048)         92       REAL NU(8195)         93       INTEGER PAPER         94       COMMON COMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPOD,NABORT,RESOL,         95       INDMU,DELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN         96       PAPER=6         97       NP=0         98       NZ=0         99       NM=0         90       D0 4 [=1,NUM         91       IF(FX(1))5,6,7         92       S         93       NV=0         94       CONTON         95       NM=0         96       NZ=0         97       NP=0         98       NZ=0         99       NM=0         91       IF(FX(1))5,6,7         92       S         93       ND=0         94       6         95       ND=0         96       NZ=NZ+1         97       GO TO 4         98       CONTINUE         98	37	С	***** ENSURE THAT SAMPLE AND REFERENCE DATA ARE TRANSFORMED WITH
<pre>89 SUBROUTINE CASJUG(F,FX,NUM,FINT,NU,*,*) 90 DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048) 91 1,S(2048) 92 REAL NU(8195) 93 INTEGER PAPER 94 COMMON COMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPOD,NABORT,RESOL, 95 INONU,DELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN 96 PAPER=6 97 NP=0 98 NZ=0 99 NM=0 90 D0 4 I=1,NUM 91 IF(FX(I))5,6,7 92 S NM=NM+1 93 GO TO 4 94 CONTINUE 95 GO TO 4 96 A NZ=NZ+1 97 CONTINUE 98 C ***** FOR SPECTRA TO BE RATIDED AGAINST EARLIER SPECTRA SET 99 C ***** FOR SPECTRA TO BE RATIDED AGAINST EARLIER SPECTRA SET 99 C ***** FOR SPECTRA TO BE RATIDED AGAINST EARLIER SPECTRA SET 99 C ***** FOR SPECTRA TO BE RATIDED AGAINST EARLIER SPECTRA SET 99 C ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN 10 C #X*** ON EACH ***** 11 GO TO (1,2,3),MODE 12 Z GO TO(1,70),111S 13 TO IF(NP=NM)71,72,72 14 T1 NROSS=2*NP+NZ 15 GO TO 73 16 T2 NROSS=2*NP+NZ 17 NFS=2*N 18 IF(NROSS=NFS)74,41,41 19 T4 WRITE(PAPER,201) MODE,MODE3 20 Z FORMAT(1H0,'INSUFFICIENT POINTS TAKEN. MODE=',14,'NMODE3=',14) 21 WRITE (PAPER,204)MODE,MODE3 22 41 WRITE (PAPER,204)MODE,MODE3 23 Z04 FORMAT(1H0,'DATA IS COMPATIBLE. MODE=',14,'NMODE3=',14)</pre>	88	C	*****THE SAME NUMBER OF POINTS. *****
0       DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048)         91       1,S(2048)         92       REAL NU(8195)         93       INTEGER PAPER         94       COMMON COMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPOD,NABORT,RESOL,         95       NONU,DELX,LPAGE,XPAGE,NO,MOVE,XMAX,XMIN         96       PAPER=6         97       NP=0         98       NZ=0         99       NM=0         30       D0 4 I=1,NUM         31       IF(FX(1))5,6,7         32       G0 TO 4         34       6         40       NZ=NZ+1         35       G0 TO 4         36       T         37       NP=NP+1         37       A CONTINUE         38       C         39       NZ=NZ+1         30       G0 TO 4         34       6         36       7         4       CONTINUE         37       GO TO 4         38       C         4       GO TO (1,2,3),MODE         37       IF(PP-NN)T1,72,72         38       GO TO 73         39       IF(NROSS=2*NP+NZ         3	89.	· · ·	SUBROUTINE CASJU6(F,FX,NUM,FINT,NU,*,*)
91       1,S(2048)         92       REAL NU(8195)         93       INTEGER PAPER         94       COMMON COMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPOD,NABORT,RESOL,         95       1NONU,DELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN         96       PAPER=6         97       NP=0         98       NZ=0         99       NM=0         30       D0 4 I=1,NUM         31       IF(FX(1))5,6,7         25       NM=NM+1         33       G0 T0 4         34       G0 T0 4         35       G0 T0 4         36       NZ=NZ+1         37       CONTINUE         38       C         74       CONTINUE         37       GO T0 4         38       C         39       NEONTINUE         30       GO T0 4         31       GO T0 4         32       CO T0 4         33       GO T0 4         34       GO T0 (1,2,3),MODE         35       GO T0 (1,2,3),MODE         36       T IF(NP-NN'T1,72,72         37       NFS=2*NP+NZ         37       NFS=2*NP+NZ         37 <t< td=""><td><del>9</del>0</td><td></td><td>DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048)</td></t<>	<del>9</del> 0		DIMENSION FTDATA(16388),FINT(8193),F(9000),FX(9000),INV(2048)
22       REAL NU(8195)         33       INTEGER PAPER         34       COMMON COMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPOD,NABORT,RESOL,         35       INDNU,DELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN         36       PAPER=6         37       NP=0         38       NZ=0         39       NM=0         30       D0         31       IF(FX(1))5,6,7         32       GO TO 4         33       GO TO 4         34       6         35       GO TO 4         36       NP=NP+1         37       Y=NP+1         36       GO TO 4         37       NP=NP+1         38       NZ=0         39       GO TO 4         39       GO TO 4         30       GO TO 4         316       7         317       NP=NP+1         318       C         319       C         319       C         329       C         320       CO 11,2,3,MODE         321       CO 11,70,1,115         323       CO 10 73         324       GO TO 73         325       <	91		1,5(2048)
93       INTEGER PAPER         94       COMMON COMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPOD,NABORT,RESOL,         95       INONU,DELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN         96       PAPER=6         97       NP=0         98       NZ=0         99       NM=0         30       D0 4 1=1,NUM         31       IF(FX(1))5,6,7         32       S         33       G0 TO 4         34       AZ=0         35       NM=NM+1         36       GO TO 4         37       NP=NP+1         38       GO TO 4         39       C         39       C         30       GO TO 4         31       GO TO 4         32       GO TO 4         33       GO TO 4         34       C         35       GO TO 4         36       Y         37       Y         38       Y         39       C         4       CONTINUE         38       C         4       CONTINUE         39       C         4       TO (1,2,3),MODE	92		REAL NU(8195)
94       COMMON COMP(20),TITLE(20),MODE,ITIS,NMODE3,NAPOD,NABORT,RESOL,         95       INONU,DELX,LPAGE,XPAGE,NG,MOVE,XMAX,XMIN         96       PAPER=6         97       NP=0         98       NZ=0         99       NM=0         50       DO 4 [=1,NUM         51       IF(FX(1))5,6,7         52       NM=NM+1         53       GO TO 4         54       6         55       GO TO 4         56       GO TO 4         57       Y=NP=NP+1         58       C         59       C         50       GO TO 4         516       GO TO 4         52       GO TO 4         53       GO TO 4         54       C         57       Y=X=X*         58       C         59       C         59       C         50       THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         50       TO (1,2,3),MODE         52       GO TO (1,2,3),MODE         52       GO TO 73         53       GO TO 73         54       GO TO 73         56       TF (NROSS=NFS)	93	· · ·	INTEGER PAPER
95       INDRO, DELX, LPAGE, NG, MOVE, XMAX, XMIN         96       PAPER=6         97       NP=0         98       NZ=0         99       NM=0         50       DO 4 J=1,NUM         51       IF(FX(I))5,6,7         52       S         53       GO TO 4         64       NZ=NZ+1         55       GO TO 4         64       NZ=NZ+1         55       GO TO 4         56       GO TO 4         74       CONTINUE         75       GO TO 4         76       YPENP+1         77       4         74       CONTINUE         75       GO TO 4         76       YMENCH         77       YPENP+1         77       4         70       NPENP+1         71       GO TO (1,2,3), MODE         72       GO TO (1,2,3), MODE         72       GO TO (1,2,3), MODE         73       NFS=2*NP+NZ         74       NROSS=2*NP+NZ         75       GO TO 73         76       TF(NPOSS=NFS)74,41,41         77       NFS=2*N         78       <	94		COMMON COMP(20), TITLE(20), MODE, ITIS, NMODE3, NAPOD, NABORT, RESOL,
96       PAPER=6         97       NP=0         98       NZ=0         99       NM=0         50       D0 4 i=1,NUM         51       IF(FX(I))5,6,7         52       S         53       G0 TO 4         54       A         55       G0 TO 4         56       G0 TO 4         57       A         56       G0 TO 4         57       A         57       GO TO 4         58       G0 TO 4         59       GO TO 4         50       GO TO 4         57       4         58       C         59       C         50       CO TO TA         50       CO TO TINUE         50       CO TO TA         50       CO TO TA         51       GO TO TO TA, ANDE         52       GO TO TA         52       GO TO TA         53       GO TO TA         54       TH (NP-NM)71,72,72         54       TA NROSS=2*NP+NZ         55       GO TO 73         56       GO TO 73         57       FORMAT(1HO,*IN	95	•	INUNU, DELX, LPAGE, XPAGE, NG, MUVE, XMAX, XMIN
98       NZ=0         99       NM=0         00       D0 4 I=1,NUM         01       IF (FX(I))5,6,7         02       5         03       G0 T0 4         04       6         05       G0 T0 4         06       7         07       A         08       07         09       NPENP+1         07       4         07       4         08       ******         09       C         ******       FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C         *****       FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C         *****       FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C         *****       FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         00       C         *****       FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         00       C       *****         10       C       *****         11       GO TO (1,2,3),MODE         12       GO TO 73         13       TO IF (NP-NM)71,72,72 <td>36</td> <td></td> <td></td>	36		
70       NZ=0         99       NM=0         50       D0 4 I=1,NUM         11       IF(FX(I))5,6,7         52       5         72       5         NM=NM+1         33       GO TO 4         64       6         75       GO TO 4         76       7         76       7         77       4         70       4         71       4         72       5         74       CONTINUE         75       GO TO 4         76       7         77       4         70       7         70       8         71       7         70       7         70       17         70       17         71       NROSS=2*NP+NZ         72       GO TO 73         73       NFS=2*N         74       WRITE (PAPER,201) MODE,NMODE3         70       17         74       WRITE (PAPER,201) MODE,NMODE3         70       201         74       WRITE (PAPER,204)MODE,NMODE3         75       204 </td <td>28</td> <td></td> <td></td>	28		
30       D0 4 1=1,NUM         31       IF(Fx(1))5,6,7         32       G0 T0 4         34       6         36       G0 T0 4         36       G0 T0 4         37       G0 T0 4         38       G0 T0 4         39       G0 T0 4         39       G0 T0 4         30       G0 T0 4         31       G0 T0 4         36       G0 T0 4         37       4         CONTINUE       Sec         38       C ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         39       C ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         10       C ***** ON EACH *****         11       G0 T0 (1,2,3),MODE         12       G0 T0 (1,2,3),MODE         12       G0 T0 (1,70,TITS         13       70         14       71         15       G0 T0 73         16       72         17       3         18       IF(NROSS=NFS)74,41,41         19       74         19       74         10       FORMAT(1H0, 'INSUFFICIENT POINTS TAKEN.         11       G0 T0 42 <td>20</td> <td>· · ·</td> <td>NZ = 0</td>	20	· · ·	NZ = 0
1       IF (FX(I))5,6,7         2       5       NM=NM+1         03       GO TO 4         04       6       NZ=NZ+1         05       GO TO 4         06       7       NP=NP+1         07       4       CONTINUE         08       C       ****** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C       ****** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         10       C       ****** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         10       C       ****** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         10       C       ****** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         10       C       ****** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         10       C       ****** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         10       C       ****** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         11       GO TO (1,2,3),MODE       [12       2         12       GO TO 73       [14         13       70       IF (NPONS=2*NP*NZ         14       71       NROSS=2*NP+NZ         15       GO TO 42       [14]         16       72	50		DO 4 I=1.NUM
5       NM=NM+1         03       GO TO 4         04       6       NZ=NZ+1         05       GO TO 4         07       4       CONTINUE         08       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         08       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         10       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         10       C       ****** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         11       GO TO (1,2,3), MODE       1         12       GO TO 73       1         13       TO IF (NP-NM)71,72,72       1         14       TO NESS=2*NP+NZ       1         16       T2 NROSS=2*NF\$\$774,41,41<	01	•	IF(FX(1))5,6,7
3       GO TO 4         34       6       NZ=NZ+1         35       GO TO 4         36       7       NP=NP+1         37       4       CONTINUE         38       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         39       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         30       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         30       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         31       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         32       C       ****** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         33       CONTINUE       Set	)2	5	NM = NM + 1
04       6       NZ=NZ+1         05       GO TO 4         06       7       NP=NP+1         07       4       CONTINUE         08       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         01       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         00       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         01       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         02       GO TO (1,2,3),MODE       C         12       GO TO (1,2,3),MODE       C         13       70       IF (NP-NM)71,72,72         14       71       NROSS=2*NP+NZ         15       GO TO 73       C         16       72       NROSS=2*NM+2*NZ         17       73       NFS=2*N         18       IF (NROSS=NFS)74,41,41         19       74       WRITE (PAPER,201) MODE,NMODE3         20       201       FORMAT(1HO, 'INSU	03		GO TO 4
D5       GO TO 4         J6       7       NP=NP+1         D7       4       CONTINUE         D8       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         D9       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         D9       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         D9       C       ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         10       C       ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         10       C       ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         10       C       ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         10       C       ***** ON EACH *****         11       GO TO (1,2,3), MODE         12       Z       GU TU(1,70), ITIS         13       70       IF (NP-NM)71,72,72         14       71       NROSS=2*NP+NZ         15       GO TO 73         16       TF (NROSS=NFS)74,41,41         17       73       NFS=2*N         18       IF (NROSS=NFS)74,41,41         19       74       WRITE (PAPER,201) MODE,NMODE3         20       201       FORMAT(1HO,'INSUFFICIENT POINTS TA	)4	6	NZ=NZ+1
36       7       NP=NP+1         37       4       CONTINUE         38.       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         39       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         39       C       ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         10       C       ***** ON EACH *****         11       G0 TO (1,2,3),MODE         12       2       GU TO(1,70),ITIS         13       70       IF (NP-NM)71,72,72         14       71       NROSS=2*NP+NZ         15       GO TO 73         16       72       NROSS=2*NP+NZ         17       73       NFS=2*N         18       IF (NROSS-NFS)74,41,41         19       74       WRITE (PAPER,201) MODE,NMODE3         20       201       FORMAT(1H0,'INSUFFICIENT POINTS TAKEN.       MODE=',I4,' NMODE3=',I4)         21       GO TO 42       22       41       WRITE (PAPER,204)MODE,NMODE3         23       204       FORMAT(1H0,'DATA IS COMPATIBLE.       MODE=',I4,' NMODE3=',I4)	<b>)5</b> .		GO TO 4
07       4       CONTINUE         08       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         09       C       ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         10       C       ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         10       C       ***** ON EACH *****         11       GO TO (1,2,3), MODE         12       2       GU TU(1,70), ITIS         13       70       IF (NP-NM)71,72,72         14       71       NROSS=2*NP+NZ         15       GO TO 73         16       72       NROSS=2*NM+2*NZ         17       73       NFS=2*N         18       IF (NROSS=NFS)74,41,41         19       74       WRITE (PAPER,201) MODE,NMODE3         20       201       FORMAT(1HO,'INSUFFICIENT POINTS TAKEN.       MODE=', I4,' NMODE3=', I4)         21       GO TO 42       22       41       WRITE (PAPER,204)MODE,NMODE3         23       204       FORMAT(1HO,'DATA IS COMPATIBLE.       MODE=', I4,' NMODE3=', I4)	76	7	NP=NP+1
38.       C       ***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET         39       C       ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         10       C       ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         10       C       ***** ON EACH *****         11       GO TO (1,2,3),MODE         12       2       GO TO (1,70),ITIS         13       70       IF (NP-NM)71,72,72         14       71       NROSS=2*NP+NZ         15       GO TO 73         16       72       NROSS=2*NP+NZ         17       73       NFS=2*N         18       IF (NROSS=NFS)74,41,41         19       74       WRITE (PAPER,201)         19       74       WRITE (PAPER,201)         19       74       WRITE (PAPER,201)         201       FORMAT(1H0, 'INSUFFICIENT POINTS TAKEN.       MODE=', I4, ' NMODE3=', I4)         21       GO TO 42       22         22       41       WRITE (PAPER,204)MODE,NMODE3         23       204       FORMAT(1H0, 'DATA IS COMPATIBLE.       MODE=', I4, ' NMODE3=', I4)	27	. 4	CONTINUE
J9       C       ***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN         10       C       ***** ON EACH *****         11       GO TO (1,2,3),MODE         12       2       GU TU(1,70),ITIS         13       70       IF (NP-NM)71,72,72         14       71       NROSS=2*NP+NZ         15       GO TO 73         16       72       NROSS=2*NM+2*NZ         17       73       NFS=2*N         18       IF (NROSS=NFS)74,41,41         19       74       WRITE (PAPER,201) MODE,NMODE3         20       201       FORMAT(1HO,'INSUFFICIENT POINTS TAKEN. MODE=',14,' NMODE3=',14)         21       GO TO 42         22       41       WRITE (PAPER,204)MODE,NMODE3         23       204       FORMAT(1HO,'DATA IS COMPATIBLE. MODE=',14,' NMODE3=',14)	38	C	***** FOR SPECTRA TO BE RATIOED AGAINST EARLIER SPECTRA SET
10       C       ***** ON EACH *****         11       GO TO (1,2,3),MODE         12       2       GO TO (1,70),ITIS         13       70       IF (NP-NM)71,72,72         14       71       NROSS=2*NP+NZ         15       GO TO 73         16       72       NROSS=2*NM+2*NZ         17       73       NFS=2*N         18       IF (NROSS=NFS)74,41,41         19       74       WRITE (PAPER,201) MODE,NMODE3         20       201       FORMAT(1H0,'INSUFFICIENT POINTS TAKEN. MODE=',I4,' NMODE3=',I4)         21       GO TO 42         22       41       WRITE (PAPER,204)MODE,NMODE3         23       204       FORMAT(1H0,'DATA IS COMPATIBLE. MODE=',I4,' NMODE3=',I4)	<u> </u>	C	***** THINGS UP SO THAT WE HAVE THE SAME NUMBER OF POINTS TAKEN
GU TU (1,2,3),MUDE         I2       GU TU(1,70),ITIS         I3       70       IF (NP-NM)71,72,72         I4       71       NROSS=2*NP+NZ         I5       GO TO 73         I6       72       NROSS=2*NM+2*NZ         I7       73       NFS=2*N         I8       IF (NROSS=NFS)74,41,41         I9       74       WRITE (PAPER,201)         MODE,NMODE3       201         FORMAT(1H0,'INSUFFICIENT POINTS TAKEN.       MODE=',I4,' NMODE3=',I4)         21       GO TO 42         22       41       WRITE (PAPER,204)MODE,NMODE3         23       204       FORMAT(1H0,'DATA IS COMPATIBLE.	10	ι L	***** UN EACH *****
<pre>12 2 GO TO(1,70),1115 13 70 IF(NP-NM)71,72,72 14 71 NROSS=2*NP+NZ 15 GO TO 73 16 72 NROSS=2*NM+2*NZ 17 73 NFS=2*N 18 IF(NROSS=NFS)74,41,41 19 74 WRITE(PAPER,201) MODE,NMODE3 20 201 FORMAT(1H0,'INSUFFICIENT POINTS TAKEN. MODE=',14,' NMODE3=',14) 21 GO TO 42 22 41 WRITE (PAPER,204)MODE,NMODE3 23 204 FORMAT(1H0,'DATA IS COMPATIBLE. MODE=',14,' NMODE3=',14)</pre>	11	· · · · · · · · · · · · · · · · · · ·	
14       71       NROSS=2*NP+NZ         15       GO TO 73         16       72       NROSS=2*NM+2*NZ         17       73       NFS=2*N         18       IF(NROSS=NFS)74,41,41         19       74       WRITE(PAPER,201) MODE,NMODE3         20       201       FORMAT(1H0,'INSUFFICIENT POINTS TAKEN.       MODE=',I4,' NMODE3=',I4)         21       GO TO 42         22       41       WRITE (PAPER,204)MODE,NMODE3         23       204       FORMAT(1H0,'DATA IS COMPATIBLE.       MODE=',I4,' NMODE3=',I4)	13	70	U TULL + TULL + TULL S TE /ND-NM \71 - 72 - 72
11       INK033-2+NF +N2         15       GO TO 73         16       72       NROSS=2*NM+2*NZ         17       73       NFS=2*N         18       IF(NROSS-NFS)74,41,41         19       74       WRITE(PAPER,201) MODE,NMODE3         20       201       FORMAT(1H0,'INSUFFICIENT POINTS TAKEN. MODE=',I4,' NMODE3=',I4)         21       GO TO 42         22       41       WRITE (PAPER,204)MODE,NMODE3         23       204       FORMAT(1H0,'DATA IS COMPATIBLE. MODE=',I4,' NMODE3=',I4)	LJ IÅ	70	
<pre>16 72 NROSS=2*NM+2*NZ 17 73 NFS=2*N 18 IF(NROSS=NFS)74,41,41 19 74 WRITE(PAPER,201) MODE,NMODE3 20 201 FORMAT(1H0,'INSUFFICIENT POINTS TAKEN. MODE=',14,' NMODE3=',14) 21 GO TO 42 22 41 WRITE (PAPER,204)MODE,NMODE3 23 204 FORMAT(1H0,'DATA IS COMPATIBLE. MODE=',14,' NMODE3=',14)</pre>	15	· · ·	
<pre>17 73 NFS=2*N 18 IF(NROSS-NFS)74,41,41 19 74 WRITE(PAPER,201) MODE,NMODE3 20 201 FORMAT(1H0,'INSUFFICIENT POINTS TAKEN. MODE=',I4,' NMODE3=',I4) 21 GO TO 42 22 41 WRITE (PAPER,204)MODE,NMODE3 23 204 FORMAT(1H0,'DATA IS COMPATIBLE. MODE=',I4,' NMODE3=',I4)</pre>	16	72	NRNSS=2*NM+2*N7
<pre>IF (NROSS-NFS)74,41,41 IF (NROSS-NFS)74,41,41 IF (NROSS-NFS)74,41,41 IF (PAPER,201) MODE,NMODE3 20 201 FORMAT(1H0,'INSUFFICIENT POINTS TAKEN. MODE=',14,' NMODE3=',14) 21 GO TO 42 22 41 WRITE (PAPER,204)MODE,NMODE3 23 204 FORMAT(1H0,'DATA IS COMPATIBLE. MODE=',14,' NMODE3=',14)</pre>	17	72	$NFS=2 \times N$
<pre>19 74 WRITE(PAPER,201) MODE,NMODE3 20 201 FORMAT(1H0,'INSUFFICIENT POINTS TAKEN. MODE=',14,' NMODE3=',14) 21 GO TO 42 22 41 WRITE (PAPER,204)MODE,NMODE3 23 204 FORMAT(1H0,'DATA IS COMPATIBLE. MODE=',14,' NMODE3=',14)</pre>	18		TE(NR0SS-NES)74.41.41
<pre>20 201 FORMAT(1H0,'INSUFFICIENT POINTS TAKEN. MODE=',I4,' NMODE3=',I4) 21 GO TO 42 22 41 WRITE (PAPER,204)MODE,NMODE3 23 204 FORMAT(1H0,'DATA IS COMPATIBLE. MODE=',I4,' NMODE3=',I4)</pre>	19	74	WRITE(PAPER, 201) MODE, NMODE3
<pre>21 GO TO 42 22 41 WRITE (PAPER,204)MODE,NMODE3 23 204 FORMAT(1H0,'DATA IS COMPATIBLE. MODE=',I4,' NMODE3=',I4)</pre>	20	201	FORMAT(1H0, INSUFFICIENT POINTS TAKEN, MODE= 1.14. NMODE3=1.14)
<pre>22 41 WRITE (PAPER,204)MODE,NMODE3 23 204 FORMAT(1H0,'DATA IS COMPATIBLE. MODE=',I4,' NMODE3=',I4)</pre>	21		GO TO 42
23 204 FORMAT(1H0, 'DATA IS COMPATIBLE. MODE=', I4, ' NMODE3=', I4)	22	41	WRITE (PAPER, 204) MODE, NMODE3
	23	204	FORMAT(1H0, 'DATA IS COMPATIBLE. MODE=', I4, ' NMODE3=', I4)

			<b>~69~</b>
4	· · · · ·		<u>GO TO 15</u>
5.		42	GO TO (44,44,47),MODE
6		47	IF(NMODE3 - 1)48,48,43
27		48	NMODE3 = NMODE3 + 1
8		44	NABORT=2
29			MODE = 1
30			
) 1. : つ		2	$\mathbf{E} = \mathbf{E} = $
12 : 13	. · ·	43	WRITE (PAPER 205) NMODES
4		205	FORMAT(1H0, 'NMODE3=', 14, ' SAMPLE DATA NOT COMPATIBLE WITH REFERE
5			LE DATA. RESUBMIT UNDER MODE=1 THIS DATA IGNORED!)
6			NMODE3 = NMODE3 + 1
7	•.		RETURN 2
8		C	*****DEFINE KNP,KNZ,KNM FOR SUBSEQUENT CALCULATIONS *****
9		1	KNP=NP
·0		· .	KNZ=NZ
·1			KNM=NM
-2		15	IF (KNP-KNM)9,9,10
3		9	M = KNP + KNZ
-4 E		10	
-9 -6	11	10	
7	·.•	11	NOD = ND + N7 + 1
8			MEND=M-2×KNZ
9		С	*****NAPOD=1,APODISE; NAPOD=2 DON'T APODISE *****
0			GO TO (27,28), NAPOD
1		27	DO 21 I=1,14
2		· · ·	FTDATA(I) = F(NOP-I) * (1 - (I-1) / M)
3		21	CONTINUE
4		20	
5	۰.	20	$\frac{1}{1} \frac{1}{1} \frac{1}{1} = \frac{1}{1} \frac{1}{1} = \frac{1}{1} \frac{1}{1} \frac{1}{1} = \frac{1}{1} \frac{1}{1} \frac{1}{1} = \frac{1}{1} \frac{1}{1} \frac{1}{1} \frac{1}{1} = \frac{1}{1} \frac{1}{1} \frac{1}{1} \frac{1}{1} = \frac{1}{1} $
7		30	CONTINUE
Ŕ		29	N = (M + M E ND) / 2
q		<b>L</b> /	DO(22) I=1.15
σ			
1		•	NMIS=2*(2**1)-2*N
2			IF (NMIS)22,24,23
3	•	22	CONTINUE
4		23	DO 25 I=1,NMIS
5			FTDATA(M+I)=0.0
6		25	
1		24	GU TU (31,32),NAPUD
0 0		21	$\frac{1}{20} = 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1$
0	·, •	26	CONTINUE
ĩ		20	60 TO 34
	·	32	DO 33 1=1.MEND
3		-	FTDATA(M+NMIS+I)=F(MNEG-I)
4		33	CONTINUE
5	•	34	NPDINT=N + NMIS/2
6	<i>.</i>	·	LNPOI=2*NPOINT
7		· _ ·	NONU = NPOINT
		. <b>-</b>	
÷	· .	and the Market	

			a statut de la complete de la <b>-70-</b> de la complete de
		• •	
	· · ·	•	
78		C	UNPOI (=2*2**1FI)PUINIS READY IN FIDATA FOR RHARM.COEFFICIENTS
79		- C	RETURNED FROM RHARM IN FTDATA, LNPOI+2VALUES. CALCULATE INTENSITY
80		C	FINT AT NUNU FREQUENCIES FROM THIS
81			CALL RHARM(FIDATA, IFT, INV, S, IFERR)
82		•	MFIN = LNPUI + 2
83			
04 05		209	$PURMATTINU_{9}^{*}N = \frac{149}{9} PUINT = \frac{149}{9} PUI = 14$
86		· .	0 - 0 DO 35 I-3 MEIN 2
87	t in	<b>.</b>	
88			FINT(J) = SORT(FTDATA(T) * * 2 + FTDATA(T+1) * * 2)
89		35	CONTINUE
90			***** CALCULATE RESOLUTION, AND FREQUENCIES AT WHICH INTENSITIES
91		С.	**** CALCULATED. *****
92			RESOL = 10000/(N*DELX)
93			GO TO (53,52), NAPOD
94		53	RESOL=RESOL*2**.5
95		52	DELNU=5000.0/(NPOINT*DELX)
96		C	***** PRINT OUT UNUSED DATA ****
97		200	WRITE(PAPER,200) NMIS,NAPUD
98		200	FURMAILINU, 'THE FULLUWING FX PUINTS WERE NUT NUT USED IN THE TRA
99			2 NOT ADODISE)1)
00	•	· .	Z NOT AFODISE) / MDONE~NOP_M~1
<u>n</u> 2-		, · · · · · · · · · · · · · · · · · · ·	
03		•.	WRITE(PAPER $\cdot$ 207) EX(1) $\cdot$ EX(MPONE)
04		46	CONTINUE
05		61	IF (MNEG.GT.NUM)G0 TO 62
06			WRITE(PAPER, 207) FX(MNEG), FX(NUM)
07		45	CONTINUE
08		207	FORMAT(1H0,F9.4, ' TO ',F9.4)
09		62	WRITE(PAPER,208) LNPOI,NONU,DELNU,RESOL
10		208	FORMAT(1H0,15, ' POINTS USED IN TRANSFORM, INTENSITIES CALCULATED
11			1 ', I4, ' FREQUENCIES', F6.3, 'WAVE/CM APART. RESOLUTION IS ABOUT'
12			2F6.3, WAVE/CM')
13			GU IU (36,37,38), MUDE
14 15		50	
16		39	CONTINUE
17			GO TO 40
18		37	GO TO (36,40),ITIS
19		38	IF (NMODE3-1)36,40,40
20		40	RETURN 1
21		· · ·	END
22		С	***** SUBROUTINE TO PLOT RATIO OR INTENSITY AS A
23		C	***** FUNCTION OF WAVE NUMBER (1/CM) *****
24		• •	SUBROUTINE WBPLOT (XFN,YFN,NDATA)
25			DIMENSION XFN(8195), YFN(8195), XA(8195), YA(8195), XB(8195), YB(8195)
26	_		CUMMUN COMP(20), LITLE(20), MODE, ITIS, NMODE3, NAPOD, NABORT, RESOL,
21		· .	INUNU, DELX, LPAGE, XPAGE, NG, MOVE, XMAX, XMIN
28		· ··· ··· ·	
27	•.		$\frac{1}{1} \frac{1}{1} \frac{1}$
21		•	
	·	······	
		. ·	

		-71-
32		XA(I)=XFN(I)
33		YA(I) = YFN(I)
34	51	CONTINUE
35	63	WRITE(6,32)XA(LDATA)
36	32	FORMAT(1HO, 'THE MAXIMUM FREQUENCY ON PLOT 1S ', F8.4)
37 -	÷	MDATA=0
38		DO 52 I=1,LDATA
39		MDATA=MDATA+1
40	· · · · ·	IF(XA(I).GE.XMIN) GO TO 54
41	52	CONTINUE
42	•	WRITE(6,210)
43	210	FORMAT('NO PLOT')
44	· · ·	CALL PLOTND
45		WRITE(6,258)NG
46	258	FORMAT(1H0,14, 'GRAPHS PLOTTED')
47	· · · · · · ·	STOP 4
48	54	WRITE(6,501)XA(MDATA)
49	501	FORMAT(1HO, 'THE LOWEST FREQUENCY PLOTTED IS ' F8.4)
50		LMDATA=LDATA-MDATA
51		DO 55 I=1,LMDATA
52		XB(I)=XA(MDATA+I)
53		YB(I) = YA(MDATA+I)
54	55	CONTINUE
55		XPAGE = (XA(LDATA) - XA(MDATA+1)) / LPAGE+2.0
56	•	IF(XPAGE.GT.52.0) GD TD 20
57		WRITE(6,62)LPAGE
58	62	FURMAT(IHO, 'UN X AXIS THE SCALE IS', I4, 'RC PER INCH')
59		WRITE(0,111)XPAGE
60	111	
01 27		
62	C is	2D-10●0 2D-10●0
64	v	CALL SCALE(VB + MDATA + SH + VMIN + DV + 1)
65		TE (MODE EQ 1) CO TO 8
66		$C\Delta I = \Delta X I S (0, 0, 0, 0, 5 H R \Delta T I 0, 5, SH, 90, 0, YM I N, DY)$
67 ·		GO TO 9
58	8	$\frac{1}{1} \frac{1}{1} \frac{1}$
69	ĩ	***** DRAW ERECHENCY AYIS *****
70-	$\tilde{9}$	7PAGE=LPAGE
71		CALL AXIS $(0, 0, 0, 0, 1)$ HWAVE PER $(M, -1)$ SW $(0, 0, 1)$ MIN $(7PAGE)$
72		DO 11 $I=1 \cdot I$ MDATA
73		XB(I) = (XB(I) - XMIN) / 7 PAGE
74		CONTINUE
75	C	**** WRITE TITLE ****
76		X = XPAGE - 10.0
77		Y=\$H-0.35
78		CALL SYMBOL(X,Y,0.12,TITLE,0.0,80)
79		Y=SH-0.75
80-	· · · · · · · · · · · · · · · · · · ·	CALL SYMBOL (X, Y, 0.12, COMP, 0.0, 80)
B1	· · · ·	CALL PLOT(0.0,0.0,3)
82	С	**** PLOT GRAPH *****
B3		CALL LINE(XB,YB,LMDATA,1)
84		CALL PLOT(XPAGE,0.0,-3)
85	23	RETURN

	••	-72-	
:: <sup>•</sup>	• .		
86	20	LPAGE=2%LPAGE	
87		GO TO 61	•
88		END	·
90	L <sub>.</sub>	SUBROUTINE FUREAR FAPE UUTPUT	
<del>7</del> 1		DIMENSION IT(27024), OU(9008), XS16(9000), IK(200)	
92		COMMON COMP(20), TITLE(20), MODE, ITIS, NMODE3, NAPOD, NABORT, RESOL	•
93		1NONU, DELX, LPAGE, XPAGE, NG, MOVE, XMAX, XMIN	
94 25		$\frac{\text{KEAL} \text{IPINF}(6)}{\text{DO} 33 \text{ K}=1.200}$	
96		CALL PTAPE(I)	
97	· .	I K (K) = I	
38		IF(IK(K).EQ.0) GO TO 33	
99 20	22		
)1	14	M=0	· · · · · · · · · · · · · · · · · · ·
20	•••	LAST = 8888	-
)3		DO 10 J=1,27024,3	••
)4 )5	· .	CALL PIAPE(I)	
)6	· · ·	IF(IT(J).EQ.256)GO TO 19	
<u>)</u> 7	یہ بندہ است میں ریپر د رہ	IF(IT(J).E0.512)GO TO 21	
28			
79 10		CAST=99999	
11	22	IF(IT(J).EQ255)GO TO 4	
12	81	IF(IT(J).GE.128)GO TO 5	
13	4	J=J-3 CO TO 10	
15	5	M=M+1	
16	· · · · · · · · · · · · · · · · · · ·	11(J) = 11(J) - 128	
17	: .	CALL PTAPE(I)	
10		$\frac{\Gamma(J+I)=I}{\Gamma(J+I)}$	
20		IT(J+2)=I	
21	· ·	DO 7 N=1,3	
22	· · · · ·	K=J+N-1 IE(IT(K) CE 64) IT(K)-IT(K)-64	
24	•	$IF(IT(K) \cdot EQ \cdot 32) IT(K) = 0.0$	
25	· · · · · · · · · · · · · · · · · · ·	IF(IT(K).GE.16)GO TO 8	
26	0		
21	8		
29	7	CONTINUE	
30	,	$OU(M) = 256 \times IT(J) + 16 \times IT(J+1) + IT(J+2)$	
31	10	CONTINUE	
って えて	19	GU TU 90 . M=M+1	•
34	1/	OU(M)=5555.0	
35	90	DO 3 I=1,6	
36		IPINF(I)=0U(I)	
57 38	2 94	CUNTINUE DD 6 K=9.M	
39		XS16(K-8)=OU(K)	
÷			
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					-73-		<b>.</b>	· · · · · · · · · · · · · · · · · · ·		•
+0 +1 +2	6 100	CONTIN RETURN END	U'E				<u>.</u>	· · · · · · · · · · · · · · · · · · ·	· · ·	***
JF	FILE				·					
10F	F						• •			
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