

SHIFT MEASUREMENTS OF THE STARK-BROADENED
IONIZED HELIUM LINES AT 1640 AND 1215 Å

by

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ABSTRACT

Title of Dissertation: SHIFT MEASUREMENTS OF THE STARK-BROADENED
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Time-resolved measurements were made of the shifts of the ionized helium lines at 1640 Å ($n = 3 \rightarrow 2$) and 1215 Å ($n = 4 \rightarrow 2$), and of the Stark profile of the λ 1215 Å line. An electromagnetic shock tube was used as a light source. The plasma conditions corresponded to electron temperatures of ~ 3.5 eV and electron densities of 0.8 to $1.8 \times 10^{17} \text{ cm}^{-3}$. The measured shifts fell between two previous estimates of plasma polarization shifts. The measured Stark width of the λ 1215 Å line was up to 30% greater than the theoretical width.

DEDICATION

To my wife, Nita, who kept my nose to the grindstone.

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CHAPTER I

INTRODUCTION

Spectroscopy has long been recognized as an important diagnostic tool for both astrophysical plasmas, where it is often the only method available, and in the laboratory where, unlike many methods, it does not disturb the plasma under study.

The considerable theoretical and experimental efforts in this field have resulted in good understanding of the pressure broadening and shifts of spectral lines due to the Stark effect of nearby charged perturbers. Particular attention has been paid to the lines of hydrogen and the hydrogenic ions, for which the quasistatic and impact theories predict considerable broadening but no shifts. However, in 1962, Berg et al reported¹ a blue shift for the He II 4686 line, which they attributed to the reduction of the Coulomb potential of the nucleus by the polarization of the plasma near the radiating ion. Later measurements² demonstrated this "shift" had been simulated by some unresolved Si III lines on the blue wing of the helium line. Greig et al. then reported blue shifts of the He II 304 line.³ Subsequent photographic measurements^{4,5} did not verify the shift of the 304 line, but higher series members (256, 243, etc.) had blue shifts which could have been due to plasma polarization. The most recent measurement⁶ showed blue shifts for the 256 and 243 lines, with a greater shift for the 304 line, in agreement with Greig's result.

The polarization shift is expected to be important for high-Z ion lines and may limit wavelength accuracies in, for example, laser-produced plasmas. The theoretical treatments of this effect have

been unsatisfactory,^{7,8} and no attempts have been made to measure shifts of the "Balmer" (or "second Lyman") series lines of ionized helium, at 1640, 1215, 1084 ... Å. The primary aim of this experiment was to look for such shifts, and investigate their possible dependence on plasma conditions. A secondary purpose was to measure the Stark broadening of the higher series members, to check the theoretical calculations.^{9,10}

A T-tube was chosen as a source because it produces a fairly homogeneous plasma⁶ near local thermal equilibrium (LTE),^{11,12} at a density and temperature suitable for the emission of ionized helium lines. The line positions were measured relative to nearby impurity lines. Plasma conditions were determined from photoelectric measurements of the He II 4686 line, and plasma reproducibility was checked by monitoring the total intensities of the 4686 line and the continuum near 4976 Å.

The first chapter of this dissertation has served as an introduction. In Chapter 2 some of the relevant results of plasma spectroscopy are presented. A description of the experimental apparatus and method appears in Chapter 3. The experimental results, with a discussion of them and possible errors, are in Chapter 4.

CHAPTER II

THEORETICAL BACKGROUND

A. Line Intensities

The relative intensities of emission lines depend on the population densities of atoms in the upper state and the probability of radiative transition to the corresponding lower state.

In equilibrium, the density N_z of ions of charge Z is related to the electron density N_e and the density of atoms in the next lower ionization stage according to the Saha equation¹³

$$\frac{N_e N_z}{N_{z-1}} = 2 \frac{Z_z(T)}{Z_{z-1}(T)} \left(\frac{m_e \kappa T}{2\pi\hbar^2} \right)^{3/2} \exp \left(-\frac{E_\infty^{z-1} - \Delta E_\infty^{z-1}}{\kappa T} \right) . \quad (2-1)$$

Since nearly all the atoms are in the ground state, the partition function $Z_z(T)$ can usually be replaced by the statistical weight g_z of the ground state. In this case, $\ell=0$, and we have $g_z = 2S+1$ (1 for H^+ , He^0 , and He^{++} ; 2 for H^0 and He^+). The correction ΔE_∞^{z-1} to the ionization energy E_∞^{z-1} due to Coulomb interactions in the plasma is¹³

$$\Delta E_\infty^{z-1} = \frac{Z e^2}{4\pi\epsilon_0 \lambda_D^2} , \quad (2-2)$$

where λ_D is the plasma Debye length¹⁴

$$\lambda_D = \left(4\pi \sum_i \frac{N_i q_i^2}{k T_i} \right)^{-1/2} , \quad (2-3)$$

where N_i is the density of particles with charge q_i . Plots of helium ionization stage concentrations as functions of temperature appear in Fig. 2-1. Plots of λ_D and other plasma properties appear in Fig. 2-2,

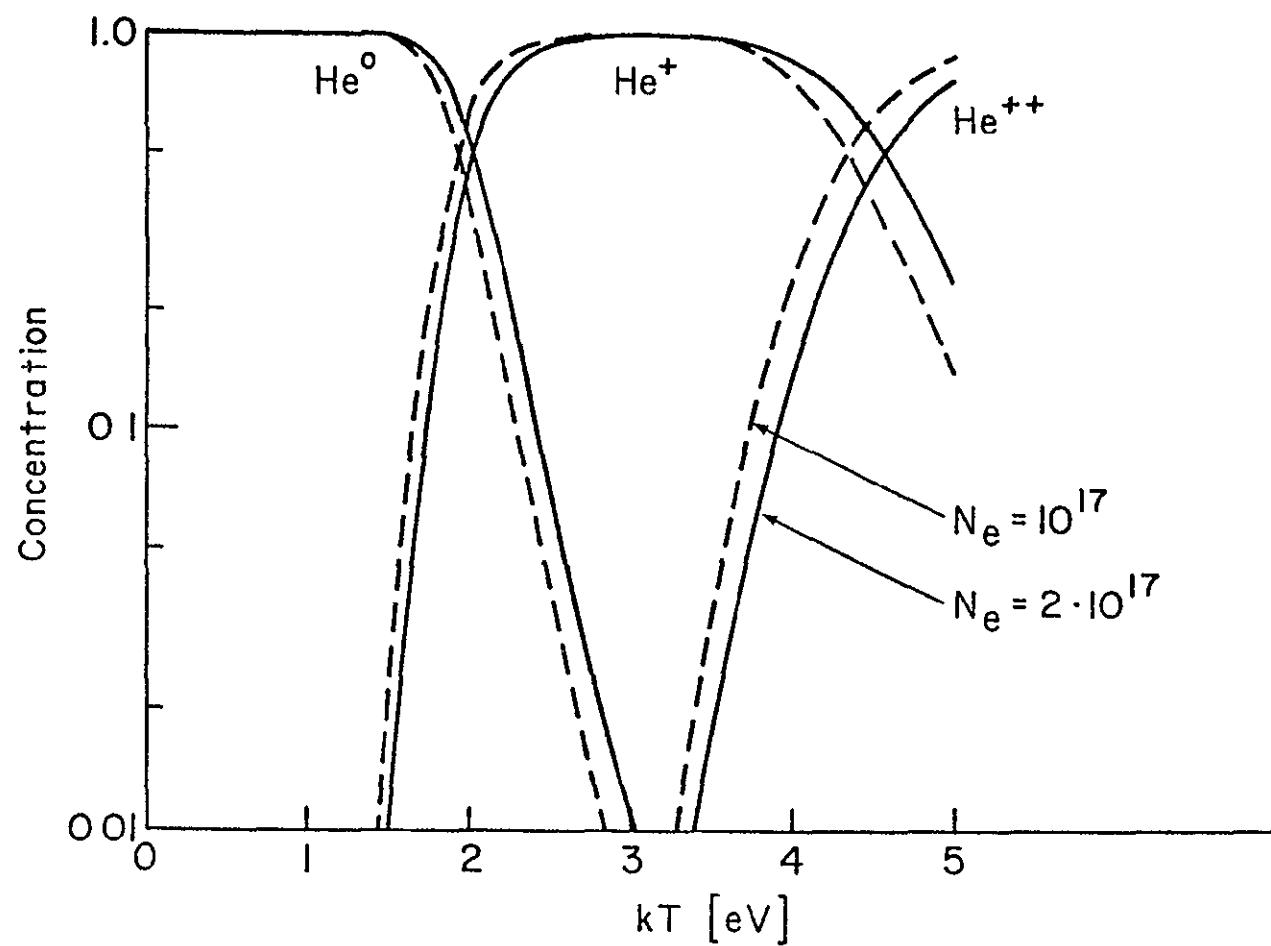


Fig. 2-1 Calculated helium ionization stage concentrations

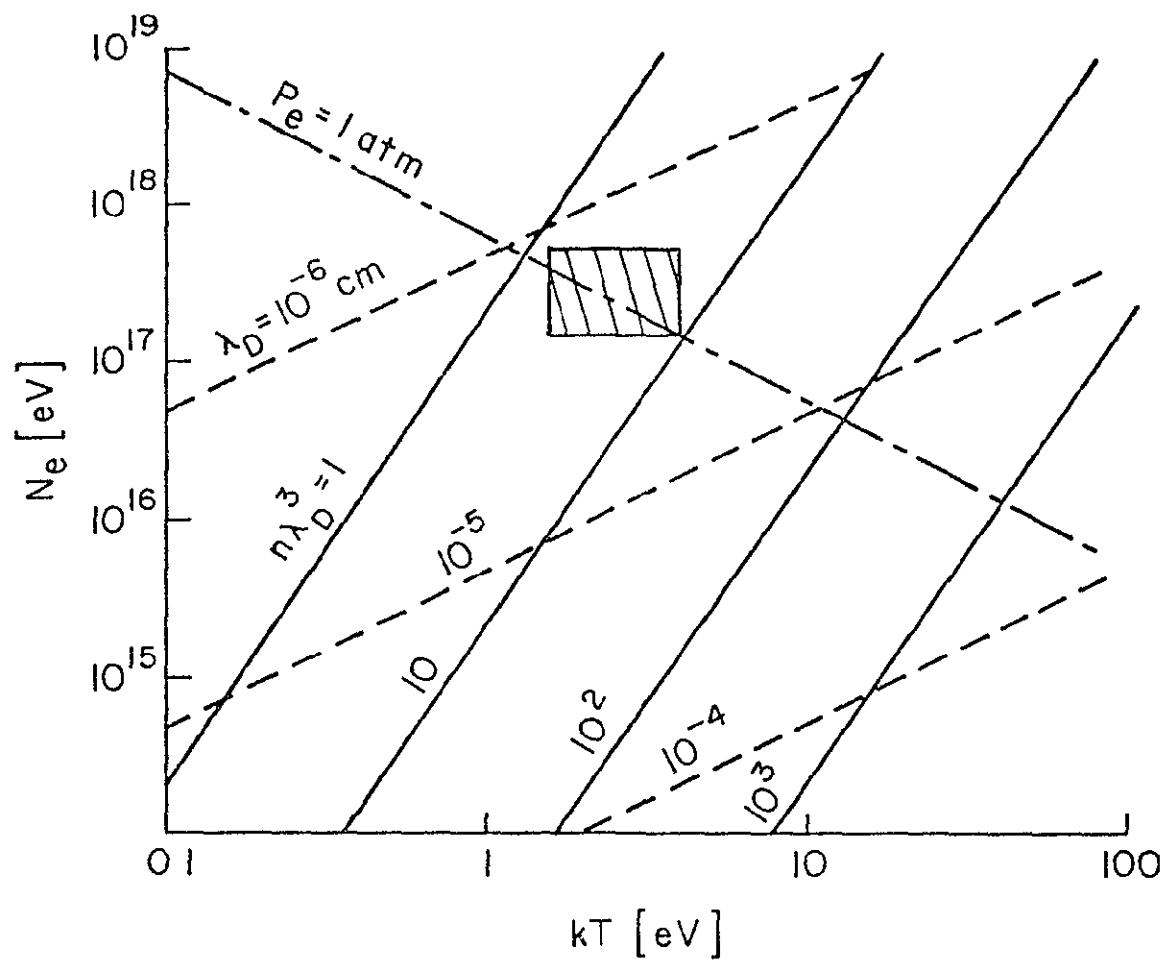


Fig. 2-2 Calculated conditions for a pure helium plasma

where the shaded region is typical of T-tubes. Note that the plasma approximation $N_e \lambda_D^3 \gg 1$ (indicating many particles in a Debye sphere) is only marginally satisfied.

The population densities N_{nLS} of the state (n,L,S) of a given ionization stage is given by the corresponding Boltzmann factor¹³

$$N_{nLS} \propto g_{nLS} \exp \left(-\frac{E_{nLS}}{kT} \right), \quad (2-4)$$

together with the normalization condition. The exponential term is nearly always much less than one for excited states, justifying the earlier statement that most atoms are in the ground state. Note that an isolated atom has an infinite number of bound states, whose energies tend to the ionization energy E_∞^2 . When the atom is embedded in a plasma, however, the ionization energy is reduced as described above, and only a finite number of bound states remain.

Treating an atom as an electric dipole radiator, the transition probability per unit time for spontaneous emission is¹³

$$A_{lu} = \frac{4e^2 \omega^3}{3\hbar c^3 [4\pi\epsilon_0]} g_l \sum_i |\langle l | x_i | u \rangle|_{av}^2, \quad (2-5)$$

which is tabulated for many spectral lines.¹⁵ The sum is over the components of the coordinate vector of the radiating electron, and the average is over possible final states. Multiplying by the energy $\hbar\omega$ of the photon, and using (2-4) to relate the upper state population density to the ground state population density N_g (with statistical weight g_g) we find the total power per unit volume spontaneously radiated in the given line to be¹³

$$P_{lu} = 2\pi\hbar c \frac{N_g A_{lu}}{\lambda} \frac{g_u}{g_g} \exp \left(-\frac{E_u}{kT} \right). \quad (2-6)$$

Since the line intensities are proportional to the concentration of atoms in the appropriate ionization stage, the intensity ratio of lines of different ionization states is an extremely sensitive function of temperature (see Fig. 2-3), and can be used to measure the temperature. Note, however, that this measurement depends strongly on the assumption of local thermal equilibrium, which can require a long time and considerable distance to establish between states with very different energies.

B. Continuum Intensities

Plasmas emit continuum radiation due to radiative recombination (inverse photoionization), bremsstrahlung, and the formation of negative ions. A pseudo-continuum results when the Stark profiles of nearby lines overlap.

The extremely weak bremsstrahlung radiation due to ion-ion and nonrelativistic electron-electron collisions can be neglected. That due to electron collisions with ions of charge z is given by¹⁶

$$\frac{\epsilon_{\omega}^{ei}}{\omega} = \frac{16\pi e^6}{3c^2 \sqrt{6\pi m_e^3}} \frac{N_e N_z}{\sqrt{kT_e}} z^2 G_z(\omega, T_e) , \quad (2-7)$$

where G_z is the free-free Gaunt factor, which is usually of order one.¹⁷

The radiation from electron-neutral collisions (approximated by elastic, billiard-ball type interactions) is given by¹⁶

$$\frac{\epsilon_{\omega}^{e0}}{\omega} = \frac{32e^2}{3c^3 (2\pi m)^{3/2}} N_e N_0 (\kappa T_e)^{3/2} G_0(\omega, T) . \quad (2-8)$$

When an ion captures a free electron, the binding energy and the electron's kinetic energy are given to a photon. For recombination into a given orbital (n, L, S), the photon then has the minimum energy

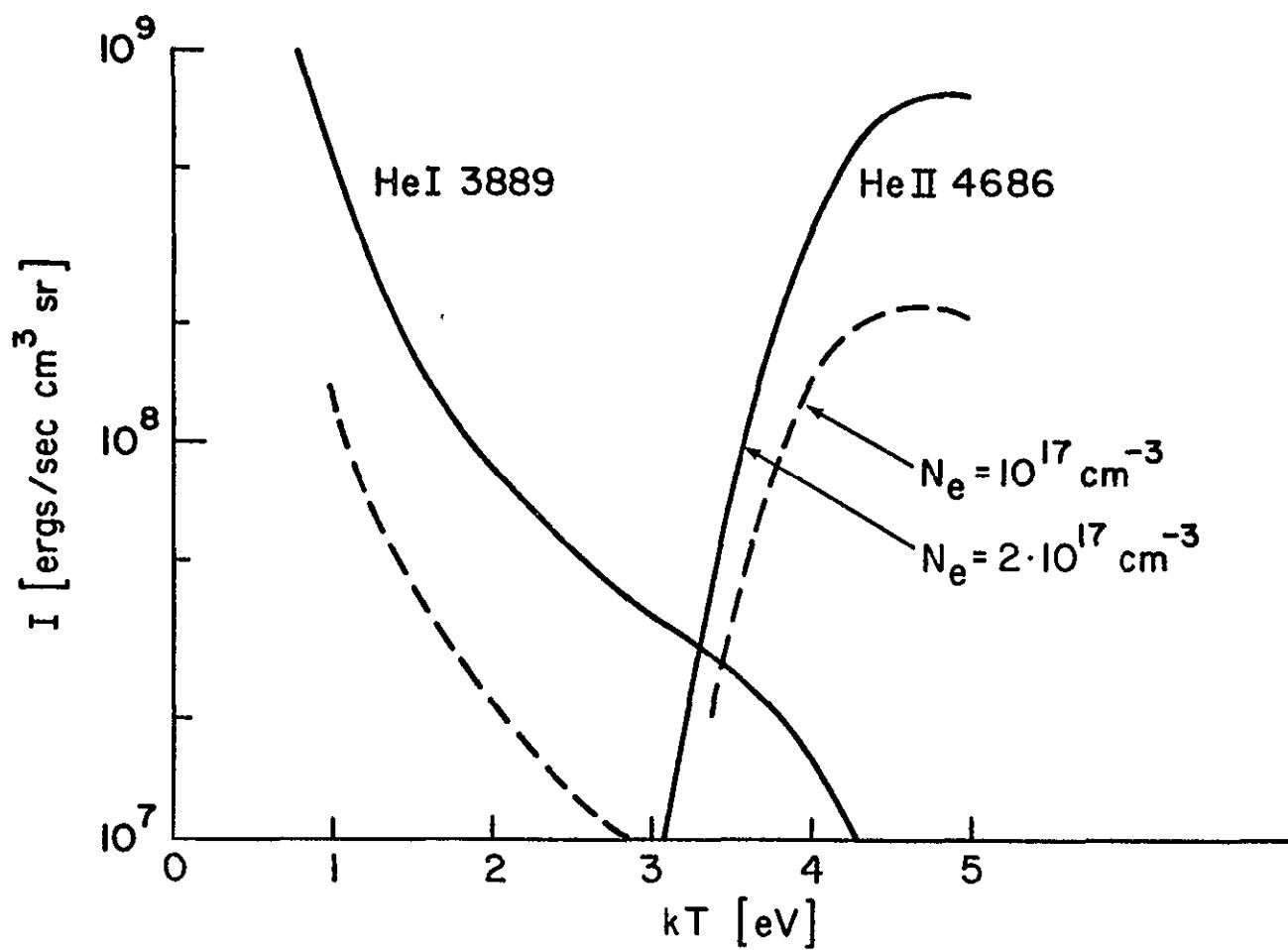


Fig. 2-3 Calculated helium line intensities

$$\hbar\omega = E_{z-1,\infty} - E_{z-1,n} . \quad (2-9)$$

Viewed another way, this restricts the possible final states for the electron for a contribution to the continuum at a given frequency.

The recombination continuum is then, by detailed balancing,¹⁶

$$\epsilon_w^R = \frac{2\pi\hbar^4}{c^2} \frac{N_e N_{z,1} \omega^3}{(2\pi m k T_e)^{3/2}} \exp\left(-\frac{\hbar\omega}{kT_e}\right) \sum_n \frac{g_{z-1,n}}{g_{z,1}} \sigma_{z-1,n}, \quad (2-10)$$

where $\sigma_{z-1,n}$ is the photoionization cross section^{18,19}, $g_{z-1,n}$ and $g_{z,1}$ are statistical weights, and the sum runs from the lowest allowed state to the highest bound state (i.e., with energy less than the reduced ionization energy calculated from (2-2)).

Some electronegative atoms (H, N, O, C, etc.) can capture a free electron and form a negative ion, while emitting a continuum as in recombination. The spectral emission coefficient is, similarly,¹⁶

$$\epsilon_w^- = \frac{2\pi\hbar^4 \omega^3}{c^2 (2\pi m k T_e)^{3/2}} N_a N_e \frac{g^-}{Z_0(T_e)} \sigma^-(\omega) \exp\left(\frac{E_a - \hbar\omega}{kT_e}\right), \quad (2-11)$$

where g^- is the statistical weight of the negative ion (which usually has only one bound state), Z_0 is the partition function of the neutral atom, E_a is the binding energy of the new electron (generally less than 2 eV), and σ^- is the cross section for the inverse process of photodetachment.²⁰ This process is unimportant in hot plasmas, where the density N_a of neutral atoms is low.

The pseudo-continuum of lines is generally important only for hydrogenic atoms, which are subject to the linear Stark effect, and then only near a series limit. The last clearly distinguishable line of a series is then given by the Inglis-Teller limit.²¹

Since both line and continuum intensities increase with electron

density, but scale differently with temperature, the ratio of the line intensity to that of the nearby continuum can be used to measure the temperature.

C. Radiation Transfer

In previous sections we have discussed the spectral emission coefficient ϵ_{ω} of the plasma, expressed as power radiated per unit solid angle, frequency interval, and volume. The experimentally measurable quantity is I_{ω} , the power radiated per unit solid angle, frequency interval, and surface area of plasma observed. In the simplest situation, i.e., neglecting scattering, it obeys the differential equation¹³

$$\frac{d}{dx} I_{\omega} = \epsilon_{\omega} - k' I_{\omega} , \quad (2-12)$$

where k' is the effective absorption constant, equal to the actual absorption constant minus the induced emission. ϵ_{ω} includes only the spontaneous emission. If the plasma is in LTE, the emission follows Kirchoff's law¹³

$$\epsilon_{\omega} = k' B_{\omega}(T) , \quad (2-13)$$

where B_{ω} is the Planck function. If we further assume the plasma to be homogeneous, the solution of (2-12) is

$$I_{\omega}(\ell) = B_{\omega}(T) [1 - \exp(-k' \ell)] . \quad (2-14)$$

The quantity $k' \ell$ is the "optical depth", and if $k' \ell \ll 1$, the equation reduces to

$$I_{\omega}(\ell) = B_{\omega}(T) k' \ell = \epsilon_{\omega} \ell , \quad (2-15)$$

as expected. In the opposite limit, $k_B \omega \gg 1$, the plasma radiates as a blackbody. Stellar atmospheres have great optical depth at almost all wavelengths, while laboratory plasmas are normally optically thin except possibly near the centers of some resonance lines.

D. Line Broadening

Spectral line broadening in a plasma is a complex phenomenon, and no attempt is made here to discuss all the results of investigations in atomic spectroscopy,²² astrophysics²³ , and plasma spectroscopy.^{10,13} Only a physical picture of the various effects is presented.

Let the (frequency-space) spectral line profile $I(\omega)$ be proportional to the light intensity between ω and $\omega + d\omega$, subject to the normalization condition

$$\int_{-\infty}^{\infty} I(\omega) d\omega = 1 . \quad (2-16)$$

These spectral intensities are the squares of the corresponding Fourier components $C(\omega)$:

$$I(\omega) = |C(\omega)|^2 , \quad (2-17)$$

where $C(\omega)$ is the Fourier transform of the amplitude $f(t)$

$$C(\omega) = \sqrt{\frac{1}{2\pi}} \int_{-\infty}^{\infty} e^{i\omega t} f(t) dt . \quad (2-18)$$

Since each atom emits light for only a short time, the light from an ensemble is not monochromatic. It is physically reasonable to assume that $f(t)$ for one atom has the exponentially decaying form²⁴

$$f(t) = \begin{cases} 0 & t < 0 \\ \sqrt{2\gamma} e^{i\omega_0 t} e^{-\gamma t} & t > 0 \end{cases} , \quad (2-19)$$

which satisfies the normalization condition

$$\int_{-\infty}^{\infty} |f(t)|^2 dt = 1 , \quad (2-20)$$

and has the Fourier components

$$C(\omega) = \sqrt{\frac{\gamma}{\pi}} \frac{-i}{\omega_0 - \omega + i\gamma} , \quad (2-21)$$

leading to the Lorentz or dispersion profile

$$I(\omega) = |C(\omega)|^2 = \frac{\gamma}{\pi} \frac{1}{(\omega_0 - \omega)^2 + \gamma^2} . \quad (2-22)$$

The half-half width γ , the frequency separation at which the intensity is half the maximum, is given by the sum of the transition rates for transitions originating from either the upper or lower state of the line¹³

$$\gamma_{lu} = \sum_u A_{u'u} + \sum_l A_{l'l} . \quad (2-23)$$

Since atomic excited states have relatively long lifetimes ($A_{lu} < 10^9 \text{ sec}^{-1}$), this natural broadening is almost always smaller ($\Delta\lambda < 10^{-40} \text{ Å}$) than the other effects we will discuss. It can of course be derived rigorously from the quantum theory of radiation.²⁵

When the energy levels of the radiating atoms are well separated, compared to mean thermal energies, electron collisions rarely exchange energy with the radiator, but change the polarization or phase of the emitted light. Although this approximation does not hold, for example, for neutral helium^{7,13} (where there are nearby perturbing levels with the same n but different L), it is well satisfied for hydrogenic atoms. Assuming the light to be monochromatic between collisions, we have a sinusoidal wave train of duration τ , with the Fourier components

$$C_T(\omega) = \sqrt{\frac{1}{2\pi}} \int_0^\tau e^{i\omega_0 t} e^{-i\omega t} dt = \frac{e^{\frac{i(\omega_0 - \omega)\tau}{2}} - 1}{\frac{i(\omega_0 - \omega)}{2\pi}}, \quad (2-24)$$

producing the intensity

$$I_\tau(\omega) = \frac{\sin^2\left(\frac{1}{2}(\omega_0 - \omega)\tau\right)}{2\pi\left(\frac{1}{2}(\omega_0 - \omega)\tau\right)^2}. \quad (2-25)$$

If the probability per unit time γ_c of a collision is constant, the intervals between collisions have the Poisson distribution

$$P(\tau)d\tau = \gamma_c e^{-\gamma_c \tau} d\tau. \quad (2-26)$$

Weighting the intensities (2-25) by the corresponding probabilities, we again arrive at the dispersion profile (2-22), now with width r_c .

The frequency of light emitted by a moving atom is Doppler-shifted according to

$$\omega = \omega_0 \frac{1 - \frac{v_{||}}{c}}{\sqrt{1 - \frac{v^2}{c^2}}} = \omega_0 \left(1 - \frac{v_{||}}{c}\right). \quad (2-27)$$

Assuming the atoms have a Maxwellian distribution of velocities,

$$f_M(v)dv = \left(\frac{m_i}{2\pi k T_i}\right)^{3/2} \exp\left(-\frac{m_i v^2}{2k T_i}\right) dv, \quad (2-28)$$

the collection will emit light with the Doppler or Gaussian line profile^{13,26}

$$I_D(\omega) = \frac{1}{\Delta\omega_D} \sqrt{\frac{1}{2\pi}} \exp\left(-\frac{(\omega_0 - \omega)^2}{2\Delta\omega_D^2}\right), \quad (2-29)$$

where the characteristic width is

$$\Delta\omega_D = \sqrt{\frac{\frac{k T_i}{m_i c^2}}{2}}, \quad (2-30)$$

and the Doppler half-half width is $\sqrt{\ln 4} \Delta\omega_D$.

In contrast to the fast electron impacts, nearby ions can usually be considered stationary, and supply only perturbing electric fields. These fields perturb the energy levels (each labeled by n, L, S, and J) of the radiating atom and usually split them into several sublevels, each a linear combination of states of different magnetic quantum number m_j .¹⁶ Transitions between such sublevels of different principal quantum number give rise to the Stark components of a line. Since the operator $-q_e \vec{r}_e \cdot \vec{E}$, expressing the interaction of the electric field and a given electron, has odd parity (therefore no diagonal elements), there is usually no first-order interaction, and second-order perturbation theory is used. In the hydrogenic case, however, the terms (labeled only by n) are degenerate, and a linear effect is found. This problem is most conveniently solved in the parabolic coordinates (ξ, η, ϕ):

$$\begin{aligned}\xi &= r+z \\ \eta &= r-z \\ \tan\phi &= y/x \\ (r^2 &= x^2 + y^2 + z^2) ,\end{aligned}\tag{2-31}$$

where the unperturbed wavefunction is²⁷

$$\begin{aligned}\Psi(n_1 n_2 m | \xi \eta \phi) &= e^{-\frac{\xi+\eta}{2n}} \xi^{m/2} \eta^{m/2} U_{n_1}(\xi) V_{n_2}(\eta) \frac{e^{im\phi}}{\sqrt{2\pi}} \\ n &\equiv n_1 + n_2 + |m| + 1 = 1, 2, \dots \\ m &= 0, \pm 1, \dots, \pm(n-1) ,\end{aligned}\tag{2-32}$$

and the energy, correct to second order in field strength, is²⁷
(in units of $m_e e^4 / \hbar^2$)

$$c(n_1 n_2 m, F) = -\frac{1}{2} \frac{z^2}{n^2} + \frac{3}{2} \frac{n(n_1 - n_2)}{z} |\vec{F}|$$

$$-\frac{1}{16} \frac{n^4}{z^4} [17n^2 - 3(n_1 - n_2)^2 - 9m^2 + 19] |\vec{F}|^2 \quad (2-33)$$

For a first approximation, we may assume the ions in the plasma are uncorrelated. In this case, they produce an electric field F with the Holtsmark distribution^{10,28}

$$H\left(\frac{F}{F_0}\right) = \frac{2}{\pi} \frac{F}{F_0} \int_0^{\infty} \exp(-x^{3/2}) \sin\left(\frac{F}{F_0} x\right) x dx, \quad (2-34)$$

plotted in Fig. 2-4, where the Holtsmark normal field strength produced by perturbers with density N_p and charge q_p is¹⁰

$$F_0 = 2\pi \left(\frac{4}{15} N_p\right)^{2/3} q_p \quad (2-35)$$

Integrating the energies (2-33) over the distributions (2-34) for each level (though the effects on the upper level usually predominate) we arrive at the Holtsmark profile, shown for the hydrogen line H_β in Fig. 2-5. Profiles of lines subject to the linear Stark effect are usually expressed in terms of the reduced wavelength separation, defined by^{10,13}

$$\alpha = \left| \frac{\Delta\lambda}{F_0} \right|. \quad (2-36)$$

Note that where there is no unshifted Stark component (as in hydrogen transitions $n=4 \rightarrow 2$ or $3 \rightarrow 1$), the low probability of very small fields (since $H(0) = H'(0) = 0$) gives a line profile with a central dip, usually partly filled by other effects.

Finally, observed profiles are broadened by the instrument response function of the observing monochromator. According to physical optics,

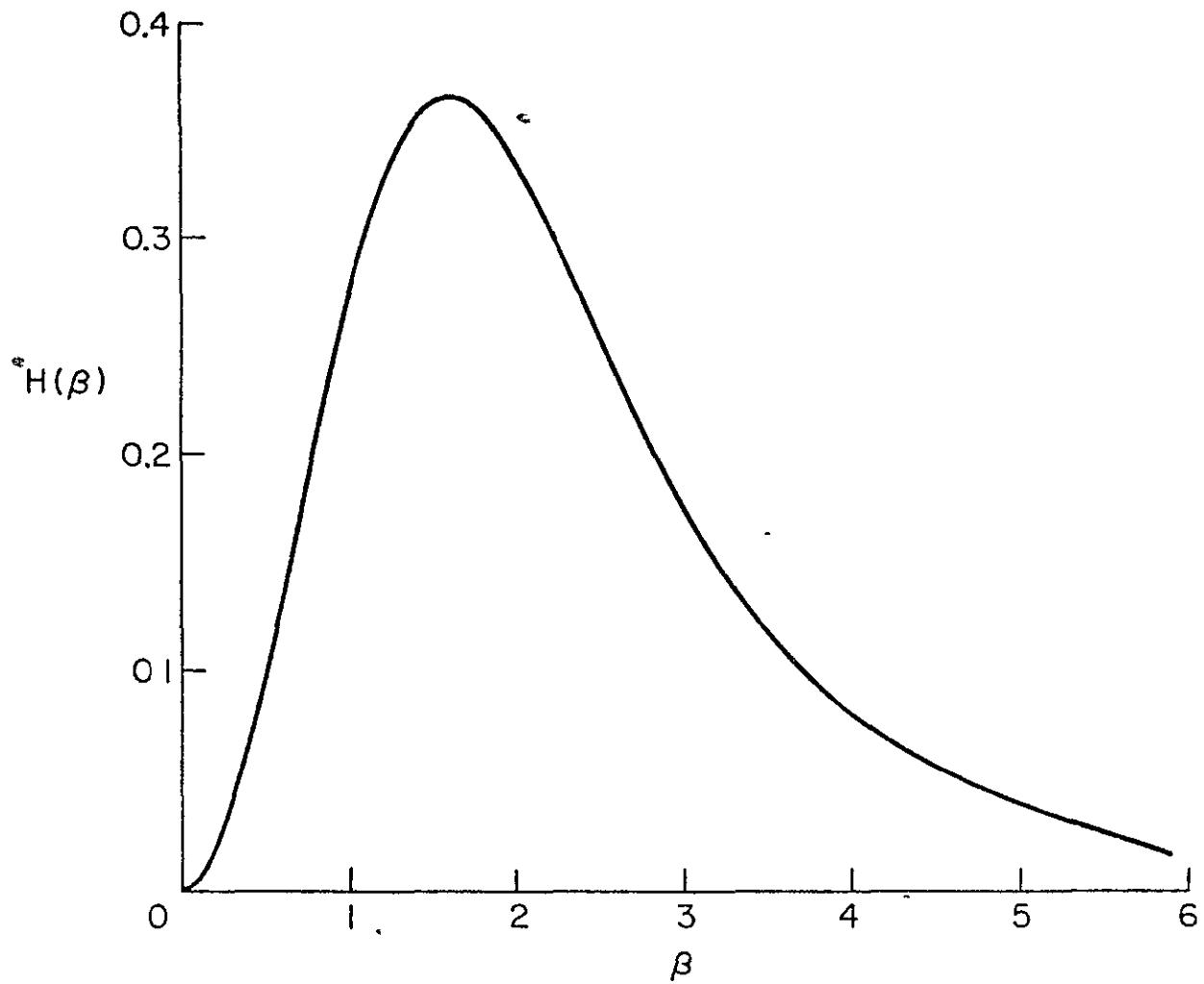


Fig. 2-4 Holtsmark field strength distribution

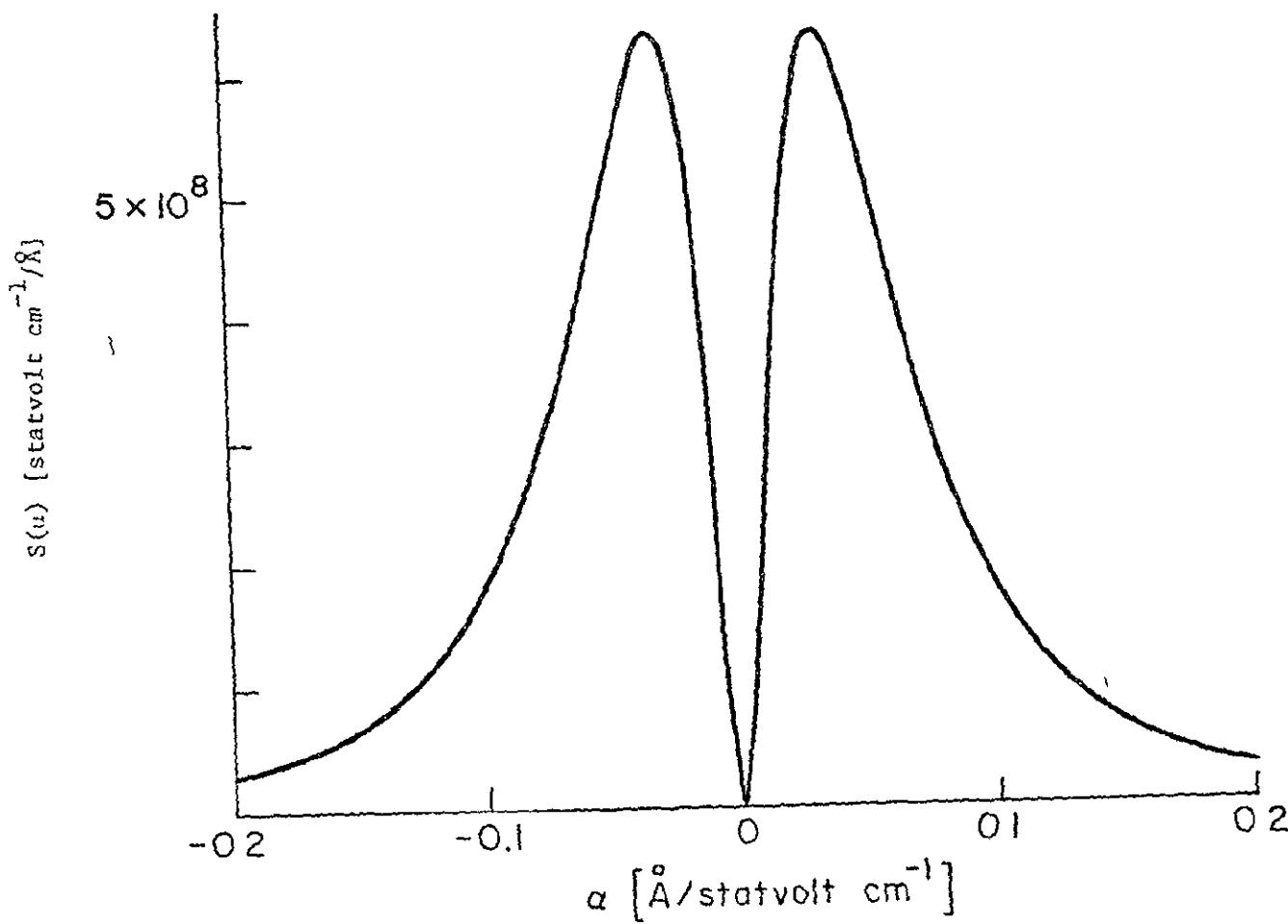


Fig. 2-5 Holtsmark profile for the H_S line
(broadened only by statistically uncorrelated ions)

it is a profile like (2-29) folded with the two rectangular slit functions, plus a constant background. With wide slits, Gaussian or triangular profiles are good approximations.

The profile of a line broadened by two independent effects is the convolution of the two profiles,

$$I(x) = I_1(x) \otimes I_2(x) = \int_{-\infty}^{\infty} I_1(x') I_2(x' - x) dx' , \quad (2-37)$$

and if we assume all of these effects are independent, we may find our theoretical profile by convolving all the profiles:

$$I_{\text{theory}} = I_{\text{natural}} \otimes I_{\text{electron}} \otimes I_{\text{Doppler}} \otimes I_{\text{ion}} \otimes I_{\text{instrument}} . \quad (2-38)$$

This assumption of statistical independence is reasonable for plasmas, because, e.g., collisions leading to significant changes of radiator velocities (Doppler effect) usually involve ions whose direct contribution (Stark effect) is insensitive to ion and radiator velocities.

E. Validity of LTE

A plasma is in local thermal equilibrium (LTE) if, locally and instantaneously, all quantum state population densities (except for photon states) correspond to a system in complete thermal equilibrium (CTE) which has the same mass density, energy density, and chemical composition.¹³ Departures from LTE occur when some transitions have unbalanced rates, so that some (generally low-energy) states are over- or under-populated when compared to the corresponding CTE system. In optically thin plasmas, where the rates of radiative excitation (photoexcitation and photoionization) are negligible compared to

those of radiative de-excitation (spontaneous emission and radiative recombination), the lower-energy states will be overpopulated unless collisional processes dominate radiative ones. That is, populations will be within $\sim 10\%$ of LTE if collisional processes are about an order of magnitude more important than radiative ones. Since collision cross sections are generally larger, and energy gaps smaller, for excited states, LTE is most easily satisfied for them. An estimate of the electron density required for the hydrogenic level n to be within $\sim 10\%$ of LTE with respect to the ion density is¹³

$$N_e > (7 \cdot 10^{18} \text{ cm}^{-3}) \frac{z^7}{n^{17/2}} \left(\frac{\kappa T}{z^2 E_H} \right)^{1/2} \quad (2-39)$$

The largest gap between atomic energy levels is generally between the ground and the first excited states, so the requirements for LTE for the ground state are usually the most restrictive. Near LTE, the largest transition rates are those to and from the first excited state, and collisional rates can be expected to dominate if¹³

$$N_e > (9 \times 10^{17} \text{ cm}^{-3}) \left(\frac{E_2}{E_H} \right)^3 \left(\frac{\kappa T}{E_h} \right)^{1/2}. \quad (2-40)$$

It often happens that the resonance line is optically thick, so that radiative de-excitation of the first excited state is balanced by photoexcitation. The resonance line profile is generally dominated by Doppler broadening (for N_e sufficiently low that electron collisions cannot maintain LTE), so its optical depth can be estimated by¹³

$$k'_{\text{reson}} d \approx (2 \cdot 10^{-10} \text{ cm}) f_{12} \lambda_{12} \left(\frac{\Delta E_H}{\kappa T} \right)^{1/2} N_{a,1}^{z-1} d \quad (2-41)$$

where the resonance line has wavelength λ_{12} and absorption strength f_{12} , and the atoms of interest have atomic weight A and ground state density

$N_{a,1}^{z-1}$. If the optical depth of the resonance radiation is greater than ~ 20 , the requirement (2-40) can be relaxed by about an order of magnitude.¹³

The validity of LTE for ionization stage populations in stationary plasmas usually need not be checked separately, since the excited states of a given stage are well connected with the ground state of the next ionization stage.

In transient plasmas, populations may depart from LTE if equilibrium times are long compared to the times over which plasma parameters change. The lowest transition rates for given stage usually involve the collisional excitation of atoms in the ground state. Assuming hydrogenic behavior, the equilibrium time is then estimated by¹³

$$T_1^{z-1} \approx \frac{(1.1 \times 10^7 \text{ sec cm}^{-3}) z^3}{f_{21} N_e} \left(\frac{N_a^z}{N_a^z + N_a^{z-1}} \right) \frac{E_2^{z-1,a}}{z^2 E_H} \left(\frac{\kappa T}{z^2 E_H} \right)^{1/2} \exp \left(\frac{E_2^{z-1,a}}{r T} \right) \quad (2-42)$$

where $E_2^{z-1,a}$ is the energy of the first excited state and the term in brackets is the fraction of atoms or ions that must be excited into the next ionization stage. If only partial LTE is required (i.e., the state with principal quantum number n is in equilibrium with higher states) the equilibrium time is much shorter, and is estimated by¹³

$$T_n^{z-1} \approx \frac{(4.5 \times 10^7 \text{ sec cm}^{-3}) z^3}{n^4 N_e} \left(\frac{\kappa T}{z^2 E_H} \right)^{1/2} \exp \left(\frac{2z^2 E_H}{n^3 \kappa T} \right).$$

CHAPTER III

EXPERIMENTAL METHOD

A. Apparatus

A.1 T-tube and circuit. The plasma studied in this work was produced in a T-tube similar to those developed by Kolb^{29,30} and used in several previous experiments at the University of Maryland³¹⁻³⁶ and elsewhere.^{37,38} In this device, illustrated in Fig. 3-1, an aluminum (alloy 2024-T4) electrode was sealed into either end of the top of a T-shaped tube of high-temperature glass with inside diameter of 16 mm. This tube was filled with the test gas at a pressure near .5 Torr (70 Pascals). A current flowed across the 16 mm gap between the electrodes, ionized the gas and ohmically heated it, then returned via a backstrap above the T. The backstrap current created a transverse magnetic field in the current-carrying plasma, and pressure and Lorentz force accelerated it down the leg of the T. This luminous front traveled 12 cm down the tube at several cm/ μ sec and struck an adjustable reflecting plate, where some of its directed motion was converted to random thermal motion. Longer expansion tubes and higher fill pressures are required for the formation of a separated shock, but this device produced the high temperatures (3.5 eV) and electron densities ($2 \cdot 10^{17} \text{ cm}^{-3}$) needed to excite ionized helium lines. The decaying plasma lasted approximately one μ sec

The circuit used appears in Fig. 3-2. The relatively modest energy needed by the tube was supplied by a .5 μ F capacitor charged to 40 kV (thus storing 400 J). When charged, this capacitor was disconnected

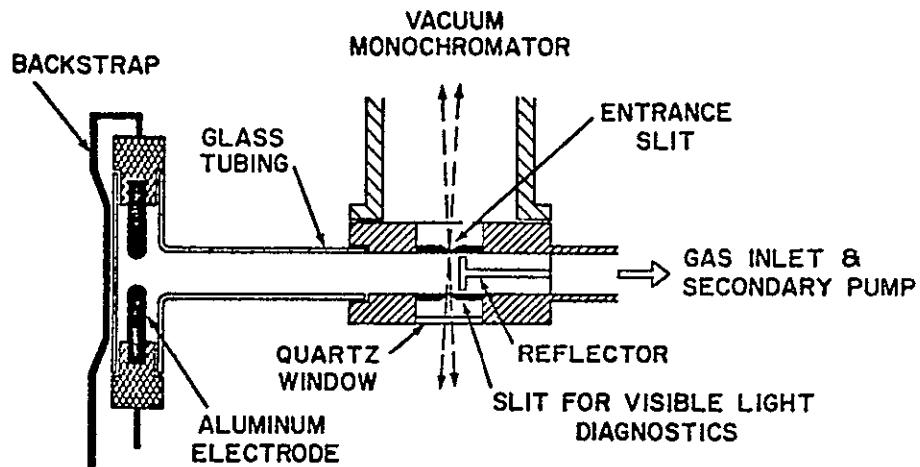


Fig. 3-1 T-tube schematic

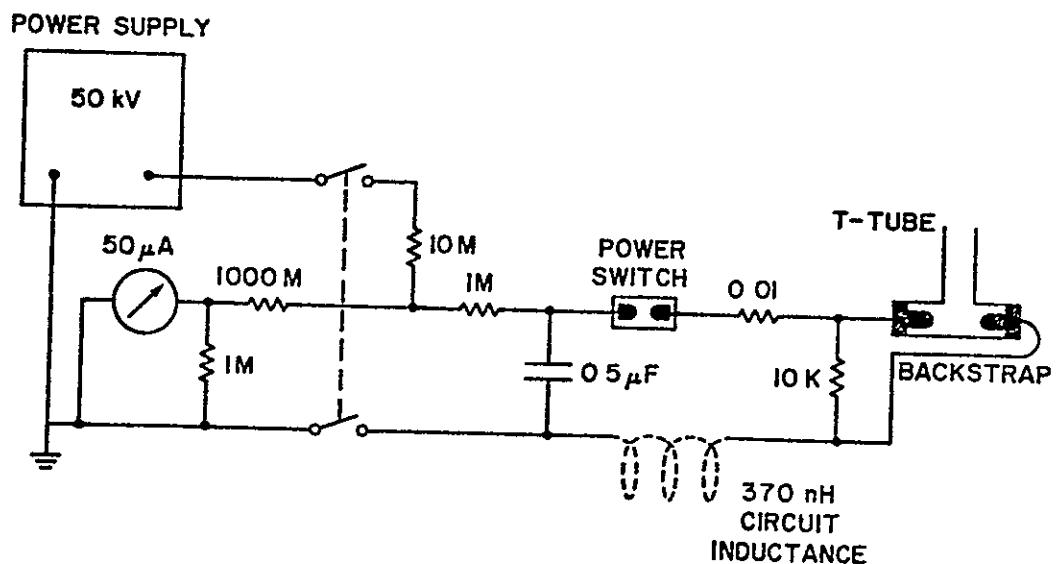


Fig. 3-2 Experiment circuit diagram

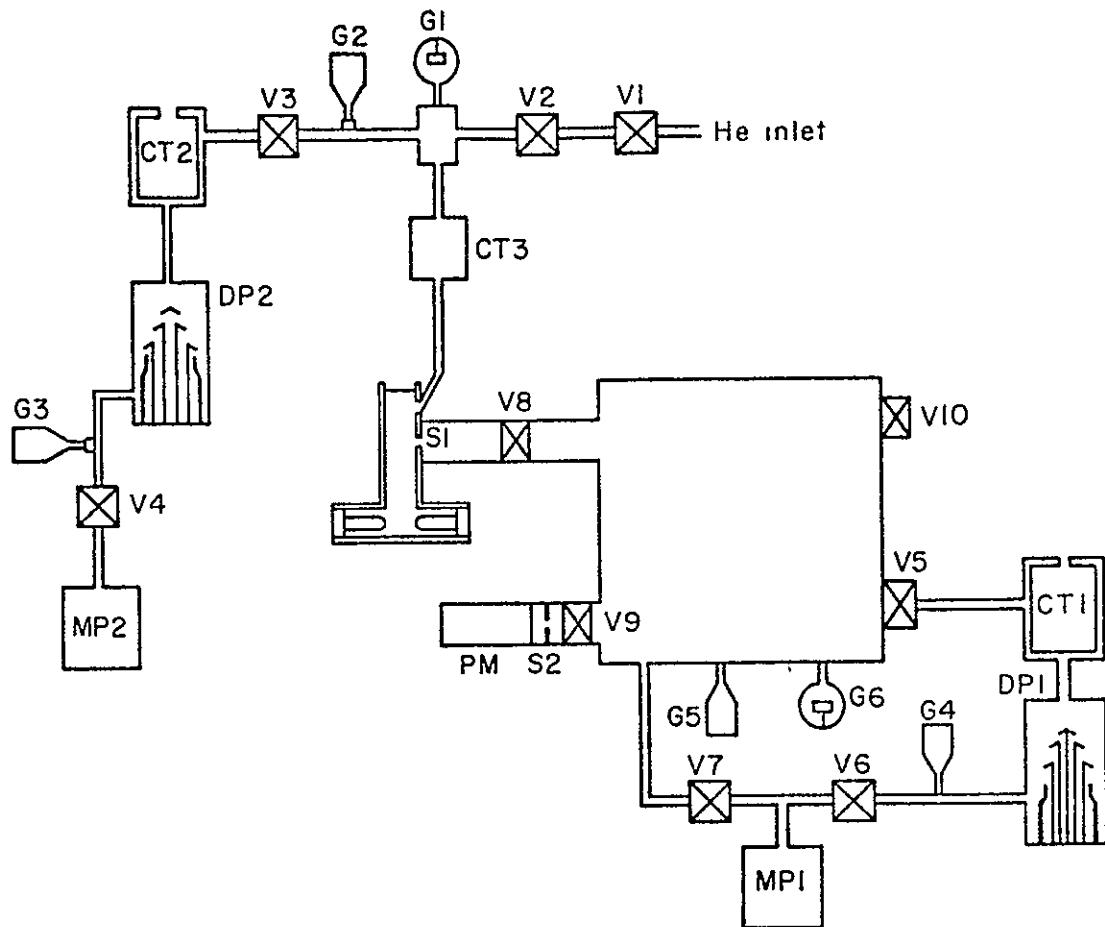
from both the high voltage supply and ground, preventing discharges from either electrode to the monochromator. The high-voltage circuit was enclosed by a copper shield to reduce electromagnetic interference.

To start the discharge, the nitrogen in a two-electrode pressure switch (initially at 30 PSI above atmospheric) was released until its dielectric strength was low enough for electron cascade. Since nitrogen was used, no ozone or nitrogen oxides were formed, as in a discharge in air. The poor control over discharge timing was no problem, since the discharge itself triggered the recording system.

The measured quarter-cycle time was .675 μ sec, indicating a total circuit inductance of 370 nH. A carbon resistor of about .01 Ω damped out the oscillations after two cycles.

The vacuum system is shown in Fig. 3-3. During the experiment, valve V3 was closed, while shut-off valve V1 and leak valve V2 were opened, so the test gas flowed from the inlet, through liquid nitrogen cold trap CT3, into the T-tube. It then leaked into the monochromator through entrance slit S1, and was removed by pumps DP1 and MP1. V2 was adjusted so the leak rates into and out of the T-tube balanced, and the pressure, measured by thermistor gauge G2, stayed at the desired value.

Between experimental runs, the T-tube was isolated by closing slit valve V9 and shut-off valve V1, and kept clean by the small diffusion pump DP2. Cold trap CT2 was cooled by a conventional refrigeration system and valves V3 and V4 were solenoid-controlled, so this secondary pumping system could operate unattended. Since the small pump was not forced to pump through a slit, it proved more effective than the large pump at outgassing the T-tube and associated plumbing.



- G1 ionization gauge Veeco RG-83
 G2,G3 thermistor gauge CVC GT-340A
 G4,G5 Gauge thermocouple
 G6 Gauge cold cathode discharge
 V1 Metering valve, 1/4 in.
 V2 Screw valve Veeco, 3/8 in.
 V3 Solenoid valve Veeco, 3/4 in.
 V4 Solenoid valve Veeco, 3/4 in.
 V5 Gate valve
 V6 Solenoid valve
 V7 Solenoid valve
 V8 Entrance slit valve
 V9 Exit slit valve
 V10 Air inlet valve
 DP1 Diffusion pump, NRC, 6 in.
 DP2 Diffusion pump, 2 in.
 CT1 Liquid nitrogen cold trap
 CT2 Freon cold trap
 CT3 Liquid nitrogen cold trap
 MP1 Fore pump DuoSeal 1397
 MP2 Fore pump DuoSeal serial 16025-2
 S1 Entrance slit
 S2 exit slit
 PM photomultiplier tube

Fig. 3-3 Schematic of vacuum system

A.2 VUV monochromator and detector. The optical arrangement is shown in Fig. 3-4. A McPherson 225 one-meter monochromator scanned the ultraviolet lines shot-to-shot. Its 50 μ entrance slit was flush with the wall of the T-tube, about .5 mm from the reflector. Since the plasma conditions changed sharply as the reflector was moved, the position was chosen which gave the most reproducible plasma. A 1200 lines/mm Pt-coated grating, with speed about f/13.6, focused the light onto a 30 μ exit slit, for a measured reciprocal dispersion of 8.3 $\text{\AA}/\text{mm}$ (4.2 $\text{\AA}/\text{mm}$ in second order) and an approximately Gaussian instrument response function of width $\sim .41 \text{\AA}$ ($\sim .19 \text{\AA}$ in second order). The light then fell on a p-terphenyl coated disc, causing it to fluoresce.³⁹ These visible photons left the vacuum chamber through a quartz window and were detected by an EMI 6522 photomultiplier. For some work, a 2 mm thick MgF_2 filter was placed between the exit slit and the fluorescent screen to remove light from second order, since it transmitted 40% of the light at 1215 \AA but essentially none below 1100 \AA .⁴⁰ The exit slit, screen, and PM tube were replaced by a film holder for photographic work. The instrument function and wavelength calibration were checked using a low-pressure Tanaka lamp.

A.3 Visible monochromators and detectors. For diagnosis of the plasma conditions, three Jarrell-Ash visible-light monochromators were used. One 1/2-meter focal length monochromator, with instrument width .4 \AA , scanned the He II 4686 line shot-to-shot to determine the electron density (from line width)¹⁰ and temperature (from line: continuum ratio)⁴¹. The reproducibility of the plasma was monitored on each shot by two 1/2-meter instruments, one for the continuum at 4976 \AA

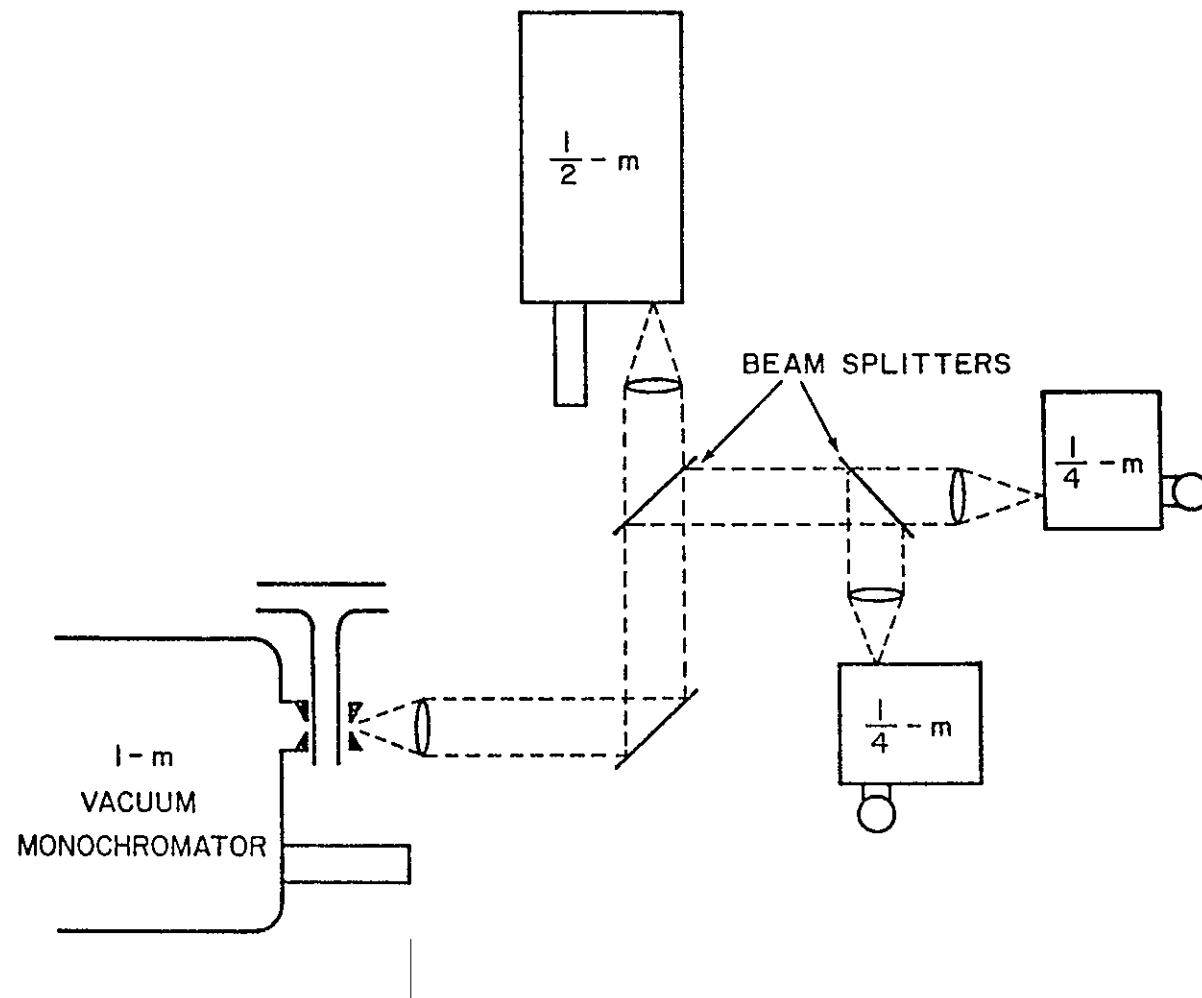


Fig. 3-4 Schematic of optical arrangement

(sensitive to electron density), and one for the He II 4686 line (sensitive to temperature, and used for later data processing).

PM tube response was checked using neutral density filters and pulses from a light emitting diode, and was found linear for signals of up to .2 V (1.1 mA) with a PM supply voltage of 900 V.

Each PM tube housing was insulated from its monochromator, and signals were taken from both the anode (negative pulse) and last dynode (positive pulse), carried by shielded, coaxial cables terminated by 90Ω resistors, subtracted to suppress noise, amplified, digitized, and stored electronically. For details on the waveform recorder, see Appendix A.

B. Data Reduction

The best-fit values of the four parameters (line intensity I , line position λ_0 , background intensity B , and electron density N_e) are found using the following procedure. Assume we have the n measurements $y_i(\lambda_i)$ and the corresponding theoretical intensities $T_i = \frac{1}{F_0} T\left(\frac{|\lambda_i - \lambda_0|}{F_0}\right)$, where $T(\alpha)$ is the theoretical profile after convolution with the instrument profile $G(\alpha)$

$$T(\alpha) = \int_{-\infty}^{\infty} S(\alpha - \alpha') G(\alpha') d\alpha' , \quad (3-1)$$

and the instrument function has been transformed into α -space. The best-fit values minimize the sum

$$\sigma^2 = \frac{1}{n-4} \sum_{i=1}^n [y_i - (IT_i + B)]^2 , \quad (3-2)$$

giving the conditions

$$\frac{\partial}{\partial I} \sigma^2 = \frac{\partial}{\partial B} \sigma^2 = 0 ,$$

so I and B are found by solving the linear system

$$\begin{pmatrix} \sum T_i^2 & \sum T_i \\ \sum T_i & n \end{pmatrix} \begin{pmatrix} I \\ B \end{pmatrix} = \begin{pmatrix} \sum y_i T_i \\ \sum y_i \end{pmatrix} . \quad (3-3)$$

The computer program "guesses" an electron density to use for the transforming of the instrument function, convolves the theoretical and instrument profiles, then finds σ^2 from (3-2) (subject to (3-3)) for many values of N_e and λ_0 . When the best values are found, the new N_e is used to again transform the instrument function. The entire convolution and fit are repeated until successive values of N_e are sufficiently close, e.g., within 2% of each other. A general discussion of least-square fitting when the functional parameters do not occur linearly (e.g., λ_0 and N_e) appears as Appendix B. Details on the computer programs appear in Appendix C.

CHAPTER IV

RESULTS AND DISCUSSION

A. Results

Examples of photoelectric measurements of the emission profiles of the ionized helium lines at 4686, 1640 and 1215 Å are shown in Figs. 4-1 through 4-3. In each case, the solid line is the best-fit theoretical curve of Kepple,^{9,10} convolved with the instrument profile (taken to be Gaussian), Dashed lines are the best-fit continuum levels, determined primarily by points far from line center, which are not shown. Crosses represent points not used in the best-fit procedure.

The 4686 line was found to be unshifted, as in previous experiments.² Its profile was in good agreement with theory, and the plasma electron density and temperature were deduced from its width and line:continuum ratio, respectively.

The position of the 1640 line was measured relative to the Al II 1670 line, and a fairly constant red shift of .11 Å was found. These shift measurements can be found in Table 4-1 and Fig. 4-4. No conclusions could be drawn about the Stark width of this helium line, because the observed profile was dominated by instrument broadening.

The relative positions of the He II 1215 and Si III 1210 lines were measured photoelectrically. The helium line was found to have a red shift of approximately .19 Å, increasing as the density and temperature fell at the end of the discharge. The halfwidth of the 1215 line was also determined as a part of the best-fit procedure.

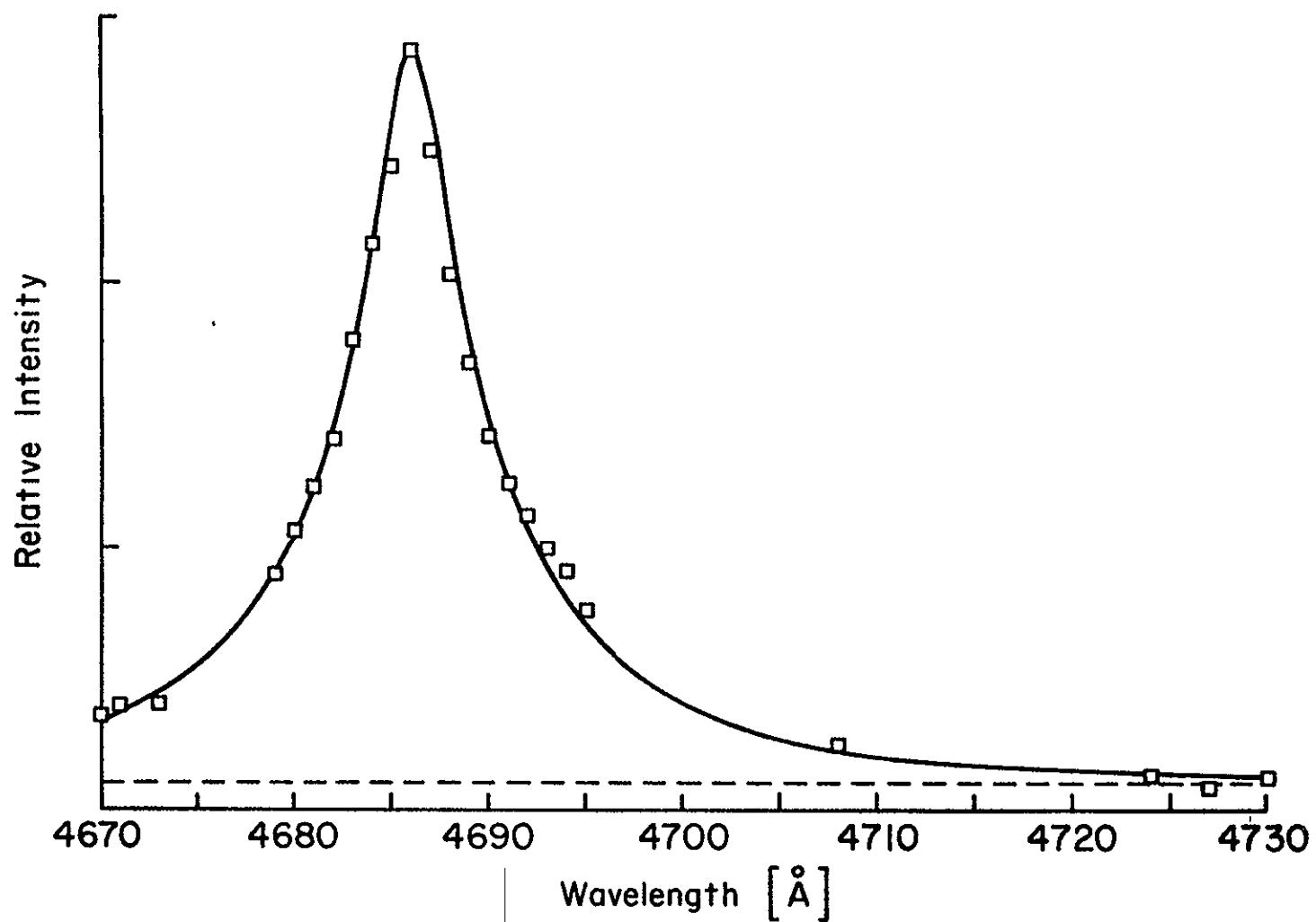


Fig. 4-1 Measured and best-fit profile for He II λ 4686 Å line

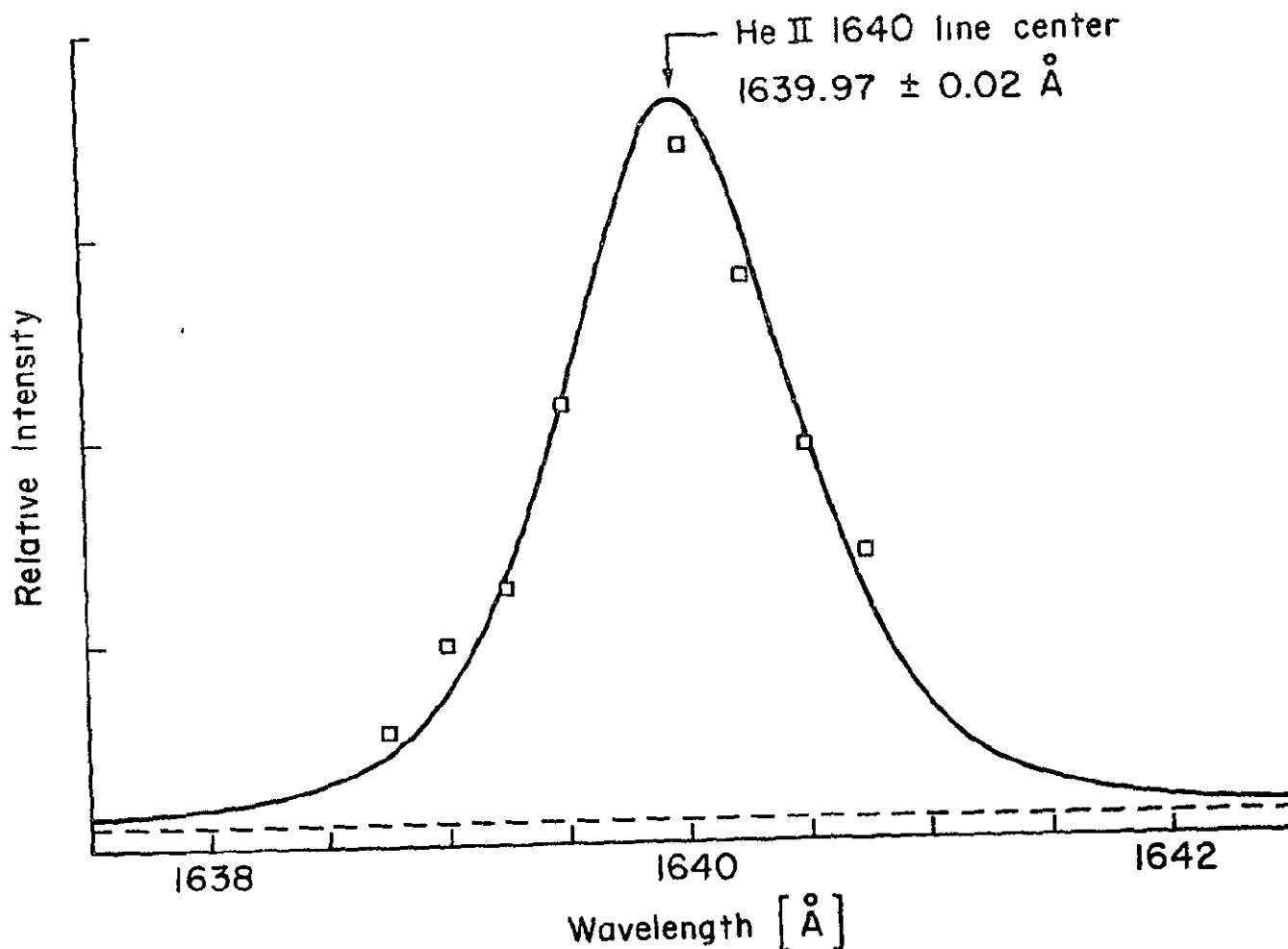


Fig. 4-2 Measured and best-fit profile for He II λ 4686 line

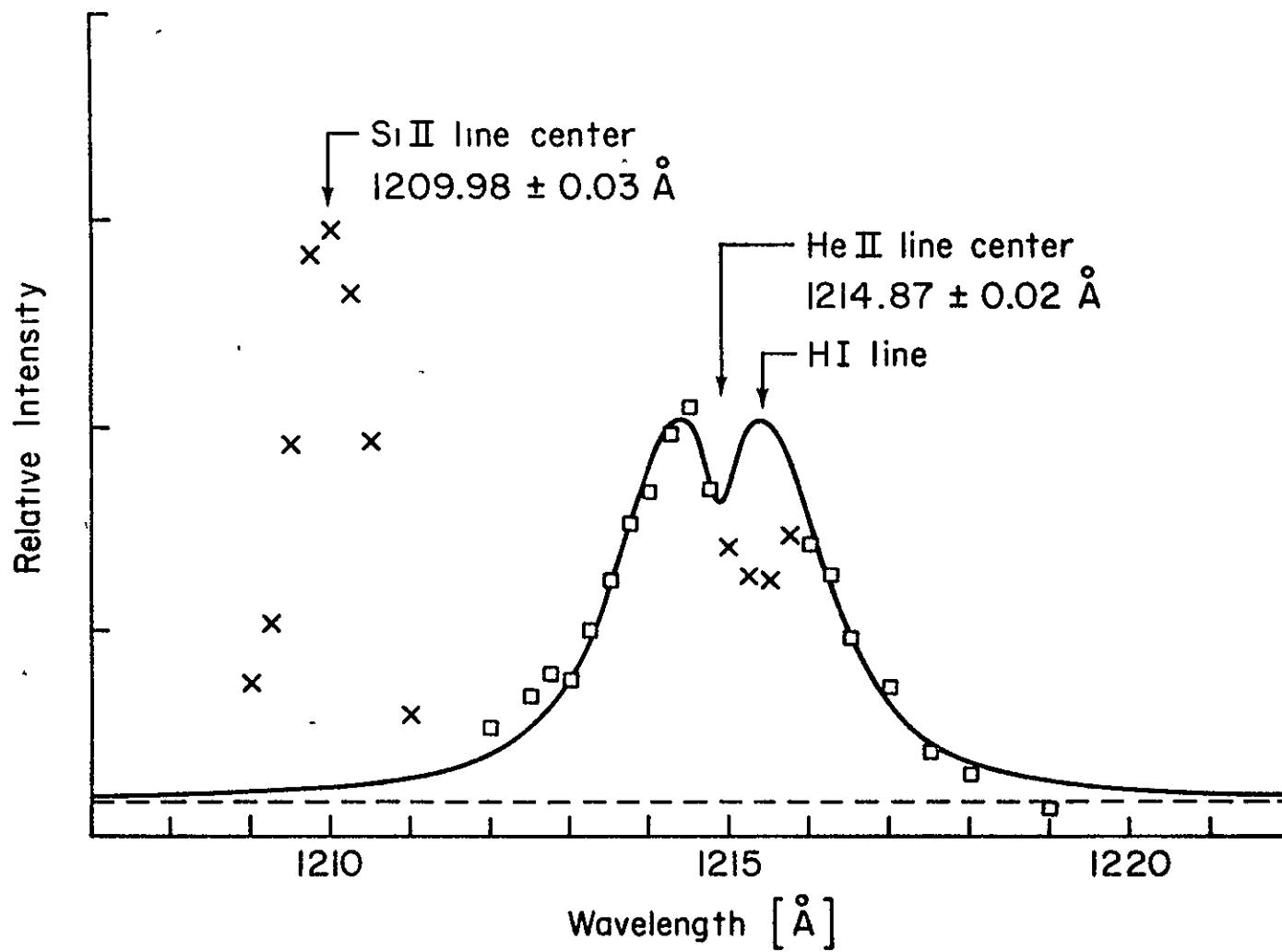


Fig. 4-3 Measured and best-fit profile for He II λ 1215 line

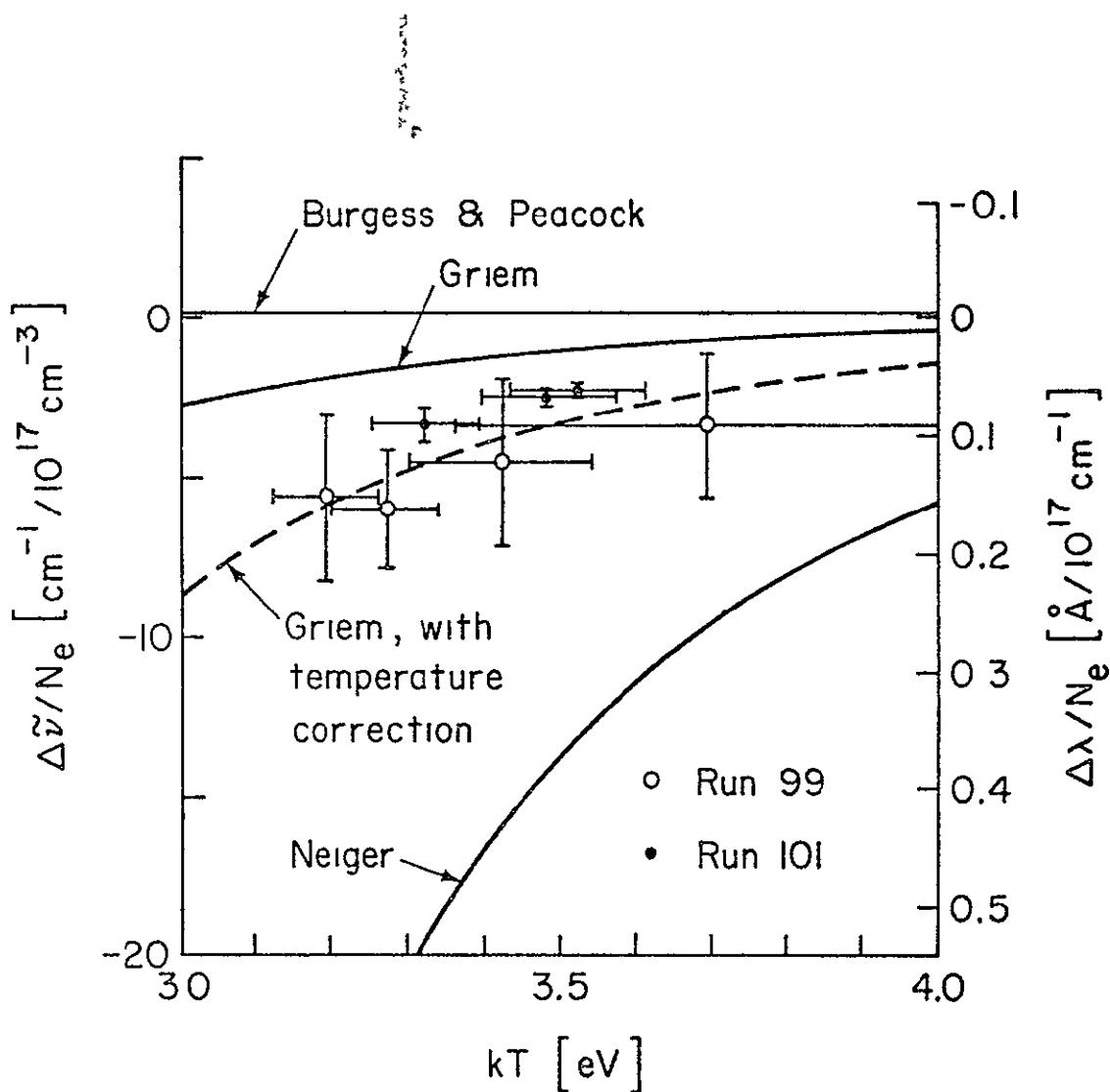


Fig. 4-4 Estimated and measured shifts of He II λ 1640 \AA line

	t [μsec]	V _{monitor} [mV]	κT [eV]	N _e [10 ¹⁷ cm ⁻³]	λ _{Al} [Å]	λ _{He} [Å]	Δλ [Å]	Δλ/N _e [Å/10 ¹⁷ cm ⁻³]
unshifted								
Run 101	3.938	28.6	3.52±.09	1.83±.05	1669.53±.01	1639.17±.01	.11±.01	.060±.005
	4.028	24.3	3.48±.09	1.67±.05	1669.54±.01	1639.18±.01	.11±.01	.066±.006
	4.104	20.6	3.32±.07	1.35±.05	1669.54±.02	1639.19±.01	.12±.02	.089±.015
Run 99	3.912	54.3	3.69±.33	1.42±.04	1670.32±.08	1639.98±.02	.13±.08	.09±.06
	4.004	46.1	3.42±.12	1.20±.03	1670.30±.08	1639.97±.02	.14±.08	.12±.07
	4.089	39.2	3.27±.07	1.02±.03	1670.31±.05	1640.00±.02	.16±.05	.16±.05
	4.146	33.3	3.19±.07	.94±.03	1670.32±.07	1639.99±.02	.14±.07	.15±.07

Table 4-1 Plasma Conditions, Shifts of HeII λ 1640 Å

These data are shown in Fig. 4-5 and Table 4-2.

B. Discussion of Possible Errors

B.1 Impurity Lines. Photographs of spectra near each of the helium lines showed many Si, O, and Al lines. The Jarrell-Ash 1/2-m monochromator could easily resolve the Si III and O II lines near He II 4686, and photoelectric scans were made using points between these impurity lines (see Fig. 4-6).

A survey spectrum was taken near the 1640 line using Kodak SWR film in the camera attachment for the McPherson 225 vacuum monochromator (see Fig. 4-7). Many Si, O, and Al lines were identified, in both first and second orders. Fortunately, none of these obscured the 1640 line. The nearby Al II 1670 line, chosen as the wavelength standard for position measurements of the 1640 line, was partially obscured by second order lines of O II and O III. Photographs using an MgF_2 filter were then taken, which showed no further problems with impurity lines. To eliminate second order lines during photoelectric scans, the filter was placed between the exit slit and the scintillating disc.

A photographic spectrum near 1215 Å showed many O II, O III, O IV Si III, and Si IV lines, including the second order O IV 608 line on the red wing of the helium line (see Fig. 4-8). To eliminate these, the MgF_2 filter was again used for both photographic and photoelectric runs.

The resonance lines of N II at 1084 Å prevented any observation of the next member of the He series, while the He II 1025 line proved too weak for reliable observation.

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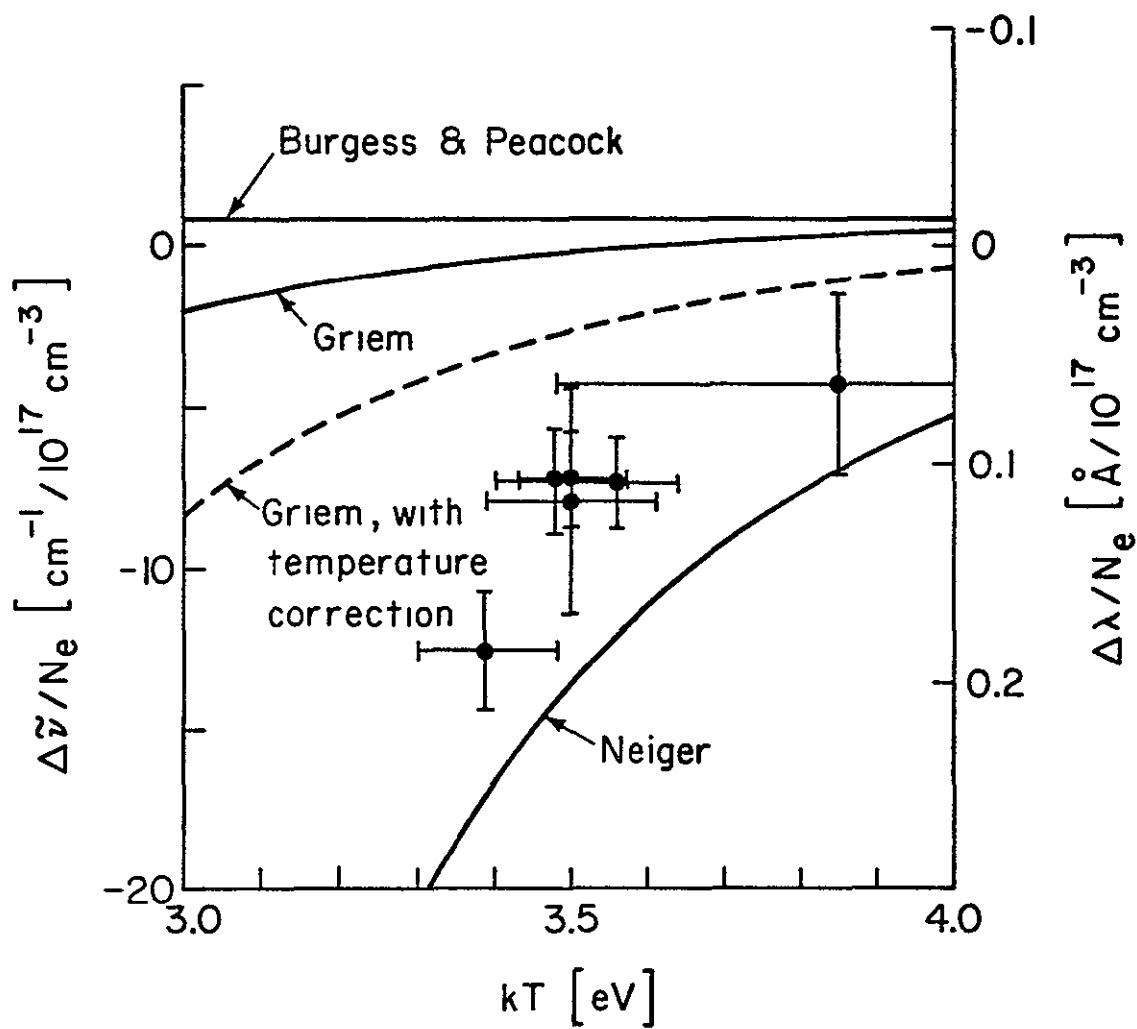


Fig. 4-5 Estimated and measured shifts of He II λ 1215 \AA line

t [μ sec]	κT [eV]	$\lambda_{\text{HHW}, 4686}^{\text{exp}}$ [\AA]	N_e [10^{17} cm^{-3}]	$\lambda_{\text{HHW}, 1215}^{\text{theory}}$ [\AA]	$\lambda_{\text{HHW}, 1215}^{\text{exp}}$ [\AA]	$\frac{\lambda_{\text{HHW}, 1215}^{\text{exp}}}{\lambda_{\text{HHW}, 1215}^{\text{theory}}}$	$\Delta\lambda$ [\AA]	$\Delta\lambda/N_e$ [$\text{\AA}/10^{17} \text{ cm}^{-3}$]
3.864	$2.23 \pm .07$	$4.61 \pm .12$	$2.23 \pm .07$	$1.97 \pm .05$	$2.06 \pm .09$	$1.05 \pm .05$	$.14 \pm .09$	$.063 \pm .041$
3.948	$1.93 \pm .05$	$4.09 \pm .09$	$1.93 \pm .05$	$1.75 \pm .03$	$1.96 \pm .06$	$1.12 \pm .04$	$.21 \pm .04$	$.109 \pm .021$
4.040	$1.77 \pm .05$	$3.80 \pm .09$	$1.77 \pm .05$	$1.63 \pm .03$	$1.95 \pm .05$	$1.20 \pm .04$	$.19 \pm .04$	$.107 \pm .023$
4.122	$1.66 \pm .05$	$3.60 \pm .09$	$1.66 \pm .05$	$1.54 \pm .04$	$1.88 \pm .06$	$1.22 \pm .05$	$.18 \pm .04$	$.108 \pm .024$
4.191	$1.62 \pm .06$	$3.53 \pm .11$	$1.62 \pm .06$	$1.51 \pm .05$	$1.88 \pm .06$	$1.25 \pm .06$	$.19 \pm .04$	$.117 \pm .052$
4.245	$1.46 \pm .07$	$3.24 \pm .13$	$1.46 \pm .07$	$1.38 \pm .06$	$1.82 \pm .05$	$1.32 \pm .07$	$.27 \pm .04$	$.185 \pm .027$

Table 4-2 Plasma Conditions, Shifts and Widths of HeII $\lambda 1215 \text{ \AA}$

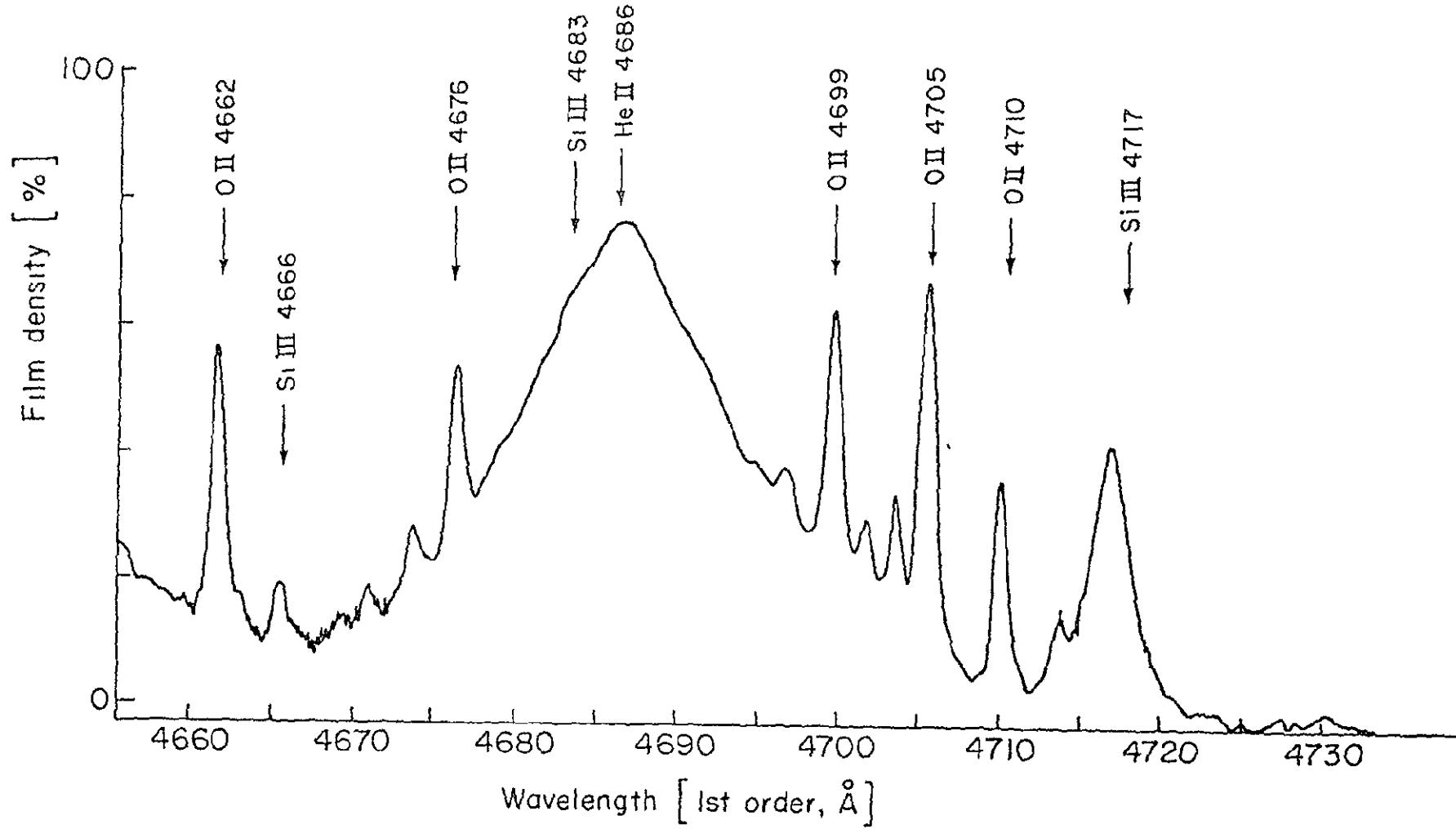


Fig. 4-6 Densitometer scan of spectrum near He II λ 4686 \AA line

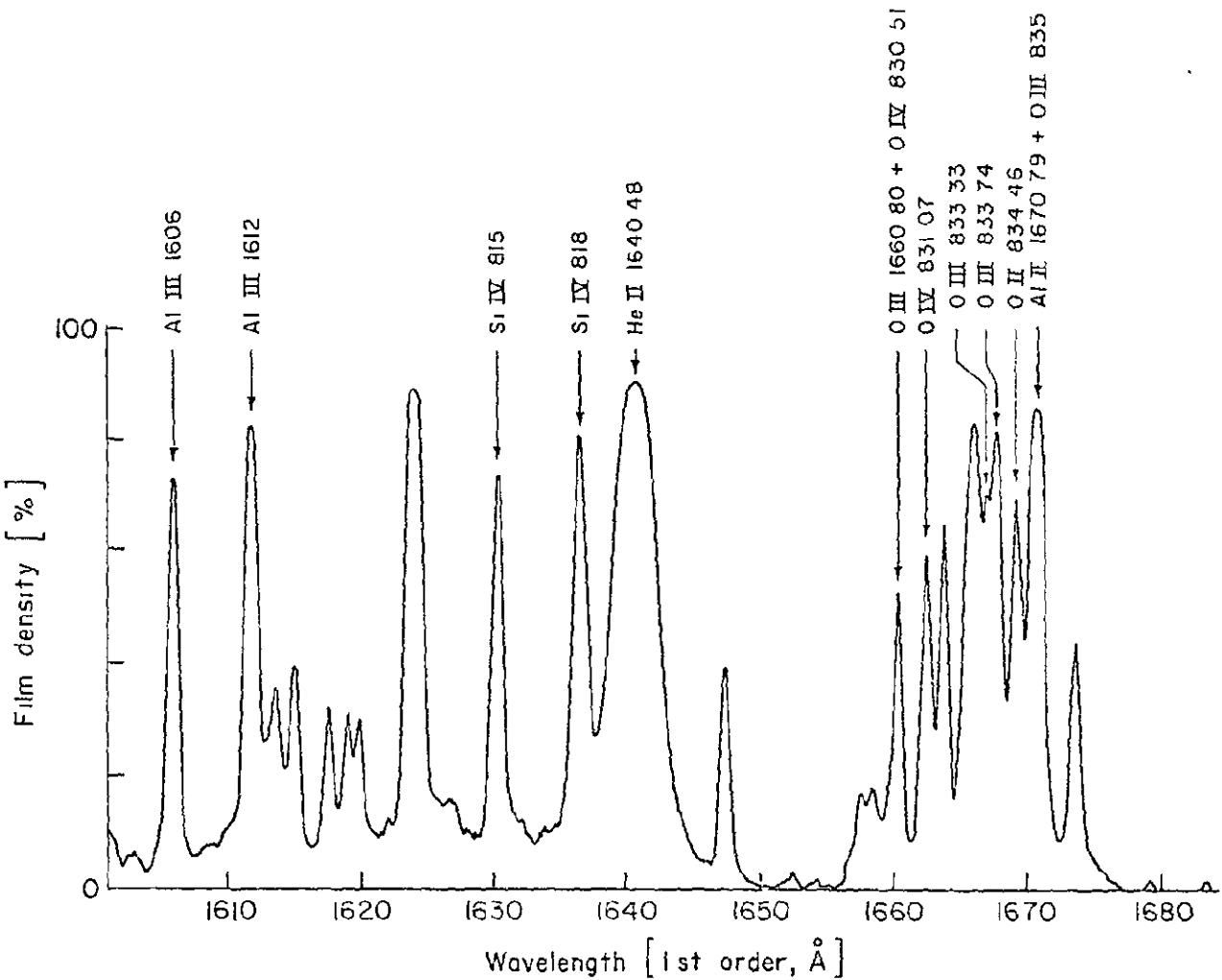


Fig. 4-7 Densitometer scan of spectrum near He II λ 1640 \AA line

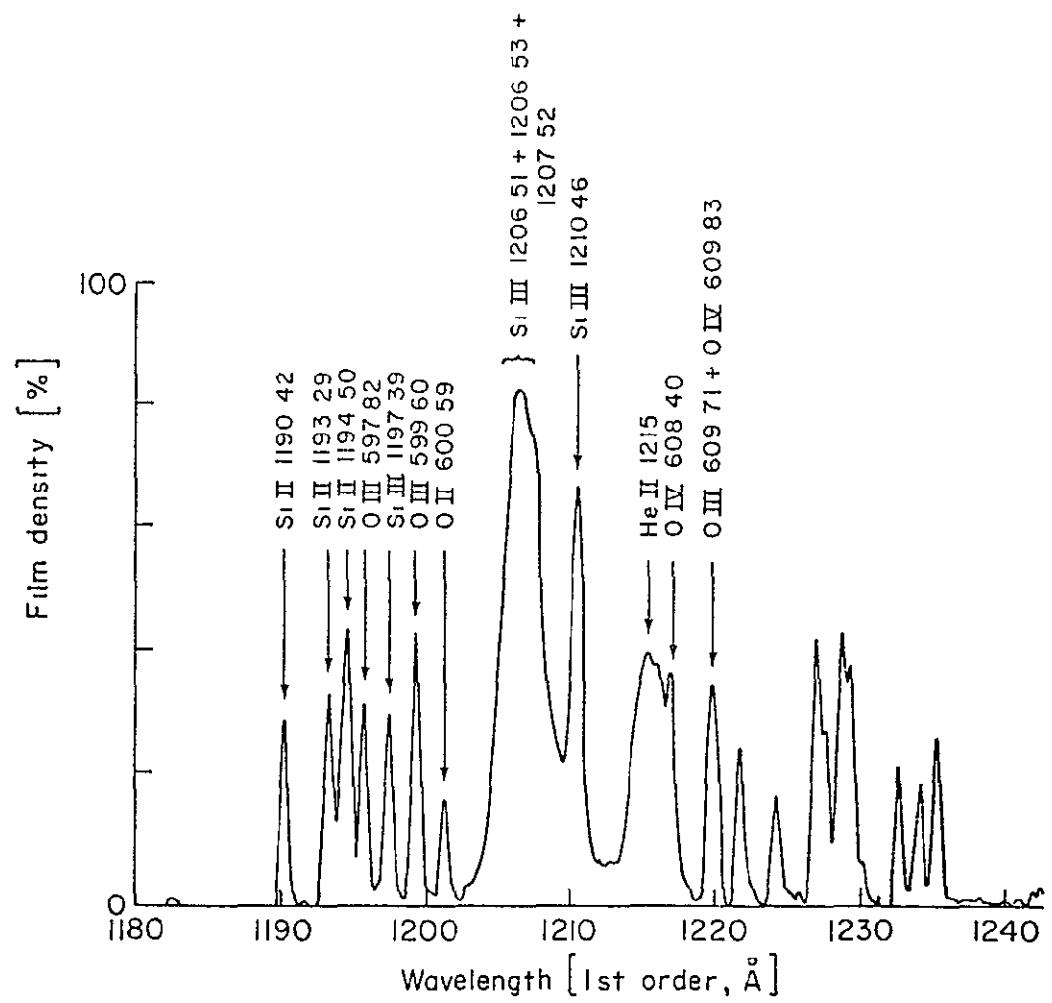


Fig. 4-8 Densitometer scan of spectrum near He II λ 1215 Å line

B.2 Wavelength Standards. All line position measurements were made relative to nearby impurity lines, and the accuracy of this procedure had to be verified. The Stark shifts of these ion lines are expected to be small⁴² (just as their widths are small), but a plasma polarization shift certainly cannot be ruled out a priori. To check for such shifts, several line position measurements were made on a Grant comparator-microphotometer. The second-order lines were found to be shifted with respect to the first-order lines by .10 Å, but otherwise, shifts were less than the measurement accuracy of .05 Å. This is consistent with previous measurements,³ in which no shifts were found for the O III and N III lines near 300 Å. In photoelectric (time-resolved) studies, no absolute shifts of the reference lines were measured as the plasma cooled, also arguing against substantial absolute shifts. Only the statistical errors in the measured shifts are indicated in the tables and figures

The monochromator wavelength scale was checked by measuring photographically the wavelength displacement between settings corresponding to the centers of the helium and reference lines. The errors in both cases were less than the setting error of 0.02 Å

B.3 He II 1215 Asymmetry. The helium 1215 line was expected to have a symmetric, double-peak profile (like that of H_β), but photoelectric scans showed only the peak on the blue side (see Fig 4-3). This was interpreted as showing reabsorption by hydrogen in a cooler boundary layer, since the hydrogen Lyman-α line lies .50 Å to the red of the (unshifted) helium line center. To check this explanation, two scans were made, using mixtures of helium plus 0.5% hydrogen, and helium plus 1.0% deuterium, respectively. The amount of absorption increased with the increasing admixture of hydrogen, and, in the case of the deuterium, the dip shifted to the blue, as expected

The residual concentration of hydrogen was estimated from these runs to be approximately 0.2% Since natural, Doppler, and Stark broadening are all very small for the hydrogen line ($<1 \text{ \AA}$), points near the dip were merely excluded from the fitting procedure.

B.4 Departure from LTE. Temperature determination from a helium ion line:continuum ratio requires that LTE holds also for the ion ground state populations, so that the line intensity (proportional to the population in the excited state) and the continuum intensity (due mainly to recombination radiation) both have their equilibrium values. The equilibration time for atomic states can be estimated from (2-42) to be only a few nanoseconds, for both neutral and ionized helium On the other hand, the recombination times (into the ground states) are estimated to be^{43,44} 2 μsec for formation of singly ionized helium and 20 μsec for neutral helium Singly and doubly ionized states are, then, expected to be overpopulated, simulating a temperature higher than the true electron temperature.

For the validity of complete LTE in a stationary plasma with temperatures near those in the experiment, Eq. (2-11) gives an optical depth of ~ 150 , for the resonance line (He II $\lambda 304 \text{ \AA}$). We are thus justified in relaxing (2-40) by an order of magnitude, and the electron density required for complete LTE is $N_e \sim 1.4 \times 10^{18} \text{ cm}^{-3}$, which is not reached in the experiment. On the other hand, the requirement (2-39) for partial LTE for the level $n=4$ (upper state of the 4686 \AA line) is easily satisfied.

Since the actual electron density is about an order of magnitude lower than that required for complete LTE, and the continuum intensity is proportional to the electron density while the line intensity is not, we estimate that the line:continuum ratio may be too high by an order of magnitude, compared with the LTE value at the true

temperature. This yields ⁴¹ a temperature (~ 3.5 eV) that is too high by about .5 eV. Similarly, if the neutral excited state population density were too low by an order of magnitude, the intensity ratio of an ionized and a neutral line would overestimate the temperature by about .5 eV. A measurement of the intensity ratio of the He II 4686 and the He I 3889 lines was performed, yielding temperatures near 4.1 eV. Since the two effects (overpopulation of singly ionized states due to recombination relaxation during the rapid cooling, and overpopulation of excited states of He II due to low collision rates) are additive, the true electron temperature is estimated to be less than the lower figure by $\sim 20\%$, i.e., near 3.0 eV.

A previous measurement³⁸ of the absolute intensity of the He II 4686 line in a shock-tube plasma at $N_e \approx 10^{17} \text{ cm}^{-3}$ indicated the populations of the lower excited states of the ion deviate by perhaps a factor of 4 from LTE. However, measurements of temperature in the same experiment by Thompson scattering of laser light (which does not depend on LTE for atomic states) and the intensity ratios of the He II 4686 and He I 5876 lines showed good agreement.

B.5 Summary of Errors. Possible errors in the determination of electron density were judged to be 5% due to statistical fluctuations and 10-15% due to theoretical uncertainties.¹⁰ Errors in temperature measurements were estimated to be .1 eV statistical and .2 eV theoretical (after applying the 20% correction). These possible diagnostic errors were not judged to endanger the principal conclusions of the work. The tables and figures indicate only statistical errors.

Errors in the measurements of the shifts were .05 Å or less due to statistical fluctuations. Systematic errors due to the shift of the

reference lines could not be ruled out, but were shown to be less than .05 Å and are expected to be smaller.

C. Discussion of Results

As mentioned in the Introduction (Chapter I), previous shift measurements of He ion lines have concentrated on the Lyman-series lines ($n_{lower} = 1$). In principle, these measurements can be used to calculate the energy level perturbations, and the shifts of the "Balmer"-series lines can be found in turn. Since the agreement between the various measurements is so poor, little is learned in this way

The polarization shift is difficult to treat theoretically, and only estimates have been made thus far. Conceptually, the radiating ion is expected to attract plasma electrons, which partially screen the nuclear charge seen by the optical electron. A simple classical argument³ gives the wavelength (or wavenumber) shifts of the Lyman-series lines to be

$$\frac{\Delta\lambda}{\lambda_0} = - \frac{\Delta\tilde{v}}{\tilde{v}} = - \frac{8}{3} \pi \frac{N_e a_0^3 n^2 (n^2 + 1)}{z^4} \exp\left(\frac{V}{kT}\right) ,$$

where a_0 is the radius of the first Bohr orbit: $a_0 = \hbar^2/m e^2$, and V is the interaction energy between the perturbing plasma electron and the radiating ion. Since the wave packet of the perturbing electron will be comparable in size to the atom, Griem proposes¹ to use the averaged interaction $V = e^2/r$, where r is the characteristic distance between the nucleus and the optical electron. $r = n^2 a_0 / z$.

Neiger proposes⁶ the modified formula $V = (3/2)e^2/r$, which is the electrostatic energy of a uniform sphere of charge e and radius r

in the field of an equal but opposite charge at its center. Burgess and Peacock argue⁴⁵ that the density of electrons near an ion is low enough that their velocities are not in equilibrium with the surrounding plasma, being directly related to their electrostatic energies. They suggest using the interaction energy at the average perturber-perturber distance, $V = e^2 N_e^{1/3}$. Note that all these estimates predict blue shifts (for the Lyman-series lines) proportional to N_e , but decreasing with temperature (since, at high temperature, the electron's thermal energy is large compared with the electron-ion interaction energy, and it doesn't see the potential well). Denoting by V_n the chosen interaction energy when the optical electron has principal quantum number n , and expressing the unperturbed energy levels in term of the Rydberg constant R , we find, for the wavenumber shifts of the "Balmer"-series lines,

$$\Delta \tilde{v} = \frac{8}{3} \pi \frac{N_e a_0^3}{z^2} R \left\{ (n^4 - 1) \exp\left(\frac{V_n}{kT}\right) - (2^4 - 1) \exp\left(\frac{V_2}{kT}\right) \right\} .$$

This can be converted to a wavelength shift by multiplying with λ_0^2 , or an energy shift by multiplying by hc . Shifts predicted by each of these choices for V ($ze^2/n^2 a_0$, $3/2 ze^2/n^2 a_0$, and $e^2 N_e^{1/3}$) are plotted in Figs. 4-4 and 4-5. For both lines, Burgess and Peacock predict very small blue shifts, nearly independent of temperature. Griem's estimate gives somewhat larger shifts, while the stronger interaction proposed by Neiger gives large shifts with strong temperature dependence. Using the measured values of the temperature, the data are consistent with an interaction energy between those of Griem and Neiger, while Burgess and Peacock underestimate the shifts. To illustrate the effect of the systematic error discussed above in the temperature

measurement, the shift predicted by Griem's formula was recalculated using a 20% lower temperature, the results being shown as the dashed curve in Figs. 4-4 and 4-5. After this correction, his interaction energy gives the best fit to the data.

The halfwidth of the 1215 Å line was up to 30% greater than that calculated by Kepple.^{9,10} This is to be compared to a previous theta-pinch experiment,⁴⁶ in which the ratio of the widths of the 4686 and 1215 Å lines agreed with the calculated value. However, this experiment was done at a substantially higher temperature, $T_e \gtrsim 10$ eV, so that the difference may not be significant.

D. Conclusions and Suggestions

Shifts have been measured of the first two lines of the "Balmer" series of ionized helium. They are consistent with a plasma polarization shift, where the interaction energy between the radiating ion and the plasma electrons is between those proposed by Griem and Neiger and probably closer to the former.

The Stark width of the 1215 Å line of ionized helium has been measured, and found to be up to 30% greater than calculated by Kepple,^{9,10} and increasing as the temperature and density of the plasma decreased at the end of the discharge. This is perhaps due to an increased interference by the 1215 Å line of hydrogen.

Further studies of the plasma polarization shift might include more careful measurements of shifts of the hydrogenic spectra of heavier atoms, e.g., C VI 33.8 Å. Previous measurements³⁹ showed no shifts, but with a possible error of .05 Å. (In this connection, it is interesting to note that measured center wavelengths⁴⁷, e.g.,

of helium-like copper (Cu XXVIII) are slightly below theoretically predicted values.) An attempt might also be made to observe shifts of the higher "Balmer"-series members of ionized helium, perhaps in a Z-pinch or θ -pinch, with their greater optical depth.

APPENDIX A

WAVEFORM RECORDER

To reduce the error and delay of manual data taking with the usual Polaroid oscilloscopes, a waveform recorder was designed and built for this experiment (Fig. A-1). The signal from one of the PM tubes is amplified and applied simultaneously to 31 comparators. A voltage divider provides reference voltages for the comparators, so for a given signal voltage some of the comparators will be "on" and the rest "off". Integrated circuits accept the output of all the comparators, count the number "on", calculate the corresponding 5-bit binary number, and store it in a 5 bit by 64 word random access memory. When triggered, control circuits advance the memory address counter and give write commands once every 100 nanoseconds (or selectable, slower rates) for a total of 64 cycles. It then switches to "playback" mode, supplying the stored numbers, each in turn, to a digital-to-analog converter. This analog signal is a reconstructed version of the original signal, and can be displayed on an oscilloscope.

The recorder consists of five such analog-to-digital converters and memories, plus two digital-to-analog converters, so 5 signals can be recorded, then any two displayed simultaneously.

If the waveform is acceptable, the investigator may set the twelve "fixed data" thumbwheel switches and initiate recording. The shot number (incremented each time the device is triggered), the fixed data, and the contents of all 5 digital memories are written to a 9-track magnetic tape for later computer processing. The waveform recorder then

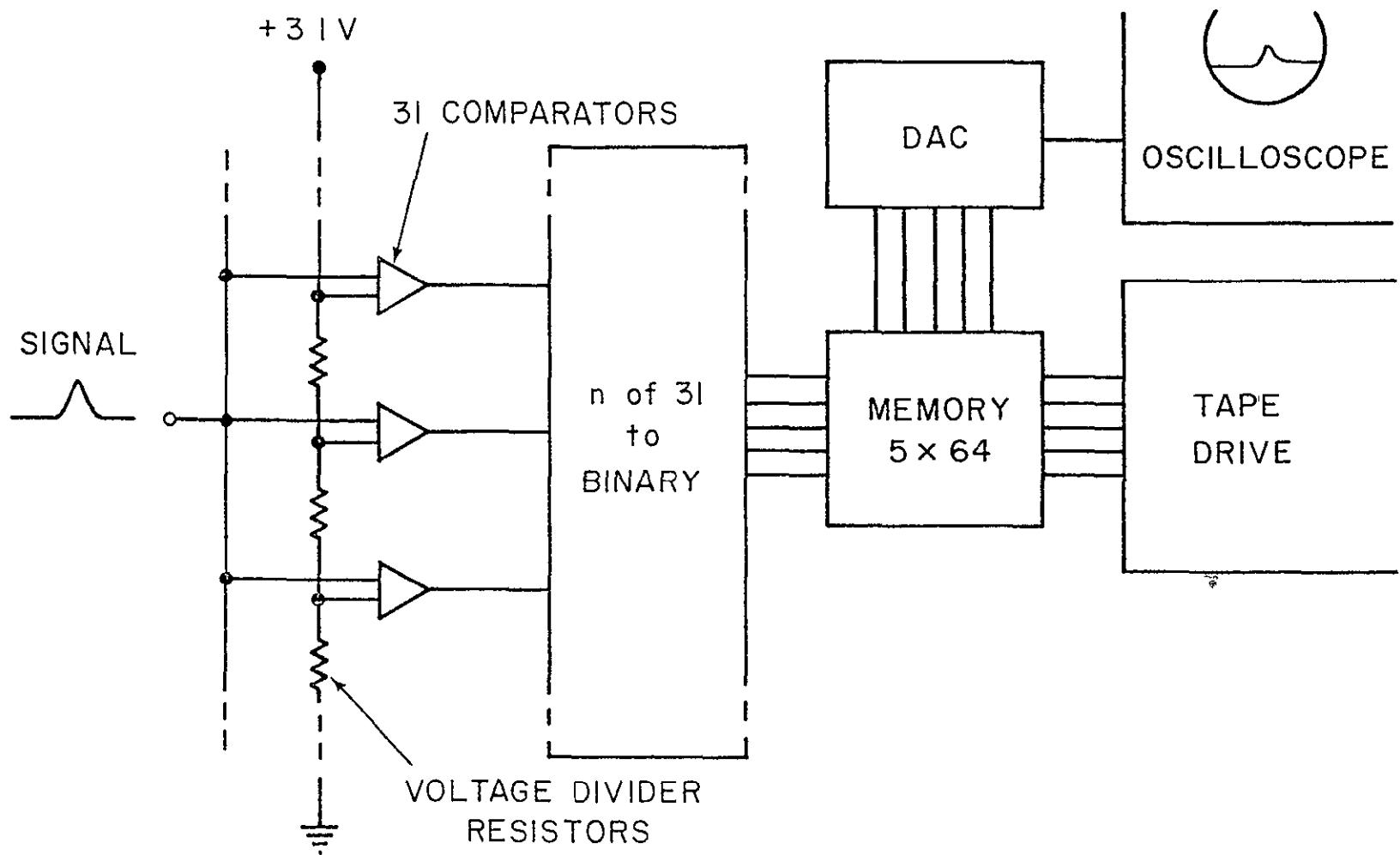


Fig. A-1 Block diagram of waveform recorder

reverts to "ready" mode, waiting for the next trigger pulse. If the shot was unacceptable (due to switch misfire or abnormal time history of a monitor signal, for example), recording can be bypassed.

Details on operation procedures and performance specifications of the waveform recorder appear in the following instruction sheet.

Digital Data Acquisition System
Instruction Manual

1. General Information

The Digital Data Acquisition System (DDAS) is a high speed analog to digital converter and memory. It can record 64 data samples on each of 5 channels, with a sample interval as short as 100 nsec. These stored samples can be displayed on an oscilloscope and recorded onto a 9-track magnetic tape.

2. Technical Specifications

sample rate, once every	.1, .2, .5, 1., 2., 5., 10, or 20 μ sec.
internal amplifier risetime	80 nsec
useful signal range	0 to + 32 V
maximum signal range	-1 to +1 V.
resolution	3.1% of full scale
channels	5
signal input impedance	50 Ω
trigger level	+1.1 V
max trigger signal range	-.6 to +5 V.
trigger input impedance	1M Ω
playback sweep output	22.7 Hz sawtooth, 0-2.6 V
analog output	0-5 V
enabling circuit	enabled if external circuit resistance is less than 100 Ω
mating input amplifier	Tektronix type 127 preamp power supply, with matching Tektronix oscilloscope preamp.
mating digital tape deck	Cipher model 70M-360, producing 800 BPI, 9-track, IBM-compatible magnetic tapes.
magnetic tape record	329 bytes of 8 bits each... 6 bytes (BCD, 2 digits/byte) fixed data from thumbwheel switches 3 bytes (BCD, 4 low order bits) experiment count 320 bytes (binary, 5 low order bits) data, grouped by time

3. Installation

For optimum protection against radio frequency interference, the unit should be mounted in a shielded 19 in. relay rack. Several inches clearance below the unit are necessary for ventilation.

4. Operation

The Cipher tape deck should never be switched on unless the DDAS is on, so the proper logic inputs are provided.

1. Turn on the DDAS and associated preamplifiers. Allow preamps to warm up
2. If a tape is desired, turn the tape deck on and load a tape. The "RECODER READY" lamp should light.
3. Switch the operating mode to "AUTO SEQUENCE", switch to "TRIGGER ENABLE INT", and press "RECORD BYPASS". The "ENABLED" lamp should light
4. Switch "DISPLAY CHANNEL SELECT" to "1". The "A-D DISPLAY" lamps are now displaying, in binary digital form, the signal on channel 1.
5. Ground the channel 1 preamp input. Advance the preamp "vertical position" control until all display lamps are lit. If this cannot be done, adjust the 127 preamp power supply "DC level" (on top of case).
6. Back off the "vertical position" control until all lamps just go out. The zero level is now adjusted. Repeat steps 4-6 for the remaining channels now, and frequently during the experiment
7. Connect the trigger and signal cables. If an "enable" circuit cable is to be used, connect it and switch to "TRIGGER ENABLE EXT". Set the desired sampling interval. When triggered (by a signal or by using the "MAN TRIGGER" button) the unit will record its 64 samples of each channel and increment the "EXPERIMENT COUNT".
8. If a visual monitor is desired, connect the "PLAYBACK SWEEP" to the "EXT HORIZ IN" jack of an oscilloscope, and one or both of the "ANALOG OUTPUT"'s to the vertical amplifier inputs. Set "ANALOG CHAN SELECT" to the desired channels.
9. When a signal is recorded, the unit will automatically switch to playback mode, the corresponding mode lamp will light, and the stored waveforms will be displayed on the oscilloscope.

10. If a recording is desired, set the desired "FIXED DATA", and press "RECORD DATA". Otherwise, press "RECORD BYPASS". The unit is again ready to record a set of signals. The unit may be switched to "MAN PLAYBACK" to again display the recorded signals.
11. After experiment has been completed, press "EOF" several times, and rewind and unload the tape.
12. Turn the tape deck off, then the DDAS and other equipment.

Alternate operating modes are provided for diagnostic purposes. In "SINGLE STEP PLAYBACK" mode, the contents of one word in memory, corresponding to the "DISPLAY CHANNEL SELECT" setting and the octal address shown under "MEMORY ADDRESS", are displayed under "MEMORY DISPLAY" and appear at the "ANALOG OUTPUT" jacks. The associated pushbutton steps to the next sample.

In "MAN SAMPLE" mode, the unit stores samples one at a time, when the "SAMPLE STROBE" pushbutton is pressed. The unit must be enabled and triggered before sampling can begin.

In "CAL" mode, the analog to digital converters operate continuously and any of them can be displayed on the "A-D DISPLAY" lamps.

APPENDIX B

STATISTICS

In most experiments the investigator assumes a functional form governing his data which has several parameters, and the object of his experiment is to determine the values of the parameters. If there is only one parameter, the quoted result might be

$$\alpha = \alpha^* \pm \sigma ,$$

where α is the true value (usually unknown), α^* is the "best" value which can be determined using the data, and σ indicates the error in α^* . We usually mean by σ the mean square deviation of the data from the best value

$$\sigma^2 = \overline{(x_1 - \alpha^*)^2} , \quad (B-1)$$

where the x_1 are the results from several similar experiments. It is necessary to extend this to the case of several parameters and specify a way of calculating the quoted values.

Assume the functional form is

$$y = f(\alpha, x) , \quad (B-2)$$

where x is the independent variable, y the dependent variable, and the α_1 are parameters. We define the error function⁴⁸

$$M(\alpha) = \sum_{k=1}^n \frac{(y_k - f(\alpha, x_k))^2}{\sigma(x_k)^2} , \quad (B-3)$$

and let the "best" α be that value α^* which minimizes M . We find it by solving the set of m equations

$$\left. \frac{\partial M(\hat{a})}{\partial a_i} \right|_{\hat{a}=\hat{a}^*} = 0 \quad (B-4)$$

The errors in these parameters are given by the elements of the variance-covariance matrix⁴⁸

$$\sigma_{ij} = \sqrt{(a_i - a_i^*)(a_j - a_j^*)}, \quad (B-5)$$

which can be calculated from⁴⁸

$$\sigma_{ij} = (H^{-1})_{ij} \quad H_{ij} = \frac{1}{2} \frac{\partial^2 M(\hat{a})}{\partial a_i \partial a_j}. \quad (B-6)$$

The variance of one of the parameters is then $\sigma_1^2 = \sigma_{11}$, and the correlation matrix is⁴⁹

$$C_{ij} = \frac{\sigma_{11}}{\sigma_i \sigma_j} \quad (B-7)$$

If all the $\sigma(x_k)$ have a common value σ , the solution of (B.4) is independent of that value. After this least square solution is found, σ can be calculated using

$$\sigma^2 = \frac{1}{n-m} \sum_{k=1}^n [y_k - f(\hat{a}; x_k)]^2, \quad (B-8)$$

where we divide by $n-m$ because after the parameters $a_1 \dots a_m$ have been calculated from the data, only $n-m$ degrees of freedom remain.

If $f(a; x)$ is linear in its parameters, the calculations are, of course, much simpler, since (B-4) is then a linear system which can be solved exactly. Failing this, a search must be performed in \hat{a} space for the best value.

APPENDIX C

PROGRAMS

The data read from the waveform recorder tapes are processed by several programs, each accepting an input file plus control or data cards, and producing one or more output files. The last programs, PROFILE, VPLOT, and THEORY, also print their results. Other programs are available to read and list each file for debugging. All mainline programs were written in FORTRAN for use on a Univac 1108 computer with the EXEC-8 operating system. Intermediate files are "direct-access" files on disc or drum storage, like those developed by IBM for their computers,⁵⁰ but not defined within ANS FORTRAN. Other nonstandard features used include PARAMETER statements and FORTRAN procedures.⁵¹

The first program, REVERT, uses the assembly-language subroutine TREAD to read the 9-track tape produced by the waveform recorder. The tape record format is shown in Fig. C-1. REVERT assumes the scale settings of the input amplifiers and the sample rate of the recorder were set on the "fixed data" thumbwheel switches. The alphanumeric file header (a prose description of the run), number of channels used, and wavelength for each channel and shot number are read from cards. The file header is written into the output file, copied by later programs, and identifies all printed output. Specified shots may be dropped at this point.

Since the waveform recorder stores 6.4 μ sec of the signal, while the plasma lasts only about one μ sec, REVERT tries to select only the useful part of each signal. The first twelve records are read, the average time T_{\max} of the maximum of the monitor signal is found, and the tape is

rewound. Each record is then read, and the data for eight samples, starting at time T_{\max} , are scaled and written to the output file, with format shown in Fig. C-2. An end-of-file marker is written after the last record.

During the experiment, the light is sometimes attenuated to prevent PM tube saturation, and PARAM corrects the measured intensities to account for this. Since PROFILE requires that the monitor signal be strictly decreasing, PARAM also chooses a decreasing portion of each signal and discards the rest. The output record format is shown in Fig. C-3.

BSORT sorts the records, first on wavelength, then on shot number. Experimental points can be taken in any order, but in this step all data for a given wavelength are collected. The format of the records is unchanged by BSORT.

PROFILE unfolds the data, recorded as intensity as a function of time at different wavelengths, into intensity as a function of wavelength (a line profile) at different times. Since the ionized helium line intensities are sensitive to temperature, all data for one profile must be taken under the same plasma conditions. PROFILE does this by taking all the data for equal monitor signal (from the total intensity of the He II 4686 line). The time at which the monitor signal decays to this level is found, and the shot is discarded if this time is further than 1.73 standard deviations from the mean. Similarly, any intensities at a given wavelength which differ from the mean by more than 1.8 standard deviations are discarded. Profiles are then found for successively lower monitor intensities (therefore later times). The means and standard deviations of intensities at each wavelength go to one file (shown in Fig. C-4), which VPLOT uses to make a printer-plot of the line

profile. All undeleted data points are written to a second file (shown in Fig. C-5), used for fitting.

The actual least-squares fit is done by THEORY. As described in the section on data reduction, the convolution of the theoretical line profile with the instrument response function is done first, in alpha space, using an assumed electron density. The instrument function is assumed Gaussian, so the convolution integrals are done using the Gaussian-Hermite 3-point quadrature formula.⁵² This profile is fit to the experimental data and a new electron density is found. The convolution and fit are repeated until the electron density converges, usually within four iterations. Each of these fits requires a search for the values of the four parameters (line intensity I, background intensity B, line center λ_0 , and electron density N_e (line width)) that minimize the mean square deviation σ^2 of the fitting function from the experimental points. The subroutine ZXPOWL, from the International Mathematical and Statistical Library (IMSL)⁵³ uses the function-minimization algorithm described by Zangwill^{54,55} to find the best-fit values of λ_0 and N_e . For each trial values of λ_0 and N_e , it calls the subroutine FUNCT3, which in turn calls other subroutines to calculate the best values of the two linear parameters, and the corresponding σ^2 , using standard methods.

When the best values of all four parameters are found, subroutine FUNCT2 finds the second derivative matrix of σ^2 numerically, inverts it, and normalizes it to get the standard deviations and correlation matrix of the best-fit parameters. If the line is He II 4686, it uses the line:continuum ratio to calculate the plasma temperature Sub-

routine TPLOT plots the average of the experimental points at each wavelength, the best-fit theoretical profile, and the background level. The entire procedure is repeated for each profile, but since the line center and electron density are carried over each time, subsequent fits converge rapidly.

	6 bytes	3 bytes	320 bytes	
	FIXED	COUNT	DATA	
FIXED			6 bytes BCD, 2 characters/byte	data from thumbwheel switches
COUNT			3 bytes BCD, 1 character/byte	shot number
DATA			320 bytes binary number, 1/byte	data, grouped by time
total. 329 8-bit bytes/record (excluding parity and check bits)				

Fig. C-1 Record format of waveform recorder tape

	2 words	1 word	1 word	16 words	
	LABEL	SCALE	COUNT	T ₁ Y ₁ T ₂ Y ₂ ... T ₈ Y ₈	
LABEL	2 words, FIELDATA				First 5 characters are the wavelength in Å (decimal point assumed before last character). Next 3 characters are the shot number
SCALE	1 word, real (R)				Amplification on preamplifier (V/div)
COUNT	1 word, integer				Shot number (same as above).
T _i	1 word, R				Time of sample (usec. after trigger pulse)
Y _i	1 word, R				Signal amplitude (V)
total: 20 words/ record					

Fig. C-2 Format of data record written by REVERT

2 words	1 word	1 word	1 word	8 words	8 words
LABEL	SCALE	COUNT	POINTS	$T_1 T_2 \dots T_8$	$Y_1 Y_2 \dots Y_8$

LABEL, SCALE, COUNT, T_i , Y_i as before

POINTS 1 word, integer Number of data points (always 8)

total. 21 words/record

Fig. C-3 Format of data record written by PARAM or BSORT

1 word	36 words	36 words	36 words
MONITOR	WAVELENGTH	AVERAGE	SIGMA

MONITOR 1 word, R Intensity of monitor for this profile

WAVELENGTH 36 words, R Wavelengths (\AA)

AVERAGE 36 words, R Average of signal intensities at corresponding wavelength .

SIGMA 36 words, R Standard deviation of signal intensities

total: 109 words/record

Fig. C-4 Format of plot-file data record written by PROFILE

1 word	55 words	36 words	36 words	$28 \times 36 = 1008$ words
MONITOR	BLOCK	NUMBER	WAVELENGTH	INTENSITY

MONITOR 1 word, R Intensity of monitor signal for this profile

BLOCK 54 words, integer (currently not used)

NUMBER 36 words, R number of shots at this wavelength

WAVELENGTH 36 words, R Wavelengths

INTENSITY 1008 words, R INTENSITY (I,J) is the signal for the Jth shot at wavelength WAVELENGTH(I)

total: 1135 words/record

Fig C-5 Format of fit-file data record written by PROFILE.

A Note on Program Documentation

A code is used to describe the parameters of some subroutines.

For example, in TIM,

INT R,I Given intensity ,

the R indicates INT is real (single precision floating point) and the I means it's used only for input (i.e., the subroutine doesn't change its value). Possible parameter modes are:

F single precision floating point

DP double precision floating point

I integer

S statement number, for alternate return

L logical

C complex,

and possible uses are:

I input only (unchanged)

O output only (changed, contains useful information)

IO input and output

W work area (changed, not meaningful on return).

Programs Listed

REVERT

TREAD*, OPT*

PARAM

BSORT

STORES, START, SADD, SDROP, HADD, HDROP, ADDTO,

FINDTO, EPUSH, EPOP

PROFILE

TIM, INTENS, LOOKUP, YESNO*

VPLLOT

THEORY

DBANK, GROUP, FETCHS, FUNCT3, FUNCT2, TPLOT,

AXISN**, NEWS, NEWT, NEWU, SIGMA, SYMSLV**, VALUE**

* Programs in UNIVAC Assembly Language.

** These programs may be of general interest

```

***** REVERT *****

205373JIM@WORKSPACE% (1).REVERT
1   C
2   C      NAME...
3   C          REVERT
4   C
5   C      PURPOSE...
6   C          TO ACCEPT A TAPE PRODUCED BY THE DIGITAL DATA ACQUISITION
7   C          SYSTEM AND PRO UCE A FILE ACCEPTABLE TO PROGRAM 'PARAM'.
8   C
9   C      USAGE...
10  C          QXQT REVERT      (NOT Q.REVERT)
11  C          <DATA CARDS>
12  C
13  C          OPTIONS:
14  C          'L' PRINTS INFORMATION FROM DATA CARDS AND FIXED DATA
15  C          FROM TAPE RECORDS (THUMBWHEEL SWITCHES)
16  C          'N' IGNORES IMPROPER SCALE OR INTERVAL FROM TAPE
17  C          RECORD HEADER...NO MESSAGES
18  C          'R' OMIT INITIAL REWIND (DEFAULT: REWIND TAPE BEFORE
19  C          READING)
20  C
21  C      INPUT...
22  C          DATA TAPE WITH NAME 'INTAPE', PRODUCED BY THE DIGITAL DATA
23  C          ACQUISITION SYSTEM
24  C          DATA FROM THUMBWHEEL SWITCHES IS INTERPRETED AS FOLLOWS:
25  C          DIGITS 1-5...SCALE (V/DIV) FOR CHANNELS 1-5
26  C          DIGIT 6...SAMPLE INTERVAL (MICROSEC)
27  C              SETTING  0    1    2    3    4    5    6    7    8    9
28  C              MEANING ILLEGAL .005 .01 .02 .05 .1 .2 .5 1. 2.
29  C              .005 .LE. SCALE .LE. 2.
30  C              .05 .LE. INTERVAL .LE. ?
31  C              INTERVAL SPECIFIED ON CARD 3 SUPERCEDES DIGIT 6.
32  C              A WARNING IS PRINTED IF INTERVAL ISN'T .1 MICROSEC.
33  C
34  C          THE FOLLOWING DATA CARDS:
35  C          CARDS 1 AND 2...
36  C          (72A1/72A1) ALPHANUMERIC FILE HEADER IMAGES
37  C          CARD 3...
38  C              (I5) NUMBER OF CHANNELS BEING USED
39  C              (F5,0) SAMPLE INTERVAL IN MICROSECONDS
40  C              (I5) MONITOR SIGNAL CHANNEL (IF BLANK, THE PROGRAM
41  C                  USES THE FIRST CHANNEL WITH BLANKS IN THE
42  C                  WAVELENGTH SPECIFICATION COLUMNS OF CARD 4.)
43  C              (I5) STARTING SAMPLE NUMBER (IF BLANK, THE PROGRAM
44  C                  READS THE FIRST 12 RECORDS AND USES THE
45  C                  AVERAGE OF THE MAXIMA OF THE MONITOR.)
46  C          CARDS 4-N
47  C              (I5) (SORTED BY SHOT #, INCREASING)
48  C              (I5) FIRST SHOT NUMBER OF A GROUP OF SHOTS WITH
49  C                  THIS SET OF WAVELENGTH SETTINGS.
50  C              (SF5,1) WAVELENGTHS IN ANGSTROMS FOR EACH CHANNEL
51  C                  BLANK FIELD INDICATES A MONITOR CHANNEL
52  C          CARD N+1...
53  C              *EOF* IN FIRST FIVE COLUMNS
54  C          CARDS N+2 - M
55  C              (I5) SHOT NUMBER WITH INCORRECT SCALE #
56  C              (SF5,4) NEW SCALE #'S (BLANKS FOR CORRECT ONES)
      CARD M+1...

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***** REVERT *****

57      C      *EOF * IN FIRST FIVE COLUMNS
58      C
59      C      OUTPUT...
60      C      IN FILE 10, A FORTRAN RANDOM-ACCESS FILE ACCEPTABLE
61      C      TO PROGRAM 'PARAM'
62      C
63      C      DATA RECORD FORMAT: LABEL(2),SCALE,NSHOT,T1+Y1,T2+Y2 ... T8+Y8
64      C      TOTAL: 20 WORDS
65      C
66      C      SUBPROGRAMS REQUIRED...
67      C
68      C      BEGIN
69      C      OPT
70      C      TREAD
71      C
72      C      PARAMETER POINTS=9
73      C      PARA IETER NPTS=50
74      C      PARAMETER MSAD=15
75      C      PARA METER ICHAN=4
76      C      PARAMETER MRCN=1000
77      C      PARAMETER NWORDSS=5+POINTS+POINTS
78      C      INTEGER HEADER,CARD
79      C      LOGICAL VARIED,SGIVEN
80      C      LOGICAL OPT,QUIET,LONG
81      C      DIMENSION SCALE(9),HEADER(12),SAVFL(IPTS,"ICHAN"),RECORD(N,ORDS),
82      C      -      IREC(NNO+DS),XSHOT(MPTS),W(MCHAN),LSHOT(IBAD),
83      C      -      GOOD(MAAD,"ICHAN")
84      C      DATA SCALE/.005,.01,.02,.05,.1,.2,.5,1,.2./
85      C      DATA IER4/0/
86      C      EQUIVALENCE (RECORD(1),INFC(1)),(HEADER(1),RECORD(1))
87      C      DATA JPTS, NFILE, ENDREC, NRD, CARD, WAPNED, SGIVE,
88      C      -      / 1, 10,*EOF *, 9,      5,.FALSE.,.FALSE./
89      C      DATA ICHAN, MPTS, MRCN, MAD
90      C      -      / MCHAN, MPTS, IREC, MAD/
91      C      COMMU, NSHOT,NUM(12),ISIV(5,64)
92      C      CALL BEGIN('REVERT 1.23 w')
93      C      QUIET=OPT('N')
94      C      LONG=OPT('L')
95      C      IF(.NOT.OPT('P'))CALL REWID
96      C      DEFINE FILE ,FILE(MRC),N=ORDS+1,IREC)
97      C      NREC=1
98      C
99      C      TRANSFER HEADER INFORMATION
100     C      DO 10 I=1,2
101     C      READ(CARD,810,END=105)HEADER
102     C      810 FORMAT(12A6)
103     C      IF(LONG)PRINT 812,HEADER
104     C      812 FORMAT(1X,12A6)
105     C      10 WRITE(INFILE,'(I=EC)HEADER'
106     C
107     C      WE ALWAYS ENTER THE MAXIMUM NUMBER OF DATA POINTS
108     C      IREC(5)=POINTS
109     C
110     C      READ NUMBER OF CHANNELS IN USE, SAMPLE INTERVAL,
111     C      MONITOR CHAN #, AND STARTING CHANNEL #
112     C      READ(CARD,820,END=106)NCHAN,SAMPLE,MONIT,KTIME
113     C      820 FORMAT(15,F5.0,2I5)

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***** REVLRIT *****

114      IF(NCHAN.GT.NCHAN .OR. NCHAN.LT.0)GO TO 108
115      IF(SAMPLE.EQ.0.)GO TO 12
116      IF(SAMPLE.LT..05 .OR. SAMPLE.GT.2.)GO TO 110
117      SGIVER=.TRUE.
118      12 IF(MONIT.LT.0 .OR. MONIT.GT.NCHAN)GO TO 112
119      15 IF(KTIME.LT.0 .OR. KTIME.GT.57)GO TO 114
120      18 IF(LONG)PRINT 815,NCHAN,SA IPLF+MONIT,KTIME
121      815 FORMAT(1X//1X,I2,' CHANNELS USED',',F6.2,' USEC SAMPLE INTERVAL'
122      -           ' CHANNEL',I2,' IS MONITOR. STARTING CHANNEL IS',I4)
123
124      C          READ WAVELENGTHS FOR EACH SHOT NUMBER
125      IF(LONG.AND. .NOT.OPT('Y'))PRINT 825
126      825 FORMAT(1X//' SHOT #   WAVELENGTHS')
127      DO 23 NPTS=1:PTS
128      READ(CARD,830,END=25)KSHOT(NPTS),(WAVEL(NPTS,M),M=1,NCHAN)
129      830 FORMAT(15.5A5)
130      DO 20 M=1,NCHAN
131      20 DECODE(832,WAVEL(NPTS,M))W(M)
132      832 FORMAT(F5.1)
133      23 IF(LONG.AND. .NOT.OPT('Y'))PRINT 835,KSHOT(NPTS),(W(M),M=1,NCHAN)
134      835 FORMAT(1X,I5,2X,F9.2)
135      GO TO 116
136      25 KSHOT(NPTS)=10000
137      NPTS=NPTS-1
138      DO 28 NBAD=1:NBAD
139      READ(CARD,836,END=30)LSHOT(NBAD),(GOOD(NBAD+M),M=1,NCHAN)
140      836 FORMAT(15.5F5.4)
141      28 CONTINUE
142      GO TO 117
143      30 LSHOT(NBAD)=10000
144      NBAD=NBAD-1
145      IF(MONIT.NE.0)GO TO 40
146
147      C          WE WEREN'T TOLD THE MONITOR CHANNEL #...
148      C          FIGURE IT OUT (PLANKS IN THE WAVELENGTH FIELD)
149      DO 35 MONIT=1,NCHAN
150      IF(WAVEL(1,MONIT).EQ.0)GO TO 40
151      35 CONTINUE
152
153      C          THERE'S STILL NO MONITOR CHANNEL SPECIFIED...
154      C          USE CHANNEL 1
155      PRINT 901
156      901 FORMAT(* NO MONITOR SPECIFIED...USING CHAN. 1*)
157      MONIT=1
158      40 IF(KTIME.NE.0)GO TO 58
159
160      C          WE WEREN'T TOLD WHICH TIME TO START WITH...
161      C          FIND AVERAGE TIME FOR PFAK OF MONITOR SIGNAL
162      C          AMONG FIRST 12 RECORDS
163      DO 47 L=1,12
164      CALL TREAD(NS40T,KEOF)
165      IF(KEOF.NE.0)GO TO 118
166      MAX=ISIG(MONIT,1)
167      I=1
168      - DO 45 K=2,64
169      - IF(ISIG(MONIT,K).LE.MAX)GO TO 45
170      I=K

```

```

***** REVERT *****

171      MAX=ISIG(ADJNT,K)
172      CONTINUE
173      KTI=KTI+1
174      KTIME=MINT(57,KTIME/12)
175      CALL REWIND
176      IF(OPT('Z'))STOP
177      INREC=0
178      MSHOT=0
179      IF(LONG)PRINT 838
180      838 FORMAT(1X//' RECORD SHOT #    FIXED DATA')
181      DO 82 L=1,NRCD
182
183      C          READ A RECORD
184      CALL TREAD(NSHOT,KEOF)
185      IF(KEOF.NE.0)GO TO 85
186      MSHOT=MSHOT+1
187      IF(LONG)PRINT 840,MSHOT,NSHOT,NUM
188      840 FORMAT(1X,I4,I9+X,5I2+2X,I2,2X,6T2)
189      INREC=INREC+1
190
191      C          FIND THE WAVELENGTH INFO FOR THIS SHOT NUMBER
192      IF(NSHOT.LT.KSHOT(JPTS))JPTS=1
193      ISTOP=NPTS-JPTS+1
194      DO 62 I=1,ISTOP
195      IF(NSHOT.LT.KSHOT(JPTS+1))GO TO 63
196      JPTS=JPTS+1
197      63 CONTINUE
198      DO 82 M=1,NCHAN
199
200      C          LOAD DATA FROM ONE CHANNEL INTO A RECORD
201
202      C          DISCARD DATA IF DESIRED
203      IF(WAVEL(JPTS,M).EQ.'9999 '+.OR.=WAVEL(JPTS,M).EQ.'99999')GO TO 82
204
205      C          PICK UP SCALE # FROM RECORD HEADER
206      IS=NUM(M)
207      IF(OPT('a'))IS=NUM(M-1)
208      IF(IS.GT.0 .AND. IS.LT.9)GO TO 65
209      IF(.NOT.QUIET)PPI/T 902,INREC,NSHOT,M,TS
210      IERR=ERR+1
211      902 FORMAT(' TAPE RECORD',I4,', SHOT',I5,', CHANNEL',I2,
212      -        '...SCALE # OUT OF RANGE:',I5/
213      -        ' USING .005 V/DIV')
214      IS=1
215      65 K=KTIME
216
217      C          SUBSTITUTE CORRECT AMPLIFICATION IF NEEDED
218      AMPLFY=SCALE(IS)
219      66 IF(LSHOT(JBAD).EQ.1000Q)GO TO 68
220      IF(NSHOT.LT.LSHOT(JBAD))JBAD=1
221      IF(NSHOT.LT.LSHOT(JBAD+1))GO TO 67
222      JBAD=JBAD+1
223      GO TO 66
224      67 IF(NSHOT.EQ.LSHOT(JBAD) .AND. GOOD(JBAD,M).NE.0.0)
225      -        AMPLFY=GOOD(JBAD,M)
226      68 IF(SGIVEN)GO TO 71
227      C

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***** REVERT *****

228      C          PICK UP SAMPLE INTERVAL FROM RECORD HEADER
229          IF=NU,(6)
230          IF(IF.GT.3 .AND. IT.LE.9) GO TO 70
231          NERR=NERR+1
232          IF(.NOT..JECT)PRINT 903,INREC,NSHOT,IT
233          903 FORMAT(' TAPE RECORD',I4,', SHOT',I5,
234          -     '...SAMPLE INTERVAL # OUT OF RANGE:',I5/
235          -     ' USING .1 MICROSEC')
236          IT=2
237          70 SAMPLE=SCALE(IT)
238
239      C          GIVE ONE WARNING IF INTERVAL ISN'T .1 US
240          71 IF(SAMPLE.EQ..1 .OR. WARNED)GO TO 72
241          NERR=NERR+1
242          WARNED=.TRUE.
243          PRINT 904,INRFC,NSHOT,SAMPLE
244          904 FORMAT(' TAPE RECORD',I4,', SHOT',I5,'...SAMPLE INTERVAL LOW',
245          -     F5.2,' MICROSECONDS')
246
247      C          TRANSFER DATA POINTS
248          72 TIME=K*SAMPLE
249          DO 75 KK=7,1,-CRDS/2
250          RECORD(KK-1)=TIME
251
252      C          WE MAKE A CORRECTION OF A FACTOR OF 10 BECAUSE
253      C          THERE ARE TWO EXTRA AMPLIFIERS IN THE DATA SYSTEM
254          RECORD(KK)=.1*ISIG(M,K)*AMPLFY
255          K=K+1
256          75 TIME=TIME+SAMPLE
257
258      C          SET UP OUTPUT RECORD HEADER
259          ENCODE(850,IREC)A=AVAL(JPTS,M),NSHOT
260          850 FORMAT(A5,I3)
261          RECORD(3)=AMPLEY
262          IREC(4)=NSHOT
263          WRITE(INFILE,IREC)RECORD
264          82 CONTINUE
265          GO TO 124
266
267      C          END OF FILE...QUITTING TIME
268          85 PRINT 860,NSHOT,IDEC
269          860 FORMAT(1X,I6,' SHOTS PROCESSED'/1X,I6,' RECORDS WRITTEN')
270          IF(.NOT..ERF.GT.0)PRINT 905,LRH
271          905 FORMAT(1X,I6,' ERRORS OR TRAPINGS')
272          GO TO 199
273
274      C          COMPLAIN
275          106 PRINT 906
276          906 FORMAT(' HEADER CARDS ARE MISSING')
277          GO TO 199
278          108 PRINT 908,ICHAN,4*CHAN
279          908 FORMAT(' NUMBER OF CHANNELS',I5,', IS OUT OF RANGE 1 TO',I2)
280          GO TO 199
281          110 PRINT 910,SAMPLE
282          910 FORMAT(' SAMPLE INTERVAL OF',G15.5,' IS BAD'
283          -     ' USING TAPE RECORD HEADERS')
284          GO TO 12

```

```
***** REVERT *****  
285      112 PRINT 912,MONIT  
286      912 FORMAT(' GIVEN MONITOR CHANNEL #,*,IS,* IS BAD')  
287          IONITE=0  
288          GO TO 15  
289      114 PRINT 914,KTIME  
290      914 FORMAT(' GIVEN STARTING CHANNEL #,*,IS,* IS BAD')  
291          KTIME=0  
292          GO TO 13  
293      116 PRINT 916,FMPTS  
294      916 FORMAT(' THERE ARE MORE THAN',I3,' WAVELENGTH CARDS')  
295          GO TO 199  
296      117 PRINT 917,MMBAD  
297      917 FORMAT(' THERE ARE MORE THAN',I3,' CORRECTION CARDS')  
298          GO TO 199  
299      118 PRINT 918  
300      918 FORMAT(' FEWER THAN 12 SIGNALS ARE PRESENT')  
301          GO TO 199  
302      124 PRINT 924,4MPCD  
303      924 FORMAT(' MORE THAN',I5,' TAPE RECORDS...QUITTING')  
304      C  
305      C           CLOSE OUTPUT FILE  
306      199 WRITE(1,FILE*NREC)ENDREC  
307          STOP  
308          END
```

QWORK.EJCT

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***** REVERT (Sample data) *****

@XOT,L .REVERT

Long printout is wanted.

HL DATA OF WED 19 NOV 75...PRESSURE=.851=.50T=2.7V, REFLECTOR =.8
SCANS OF HL II 1640 AND 4686, AL II 1670 ... MFT2 FILTER RUN 101

<u>31</u>	3 channels were used.
33277 4671	
133277 4679	
273278 4681	
<u>333278 4683</u>	First shot number at these wavelengths
393279 4684	
463279 4685	
<u>333280 4686</u>	Channel 1 set at 3280.0 Å
393280 4687	
693281 4688	Channel 2 set at 4688.0 Å
763305 4689	
849999 0000	Discard data for channel 2, shots 84-92.
9333385 4692	
9633385 4690	
1013339 4692	Channel 3 is for monitor signal.
10833395 4695	
1163340 4724	
1223340 4730	

@EOF

<u>76</u> .005	Shot 76 had wrong amplifier setting recorded
77 .005	
<u>78</u> .006	Channel 1 amplification was .005 V/div
79 .007	Channel 2 amplification was correctly recorded

@FOR

@XOT,A .PARAM
.151, 2276., 3202.
.294, 4670., 4696.

Some signals were attenuated
Attenuation factor was .151.
Signals for 4670 Å through 4696 Å were attenuated

@EOF

```

***** REVERT (TREAD) *****

205373JIM400KSHALE$().TREAD
1   .
2   .      NAME...
3   .          DATATAPE
4   .
5   .      PURPOSE...
6   .          TO READ THE HIGH SPEED DATA ACQUISITION SYSTEM TAPE.
7   .
8   .      CALLING SEQUENCE...
9   .
10  .
11  .
12  .      BUFFER 333 WORD DATA INPUT BUFFER, INTEGER
13  .          BUFFER(1) IS THE EXPERIMENT COUNT
14  .          BUFFER(2-13) ARE MISC FIXED DATA
15  .          BUFFER(14-333) ARE DATA POINTS, DIMENSIONED (5,64)
16  .          EOF      END OF FILE MARKER, SET NON-ZERO IF EOF
17  .          WAS DETECTED WHEN THIS READ WAS ATTEMPTED,
18  .          ZERO OTHERWISE.
19  .
20  .
21  .
22  .
23  .
24  .
25  .
26  .
27  .
28  .
29  .
30  .
31  .
32  .      $()     AXRS.
33  .
34  .
35  .
36  .      TREAD*    LA      A0-END.          ARE WE AT THE END OF THE FILE?
37  .          JNZ     A0+3,X11.        IF SO RETURN AT ONCE
38  .      ANOTHER   LA,U    A0+PKTT.
39  .          EK      IOWS.           FETCH A BUFFER FULL
40  .          LA      A0+PKTT+2.      PICK UP STATUS AND CHECK.
41  .          TE      A0+STATUS.    SHOULD HAVE AN AFC OF 5
42  .          J      EOF.
43  .      OKAY     SX      X1+SAVEX.
44  .          LAM    X1+0,X11.        X1 WILL POINT TO THE NEXT WORD IN THE
45  .          LA,I,U X1+1.          USER'S BUFFER ALL THROUGH THE PROGRAM
46  .
47  .
48  .
49  .      PICK UP EXPT COUNT
50  .
51  .
52  .
53  .
54  .
55  .
56  .

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***** REVERT (THEAD) *****

57      AND,U A0,017.
58      MSI,U A1,100.
59      AA    A2,A1.          EXPT COUNT IS IN A2
60      SA    A2,0,*X1.        STORE EXPT COUNT IN BUFFER
61
62      *      PICK UP MISC DATA
63
64      DL    A0,IMBUF.      SIX BYTES OF TWO CHARACTERS/BYTE
65      LR,U R2,5.
66      DSC   A0,4.
67      LOOP1  LUSC   A0,12.      BACK UP ONE DIGIT
68      AND,U A1,017.        MOVE FORWARD 3 DIGITS, PUT IN A1(3-0)
69      SA    A2,0,*X1.        MOVF LAST DIGIT TO A2(3-0)
70      DSC   A0,4.          STORE DIGIT
71      AND,U A1,017.        MOVE BACK 1 DIGIT
72      SA    A2,0,*X1.        PUT ONE DIGIT INTO A2(3-0)
73      JGD   R2,LOOP1.       STORE BCD DIGIT
74      *      DECREMENT COUNTER
75      *      GET REAL DATA
76
77      SX    X2,SAVEX+1.     X2 POINTS TO NEXT PAIR
78      LX    X2,(2,INBUF+2)  OF WORDS IN INPUT BUFFER
79      LR,U R2,34.
80      LOOP3  DL    A0,0,*X2.      MOVE 35 PAIRS OF WORDS (315 BYTES)
81      LR,U R1,8.          PICK UP TWO PACKED WORDS
82      LOOP2  LUSC   A0,8.        NINE WORDS AT A SHOT
83      AND,U A1,0377.       TRANSFER ONE BYTE TO A2(7-0)
84      SA    A2,0,*X1.
85      JGD   R1,LOOP2.
86      JGD   R2,LOOP3.
87      DL    A0,0,X2.
88      LR,U R1,4.
89      LOOP4  LUSC   A0,8.        PROCESS ONLY 5 BYTES
90      AND,U A1,0377.       TRANSFER ONE BYTE TO A2(7-0)
91      SA    A2,0,*X1.
92      JGD   R1,LOOP4.       FINISH THE LAST 5 BYTES
93      SZ    #1,X11.         CLEAR EOF FLAG
94      RETURN
95      LX    X1,SAVEX.
96      LX    X2,SAVEX+1.
97      J    3,X11.
98      *      END OF FILE OR TAPE ERROR
99
100     EOF    LA,S1 A0,PKTT+3.    TEST FIRST FOR EOF
101     TE,U A0,01.          01 MEANS END OF FILE.
102     J    B0.
103     SA    A0,END.
104     SA    A0,*1,X11.       NOTIFY THAT EOF REACHED
105     J    RETURN.          TELL CALLING PROGRAM ABOUT EOF.
106     B0    LA,H2 A0,PKTT+3.    TEST FOR WRONG RECORD LENGTH
107     TNE,U A0,74.
108     J    B1.
109     SLJ    PRINT.          LENGTH WRONG...PRINT STATUS
110     ER    ABORTS.         AND QUIT.
111     B1    LA,S1 A0,PKTT+3.    GET I/O COMPLETION STATUS CODE AGAIN.
112     TNE,U A0,00.          00 MEANS NORMAL COMPLETION. (MUST BE
113     J    OKAY.            COPIED TAPE, SINCE FRAME CT IS NORMAL)

```

***** REVERT (THEAL) *****

```

114      TE,U A0,04.          04 MEANS ABNORMAL FRAME COUNT.
115      J B2.
116      SLJ PRINT.          AFC NOT 5, SO WE PRINT STATUS AND
117      J ANOTHER.         GET NEXT RECORD.
118      B2     SLJ PRINT.          SO IF OTHER I/O ERROR...PRINT STATUS
119      ER     ABORTS.        AND QUIT.
120      .
121      .
122      .
123      PRINT   + $-$.
124      LA A0,PKTT+3.       GET THE STATUS WORD
125      LR,U R2,1.
126      E2     SA A2,I,INBUF+1.    (USEFUL ONLY ON 2ND ITERATION OF LOOP)
127      LR,U R1,S.
128      E1     AND,U A0,07.      MOVE ONE OCTAL DIGIT TO A1(2-0)
129      AA,U A1,050.        CONVERT TO FIELD DATA DIGIT
130      DSC A1,6.          MOVE INTO A2(35-30)
131      SSL A0,3.          MOVE NEXT OCTAL DIGIT TO A0(2-0)
132      JGD R1,E1.
133      JGD R2,E2.
134      SA A2,INBUF.
135      LA A0,(0104,INBUF-2).
136      ER PRINTS.
137      J *PRINT.
138      .
139      .
140      .
141      REWIND* L,U A0,R#D.
142      ER IOW$.
143      LA,S1 A0,R#D+3.      REWIND THE TAPE
144      TNZ A0.              CHECK FOR BAD STATUS
145      J RE2.
146      SLJ PRINT.          STATUS BAD...PRINT THE STATUS
147      ER ABORTS.         AND QUIT
148      RE2    S2 END.        NOTE WE AREN'T AT AN END OF FILE NOW
149      J 1,X1].
150      .
151      .
152      .
153      S(0),SAVEX RES 2.
154      PKTT  ISOT 'INTAPE',PS 74,INBUF.
155      + 'I/O STATUS '.
156      INBUF RES 74.
157      STATUS #042005000112.
158      END  + 0.
159      RWD  ISOT 'INTAPE',REWS.    SET NONZERO WHEN EOF FOUND
160      END

```

B.EJECT

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***** REVERT (OPT) *****

2053/3J1/*WORKSPACES(1).OPT
1      . NAME...
2      .
3      . OPT
4      .
5      . PURPOSE...
6      .
7      . TO OBTAIN FOR THE USER PROGRAM THE OPTIONS SPECIFIED ON
8      . THE EXECUTING STATEMENT.
9      .
10     . CALLING SEQUENCE...
11     .
12     . LOGICAL SWITCH, TEST, OPT
13     .
14     .
15     . SWITCH=OPT('U')
16     . TEST=OPT('T')
17     .
18     . SWITCH WILL HAVE THE VALUE .TRUE. IF THE 'U' OPTION WAS
19     . SPECIFIED ON THE WXGT OR WFILE.PROGRAM CARD, AND .FALSE.
20     . OTHERWISE. TEST WILL SIMILARLY INDICATE THE PRESENCE OF
21     . THE 'T' OPTION.
22 S(0) LIT.
23 S(1) AXPS.
24 OPT* TZ HAVE .          GO GET OPTIONS IF WE HAVEN'T ALREADY
25           J GET .
26 GO   LA A1,*0,X11 .
27           SSL A1,30 .
28           A1A,U A1,06 .
29           LA AU,WORD .
30           LSSL A0,10,A1 .      SHIFT CORRECT BIT TO HIGH-ORDER BIT
31           SSL A0,35 .      SHIFT TO LOW-ORDER (RESULT IS 1 OR 0)
32           J 2,X11 .        RETURN!
33 GET   SX X11,WORD .
34           ER OPTS .
35           LX X11,WORD .
36           SA A0,WORD .
37           SZ HAVE .        NOTE OPTION WORD IS PRESENT
38           J GO .
39 S(0).
40 RETURN RCS 1 .
41 HAVE + 1 .
42 WORD RES 1 .
43 END  .

```

W-EJLT

```

***** PARAM *****
205373J1M*.WORKSPACE(1).PARAM
1   C
2   C      NAME...
3   C          PARAM
4   C
5   C      PURPOSE...
6   C          TO CREATE RECORDS WITH STRICTLY DECREASING MONITOR SIGNALS
7   C
8   C      USAGE...
9   C          W.PARAM OR QXOT .PARAM
10  C
11  C      OPTIONS:
12  C          A      (QXOT ONLY) AMPLIFY SOME SIGNALS WHICH WERE
13  C          ATTENUATED WITH A NEUTRAL DENSITY FILTER
14  C
15  C          <WLLOW,WHIGH> (FREE) SIGNALS WITH WAVELENGTHS IN THE
16  C          RANGE <WLLOW,WHIGH> WILL BE AMPLIFIED BY 1/.294
17  C
18  C      INPUT...
19  C          ACCEPTS FILES CREATED BY PROGRAMS 'RECOVER' OR 'REVERT'.
20  C
21  C          RECORDS 1 & 2:
22  C          (72A1/72A1) FILE HEADER
23  C
24  C          RECORDS 3-N:
25  C          WORDS 1,2: (F5.1,I3) WAVELENGTH,SHOT #
26  C          WORD 3: (R) SCALE, VOLTS/DIV
27  C          WORD 4: (I) SHOT #
28  C          WORD 5: (I) # POINTS IN THIS RECORD
29  C          WORDS 6-13: (R) TIMES (USEC)
30  C          WORDS 14-21: (R) SIGNALS (V)
31  C          RECORD N+1:
32  C          'EOF' * IN FIRST WORD
33  C
34  C      OUTPUT...
35  C          FILE ACCEPTABLE TO PROGRAM 'BSORT'
36  C
37  C          RECORDS 1,2:
38  C          (72A1/72A1) FILE HEADER
39  C          RECORDS 3-N:
40  C          WORDS 1,2: (F5.1,I3) WAVELENGTH,SHOT #
41  C          WORD 3: (R) SCALE (V/DIV)
42  C          WORD 4: (I) SHOT #
43  C          WORDS 5-20: (R) PAIRS OF TIME (USEC), SIGNAL (V)
44  C          RECORD N+1:
45  C          'EOF' * IN FIRST WORD
46  C
47  C      SUBPROGRAMS REQUIRED...
48  C
49  C      BEGIN,OPT
50  C
51  C      PARAMETER MRCD=1000
52  C      INTEGER OUTFIL,OUTREC,TEST,END1
53  C      INTEGER HEAD(20),HIGH,VALLEY,PEAK
54  C      LOGICAL OPT
55  C      DIMENSION A(8),B(8),FACTOR(8),WLLOW(8),WHIGH(8)
56  C      EQUIVALENCE (A(1),HEAD(5)),(B(1),HEAD(13))

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***** PARAM *****
57      DATA    END1,INFILE,OUTFIL, INREC,OUTREC
58      -   /'2EOF ', 10, 15, 0, 0/
59      DIMENSION X(9),Y(9),K(8)
60      EQUIV,L,E,XE,X(1),E(1)
61      LOGIC,L,SAME
62      CALL BEGIN('PARAM 2.11 A')
63      KATTEN=1
64      IF(.NOT.OPT('A'))GO TO 5
65      PRINT 800
66      800 FORMAT(' ENTER ATTEN AND WAVELENGTH RANGE')
67      DO 3 KATTEN=1,8
68      READ 805,END=5,FACTOR(KATTEN),WLOW(KATTEN),WHIGH(KATTEN)
69      805 FORMAT()
70      WLOW(KATTEN)=WLOW(KATTEN)-.05
71      WHIGH(KATTEN)=WHIGH(KATTEN)+.05
72      IF(FACTOR(KATTEN).GT.1.)PRINT 901
73      901 FORMAT(' >1?')
74      3 CONTINUE
75      KATTEN=8
76      5 WLOW(KATTEN)=8000.
77      WHIGH(KATTEN)=7999.
78      DEFINE FILE INFILE(MRC0,1,U,I'REC)
79      DEFINE FILE OUTFIL(MRC0,20,U,OUTREC)
80      C
81      C      TRANSFER FILE HEADER
82      DO 8 J=1,2
83      READ(INFILE'J)(HEAD(I),I=1,12)
84      8 WRITE(OUTFIL'J)(HEAD(I),I=1,12)
85      C
86      C      READ A RECORD
87      10 READ(INFILE'INREC)(HEAD(I),I=1,4),H,(X(I),Y(I),I=1,N)
88      C
89      C      QUIT AT END OF FILE
90      IF(HEAD(1).EQ.END1)GO TO 90
91      AMPLFY=1.
92      C      REMOVE BAD RECORDS & CORRECT AMPLIFICATION
93      DECODE(830,HEAD)AVE
94      830 FORMAT(F5.1)
95      DO 12 KK=1,KATTEN
96      IF(WAVE.LT.WLOW(KK))GO TO 12
97      IF(WAVE.LE.WHIGH(KK))GO TO 14
98      12 CONTINUE
99      GO TO 15
100     14 AMPLFY=FACTOR(KK)
101     C
102     C      TRANSFER RECORD TO OUTPUT AREA
103     15 N=MING(N,8)
104     DO 20 I=1,N
105     A(N+1-I)=X(I)
106     20 B(N+1-I)=Y(I)/AMPLFY
107     C
108     C      SORT POINTS ON TIME
109     IF(N.LE.1)GO TO 40
110     DO 2d J=N,2,-1
111     SAME=.TRUE.
112     DO 25 I=2,J
113     IF(A(I).GE.A(I-1))GO TO 25

```

```

***** PARAM ****
114      S=A(I)
115      A(I)=A(I-1)
116      A(I-1)=S
117      S=B(I)
118      B(I)=B(I-1)
119      B(I-1)=S
120      SAME=FALSE.
121      25 CONTINUE
122      IF(SAME)GO TO 30
123      28 CONTINUE
124      '
125      C           IF THIS IS A MONITOR SIGNAL, ENSURE IT'S
126      C           MONOTONICALLY DECREASING
127      30 DECODE(840,HEAD)TEST
128      840 FORMAT(A5)
129      IF(TEST.EQ.'*)GO TO 31
130      IB=I
131      GO TO 44
132      31 DROP=0.
133      HIGH=1
134      VALLEY=1
135      PEAK=1
136      IB=0
137
138      C           FIND A LOCAL MAXIMUM
139      32 IB=IB+1
140      IF(IB.GT.N)GO TO 35
141      IF(B(IB).LE.B(N-ABS(IB+1-N)))GO TO 32
142
143      C           NOTE LOCATION OF LOCAL MAXIMUM
144      HIGH=IB
145
146      C           FIND A LOCAL MINIMUM
147      34 IB=IB+1
148      IF(IB.GT.N)GO TO 36
149      IF(B(IB).GE.B(N-ABS(IB+1-N)))GO TO 34
150
151      C           IS THIS DROP BIGGER THAN PREVIOUS BIGGEST?
152      IF(B(HIGH)-B(IB).LE.DROP)GO TO 32
153
154      C           NOTE THIS IS BIGGEST DROP
155      DROP=L(HIGH)-B(IB)
156      PEAK=IB,HIGH
157      VALLEY=IB
158      GO TO 32
159      36 IF(B(HIGH)-B(IB-1).LE.DROP)GO TO 38
160      PEAK=HIGH
161      VALLEY=IB-1
162
163      C           HAVE FOUND BIGGEST DROP...GET RID
164      C           OF POINTS BEFORE PEAK
165      38 IB=0
166      40 IB=IB+1
167      IF(IB.GE.PEAK)GO TO 42
168      A(IB)=A(PERK)
169      B(IB)=B(PERK)
170      GO TO 40

```

```
***** PARA'1 *****  
1/1      C  
1/2      C          GET RID OF POINTS AFTER VALLEY  
1/3      C          42 ID=VALLEY  
1/4      C          44 IB=IB+1  
1/5      C          IF(Ia.GT.B) GO TO 45  
1/6      C          A(ID)=A(VALLEY)  
1/7      C          B(IB)=B(VALLEY)  
1/8      C          GO TO 44  
1/9      C  
1/10     C          WRITE A RECORD  
1/11     C          45 WRITE(OUTFIL'OUTREC)HEAD  
1/12     C          GO TO 10  
1/13     C  
1/14     C          CLOSE THE FILE AND EXIT  
1/15     C          90 WRITE(OUTFIL'OUTREC)E ID1  
1/16     C          I=INREC-4  
1/17     C          PRINT 890,I  
1/18     C          890 FORMAT(15,' CURVES PROCESSED')  
1/19     C          STOP  
1/20     C          END
```

W.EJECT

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***** BSORT *****
205373JIM@WORKSI ALES(1).BSORT
1   C
2   C      NAME...
3   C          BSORT
4   C
5   C      PURPOSE...
6   C          TO SORT THE RECORDS, FIRST BY WAVELENGTH, THEN BY SHOT N.
7   C
8   C      USAGE...
9   C
10  C          W.BSORT OR QXQT.BSORT (NO OPTIONS)
11  C
12  C      SUBPROGRAMS CALLED...
13  C
14  C          BEGIN,START,SADD,SDROP,MADD,HDROP,ADDTO,FINDTO,EPUSH,EPUP
15  C
16  C      METHOD...
17  C          ON A FORWARD PASS, EACH RECORD IS READ. IF IT RANKS HIGH
18  C          ENOUGH (HIGHER THAN LEAST ONE CURRENTLY SAVED, IF THE
19  C          BUFFERS ARE FULL) IT IS SAVED AND, IF THE BUFFERS ARE FULL,
20  C          THE LEAST ONE CURRENTLY SAVED IS WRITTEN IN ITS PLACE. WHEN
21  C          THE END OF THE UNSORTED PORTION OF THE FILE IS REACHED, ALL
22  C          RECORDS BEING HELD ARE EXCHANGED WITH STORED RECORDS. THE
23  C          PROCESS IS REPEATED, IN ALTERNATING DIRECTIONS, UNTIL THE
24  C          ENTIRE FILE IS SORTED.
25  C
26  C      INCLUDE STORES,LIST
27  C      LOGICAL FOUND
28  C      DATA E1/*EOF */
29  C      DATA NFILE/15/
30  C      CALL BEGIN('BSORT 2.01 0')
31  C      DEFINE FILE NFILE(1000,20+U,NREC)
32  C      CALL START
33  C      NEXT=2
34  C      FOUND=.FALSE.
35  C      LAST=0
36  C      IREC#2
37  C      INCR#1
38  C      NPASS=0
39  C      NWRITE=0
40  C      NREAD=0
41  C      KNOWN=0
42  C      SURE=.TRUE.
43  C          BEGIN NEW SWEEP
44  C      10 CHANGE=.FALSE.
45  C      NPASS=NPASS+1
46  C          CALCULATE NEW PFCORG NUMBER
47  C      12 IREC=IREC+INCR
48  C          IF(IREC.EQ.LAST)GO TO 40
49  C          IF((KNOWN.LE.0).AND.(.NOT.SURE))GO TO 30
50  C          IF(HBASE)15,15,14
51  C      14 IF(IRLC.EQ.FROM(HBASE))GO TO 24
52  C          READ NEW RECORD
53  C      15 CONTINUE
54  C          READ(NFILE,IRFC)(R(I,BUFFER),I=1,LGH)
55  C          NREAD=NREAD+1
56  C          IF(FOUND)GO TO 20

```

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***** ISORT *****
57   C      STOP STEP IF THIS IS END OF FILE
58   IF(I(1,BUFFER).NE.E1) GO TO 20
59   FOUND=.TRUE.
60   LAST=IREC
61   RECDU=IREC-3
62   GO TO 40
63   C      ADD THIS RECORD TO SORT STACK
64   20 CONTI, UE
65   FROM(PBUFFER)=IREC
66   CALL SADD(PBUFFER)
67   BUFFER=DEMAND($89)
68   GO TO 12
69   C      WE ARE HOLDING A RECORD WE WANT TO WRITE HERE...
70   C      DO SO, THEN ADD IT TO THE SORT STACK
71   24 CONTINUE
72   WRITE(INFILE,IREC)(R(I,HBASE),I=1,LGH)
73   NWRITE=NWRITE+1
74   CALL SADD(HDROP($89))
75   IF(SJ,E) GO TO 12
76   CALL EPUSH(SDROP($99))
77   GO TO 12
78   C      THERE'S NOT ENOUGH ROOM TO DO ANY SORTING DURING
79   C      THIS SCAN...BYPASS ALL READING
80   30 IF(HBASE.LE.0) GO TO 32
81   IREC=FPO*(HBASE)
82   WRITE(INFILE,IPEC)(R(I,HBASE),I=1,LGH)
83   NWRITE=NWRITE+1
84   CALL EPUSH(HDROP($89))
85   GO TO 30
86   32 IREC=LAST
87   C      CALCULATE NEW SHEEP LIMITS
88   40 CONTINUE
89   LAST=NEXT
90   NEXT=IREC-INC+KNOWN
91   IF((.NOT.CHANGE).AND.(KNOWN.LT.0)) GO TO 88
92   KNOWN=0
93   C      RECORD DESTINATIONS OF RECORDS TO BE HELD
94   I=5BASE
95   NTO=0
96   51 IF(I)55,55,52
97   52 CONTINUE
98   CALL ADDTO(I)
99   I=UP(I)
100  GO TO 51
101  C      SET POINTERS
102  55 CONTINUE
103  J=LAST-INC+INTO
104  JT0=INTO
105  CALL FINDTO(J)
106  INC=INC+1
107  SURE=.TRUE.
108  TTOP=STOP
109  STOP=0
110  SBASE=0
111  C      WRITE SORTED RECORDS IN PROPER ORDER
112  58 IF(TTOP)74,74,60
113  60 IREC=IREC+INC

```

```

***** :ISORT *****
114      IF(IREC.EQ.FROM(TTOP)) GO TO 64
115      61 IF((I0(JTO)-IREC)*INC()62;63;64
116      62 JTO=JTO-1
117      GO TO 61
118      C          FILE RECORD THAT WAS HERE IS IN THE SORT
119      C          STACK AND CAN BE OVERWRITTEN
120      63 CONTINUE
121      WRITE(INFILE*IPEC)(R(I,TTOP),I=1,LGH)
122      NWRITE=NWRITE+1
123      64 I=DOWN(TTOP)
124      CALL EPUSH(TTOP) .
125      TTOP=I
126      GO TO 58
127      C          FILE RECORD THAT WAS HERE MUST BE HELD
128      C          AND WRITTEN BACK LATER THIS SWEEP
129      68 CONTINUE
130      READ(INFILE*IREC)(P(I,BUFFER),I=1,LGH)
131      NREAD=NREAD+1
132      WRITE(INFILE*IREC)(R(I,TTOP),I=1,LGH)
133      NWRITE=NWRITE+1
134      CALL HADD(BUFFER)
135      I=DOWN(TTOP)
136      BUFFER=TTOP
137      TTOP=I
138      GO TO 58
139      C          ASSIGN DESTINATIONS TO THE RECORDS HELD
140      74 I=HTOP
141      ITO=0
142      75 IF(I)42;82;78
143      78 ITO=ITO+1
144      FROM(I)=TO(ITO)
145      I=DOWN(I)
146      GO TO 75
147      C          GO FOR REST OF THIS SWEEP
148      82 CONTINUE
149      IF(ABS(LAST-NEXT).GT.1)GO TO 10
150      C          SORTING COMPLETE...REPORT & QUIT
151      88 CONTINUE
152      PRINT 808,RECORD,NPASS,NWRITE,NHEAD
153      808 FORMAT(15,' RECORDS SORTED'
154      -           15,' PASSES'
155      -           15,' WRITES'
156      -           15,' READS')
157      STOP
158      89 PRINT 905,NPASS
159      905 FORMAT(15,' STACKS FOULED UP BY PASS',I4)
160      STOP
161      END

```

Q.EJECT

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```

***** ASORT (SAUD) *****

205573JIM@WORKSPACE$1.SAND
1      SUBROUTINE SAND(WHERE)
2      C
3      C PURPOSE...
4      C          TO ADD A RECORD TO THE "SORTED" STACK
5      C
6      C USAGE...
7      C          CALLED BY PROGRAM "ASORT"
8      C
9      INCLUDE STORES,LIST
10     IF(SURE)KNOWN=KNOWN+1
11     IF(STOP)>5,5,10
12     STOP=WHERE
13     SBASE=WHERE
14     UP(WHERE)=0
15     DOWN(WHERE)=0
16     RETURN
17     10 IF(CMPARE(WHERE,STOP))20,15,15
18     C          ENTER RECORD AT TOP OF STACK
19     15 UP(STOP)=WHERE
20     UP(WHERE)=0
21     DOWN(WHERE)=STOP
22     STOP=WHERE
23     RETURN
24     20 CHANGE=.TRUE.
25     IF(CMPARE(WHERE,SBASE))22,22,25
26     C          ENTER RECORD AT BASE OF STACK
27     22 DOWN(SBASE)=WHERE
28     UP(WHERE)=SBASE
29     DOWN(WHERE)=0
30     SBASE=WHERE
31     RETURN
32     25 I=STOP
33     30 I=DOWN(I)
34     IF(CMPARE(WHERE,I))30,35,35
35     C          ENTER RECORD ABOVE RECORD I
36     35 J=UP(I)
37     DOWN(J)=WHERE
38     UP(WHERE)=UP(I)
39     DOWN(WHERE)=I
40     UP(I)=WHERE
41     RETURN
42     END

```

B.EJECT

***** JSORT (STORES) *****

```

205373JIM@WORKSPACES(1).STORES
1      STORES PROC
2      C
3      C      PROCEDURE NAME...
4      C      STORES
5      C
6      C      PURPOSE...
7      C      TO COMMUNICATE THE RECORD STACK INFORMATION FOR SORTING
8      C      PROGRAM "BSORT".
9      C
10     C      USED BY PROGRAMS...
11    C
12    C          BSORT,BEGIN,START,SADD,SOROP,HADD,HDROP,ADDTO,FINDTO,EPUSH,
13    C          EPOP
14    C
15    C          LL IS THE NUMBER OF RECORDS HELD IN MEMORY,
16    C          AND MUST BE AT LEAST 3
17    C      PARAMETER LL=24
18    C      PARAMETER LGH=20
19    C      IMPLICIT INTEGER (A-Z)
20    C      DEFINE RECORD(ILOC)=(P(JJJ,ILOC),JJJ=1,LGH)
21    C      COMMO, INCR,SURE,CHANGE,KNOWH,ITO,INTO,PUFFER,
22    C      STOP,HTOP,FTOP,SBASE,HBASE,
23    C      DOWN(LL),UP(LL),FROM(LL),TO(LL),R(LGH,LL)
24    C      LOGICAL SURE,CHANGE
25    END

```

***** BSORT (START) *****

```

205373JIM@WORKSPACES(1).START
1      SUBROUTINE START
2      C
3      C      PURPOSE...
4      C      TO INITIALIZE STORAGE FOR PROGRAM "BSORT"
5      C
6      C      INCLUDE STORES.LIST
7      C      SUFFE:=1
8      C      ETOP=2
9      C      DO 10 I=3,LL
10     C      DOWN(I-1)=I
11     C      DOWN(LL)=0
12     C      STOP=0
13     C      SBASE=0
14     C      HTOP=0
15     C      HBASE=0
16     C      INCR=1
17     C      RETURN
18     C      END

```

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```
***** SORT (SDROP) *****  
205573JIM>WORKSPACE(1),GO CP  
1      INTEGER FUNCTION SDROP(S)  
2      C  
3      C      PURPOSE...  
4      C          TO DROP A RECORD FROV THE "SORTED" STACK  
5      C  
6      C      USAGE...  
7      C          CALLED BY PROGRAM "SSORT"  
8      C  
9          INCLUDE STORES.LIST  
10         IF(SBASE)90,90,5  
11         5 SDROP=SBASE  
12         SBASE=UP(SUASF)  
13         IF(SBASE)10,10,15  
14         10 STOP=0  
15         RETUR.  
16         15 DOWN(SBASE)=0  
17         RETUR.  
18         90 PRINT 901  
19         901 FORMAT(' SORT STACK OVERDROPPED')  
20         RETURN 1  
21         END
```

W-EJECT

```

***** 1$ORT (H$UD) *****
205373JIM@WORKSPACE(1).HADD
1      C      SUBROUTINE HADD(WHERE)
2      C
3      C      PURPOSE...
4      C          TO ADD A RECORD TO THE 'HOLD' STACK
5      C
6      C      USAGE...
7      C          CALLED BY PROGRAM '1$ORT'
8      C
9      C      INCLUDE STORES.LIST
10     C      IF(HTOP)5,5,10
11     C          HTOP=WHERE
12     C          HBASE=WHERE
13     C          UP(WHERE)=0
14     C          DOWN(WHERE)=0
15     C          RETURN
16     C      10 IF(CMPARE(WHERE,HBASE))15,20,20
17     C          ENTER TO BOTTOM OF STACK
18     C      15 DOWN(HBASE)=WHERE
19     C          UP(WHERE)=HBASE
20     C          DOWN(WHERE)=0
21     C          HBASE=WHERE
22     C          RETURN
23     C      20 IF(CMPARE(WHERE,HTOP))25,22,22
24     C          ENTER TO TOP
25     C      22 UP(HTOP)=WHERE
26     C          DOWN(WHERE)=HTOP
27     C          UP(WHERE)=0
28     C          HTOP=WHERE
29     C          RETURN
30     C      25 I=HTOP
31     C      30 I=DOWN(I)
32     C      31 IF(CMPARE(WHERE,I))30,35,35
33     C          ENTER ABOVE ELEMENT I
34     C      35 J=JP(I)
35     C          DOWN(J)=WHERE
36     C          UP(WHERE)=UP(I)
37     C          DOWN(WHERE)=I
38     C          UP(I)=WHERE
39     C          RETURN
40     C          END

```

Q.EJECT

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```

***** D$ORT (HDROP) *****

205373JIM*WORKSPACES(1).HDROP
1      1,TECH FUNCTION HDROP(s)
2
3  C PURPOSE...
4  C   TO DROP A RECORD FRO! THE "HOLD" STACK
5
6  C USAGE...
7  C   CALLED BY PROGRAM "BSORT"
8  C
9    INCLUDE STORES,LIST
10   IF(HBASE)90,90,5
11   5 HDROP=HBASE
12   HBASE=UP(HBASE)
13   IF(HBASE)10,10,15
14   10 HTOP=0
15   RETURN,
16   15 DOWN(HBASE)=0
17   RETURN,
18   90 PRINT 902
19   902 FORMAT(' HOLD STACK OVERDROPPED')
20   RETURN 1
21   END

```

***** D\$ORT (ADTO) *****

```

205373JIM*WORKSPACES(1).ADTO
1      SUBROUTINE ADTO(I)
2
3  C PURPOSE...
4  C   TO ADD A RECORD TO THE "TO" STACK
5
6  C USAGE...
7  C   CALLED BY PROGRAM "BSORT"
8
9    INCLUDE STORES,LIST
10   STOP IF STACK IS FULL
11   NTO=NTO+1
12   IF(NTO.GT.LL)GO TO 90
13   FIND PROPER PLACE TO INSERT RECORD
14   CALL FINDTO(I)
15   MOVE REST OF RECORDS & INSEPT NEW ONE
16   J=NTO
17   16 J=J-1
18   IF(J.LE.I TO 18
19   TO(J+1)=TO(J)
20   GO TO 16
21   18 TO(I TO+1)=FROM(I)
22   RETURN;
23   ERROR...STACK OVERFLOW
24   90 PRINT 708
25   708 FORMAT(' NTO ,GT. LL')
26   STOP
27   END

```

EJECT

```

***** ISORT (FI^ITO) *****

205373JIM=WORKSPACES(1).FI^ITO
1      SUBROUTINE FI^ITO(I)
2      C
3      C PURPOSE...
4      C           SET POINTER 'ITO' TO POINT IN 'TO' STACK WHERE
5      C           A GIVEN NEW RECORD SHOULD BE INSERTED
6      C
7      C USAGE...
8      C           CALLED BY PROGRAM 'BSORT'
9      C
10     INCLUDE STORES,LIST
11     ITO=INTJ
12     5 ITO=ITO-1
13     IF(ITU)15,15,10
14     10 IF((FROM(I)-TO(ITO))*INCH)5,15+15
15     15 RETURN
16     END

```

```

***** BSORT (EPUSH) *****

205373JIM=WORKSPACES(1).EPUSH
1      SUBROUTINE EPUSH(LOC)
2      C
3      C PURPOSE...
4      C           TO STORE A LOCATION IN THE 'EMPTY' STACK
5      C
6      C USAGE...
7      C           CALLED BY PROGRAM 'BSORT'
8      C
9      INCLUDE STORES,LIST
10     DOWN(LOC)=ETOP
11     ETOP=LOC
12     RETURN
13     END

```

```

***** BSORT (EPOP) *****

205373JIM=WORKSPACES(1).EPOP
1      INTEGER FUNCTION EPOP(S)
2      C
3      C PURPOSE...
4      C           TO GET A LOCATION FROM THE 'EMPTY' STACK
5      C
6      C USAGE...
7      C           CALLED BY PROGRAM 'BSORT'
8      C
9      INCLUDE STORES,LIST   .
10     IF(ETOP)90,90,5
11     5 EPOP=ETOP
12     ETOP=DOWN(ETOP)
13     RETURN
14     90 RETURN 1
15     END

```

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***** PROFILE *****

Z0537SJIM@WORKSPACES(1).PROFILE

1   C
2   C      NAME...
3   C          PROFILE
4
5   C      PURPOSE...
6   C          TO UNFOLD THE DATA INTO INTENSITY VS WAVELENGTH CURVES
7
8   C      USAGE...
9
10  C          Q.PROFILE OR QXQT .PROFILE
11  C
12  C      OPTIONS:
13  C          A PRINT AND WRITE TO OUTPUT FILE POINTS FOR ALL
14  C          MONITOR INTENSITIES (OTHERWISE, IF < 50% OF THE
15  C          POINTS ARE ACCEPTED, THE WHOLE PROFILE IS DISCARDED)
16  C          C DISCARD POINTS WITH TIMES FOR THIS MONITOR INTENSITY
17  C          FURTHER THAN 1.6 SIGMA (DEFAULT 1.73) FROM THE MEAN.
18  C          THUS DELETING ABOUT 11% (DEFAULT 8%)
19  C          D DELETE 10 DATA POINTS (OVERPrides 'C' OPTION)
20  C          L PROVIDE FULL LISTING (OTHERWISE, ONLY A SUMMARY)
21  C          R REPORT RESULTS FOR ALL WAVELENGTHS (EVEN IF MOST
22  C          POINTS ARE DISCARDED)
23  C          S SKIP SOLE PROFILES
24  C          T GENERATE FILES FOR PROGRAM 'THEORY'
25
26  C      SUBPROGRAMS REQUIRED...
27  C
28  C          BEGIN,OPT,TIM,INTENS,LOOKUP,YESNO
29
30  C          MAXIMUM NUMBER OF WAVELENGTHS
31  C          PARAMETER LIMEXP=36
32  C          MAXIMUM NUMBER OF POINTS PER WAVELENGTH
33  C          PARAMETER LIMSH=8
34  C          OUTPUT RECORD LENGTH
35  C          PARAMETER CSIZE=360
36  C          PARAMETER CSIZE2=CSIZE+2
37  C          DIMENSION NUMSH(LIMEXP),INTEXP(LIEXP,LIMSH),LENGTH(LIMEXP)
38  C          DIMENSION BLOCK(55),EVOTE(2)
39  C          EQUIVALENCE (INTREF,BLOCK(1)),(TAVER,BLOCK(2)),(J,BLOCK(3))
40  C          INTEGER TEMP(20),GRP
41  C          DIMENSION HEADER(24),SIG(LIMEXP),ERROR(LIEXP),LABEL(20)
42  C          EQUIVALENCE (TEMP(4),RSHOT),(TEMP(5),AREF(1)),(TEMP(13),BREF(1))
43  C          EQUIVALENCE (LABEL(4),ISHOT),(LABEL(5),ALIV(1)),(LABEL(13),BLIN(1))
44  C          DIMENSION AREF(8),BREF(8),ALIN(8),BLIN(8),LOCATE(CSIZE),
45  C          LIST(CSIZE2)
46  C          LOGICAL SKIP(10),PRETURN,PRINT,OPT,CLOSE,ALL,THEORY,PRSKIP,EVERY
47  C          LOGICAL YESNO,REPORT
48  C          REAL INTENS,INT(10),INTAV(LIMEXP),LANDA,LENGTH,INTREF
49  C          REAL IBEGIN,INTEAP
50  C          EXTERNAL INTENS
51  C          INTEGER POOR,EARLY,FOUND,PCENT
52  C          INTEGER GROUP(8),FBEGIN(8),END(8),CREC,PFILE,PREC/1/,GP,TRY,OUT
53  C          INTEGER RSHOT,REFEND,REF1,CEND,CFILE,E1,POINTS,BAD
54  C          INTEGER SHOT(LIMEXP,10),TAG(LIMEXP,10),NTAG(10),LINTAG(LIMEXP)
55  C          INTEGER TFILE,TREC,TFMT
56  C          DATA (BLOCK(I),I=4,21)/18*0./

```

```

***** PROFILE *****
57      DATA INFILE, DELT,
58      -   / 15,   .1, 'REUF', 0.0,    0, 0, 16, 21, 503/
59      DATA LIST(1), ALTER,SPRLAD,EVNOTE
60      -   / 132,   .85, 3.0,   .0,   .0,   .0/
61      CALL LOGIN('PROFILE 2.41 J')
62      DEFINE FILE IFILE(1000,20,0),INREC
63      DEFINE FILE CFILE(CSIZE,20,0),CINC
64      FIND OUT WHETHER TO PRINT PROFILE OUT
65      ALL =OPT('A')
66      CLOSE =OPT('C')
67      EVERY =OPT('E')
68      PRINT =OPT('L')
69      REPORT=OPT('R')
70      PRSKIP=OPT('S')
71      THEORY=OPT('T')
72      IF(CLOSE) SPREAD=2.56
73      IF(.NOT.EVERY) GO TO 5
74      EVNOTE(1)= 'I'C'
75      EVNOTE(2)= 'LUDED '
76      5 IF(.NOT.THEORY) ITFILE=0
77      IBEGIN=0.0
78      L=0
79      K=0
80      C      SAVE FILE HEADER
81      READ(INFILE*1)(HEADER(I),I=1,12)
82      READ(INFILE*2)(HEADER(I),I=13,24)
83      C      FIND-BEGINNING AND END OF EACH GROUP
84      10 READ(INFILE*INREC)LABEL
85      IF(LABEL(1)=E0,E1)GO TO 25
86      DECODEL(800,LABEL)NP
87      800 FORMAT(A5)
88      DECODEL(803,LABEL)NP
89      803 FORMAT(15)
90      GP=GP*100
91      IF(GP.NE.)   GO TO 12
92      IBEGIN=MAX(IBEGIN,BLIN(1))
93      K=K+1
94      LOCATE(K)=NSHOT
95      12 I=0
96      15 I=I+1
97      IF(I.GT.L)GO TO 20
98      IF((97*GROUP(I).GT.GP)+0.0,(GP.GT.103*GPOUP(I)))GO TO 15
99      GO TO 19
100     C      FOUND BEGINNING OF NEW GROUP
101     20 IF(L.GE.A)GO TO 197
102     L=L+1
103     GROUP(L)=GP/100
104     FBEGIN(L)=INREC-1
105     PRINT 805, GROUP(L),FBEGIN(L)
106     805 FORMAT(1, 'FOUND GROUP: ',15, ' AT RECORD',I4)
107     IF(L.NE.1)END(L-1)=INREC-2
108     GO TO 10
109     25 IF(L.NE.0)END(L)=INREC-2
110     C      NOTE BEGINNING & END OF REFERENCE SIGNAL GROUP
111     INREC=1
112     K=0
113     00 30 KK=1,L

```

```

***** PROFILE *****
114      30 IF(GRLUP(KK).EQ.0) GO TO 32
115      GO TO 191
116      NEF1=FBEGIN(KK)
117      REFLN=LN0(KK)
118      KK=0
119      KLIM=L-1
120      IHEAD=0
121      IF(.NOT.PRINT)PRINT 806
122      806 FORMAT('0 FILES INTENSITY POINTS//'
123      -           '(VOLTS) FOUND BAD')
124      C          PRODUCE NEW FILE FOR EACH LINE PRESENT
125      DO 100 K=1,KLIM
126      C          INITIALIZE THE FILE
127      35 KK=KK+1
128      IF(KK.GT.KLIM)GO TO 190
129      IF(GROUP(KK).EQ.1)GO TO 35
130      PFILE=CFILE+K
131      CREC=1
132      JA=FBEGIN(KK)
133      JB=END(KK)
134      IF(JB-JA+1.GT.CSIZE)GO TO 190
135      DO 38 J=JA,JB
136      READ(IFILE'J)LABEL
137      38 WRITE(CFILE'CREC)LABEL
138      CEND=LREC-1
139      DEFINE FILE PFILE(14+3*L1*EXP+1,U,PREC)
140      WRITE(PFILE'1)HEADER
141      INTREF=.93*IBEGIN
142      TRY=0
143      NT=0
144      LINES=100
145      IF(.NOT.THEORY)GO TO 40
146      DEFINE FILE TFILE(13+55+(2+LIMSH)*LIMEXP,U,TRFC)
147      WRITE(TFILE'1)TFORMAT,HEADER
148      C          START NEXT MONITOR SIGNAL LEVEL
149      40 INTREF=ALTER*INTREF
150      TRY=TRY+1
151      IF(TRY.GT.20)GO TO 97
152      IF(.NOT.PASKIP)GO TO 41
153      PRINT 813,PFILE,TFILE,I'ITREF
154      IF(YESNO('WANTED?G',97))GO TO 41
155      NT=0
156      GO TO 40
157      41 AVERR=0.0
158      CREC=1
159      NSHOT=0
160      J=1
161      LENGTH(1)=2.
162      POINTS=0
163      NOMON=0
164      FOUND=0
165      POOR=0
166      BAD=0
167      OUT=0
168      EARLY=0
169      LATE=0
170      N=0

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C.2

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***** PROFILE *****

171      C          FIND MEAN & STANDARD DEVIATION OF TIMES FOR THIS
172      C          MONITOR INTENSITY.
173      C          IF(INT.GT.1)GO TO 44
174      C          WE MUST GO READ THE FILE THE FIRST TIME THROUGH
175      C          T=0.
176      C          TS=0.
177      C          DO 42 L=REF1,REFEND
178      C          READ(INFILE'L')TE 10
179      C          TA=TI,I(INTREF,AREF,BREF,$42,$42)
180      C          NT=NI+1
181      C          T=T+TA
182      C          TS=TS+TA*TA
183      C          42 CONTINUE
184      C          GO TO 50
185      C          RECORD TIMES FOR ALL MONITOR SIGNALS NOT USED
186      C          FOR THIS PROFILE
187      C          44 DO 45 L=REFEND,PEF1,-1
188      C          CALL LOOKUP(LOCATE(L+1-RLF1),I,LIST,$45)
189      C          READ(INFILE'L')TE 10
190      C          TA=TI,I(INTREF,AREF,BREF,$45,$45)
191      C          T=T+TA
192      C          NT=NI+1
193      C          TS=TS+TA*TA
194      C          45 CONTINUE
195      C          50 IF(INT.LE.1)GO TO 192
196      C          CALL EMPTY(LIST)
197      C          TAVER=T/FLOAT(NT)
198      C          TSIGMA=SORT((TS-TAVER*T)/FLOAT(NT-1))
199      C          TSIG=((TS-TAVER*T)/FLOAT(NT-1))*SPREAD
200      C          T=0.
201      C          TS=0.
202      C          NT=0
203      C          INREC=REF1
204      C          RSHOT=-2
205      C          GET ANOTHER CURVE UNLESS WE'RE AT THE END OF THE FILE
206      C          52 IF(CREC.LE.CE)GO TO 54
207      C          IF WE HAVE DATA FOR THIS WAVELENGTH, FIND AVERAGES
208      C          IF(N.GT.0)GO TO 70
209      C          IF WE HAVE DATA FOR THIS TIME GO RECORD IT
210      C          IF(J.GT.1)GO TO 81
211      C          GO TO NEXT TIME
212      C          GO TO 96
213      C          GET NEW CURVE
214      C          54 READ(CFILE'CREC)LABEL
215      C          DECODE(B12,LAMBDA)
216      C          B12 FORMAT(F5.1)
217      C          IF(AJS(LAMBDA-LENGTH(J)).LT..02)GO TO 58
218      C          IF(N.GT.0)GO TO 70
219      C          56 LENGTH(J)=LAMBDA .
220      C          N=0
221      C          NF=0
222      C          GET REFERENCE CURVE FOR THIS SHOT
223      C          58 NF=MIND(NF+1,10)
224      C          SHOT(J,NF)=NSHOT
225      C          TAG(J,NF)=' '
226      C          IF(INREC.LE.REFEND)GO TO 59
227      C          I=REF1

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      ***** PROFILE *****

228      GO TO 60
229      59 IF(LOCATE(INRFC+1-REF1),EQ,NSHOT)GO TO 63
230          I=INREC
231          60 DO 61 I=REC=REF1,REFE IC
232          61 IF(LOCATE(INRFC+1-REF1),EQ,NSHOT)GO TO 63
233          C           NO MONITOR SIGNAL FOUND FOR THIS SHOT NUMBER!
234          INREC=I
235          NO40,N=NO40N+1
236          TAG(J,NF)='N'
237          GO TO 52
238          63 READ(INFILE*INREC)TEMP
239          C           RECORD TIME AT NEXT INTENSITY
240          TA=TI*(INTREF+ALTRF,AREF,BREF,$64,$64)
241          NT=NT+1
242          T=T+TA
243          TS=TS+TA*TA
244          C           IF TIME FOR THIS MONITOR INTENSITY IS MORE THAN
245          C           1.73 (OF 1.6, UNDER 'C' OPTION) SIGMA FROM THE MEAN,
246          C           THE MONITOR SIGNAL IS BAD AND WE DISCARD THIS POINT.
247          C           THIS SHOULD, ASSUMING A GAUSSIAN DISTRIBUTION,
248          C           DELETE ABOUT 8% (OR 11%) OF THE POINTS.
249          64 TA=TI*(INTREF,AREF,BREF,$66,$193)
250          IF((TA-TAVER)**2.LT.TSIG)GO TO 65
251          POOR=POOR+1
252          TAG(J,NF)='P'
253          IF(.NOT.EVERY)GO TO 52
254          C           FOUND ONE MORE CURVE FOR THIS LEVEL..RECORD
255          65 N=N+1
256          IF(N.GT.LI-SH)GO TO 176
257          INT(N)=INTENS(TA,ALIN,BLIN,$67,$68)
258          SKIP(I)=.FALSE.
259          NTAG(N)=NF
260          GO TO 52
261          C           INTENSITY IS OUT OF RANGE OF MONITOR VALUES
262          66 OUT=OUT+1
263          TAG(J,NF)='O'
264          GO TO 69
265          C           TIME IS TOO EARLY FOR SIGNAL CURVE
266          67 EARLY=EARLY+1
267          TAG(J,NF)='E'
268          GO TO 69
269          C           TIME IS TOO LATE FOR SIGNAL CURVE
270          68 LATE=LATE+1
271          TAG(J,NF)='L'
272          IF(LATE.GT.10)GO TO 97
273          69 N=N-1
274          GO TO 52
275          C           FOUND ALL DATA FOR ONE WAVELENGTH...
276          C           CALCULATE AVERAGE INTENSITY
277          70 RETURN,.FALSE.
278          71 NI=0
279          SUM=0
280          SUMSQ=0.0
281          DO 72 I=1,N
282          IF(SKIP(I))GO TO 72
283          NN=NN+1
284          SUM=SUM+INT(I)

```

```

***** PROFILE *****
285      SUMSUM=SUM+INT(I)+INT(I)
286      I,TEAR(J,NN)=INT(I)
287      CONTINUE
288      NUMSH(J)=NN
289      IF(NN>1)79,75,73
290      73  IF(TAV(J)=SUM/N)
291          SIG(J)=(SUMSA-SUM*INTAV(J))/(NN-1)
292          C      DISCARD POINTS ONLY ONCE
293          C      IF(RETURM)GO TO 76
294          C      THROW OUT ALL POINTS FURTHER AWAY THAN 1.8 SIGMA
295          C      THIS SHOULD DELETE ABOUT 6% OF THE POINTS.
296      DO 74 I=1,N
297      IF(SKIP(I))GO TO 74
298      IF((INT(I)-INTAV(J))**2.LT.SIG(J)*3.24)GO TO 74
299      BAD=BAD+1
300      II=NTAG(I)
301      TAG(J,II)='B'
302      IF(LVLRY)GO TO 74
303      RETURN=.TRUE.
304      SKIP(I)=.TRUE.
305      74  CONTINUE
306      C      RECALCULATE MEAN & STANDARD DEVIATION IF
307      C      WE'VE THROWN OUT ANY MORE POINTS
308      C      IF(RETURM)GO TO 71
309      C      GO TO 70
310      75  INTAV(J)=SUM
311      SIG(J)=0.
312      76  SIG(J)=SORT(SIG(J))
313      IF((I,TAV(J),LT,1.E-6).OR.(N.EQ.0))GO TO 194
314      ERROR(J)=100.*SIG(J)/INTAV(J)
315      AVERH=AVERR+ERROR(J)
316      LIMTAG(J)=NF
317      POINTS=POINTS+NN
318      J=J+1
319      GO TO 80
320      79  IF(REPORT)J=J+1
321      80  FOUND=FOUND+NN
322      IF(CREC.GT.CEND)GO TO 81
323      IF(J.LE.LINEXP)GO TO 56
324      J=J-1
325      PRINT 950,J
326      980 FORMAT('0**** MORE THAN',I4,' WAVELENGTHS, REST DISCARDED ****')
327      C      DON'T BOTHER RECORDING OR PRINTING IF MORE
328      C      THAN 40% OF THE POINTS WERE THROWN OUT
329      C      81  FOUND=FOUND+(J-1)*(POOR+OUT+EAPLY+LATE)
330      C      IF(FOUND.LE.0)GO TO 195
331      PCENT=(100*(NOMON+POOR+OUT+EAPLY+LATE+BAD))/FOUND
332      J=J-1
333      IF(ALL)GO TO 82
334      IF(PCENT .GT. 40)GO TO 92
335      C      IF WAVELENGTH IS IN UV DIVIDE BY TWO
336      C      TO COMPENSATE FOR INCORRECT MCPHEARSON SCALE
337      C      82  IF(LENGTH(I) .GT. 3300.)GO TO 86
338      DO 84 I=1,J
339      84  LENGTH(I)=.5*LENGTH(I)
340      86  IF(PRINT)GO TO 87

```

```

***** PROFILE *****

342      PRINT 813,PFILE,TFILE,INTREF,FOUND,PCENT
343      813 FORMAT(1X,I2,I3,F4.3,I9,15,1H*)
344      GO TO 91
345      C          PRINT PROFILE IF REQUESTED TO
346      87 LINES=LINES+J+17
347      IF(IHEAD<LT.0)GO TO 88
348      IF(LINES>LT.57)GO TO 89
349      88 PRINT 814,HEAER
350      814 FORMAT(1H1,12A6/1H ,12A6)
351      LINES=J+19
352      89 PRINT 815,TAVER,TSIGMA,INTREF,PFILE,TFILE,FOUND,NOMON,
353      -     POOR,EVNOTE,OUT,EARLY,LATE,BAD,EVNOTE,POINTS
354      815 FORMAT(1X//' TIME =',F6.3,' +-',F5.3,' MSEC   MONITOR =',
355      -     F6.4,' V   FILES',I3,' ',I3,'//'
356      -     T10,I3,' POINTS FOUND/'
357      -     T10,I3,' HAD NO MONITOR SIGNALS (N)//'
358      -     T10,I3,' HAD POOR MONITOR SIGNALS (P)',2A6/
359      -     T10,I3,' OUT OF MONITOR RANGE (O)//'
360      -     T10,I3,' TIMES TOO EARLY (E)//'
361      -     T10,I3,' TIMES TOO LATE (L)//'
362      -     T10,I3,' SIGNALS TOO FAR FROM MEAN (B)',2A6/
363      -     T10,I3,' ACTUALLY USED//'
364      PRINT 816
365      816 FORMAT(' WAVELENGTH      I ITENSITY      ERROR',T50,'POINTS FOUND//'
366      -     '(ANGSTROMS)           (VOLTS)')
367      IHEAD=1
368      DO 90 I=1,J
369      III=LIMTAG(I)
370      90 PRINT 818,LENGTH(I),I'ITAV(I),SIG(I),ERROR(I),
371      -     (SHOT(I,II),TAG(I,II),II=1,III)
372      818 FORMAT(F10.2,F9.5,' +-',F7.5,F6.0,T35,1H%,
373      -     2X,10(I5,1A,A1))
374      AVERR=AVERR/FLOAT(J)
375      PRINT 821,AVERR
376      821 FORMAT(T17,'AVERAGE SIGMA',F6.0,T35,1H%)
377      C          WRITE INFORMATION TO FILFS
378      91 IF(J.LE.29)LENGTH(J+1)=0.
379      WRITE(PFILE*PREC)I'ITREF,LENGTH,INTAV,SIG
380      IF(THEORY)WRITE(TFILE*TAC)BLOCK, IUS,I LENGTH,INTEXP
381      GO TO 96
382      C          REPORT ONE PROFILE DISCARDED
383      92 NOPROF=NOPROF+1
384      IF(.NOT.PRINT)GO TO 96
385      C          GO TO NEXT PAGE IF THIS PAGE HAS A PROFILE ALREADY
386      IF(IHEAD.GT.0)PRINT 814
387      PRINT 825,I'ITREF,PCENT,NOMON,POOR,OUT,FARLY,LATE,BAD
388      825 FORMAT(' MONITOR =',F5.3,I5,'% DISCARDED',
389      -     I4,' N',I4,' P',I4,' O',I4,' E',I4,' L',I4,' B')
390      IHEAD=-1
391      GO TO 96
392      C          REPORT ERRORS OCCURRING WITHIN MAJOR LOOP
393      180 PRINT 901,GRUP(KK),JA,JB,CFILE,CSIZE
394      901 FORMAT(' GROUP: ',I5,' USES RFCORDS',I4,' THROUGH',I4,
395
396
397
398

```

```

***** PROFILE *****

399      -     '...TOO MANY FOR FILE',I4/
400      -     ' WHICH HOLDS',I4,' RECORDS')
401      GO TO 97
402 PRINT 902,INTREF
403 FORMAT(' MONITOR =',F5.3,', TOO FEW VALID MONITOR SIGNALS')
404      GO TO 40
405 193 I=INREC-1
406      PRINT 903,I,(TE4P(I),I=1,4),(TE4P(I),I=1,7,2),(TEMP(I),I=2,8,2)
407 903 FORMAT(' INVALID DATA IN RECORD',I3,', GROUP ',2A6,', SCALE',F6.3,
408      -     ', SHOT',I4/
409      -     1X,6F8.5/1X,8F8.5)
410 194 FOUND=FOUND+NOMON+POOR+OUT+EARLY+LATE
411 PRINT 904,J,LNGTH(J),INTAV(J),N,N
412 904 FORMAT(' ERROR ON POINT',I3,', (',F8.2,')...AV INTENS=',F8.5/
413      -     ' FOUND',I3,' POINTS, USING THE FOLLOWING',I3,1H')
414      PRINT 818,LENGTH(J),INTAV(J),SIG(J),EPPOR(J),
415      -     (SHOT(J,II),TAG(J,I1),II=1,NF)
416      PRINT 905
417 905 FORMAT(IX// PREVIOUS POINTS...))
418      PRINT 815,TAVER,TSIGMA,I ITREF,'FILE',TFILE,FOUND,NOMON,
419      -     POOR,EVNOTE,OUT,EARLY,LATE,GAD,EVNOTE,POINTS
420      GO TO 90
421 196 KKK=LISH
422      PRINT 906,KKK,J,INTAV(J),(SHOT(J,I),TAG(J,I),I=1,NF)
423 906 FORMAT(' >',I3,' CURVES FOUND FOR POINT',I3,
424      -     ' OF PROFILE...AV INTENSITY =',F8.5/
425      -     ' INCLUDING THESE:',10(1X,A1))
426      GO TO 97
427 C
428 C           TRY TO FIND 10 PROFILES IN ALL
429 96 IF(PREC.LT.13 .AND. (PCENT.LT.40 .OR. PREC.LT.4))GO TO 40
430      GO TO 97
431 C
432 C           FINISH FILE
433 C
434 97 IF(PREC.LE.14)WRITE(PFILE,PREC)E1
435 I=PREC-3
436      PRINT 830,I,NOPROF
437 830 FORMAT(16,'TOTAL OF',I4,' PROFILES ENTERED AND',I3,' DISCARDED')
438      IF(.NOT.THEGRAY)GO TO 100
439      IF(TREC.LT.41)WRITE(TFILE,TREC)E1
440      TFILE=TFILE+1
441 100 CONTINUE
442      STOP
443 C
444 C           REPORT ERRORS OCCURRING BEFORE MAJOR LOOP
445 C
446 190 PRINT 910
447 910 FORMAT(' NO CURVES FOUND FOR MAIN SIGNAL')
448      STOP
449 191 PRINT 911
450 911 FORMAT(' NO CURVES FOUND FOR REFERENCE SIGNAL')
451      STOP
452 197 PRINT 917,L,(GROUP(I),I=1,L),GP
453 917 FORMAT(' MORE THAN',I3,' GROUPS FOUND://
454      -     (8I8))
455      STOP

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***** PROFILE *****

456 END

***** PROFILE (TIM) *****

```

205373JIM**ORKSPACES(1).TIN
1      FUNCTION TIM(INT,A,B,S)
2      C
3      C PURPOSE...
4      C          TO FIND THE TIME CORRESPONDING TO A GIVEN INTENSITY
5      C
6      C USAGE...
7      C
8      C          T=TIM(INT,A,B,S80,S90)
9      C
10     C          TIM    R.O    CALCULATED TIME
11     C          INT    R.I    GIVEN INTENSITY
12     C          A      R.I    ARRAY OF TIMES
13     C          B      R.I    ARRAY OF CORRESPONDING INTENSITIES
14     C          S80   S.I    EXIT USED IF DESIRED INTENSITY IS OUTSIDE THE
15     C                      RANGE OF THE INTENSITIES IN ARRAY B
16     C          S90   S.I    EXIT USED IF GIVEN DATA IS INVALID
17     C                      (I.E., TIMES NOT INCREASING OR INTENSITIES NOT
18     C                      DECREASING)
19     C
20     C METHOD...
21     C          LINEAR INTERPOLATION.
22     C
23     REAL INT
24     DIMENSION A(8),B(8)
25     IF((A(8).LT.A(1)).OR.(B(8).GT.B(1)))RETURN 5
26     IF((INT.LT.B(8)).OR.(INT.GT.B(1)))RETURN 4
27     DO 10 I=2,8
28     IF(INT.GE.B(I))GO TO 12
29     CONTINUE
30     IF(B(I).NE.B(I-1))GO TO 15
31     TIM=A(I)
32     RETURN
33     TIM=A(I)-(A(I)-A(I-1))*(B(I)-INT)/(B(I)-B(I-1))
34     RETURN
35     END

```

W-EJECT

```

***** PROFILE (INTENS) *****
205373-1M+0K$PACE\$1).INTENS
1      REAL FUNCTION INTENS(TIME,A,B,S,$)
2      C
3      C PURPOSE...
4      C          TO FIND THE INTENSITY FOR A GIVEN TIME
5      C
6      C USAGE...
7      C
8      C          Y = INTENS(TIME,A,B,$80,$90)
9      C
10     C          TIME   R:I    GIVEN TIME
11     C          A      R:I    SAMPLE TIMES
12     C          B      R:I    SAMPLES (INTENSITIES)
13     C          $80    S:O    ERROR EXIT TAKEN IF GIVEN TIME TOO EARLY
14     C          $90    S:O    ERROR EXIT TAKEN IF GIVEN TIME TOO LATE
15     C
16     C METHOD...
17     C          LINEAR INTERPOLATION
18     C
19     DIMENSION A(8),B(8)
20     IF(TIME.LT.A(1))RETURN 4
21     IF(TIME.GT.A(8))RETURN 5
22     DO 10 I=2,8
23     IF(TIME.LE.A(I))GO TO 12
24     10 CONTINUE
25     IF(A(I).NE.A(I-1))GO TO 15
26     INTE B=B(I)
27     RETURN,
28     15 INTENS=B(I)-(B(I)-B(I-1))*(A(I)-TIME)/(A(I)-A(I-1))
29     RETURN,
30     END

```

W-EJECT

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***** PROFILE (LOOKUP) *****

205373JIM@WORKSF ACES(1).LOOKUP
 1      SUBROUTINE LOOKUP(NUMBER,I,LIST,$)
 2      C
 3      C      NAME...
 4      C      TABLE LOOKUP
 5      C
 6      C      PURPOSE...
 7      C      TO CREATE, AND LATER FIND ENTRIES IN, A SORTED TABLE OF
 8      C      INTEGERS.
 9      C
10      C      USAGE...
11      C
12      C          CALL EMPTY(LIST)           MARK LIST AS EMPTY
13      C
14      C          LIST   I,IO    WORK ARRAY (SAVED BETWEEN CALLS)
15      C                      LIST(1) SHOULD BE SET TO THE LENGTH OF THE
16      C                      ARRAY.
17      C
18      C          CALL ENTER (NUMBER,LIST,$) ADD NUMBER TO LIST
19      C
20      C          NUMBER I,I    NUMBER TO BE ADDED
21      C          $     S,I    THIS RETURN TAKEN IF LIST IS ALREADY FULL
22      C
23      C          CALL LOOKUP (NUMBER,I,LIST,$) SEARCH FOR NUMBER IN LIST
24      C
25      C          NUMBER I,I    NUMBER TO BE FOUND
26      C          I     I,O    RELATIVE LOCATION IN LIST, IF FOUND
27      C                      ZERO, IF NOT FOUND
28      C          $     S,I    THIS RETURN IS TAKEN IF NUMBER IS FOUND
29      C                      (OTHERWISE, NORMAL RETURN)
30      C
31      C      DIMENSION LIST(50)
32      C      I=0
33      C      IF(LIST(2).LT.3)RETURN
34      C      DO 20 I=3,LIST(2)
35      C      20 IF(LIST(I).EQ.NUMBER)RETURN 3
36      C      I=0
37      C      RETURN
38      C      ENTRY ENTER(NUMBER,LIST,$)
39      C      L=MAX0(LIST(?)+1,3)
40      C      IF(L.GE.LIST(1))RETURN 1
41      C      LIST(2)=L
42      C      LIST(L)=NUMBER
43      C      RETURN
44      C      ENTRY EMPTY(LIST)
45      C      LIST(2)=2
46      C      RETURN
47      C      END

```

B.EJECT

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***** PROFILE (YES10) *****

205373JIM@WORKSPACES(1).YES10
1   NAME...
2   YESNO
3
4   PURPOSE...
5       TO GET A YES OR NO ANSWER TO A QUESTION FOR
6       AN INTERACTIVE PROGRAM.
7
8   CALLING SEQUENCE...
9
10
11   LOGICAL YESNO
12
13
14   IF(YESNO("SHALL I SKIP OPTIONAL PART?Q",\$90))GO TO 40
15   CONTINUE
16
17
18   <OPTIONAL PART OF PROGRAM>
19
20
21   IF(YESNO("SHALL I REPEAT OPTIONAL PART?Q"))GO TO 20
22   <REST OF PROGRAM>
23
24
25   90 <SPECIAL SECTION FOR END-OF-FILE RETURN>
26
27   THE QUESTION MUST END WITH THE STOP CHARACTER Q (WHICH
28   ISN'T PRINTED), OR THE QUESTION WILL BE FOLLOWED BY A
29   WHOLE STRING OF TRASH, AND THE PROGRAM MAY BLOW UP. THE
30   QUESTION WILL BE PRINTED, AND THE TELETYPE WILL WAIT ON
31   THE SAME LINE FOR THE USER TO TYPE HIS ANSWER. THAT
32   ANSWER MAY START IN ANY COLUMN AND CONSIST OF ANY NORMAL
33   AFFIRMATIVE OR NEGATIVE WORD (I.E., ANY ONE I COULD THINK
34   OF WHEN I WROTE IT). THE USER MAY SUPPLY AN EOF RETURN
35   ADDRESS AS THE SECOND ARGUMENT, BUT THIS IS OPTIONAL
36   (THE PROGRAM WILL FIND IT'S WAY BACK EITHER WAY).
37
38   CONTENTS OF ALL REGISTERS EXCEPT AO ARE SAVED.
39
40   ERROR CONDITIONS...
41
42   IF THE USER'S ANSWER IS A BLANK LINE OR A CHARACTER
43   STRING THE PROGRAM DOESN'T RECOGNIZE (IT CAN BE FOOLED)
44   IT TRIES AGAIN, PRINTING ONLY "WHAT?". IT WILL REPEAT THE
45   ORIGINAL QUESTION ONE TIME IN FOUR.
46
47   IF THE RESPONSE IS EOF, THE PROGRAM USES THE ALTERNATE
48   RETURN ADDRESS, IF SUPPLIED. THIS CAN BE USED, FOR
49   INSTANCE, TO TERMINATE THE PROGRAM OR RE-ASK A
50   PREVIOUS QUESTION (THIS WAY YOU DON'T HAVE TO RE-RUN THE
51   WHOLE PROGRAM), IF THE ANSWER IS ANY OTHER CHARACTER
52   STRING BEGINNING WITH Q THE SYSTEM THINKS THE PROGRAM
53   IS TRYING TO READ A CONTROL CARD, AND ALLOWS NO FURTHER
54   READS. IN THIS CASE, OR IF EOF IS ENCOUNTERED AND NO
55   QEOF RETURN ADDRESS HAS BEEN SUPPLIED, THE PROGRAM PRINTS
56   A SHORT MESSAGE AND EXITS.

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***** PROFILE (YES JO) *****

57      /
58      S(0)    LIT .
59      S(1)    AXRS .
60      TESNO*   SA X11,PETURN .
61      DS      A1,SAVF .
62      DS      A3,SAVE3 .
63      SR      R1,SAVER1 .
64      SR      R14,SAVER14 .
65      ESDIT   PACKFT .
66      LX      X11,RETURN .
67      L,H1    A0,1,X11 . GET FIRST WORD FOLLOWING QUESTION POINTER
68      AN,U    A0,0742000 . COMPARE TO JUMP INSTRUCTION
69      S       A0,PRESENT . THIS INDICATES PRESENCE OF EOF ADDRESS
70      L       A0,0,X11 . GET ADDRESS OF USP'R'S QUESTION
71      LMJ    X11,EMSGS . AND INSERT IT INTO PRINT LINE
72      LMJ    X11,EDITX$ . END EDIT MODE & RESTORE REGISTERS
73      L,U     A4,3 . INITIALIZE QUERY COUNTER
74      ASK     L,U     A0,READPKT .
75      READ    L,U     A1,BLANKS . FILL INPUT LINE WITH BLANKS SO THE
76      LX1,U   A2,1 . PREVIOUS INPUT DOESN'T CONFUSE THE ISSUE
77      LM1,U   A2,INPUT .
78      LR,U    R1,14 .
79      BT      A2,0,*A1 .
80      ER      TREAD3 . DO A TREADS TO PRINT QUESTION & GET ANSWER
81      LSSL   A0,4 . IS REPLY ACTUALLY IN 'INFOR' FORMAT?
82      JP      A0,EXAMINE . REPLY IS PRESENT
83      LA      A0,RFANPKT+1 . INPUT IS IN 'INFOR' FORMAT...REREAD
84      ER      READS .
85      EXAMINE LX1,U   A2,0 . INITIALIZE INDEX REGISTERS
86      L,S1    A3,INPUT . IF FIRST CHARACTER IS NON-BLANK, SKIP
87      L       A0,INPUT . TO SEARCHING FOR A MATCHING WORD
88      TE,U    A3,5 . 05 IS A BLANK
89      J       MATCH .
90      LR,U    R1,14 . OK...WE'LL HAVE TO DO IT THE LONG WAY
91      LA      A1,BLANKS .
92      SNE    A1,INPUT,*A2 . FIND FIRST WORD NOT ENTIRELY BLANKS
93      J       AGAIN . OOPS...THE WHOLE LINE WAS BLANK!
94      L       A0,INPUT-1,A2 . GET THAT FIRST NON-BLANK CHARACTER
95      L,U     A3,5 . FIGURE OUT WHICH CHARACTER IT IS
96      LOOP   A1,L    A0,(077000000000) . MASK OUT LAST 5 CHARACTERS
97      TE      A1,(005000000000) . IS IT A BLANK?
98      J       LOAD   . NO...GO LOOK FOR A MATCHING WORD
99      LSSL   A0,6 . YES...TRY NEXT CHARACTER
100     JGD    A3,LOOP .
101     LOAD   DL    A0,INPUT-1,A2 . GET THE MESSAGE
102     EX      MOVE,A3 . SHIFT THE BLANKS AWAY
103     LM1,U   A2,0 .
104     MATCH   LR,U    R1,WNCOUNT . SEARCH FOR MATCHING WORD IN TABLE
105     SE      A0,TABLE,*A2 .
106     J       AGAIN . NO MATCH...ASK AGAIN
107     L       A0,A2 . FOUND A MATCH...GET INDEX
108     LSSL   A0,35 . LAST BIT IS 1 IF 'YES', 0 IF 'NO'
109     SSL    A0,35 . (SINCE A2 HAS BEEN INCREMENTED)
110     SLJ    RESTORE . RESTORE REGISTERS & RETURN
111     TZ    PRESENT .
112     J      2,X11 . RETURN TO CALL+2 IF NO EOF ADDR SUPPLIED
113     J      3,X11 . RETURN TO CALL+3, SINCE EOF ADDR PRESENT

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***** PROFILE (YES 10) *****

114 AGAIN L,U A0,AGAINPKT , PRINT THE ENTIRE QUESTION ONLY ONE TIME
115 J0,J A4,READ . OUT OF FOUR
116 L,U A4,3 .
117 J ASK .
118 EOF SLJ RFSTORF . END-OF-FILE RETURN...RELOAD REGISTERS
119 TN2 PHSENT . ACTION. ONLY IF EOF ADDR SUPPLIED
120 JP A0,*1,X11 . RETURN TO EOF ADDRESS
121 L A0,(PF 1,PRTCNT,PRTLINE) .
122 ER PRINTS . NON-EOF CONTROL CARD ENCOUNTERED...
123 ER EXITS . WE'RE FORCED TO QUIT
124 RESTORE RES 1 *ROUTINE FOR RESTORING REGISTERS
125 DL A1,SAVE .
126 DL A3,SAVE3 .
127 LR R1,SAVER1 .
128 LR R14,SAVER14 .
129 LX X11,RETURN .
130 J *RESTORE .

131 /
132 $(0) .
133 WBCK *YESNO*
134 RETURN + 0 .
135 SAVE RES 2 .
136 SAVE3 RES 2 .
137 SAVER1 RES 1 .
138 SAVER14 RES 1 .
139 PRESENT + -1 .
140 PACKET ESPKT 24,LINE *4SG*,? . IF THE USER FORGETS THE STOP
141 * CHARACTER, A ? IS THE CHARACTER MOST
142 * LIKELY TO BE FOUND BY ACCIDENT.
143 PRTLINE *CONTROL CARD FORCES PROGRAM EXIT* .
144 PRTCNT EGU $-PRTLINE . NUMBER OF WORDS IN MESSAGE
145 PF FORM 12,6,18 .
146 READPKT PF 1,22,LINE .
147 LINE RES 24 .
148 AGAINPKT PF 1,1,QUESTION .
149 +
150 +
151 QUESTION *WHAT?* .
152 INPUT RES 14 .
153 BLANKS ' ' .
154 MOVE LD$L A0,30 .
155 LD$L A0,24 .
156 LD$L A0,18 .
157 LD$L A0,12 .
158 LD$L A0,6 .
159 NOP .
160
161 TABLE *YES* . EVEN RELATIVE LOCATIONS FOR 'YES',
162 *NO* . ODD FOR 'NO'
163 'Y' .
164 'N' .
165 'QUI' .
166 'NON' .
167 'ALRIGHT' .
168 'NOPE' .
169 'YEP' .
170 'NAW' .

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```
***** PROFILE (YESNO) *****  
171      'YEA' .  
172      'NIGHT' .  
173      'RIGHT' .  
174      'NEIN' .  
175      'JA' .  
176      'NYET' .  
177      'DA' .  
178      'DUNT' .  
179      'DO' .  
180      'DON'T' .  
181      'OK' .  
182      'NOT' .  
183      'OKAY' .  
184      'IN' .  
185      'SI' .  
186      WCOUNT EQU     $-TABLE    . THE NUMBER OF WORDS IN THE TABLE  
187      END .
```

N-EJECT

```

***** VPLOT *****
205373JIM@WINKSPACES1.VPLOT
1   C      NAME...
2   C          VPLOT
3   C
4   C      PURPOSE...
5   C          TO PRODUCE A PRINTER-PLOT OF THE EXPERIMENTAL LINE PROFILE
6   C          PRODUCED BY PROGRAM 'PROFILE'.
7   C
8   C      USAGE...
9   C
10  C          QXQT .VPLOT OR .VPLOT
11  C          <FILE #>      (FREE) NUMBER OF 1ST FILE TO PLOT
12  C          <FILE #>      (FREE) NUMBER OF 2ND FILE TO PLOT
13  C          EOF
14  C
15  C          OPTIONS:
16  C          T      PLOT IS TO BE ON A TERMINAL, SO IT USES ONLY
17  C          COLUMNS 1-72.
18  C
19  C
20  C      INPUT...
21  C          DATA FILE AS PRODUCED BY PROGRAM 'PROFILE'.
22  C
23  C      SUBPROGRAMS REQUIRED...
24  C          BEGIN,OPT,NUMBER
25  C
26  C      PARAMETER LIMEXP=36
27  C      LOGICAL OPT,BATCH
28  C      REAL INTL,0,LNGTH,INTAV,IMAX,INCR,NL
29  C      DIMENSION LINE(105),HEADER(24),LENGTH(LIMEXP),INTAV(LIMEXP),
30  C          - SIG(LIMEXP)
31  C      DATA E1//EOF//MARK//11//,IZERO//0//,IONE//1//
32  C      JCOL(X)=1+IFIX(X*INCR)
33  C      CALL BEGIN('VPLOT 1.12 R')
34  C      IDIF=IONE-IZERO
35  C          FIND FILE AND READ FILE HEADER
36  C      5 NFILE=NUMBER('FILE NU.BCR??.7,29,599')
37  C      DEFINE FILE NFILE(14,1+3*LIMEXP,U,NREC)
38  C      READ(NFILE'1)HEADER
39  C          DECIDE WHETHER SMALL ('T' OPTION) OR LARGE GRAPH
40  C          ICOL=41
41  C          BATCH=.NOT.OPT('T')
42  C          IF(BATCH)ICOL=101
43  C          COL=FLOAT(ICOL-1)
44  C          LAST=' '
45  C          IF(BATCH)LAST=MARK
46  C          READ A PROFILE
47  C          8 IF(NREC.LE.14)GO TO 11
48  C          I=MAX0(U,NREC-2)
49  C          10 PRINT 805,I
50  C          805 FORMAT(1X//I3,' PROFILES')
51  C          PRINT 808
52  C          808 FORMAT(1H1)
53  C          GO TO 5
54  C          11 READ(NFILE'NREC)INTMON,LENGTH,INTAV,SIG
55  C          IF(INTMON.EQ.E1)GO TO 10
56  C          SET UP SCALING PARAMETERS

```

```

***** VPLUT *****

57      IMAX=0.
58      NL=10.
59      N=0
60      12 IF((LENGTH(N+1).LT. 1E-5),OR.(N.GE.LIMEXP))GO TO 15
61      N=N+1
62      IF(N.GE.2)NL=AMIN1(NL,LENGTH(1)-LENGTH(N-1))
63      IMAX=AMAX1(IMAX,INTAV(N)+SIG(N))
64      GO TO 12
65      15 NL=1./NL
66      IF((NL*(LENGTH(N)-LENGTH(1)).LE. 24.),AND. BATCH)NL=NL*2
67
68      C          NL IS NOW THE SCALE IN PRINT LINES PER ANGSTROM
69      TOTAL=NL*(LENGTH(N)-LENGTH(1))
70      IF(TOTAL.GT.200.)GO TO 115
71      POWER=1.
72      NP=0
73      20 IF(IMAX*POWER.GT.1.)GO TO 25
74      POWER=POWER*10.
75      NP=NP-1
76      GO TO 20
77      25 IF(IMAX*POWER.LE.10.)GO TO 30
78      POWER=POWER*.1
79      NP=NP+1
80      GO TO 25
81      30 IF(IMAX*POWER.LE.2)GO TO 35
82      IF(IMAX*POWER.LE.5.)GO TO 34
83      NT=10
84      GO TO 40
85      34 NT=5
86      GO TO 40
87      36 NT=2
88      C          PRINT GRAPH HEADER
89      40 PRINT 810,HEADER,INTMON,FILE
90      810 FORMAT(1H1,I246/1H ,I246//' MONITOR INTENSITY =',F6.4,' VOLTS',
91      -           8X,'FILE',I3/)
92      INCR=COL*POWER/FLOAT(NT)
93      PREV=LENGTH(1)
94      C          PRINT TOP BORDER
95      DO 42 I=1,ICOL
96      42 LINE(I)='-
97      L=ICOL/NT
98      DO 44 I=0,ICOL-L
99      44 LINE(I+1)='+'
100      PRINT 811,(LINE(J),J=1,ICOL)
101      811 FORMAT(27X,I05A1)
102      DO 46 I=1,ICOL
103      46 LINE(I)=' '
104      C          INSERT NEEDED BLANK LINS
105      C
106      DO 60 I=1,N
107      IF(SIG(I).LT. 0.0)GO TO 60
108      LINES=IFIX(NL*(LENGTH(I)-PREV)+.5)
109      PREV=LENGTH(I)
110      IF(LINES.GT.25)GO TO 50
111      48 IF(LINES.LE.1)GO TO 55
112      LINES=LINES-1
113      PRINT 812,MARK,LAST

```

```

***** VPLUT *****

114      B12 FORMAT(27X,A1,99A,A1)
115      GO TO 48
116      50 PRINT B12,(MARK, LAST, II=1,4)
117      PRINT B13,LAST
118      B13 FORMAT(25X,'//',T128,A1)
119      PRINT B12,(MARK, LAST, II=1,4)
120
121      C          PRINT ONE LINE OF GRAPH
122      55 LINE(1)=MARK
123      LINE(ICOL)=LAST
124      J1=JCOL(INTAV(I)+SIG(I))
125      J2=JCOL(AMAXI(B,INTAV(I)-SIG(I)))
126      DO 57 J=J2,J1
127      57 LINE(J)='*'
128      PRINT B15,INTAV(I),SIG(I),LENGTH(I),(LINE(J),J=1,ICOL)
129      B15 FORMAT(1X,F7.5,' +',F7.5,F9.2,10IA1)
130      DO 59 J=J2,J1
131      59 LINE(J)=' '
132      60 CONTINUE
133      C          PRINT LOWER BORDER
134      DO 62 I=1,ICOL
135      62 LINE(I)='--'
136      DO 64 I=0,ICOL+L
137      64 LINE(I+1)='+'+
138      PRINT B11,(LINE(J),J=1,ICOL)
139      DO 66 I=1,ICOL
140      66 LINE(I)=' '
141      C          PRINT HORIZONTAL SCALE
142      DO 68 I=0,NT
143      68 LINE(L+I+1)=IZERO+I*IDIF
144      IF(NT.NE.10)GO TO 69
145      LINE(ICOL)=IZFRO
146      LINE(ICOL+1)=IONE
147      69 IF(NP.EQ.0)GO TO 70
148      LINE(ICOL+1)=' '
149      LINE(ICOL+2)='E'
150      LINE(ICOL+3)=' '
151      IF(NP.LT.0)LINE(ICOL+3)='--'
152      LINE(ICOL+4)=IZERO+IADS(IP)*IDIF
153      NCOL=ICOL+4
154      PRINT B11,(LINE(J),J=1,NCOL)
155      GO TO 8
156      70 PRINT B11,(LINE(J),J=1,ICOL)
157      GO TO 8
158      C          QUIT
159      99 STOP
160      C          ERROR MESSAGES
161      115 PRINT 915, TOTAL
162      915 FORMAT(' GRAPH LENGTH OF ',F6.0,' LINES IS TOO LONG!')
163      GO TO 8
164      END

```

B-EJECT

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***** THEORY *****

```

205373-11 *WORKSPACES(1).THEORY
1   C
2   C      NAME...
3   C          THEORY
4   C
5   C      PURPOSE...
6   C          TO FIND THE VALUES OF THE PARAMETERS (LINE POSITION,
7   C          LINE INTENSITY, LINE WIDTH OR ELECTRON DENSITY, AND
8   C          BACKGROUND INTENSITY) WHICH BEST FIT THE THEORETICAL
9   C          PROFILE TO THE EXPERIMENTAL DATA.
10  C
11  C      USAGE...
12  C
13  C          Q.THEORY OR QXQT .THEORY
14  C          <DATA>
15  C          OPTIONS:
16  C          'D'  DELETE SOME POINTS
17  C          'N'  PRODUCE PLOTS NOW
18  C          'T'  PRODUCE FILES FOR PLOTS LATER
19  C                  (FEATURE UNTESTED)
20  C          'S'  SKIP SOME PROFILES
21  C          'Y'  PRINT DIAGNOSTIC INFO FOR EVERY POINT REQUESTED
22  C                  BY 'ZPOWL'
23  C          'Z'  PRINT DIAGNOSTIC INFO EVERY TIME 'ZPOWL'
24  C                  CHANGES SEARCH DIRECTION
25  C
26  C      DATA IMAGES:
27  C      CARD 1:(FREE) INPUT FILE 'NUMBER'
28  C      CARD 2:(FREE) OUTPUT FILE NUMBER, (ONLY WITH 'T' OPTION)
29  C      CARD 3:(FREE) WAVELENGTHS TO DELETE (ONLY WITH 'D' OPTION)
30  C      CARD 4:(FREE) LINE NUMBER
31  C          1    HE II 4686 (DENSITY 1.E17)
32  C          2    HE II 1640
33  C          3    HE II 1215
34  C          4    HE II 1025
35  C          5    HE II 4696 (DENSITY 1.E18)
36  C      CARD 5:(FREE) 'YES' IF FIT TO THIS PROFILE IS WANTED
37  C                  (ONLY WITH 'S' OPTION)
38  C      CARD 6,(FREE) 'YES' IF PLOT DESIRED, 'NO' IF NOT
39  C                  (ONLY WITH 'N' OPTION)
40  C                  (REPEAT CARDS 5 & 6 FOR REMAINING PROFILES AS NEEDED)
41  C
42  C      SUBPROGRAMS REQUIRED...
43  C
44  C          FETCHS OBTAINS THE NORMALIZED LINE PROFILE AND THEORETICAL
45  C          LINE POSITION FOR THE LINE.
46  C          ZPOWL (FROM IMSL) GENERAL FUNCTION MINIMIZER, USED TO
47  C          FIND THE NONLINEAR PARAMETERS WHICH MINIMIZE THE SUM
48  C          OF THE SQUARES OF THE DEVIATIONS OF THE EXPERIMENTAL
49  C          POINTS FROM THE THEORETICAL PROFILE
50  C          FUNCT3 HAS THE THEORETICAL PROFILE CALCULATED FOR THE
51  C          CURRENT PARAMETERS, AND OBTAINS THE MEAN SQUARE
52  C          DEVIATION OF THE DATA FROM THE NEW PROFILE.
53  C          FUNCT2 FINDS THE CORRELATION MATRIX OF THE BEST-FIT
54  C          PARAMETERS, USING THE SECOND PARTIAL DERIVATIVES
55  C          OF THE ERROR FUNCTION.
56  C          TPLOT PLOTS THE EXPERIMENTAL DATA AND THEORETICAL PROFILE

```

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***** THEORY *****

57 C      USING THE OFF-LINE PLOTTER.
58 C      AXISN,REGIN,FETCHS,IFAS,NEWT,NEWU,OPT,PLOTC,SIGMA,SYNSLV,
59 C      TPLOT,VALUF
60 C
61 C      METHOD...
62 C      ISSL ROUTINE 'ZXPOLJ' FINDS THE MINIMUM OF THE ERROR
63 C      FUNCTION (THE SUM OF THE SQUARES OF THE DEVIATIONS OF THE
64 C      FITTED FUNCTION FROM THE DATA POINTS) AS A FUNCTION OF
65 C      ITS TWO NON-LINEAR PARAMETERS. THE COVARIANCE MATRIX IS
66 C      COMPUTED AS THE INVERSE OF THE MATRIX OF SECOND PARTIAL
67 C      DERIVATIVES OF THE ERROR FUNCTION NEAR ITS MINIMUM.
68 C
69 C      INCLUDE DBANK,LIST
70 C      INCLUDE GROUP,LIST
71 C      COMMON /F3COM/, ARG2(2)
72 C      EXTERNAL FUNCT
73 C      REAL IAY
74 C      LOGICAL YESNO,KEEP,OUT,OPT,LATER,ALL
75 C      DIMENSION HEADER(24),H(30),ARG0(4),RAD(25)
76 C      DIMENSION LARFL(20)
77 C      INTEGER OUTFILE,OUTFMT,OUTREC,FILE,DRFC,TFIT
78 C      DATA EST,CLOSEF,CLOSER,EID,FPSNE,EPSI,OUTFMT,TFIT
79 C      - / 1.E-4, 1.E-4, 3.E-6,'0EOF ', .2, .02, 700, 503/
80 C      DATA LINEP
81 C      - / 0/
82 C      DATA (LABEL(I),I=1,10)/'HE II ','4686 ','HE II ','1640 ',
83 C      - 'HE II ','1215 ','HE II ','1025 ','HE II ','4686 '
84 C      IPCENT(00)=IFIX(100.*ABS(00)+.5)
85 C      CALL BEGIN('THEORY 1.74 ')
86 C      GET OPTIONS FROM CONTROL CARD
87 C      OUT=OPT('T')
88 C      LATER=.NOT.OPT('N')
89 C      ALL=.NOT.OPT('S')
90 C      SET UP PARAMETERS
91 C      10 IF(LINEP.NE.0)PRINT 820
92 C      DFILE=NUMBER('INPUT FILE?Q',7,29,$96)
93 C      DEFINE FILE DFILE(13,ISIZE,U,PREC)
94 C      IF(OUT)OUTFILE=NUMBER('OUTPUT FILE?P',7,29,$96)
95 C      IF(OUT)DEFINE FILE OUTFILE(13,ISIZE,U,OUTREC)
96 C      KEEP=.NOT.OPT('D')
97 C      IF(KLEP)GO TO 15
98 C      PRINT 800
99 C      800 FORMAT(' ENTER WAVELENGTHS TO DELETE')
100 C      READ(5,810,END=13)(BAD(NBAD),NBAD=1,25)
101 C      810 FORMAT()
102 C      NBAD=26
103 C      13 NBAD=BAD-1
104 C      IF(NBAD.EQ.0)KEEP=.TRUE.,
105 C      15 CALL FETCHS(ARG0,NA,LINE)
106 C      READ(DFILE'1')MF'T,HEADER
107 C      IF(NF'T.NE.TF'T)GO TO 97
108 C      IF(OUT)WRITE(OUTFILE'1')OUTFMT,HEADER
109 C      PRINT 820,HEADER
110 C      820 FORMAT(1H1,12A6/1Y,12A6)
111 C      LINEP=2
112 C      READ(DFILE'DREC)BLOCK,NSHOT,LENGTH,INTEXP
113 C

```

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***** THEORY *****

114      NARG=NA
115      DO 22 I=1,NARG
116      ARG(I)=ARGQ(I)
117      LINES(1)=LINF
118      IF(INT4DN.EQ.FND)GO TO 10
119      C          CHECK FOR ACCEPTABLE WAVELENGTH RANGE
120      IF(ARG(2)+BASE.LT.2*LENGTH(I)-LENGTH(NU))OR.
121      -     ARG(2)+BASE.GT.2*LENGTH(NU)-LENGTH(I)) GO TO 92
122      NU1=1
123      NU2=NU
124      IF(KEEP)GO TO 50
125      NU1=0
126      NU2=NU+1
127      38 NU1=NJ1+1
128      IF(NU1.GE.NU2)GO TO 49
129      DO 40 I=1,18BAD
130      IF(ABS(LENGTH(NU1)-BAD(I)).LT. .001)GO TO 38
131      40 CONTINUE
132      42 NU2=NU2-1
133      IF(NU1.GE.NU2)GO TO 49
134      DO 44 I=1,18BAD
135      IF(ABS(LENGTH(NU2)-BAD(I)).LT. .001)GO TO 45
136      44 CONTINUE
137      GO TO 42
138      45 HOLD=LENGTH(NU1)
139      LENGTH(NU1)=LENGTH(NU2)
140      LENGTH(NU2)=HOLD
141      N=MAX0(NSHOT(NU1),NSHOT(NU2))
142      DO 48 KSHOT=1,N
143      HOLD=INTEXP(NU1,KSHOT)
144      INTEXP(NU1,KSHOT)=INTEXP(NU2,KSHOT)
145      48 INTEXP(NU2,KSHOT)=HOLD
146      N=NSHOT(NU1)
147      NSHOT(NU1)=NSHOT(NU2)
148      NSHOT(NU2)=1
149      GO TO 38
150      49 NU2=NU
151      C          PRINT LABELLING INFORMATION
152      50 TOTAL=0
153      BOTTOM=LENGTH(NU1)
154      TOP=LENGTH(NU2)
155      AVG=0.
156      DO 51 KU=NU1,NU2
157      BOTTOM=A*INIT1(BOTTOM,LENGTH(KU))
158      TOP=A*AX1(TOP,LENGTH(KU))
159      N=NSHOT(KU)
160      TOTAL=TOTAL+N
161      DO 51 KSHOT=1,N
162      51 AVG=AVG+INTEXP(KU,KSHOT)
163      AVG=AVG/TOTAL
164      IF(AVG.LT.1.E-5)GO TO 95
165      LINEP=LINEP+13
166      IF(LINEP.LT.57-3)GO TO 53
167      PRINT 820,HEADER
168      LINEP=15
169      53 PRINT 830,TAPER,INTMON,TOTAL,BOTTOM,TOP
170      830 FORMAT(1X/' TIME:',F6.3,' MONITOR:',F6.4/

```

```

***** THEORY *****

171      - IX,IS,' POINTS, YAVELE,GTHS:,FP,2,' TO1,FD,2)
172      IF(ALL)GO TO 55
173      IF(YES)('FIT2',+96))GO TO 55
174      LINEP=LINEP-11 -
175      GO TO 20
176      C          CHECK THAT THE SYSTEM ISN'T DEGENERATE
177      55 I=NU2-NU1+1
178      IF(I.LE.'ARG+2)GO TO 93
179      C          SET UP FOR SOLUTION
180      NEVAL=0
181      DO 60 ITER=1,6
182      A1=ARG(1)
183      ARG2(1)=9.9
184      ARG2(2)=9.9
185      CALL NEWS(ARG,NARG)
186      LI IT=10
187      C          HAVE MINIMUM FOUND (USING ROUTINE FROM IMSL)
188      CALL ZXPOLW(FUNCT3,CLOSE,NARG,ARG,VALUE,LIMIT,H,IER)
189      IF(JPT('0'))PRINT 760,ARG(1),ARG(2),VALUE,IER
190      760 FORMAT(' RESULTS:',3G13.6,I4)
191
192      C          IF ELECTRON DENSITY CHANGED MUCH, REPEAT SOLUTION
193      IF(ABS(ARG(1)-A1).LT.,1*ARG(1))GO TO 65
194      60 CONTINUE
195      ITEP=0
196      A1=ARG(1)*1.E16
197      PRINT 838,ITEP,A1
198      838 FORMAT(' DENSITY DIDN''T CONVERGE AFTER',I4,' ITERATIONS, HAVE',
199      -           1PE11.3)
200
201      C          REPEAT WITH CLOSER TOLERANCES
202      65 ITER=ITER+1
203      CALL NEWS(ARG,NARG)
204      ARG2(1)=9.9
205      CALL ZXPOLW(FUNCT3,CLOSE,NARG,ARG,VALUE,LIMIT,H,IER)
206      IF(VALUE.LT..01*EST)GO TO 94
207
208      C          UPDATE ESTIMATE OF MINIMUM VALUE
209      EST=VALUE
210
211      C          FIND ERRORS IN CALCULATED PARAMETERS
212      CALL FUNCT2
213
214      C          PRINT RESULTS
215
216      PRINT 840,ITER,NEVAL,IER,H WIDTH,FP,VALUE
217      840 FORMAT(' ITERATION IS:',IS,' EVALUATIONS.',I7,' ERROR CODE:',I4/
218      -           ' HALF WIDTH:',F5.2,' FIELD STRENGTH:',F5.0,' SIGMA:',F9.4)
219      IT=IPCENT(SIG(1)/ARG(1))
220      PRINT 845,ARG(1),SIG(1),II,COVAR(1,1)
221      845 FORMAT(1HQ,T13,' FIRST FIT VALUES',T40,'CORRELATION MATRIX'/
222      -           ' ELECTRON JET ISITY:',1PE11.3,' +-',0PE8.3,I4,'%',T47,F6.2)
223      A=ARG(2)+BASE
224      PRINT 846,LABEL(2*INES-1),LABEL(2*INES),A,SIG(2),
225      -           COVAR(1,2),COVAR(2,2)
226      846 FORMAT(T2,2A6,'CENTER=',F9.2,' +-',F4.2,T47+2F6.2)
227      II=IPCENT(E(1)/INT(1))

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O      ***** THEORY *****
228      PRINT 847,INT(1),E(1),II,(COVAR(I,3),I=1,3)
229      847 FOR IAT(T13,'INTENSITY=',F7.4,'+-',Fo.4,Io,'%',T47,3F6.2)
230      II=IPCENT(E(1)/INT(2))
231      PRINT 848,INT(2),E(2),II,(COVAR(I,4),I=1,4)
232      848 FORMAT(' BACKGROUND INTENSITY=',F7.4,'+-',F6.4,Ib,'%',T47,
233      -        4F5.2)
234      IF(RATIO .LT. 1.E-5)GO TO 70
235      II=IPCENT(ERATIO(1)/RATIO(1))
236      PRINT 350,RATIO(1),ERATIO(1),II
237      850 FORMAT(1H0,T13,'LINE CONT=',F7.2,'+-',F6.2,I6,'A')
238      C      IF LINE IS HE II 4686, FIND & PRINT TEMPERATURE
239      IF(AUS(ARG(2)+BASE-4685.75).GT. 10.)GO TO 70
240      II=IPCENT(ETE*P/TEMP1)
241      PRINT 855,TEMP,ETEMP,II
242      855 FORMAT(T11,'TEMPERATURE=',F7.2,'+-',F6.2,I6,'%')
243      LINEP=LINEP+1
244      C      WRITE RESULTS TO FILE IF DESIRED
245      70 IF(OUT)WRITE(OUTFIL'OUTREC')BLOCK,NSHOT,LENGTH,INTEXP
246      ARG(1)=1.E-16*ARG(1)
247      C      PLOT NOW IF DESIRED
248      IF(LATER)GO TO 20
249      LINEP=LINEP+1
250      IF(.NOT.YESNO('PLOT?$',596))GO TO 20
251      CALL TPLOT(IMX,BOTTO,TOP)
252      PRINT 860,IMAX,BOTTOM,TOP
253      860 FORMAT('    AXIS LABELS:',F7.4,2F8.1)
254      LINEP=LINEP+1
255      GO TO 20
256      C      NOTIFY OF ERRORS
257      92 A=BASE+ARG(2)
258      PRINT 902,A,LENGTH(1),LENGTH(MU)
259      902 FORMAT(' LINE CENTER OF',F9.2,' TOO FAR FROM EXP RANGE',F9.2,
260      -        ' TO',F9.2)
261      GO TO 90
262      93 PRINT 903,I
263      903 FORMAT(T6,'ONLY',I2,' POINTS PRESENT')
264      GO TO 96
265      94 PRINT 904
266      904 FORMAT(' SIGMA SQUARED IS TOO SMALL')
267      A=1.E16*ARG(1)
268      S=0.
269      PRINT 840,ITER,IEVAL,IER,VALUE,A,S,S
270      A=ARG(2)+BASE
271      PRINT 845,LABEL(2*INES-1),LABEL(2*INES),A+S,INT(1),S
272      GO TO 20
273      95 PRINT 905,AVG
274      905 FORMAT(' ( SIGNALS AVERAGE ONLY',E13.6,')')
275      GO TO 20
276      96 IF(OUT .AND. OUTREC.LT.15)WRITE(OUTFIL'OUTREC')END
277      STOP
278      97 PRINT 907,NFMT,TFMT
279      907 FORMAT(' INPUT DATA FILE FORMAT IS',I7,' RATHER THAN',I4)
280      STOP
281      END

```

***** THEORY (DBANK) *****

```

205373JL*WORK$1.SCS(1).DBANK
1      DBANK PROC
2
3      C      PROCEDURE NAME...
4      C          DBANK
5
6      C      PURPOSE...
7      C          TO TRANSMIT THEORETICAL, EXPERIMENTAL, AND CALCULATED
8      C          INFORMATION PAST THE LIBRARY ROUTINE 'FMCG'
9
10     C
11     C      PROGRAMS USING THIS PROCEDURE...
12
13     C          FETCHS,FUNCT1,FUNCT2,NEWS,NEWT,NEWU,SIGMA,SUMF,THEORY,TPLOT
14
15     C
16     C      PARAMETER LIMSH=20
17     C      PARAMETER LIMEXP=36
18     C      PARAMETER LIMF=8
19     C      INTEGER TOTAL
20     C      LOGICAL OPT
21     C      REAL INTEXP,LENGTH
22     C      COMMON KS,KU,IU1,NU2,KSHOT,TOTAL,NEVAL,ITER,IER,EPSI,EPSNE,HHW,
23     C          NS1,NS2,F0,BASE,
24     C          ALPH1(LI'S),SALPH1(LI'S),ALPH2(LI'S),SALPH2(LIMS),
25     C          DEL(LI'S),TOL(LIMS),
26     C          ISHOT(LI'EXP),LEITH(LI'EXP),INTEXP(LIMEXP,LIMSH),
27     C          SUM(4,5),ERROR(4),P(20),Q(10)
28     C          EQUIVALENCE (BRIGHT,SUM(1,31)),(BACKGD,SUM(2,3))
END

```

***** THEORY (GROUP) *****

```

205373JLM*WORKSPACES(1).GROUP
1      GROUP PROC
2
3      C      PROCEDURE JAMF...
4      C          GROUP
5
6      C      PURPOSE...
7      C          TO COMMUNICATE PARAMETER ERROR ESTIMATES.
8
9      C      PROGRAMS USING THIS PROCEDURE...
10
11     C          THEORY,FUNCT2,NEWU
12
13     C
14     C      PARAMETER ISI7E=55+(2+LIMSH)*LIMEXP
15     C      COMMON/GROUP/ INTMON,TAVER,NU,W1,W2,NARG,TEMP,ETEMP,
16     C          LINES(10),
17     C          VALUE,HWIDTH,
18     C          ARG(4),SIG(4),INT(4),E(4),RATIO(3),ERATIO(3),COVAR(4,4)
19     C          DIMENSION BLOCK(55)
20     C          EQUIVALENCE (BLOCK(1),INTMON)
21     C          REAL INTMON,INT
END

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***** THEORY (FETCHS) *****

205373.W1.000K1NALL$1).FETCHS
1      C
2      C      SUBROUTINE FETCHS(ARG,NARG,LINES)
3      C      NAME...
4      C      FETCHS
5      C
6      C      PURPOSE...
7      C      TO DETERMINE WHICH LINE HAS BEEN SCANNED, READ IN THE
8      C      CORRESPONDING THEORETICAL PROFILE, AND INITIALIZE THE
9      C      NONLINEAR PARAMETERS.
10     C
11     C      CALLING SEQUENCE...
12     C
13     C      CALL FETCHS (ARG,NARG,LINES)
14     C
15     C      ARG    R=0      ARRAY OF NONLINEAR PARAMETERS
16     C                  ARG(1) IS THE ELECTRON DENSITY TIMES 1.E-16 .
17     C                  ARG(2) IS THE DISTANCE FROM THEORETICAL
18     C                  TO ACTUAL LINE CENTER.
19     C      NARG    I=0      NUMBER OF NONLINEAR PARAMETERS
20     C      LINES   I=0      LINE CODE NUMBER.
21     C                  1 HE II 4696 (DENSITY 1.E17)
22     C                  2 HE II 1640
23     C                  3 HE II 1215
24     C                  4 HE II 1025
25     C                  5 HE II 4696 (DENSITY 1.E18)
26     C
27     C      VARIABLES IN BLANK COMMON:
28     C      NARG    I=0      # NONLINEAR ARGUMENTS
29     C      NS1,NS2
30     C                  I=0      # ENTRIES IN ARRAYS ALPH1, SALPH1, AND
31     C                  ALPH2, SALPH2, RESPECTIVELY
32     C                  (PRESET POSITIONS)
33     C      HHW    R=0      HALF HALF WIDTH OF INSTRUMENT FUNCTION
34     C      BASE   R=0      THEORETICAL LINE CENTER MINUS 10 ANGSTROMS
35     C      ALPH1,SALPH1
36     C                  R=0      ARRAYS OF VALUES OF ALPHA & S(ALPHA)
37     C
38     C      INCLUDE DBANK,LIST
39     C      DIMENSION ARG(4)
40     C      INTEGER STHEO
41     C      LOGICAL OPT
42     C      DATA STHEO/29/,IFMT/600/
43     C      DEFINE FILE STHEO(10,2*LINES+2,U,NFEC)
44     C      READ(STHEO'1')NFMT
45     C      IF(NFMT.NE.IFMT)GO TO 90
46     C      NARG=2
47     C
48     C      START WITH AN ELECTRON DENSITY OF 10**17
49     C      ARG(1)=1.E-16*1.E17
50     C      LINES=NUMBER('LINE NUMBER?',1,9,$30)
51     C      READ(STHEO'LINES+1)BASE,1,ALPH1,SALPH1
52     C      NS1=N
53     C      NS2=NS1+1
54     C      ARG(2)=10.
55     C      BASE=BASE-10.
56     C      IF(BASE.LT.3000)GO TO 25
      HHW=.3

```

```
***** THEORY (FETCHS) *****  
57      IF(OPT('C'))HHW=.P001  
58      RETURN.  
59      25 BASE=BASE-.58  
60      HHW=.336  
61      IF(OPT('C'))HHW=.0001  
62      RETURN  
63      30 STOP  
64      00 PRINT 906,IFMT,IFMT  
65      906 FORMAT(' S(ALPHA) FILE FORMAT IS',I5,' RATHER THAN',I4)  
66      STOP  
67      END
```

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***** THEORY (FUNCT3) *****

205373.J1A **OKS*ACE,(1).FUNCT3
1      FUNCTION FUNCT3 (ARG)
2      C
3      C   PURPOSE...
4      C   TO FIND THE MEAN SQUARE DEVIATION OF THE DATA FROM THE
5      C   THEORY USING CURRENT PARAMETERS.
6      C
7      INCLUDE UBANK,LIST
8      INTEGER ERRRCT/0/
9      DIMENSION ARG(1)
10     LOGICAL OPT
11     COMMON/FSCOM/A(2),OLDVAL,OLDANG
12     C   NEEDN'T CALL NEWI UNLESS DENSITY CHANGED
13     IF(A(1).NE.ARG(1).OR.A(2).NE.ARG(2))
14     -   ANGLE=57.296*ATA(.2*(ARG(2)-A(2),ARG(1)-A(1))
15     IF(ABS(A(2)-10.).GT.20.)ERRRCT=ERRRCT+1
16     IF(ABS(ARG(1)-A(1)).LT.1.E-7*ARG(1))GO TO 10
17     IF(A(1).LT.1..OR.A(1).GT.100.)ERRRCT=ERRRCT+1
18     C   IF(ERRRCT.GE.8)GO TO 90
19     IF(BRIGHT.LT.-1.E-5)GO TO 90
20     CALL IENI(ARG,2)
21     A(1)=ARG(1)
22     CALL IENI(ARG,2)
23     FUNCT3=SIGMA(ARG)
24     IF(ANGLE.LE.0.)ANGLE=A'GLE+180.
25     IF(OPT('Z')).AND.ABS(ANGLE-OLDANG).GT..4)
26     -   PRINT 701,A,OLDVAL,OLDANG
27     IF(OPT('Y'))
28     -   PRINT 701,ARG(1),ARG(2),FUNCT3,ANGLE,BRIGHT,BACKGD
29     701 FORMAT(3G15.8,F5.0,1P2G9.3)
30     A(2)=ARG(2)
31     OLDVAL=FUNCT3
32     OLDANG=ANGLE
33     NEVAL=NEVAL+1
34     RETURN
35     90 PRINT 703
36     703 FORMAT(' *FUNCT3* FINDS UNREASONABLE ARGUMENTS (8TH TIME).')
37     PRINT 701,A,OLDVAL,OLDANG
38     PRINT 707,ARG(1),PASE,ARG(2),F0,BRIGHT,BACKGD
39     707 FORMAT(' NOW: NE=1.E16*',1PG9.3,' CFM=*,G0.3,*+',G13.6,' F0=',
40     -   G9.3/* BRIGHT,BACKGD='2G9.3)
41     DO 92 KU=N1,IU2
42     XX=LE,G17(KU)
43     YY=VALUE(DEL,TOEL,'IS2,XX-BASE=ARG(2),0)
44     Y2=0.
45     N=NSHOT(KU)
46     DO 91 KSHOT=1,N
47     91 Y2=Y2+INTEXP(KU,KSHOT)
48     Y2=Y2/N
49     92 PRINT 724,XX,Y2,YY
50     724 FORMAT(1PG14.6,2G10.2)
51     STOP
52     END

```

```

***** THEORY (FUNCT2) *****

205373JH@WORKSTATION(1).FUNCT2
1      SUBROUTINE FUNCT2
2
3      C   NAME...
4      C       FUNCT2
5
6      C   PURPOSE...
7      C       TO FIND THE EXPECTED ERRORS IN THE REST-FIT PARAMETERS.
8
9      C   CALLING SEQUENCE...
10     C
11     C       CALL FUNCT2
12
13     C   VARIABLES IN BLANK COMMON:
14
15     C       TOTAL  I=1      N DATA POINTS
16     C       EPSI   R=1      STEP IN WAVELENGTH
17     C       EPSNE  R=1      STEP IN ELECTRON DENSITY = ARG(1)
18     C       F0     R=0      HOLTSMARK FIELD STRENGTH
19     C       BASE   R=1      THEORETICAL LINE CENTER MINUS 10 ANGSTROMS
20
21     C   VARIABLES I=: COMMON /GROUP/
22
23     C       NARG   I=1      NUMBER OF ELEMENTS IN APC
24     C       ARG    R=1      ARRAY OF NONLINEAR PARAMETERS
25     C       VALUE   R=10     INPUT: SUM OF SQUARES OF DEVIATIONS
26     C                      FOR THE REST-FIT PARAMETERS. OUTPUT: SQUARE
27     C                      ROOT OF SUM OF SQUARES.
28     C       SIG    R=0      ARRAY OF EXPECTED ERRORS IN THE NONLINEAR
29     C                      PARAMETERS
30     C       LIN    R=0      ARRAY OF LINEAR PARAMETERS
31     C       E      R=0      ARRAY OF EXPECTED ERROPS OF LINEAR PARAMETERS
32     C       COVAR  R=0      UPPER TRIANGLE IS SET TO A NORMALIZED
33     C                      VARIANCE-COVARIANCE "ATRIX.
34     C       RATIO  R=0      LINE TO (100 ANGSTROM) CONTINUUM RATIO
35     C       ERATIO R=0      EXPECTED ERROR IN RATIO
36     C       TEMP   R=0      TEMPERATURE FROM THE LINE:CONTINUUM RATIO
37     C       ETEMP  R=0      EXPECTED EXPERIMENTAL ERROR IN TEMP
38     C       HWIDTH R=0      HALF HALF WIDTH OF EXPERIMENTAL LINE
39     C                      (ANGSTROMS)
40
41     C   METHOD...
42
43     C       THE VARIANCE-COVARIANCE MATRIX IS NORMALIZED BY DIVIDING
44     C       EACH ROW AND EACH COLUMN BY THE SQUARE ROOT OF THE ORIGINAL
45     C       DIAGONAL ELEMENT. THE CALCULATIONS OF FRATIO AND ETEMP MAKE
46     C       USE OF THE APPROXIMATELY KNOWN COVARIANCE MATRIX ELEMENTS.
47     C       THE TEMPERATURE IS FOUND USING THE THEORETICAL RESULTS OF
48     C       DELCROIX AND VOLONTE.
49
50     C   SUBPROGRAMS REQUIRED...
51
52     C       NEWT,NEWU,SUMF,SIGMA,SYMINV
53
54     C   DIMENSION ARGUM(4)
55     C   LOGICAL OPT
56     C   DIMENSION TATTLE(6)

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***** THEORY (FUNCT2) *****

57      DATA ::IGI/10.,RIGNE/10.,
58      REAL INT
59      INCLUDE JBANK,LIST
60      INCLUDE GROUP,LIST
61      C          GET THE FINAL VALUES OF THE SUM OF SQUARES & ERROR
62      C          MATRIX ELEMENTS
63      CALL NEWT(ARG,NARG)
64      CALL NEWU(ARG,NARG)
65      V1=SIGMA(ARG)
66      IF(OPT('Q'))PRINT 701,ARG(1),ARG(2),V1
67      701 FORMAT('0  ',2G13.6,' FIND',G12.6)
68      V1=FU,LT3(ARG)
69      IF(OPT('O'))PRINT 701,ARG(1),ARG(2),V1
70      MARKER=0
71      BEPSI=BIGI*EPSI
72      BEPSNE=BIGN*EPSNE
73      DO 10 I=1,NARG
74      10 ARGUM(I)=ARG(I)
75      CALL NEWT(ARGUM,NARG)
76      CALL NEWU(ARGUM,NARG)
77      CALL SUMF(ARGUM,NARG,SF,SFD,VALUE)
78      TATTLE(4)=VALUE
79      INT(1)=SUM(1,3)
80      INT(2)=SUM(2,3)
81      V=VALUE
82      ARGUM(2)=ARG(2)-BEPSI
83      S1=SIGMA(ARGUM)
84      IF(S1.LE.VALUE)MARKER=1
85      TATTLE(3)=S1
86      ARGUM(2)=ARG(2)+BEPSI
87      CALL SUMF(ARGUM,NARG,SF2,SFD2,S2)
88      IF(S2.LE.VALUE)MARKER=1
89      TATTLE(5)=S2
90      COVAR(2,2)=.5*(TOTAL-4)*(S1-2*VALUE+S2)/BEPSI**2
91      ARGUM(1)=ARG(1)+BEPSI/C
92      CALL NEWT(ARGUM,NARG)
93      S1=SIGMA(ARGUM)
94      IF(S1.LE.VALUE)MARKER=1
95      TATTLE(2)=S1
96      ARGUM(2)=ARG(2)
97      CALL SUMF(ARGUM,NARG,SF3,SFD3,S3)
98      IF(S3.LE.VALUE)MARKER=1
99      TATTLE(1)=S3
100     COVAR(1,2)=.5*(TOTAL-4)*(VALUE+S1-S2-S3)/(BEPSI*BEPSNE)
101     ARGUM(1)=ARG(1)-BEPSNE
102     CALL NEWT(ARGUM,NARG)
103     S1=SIGMA(ARGUM)
104     IF(S1.LE.VALUE)MARKER=1   ←CALL NEWT(ARG,NARG)
105     TATTLE(6)=S1
106     IF(MARKER.EQ.1)PRINT 702
107     702 FORMAT(' **** LEAST SQUARE SOLUTION NOT FOUND...NEARBY VALUES',
108             ' FOLLOW ****')
109     IF(MARKER.EQ.1 .OR. OPT('Q'))PRINT 707,TATTLE
110     707 FORMAT(1X,2G13.6/3G13.6/1X,G13.6/)
111     COVAR(1,1)=.5*(TOTAL-4)*(S1-2.*VALUE+S3)/BEPSNE**2
112     COVAR(1,3)=(SFD3-SFD)/BEPSNE
113     COVAR(1,4)=(SF3-SF)/BEPSNE

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***** THEORY (FUNCT?) *****

114      COVAR(2,3)=(SF07-SF0)/-EPSI
115      COVAR(2,4)=(SF2-SF)/3EFSI
116      C          COVAR(3,3), COVAR(3,4), AND COVAR(4,4) ARE SET BY
117      C          PROGRAM TRENUT
118      C
119      C          INVERT TO FIND THE VARIANCE-COVARIANCE MATRIX
120      DO 15 J=1,4
121      15 IF(OPT('Q'))PRINT 715,[COVAR(I,J),I=1,J]
122      715 FORMAT(1X,4G13.6)
123      CALL SYMHMV(COVAR,4,4,0,$60)
124      DO 18 J=1,4
125      18 IF(OPT('Q'))PRINT 715,[COVAR(I,J),I=1,J]
126      DO 20 J=1,4
127      20 DO 20 I=1,J
128      20 COVAR(I,J)=COVAR(I,J)*V
129      C          RESCALE ELECTRON DENSITY
130      ARG(1)=1.E16*ARG(1)
131      C          CORRECT REFERENCES TO DENSITY
132      C          DENSITY ACTUALLY VARIES LIKE (LINE WIDTH)**1.2
133      R=1.
134      IF(ABS(ARG(2)+BASF)-4685.75) .GT. 10.1 GO TO 25
135      R=(1.2/1.5)*(ARG(1)/1.E17)**(1.2/1.5-1.)
136      ARG(1)=1.E17*((ARG(1)/1.E17)**(1.2/1.5))
137      C          WE MUST RECALCULATE THE HOLTSHARK FIELD STRENGTH
138      C          WITH THE NEW DENSITY
139      F0=1.2503E-9*ARG(1)**.666666667
140      25 COVAR(1,1)=1.E32*COVAR(1,1)*R**2
141      COVAR(1,2)=1.E16*COVAR(1,2)*R
142      COVAR(1,3)=1.E16*COVAR(1,3)*R
143      COVAR(1,4)=1.E16*COVAR(1,4)*R
144      C          EXTRACT THE VARIANCES OF THE INDIVIDUAL PARAMETERS
145      SIG(1)=SIGN(SORT(ABS(COVAR(1,1))),COVAR(1,1))
146      SIG(2)=SIGN(SORT(ABS(COVAR(2,2))),COVAR(2,2))
147      E(1)= SIGN(SORT(ABS(COVAR(3,3))),COVAR(3,3))
148      E(2)= SIGN(SORT(ABS(COVAR(4,4))),COVAR(4,4))
149      C          FIND THE LINE-COMPUTUM RATIO & ERROR
150      RATIO=INT(1)/(INT(2)*100.)
151      ERATIO=RATIO*SQRT(ABS(COVAR(3,3)/INT(1)**2
152      - +COVAR(4,4)/INT(2)**2
153      - -2.*COVAR(3,4)/(INT(1)*INT(2)))
154      C          IF LINE IS HF II 4686, FIND TEPFRATURE & ERROR
155      IF(RATIO.LT..001 .OR. ABS(ARG(2)+BASF)-4685.75).GT.10.1 GO TO 30
156      TEMP=.208* ALOG(ARG(1))+.209* ALOG(RATIO(1))-5.10
157      T1=.208/ARG(1)
158      TL=.209/INT(1)
159      TC=-.09/INT(2)
160      ETTEMP=SQRT(ABS(T1*T1)*COVAR(1,1)
161      - +TL*TL*COVAR(3,3)
162      - +TC*TC*COVAR(4,4)
163      - +2.*TH*TL*COVAR(1,3)
164      - +2.*TH*TC*COVAR(1,4)
165      - +2.*TL*TC*COVAR(3,4))
166      C          NORMALIZE THE VARIANCE-COVARIANCE MATRIX
167      30 COVAR(1,2)=COVAR(1,2)/(SIG(1)*SIG(2))
168      COVAR(1,3)=COVAR(1,3)/(SIG(1)*E(1))
169      COVAR(1,4)=COVAR(1,4)/(SIG(1)*E(2))
170      COVAR(2,3)=COVAR(2,3)/(SIG(2)*E(1))

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***** THEORY (FUNCT2) *****
171      COVAR(2,4)=COVAR(2,4)/(SIG(2)*E(2))
172      COVAR(3,4)=COVAR(3,4)/(E(1)*E(2))
173      DO 40 J=1,4
174      40 COVAR(J,J)=1.
175      C      FIND HALF INTENSITY POINT OF EXPERIMENTAL PROFILE
176      HALF=TDEL(2)/2.
177      DO 45 KS=2,NS?
178      IF(TJEL(KS).LT.HALF)GO TO 49
179      45 CONTINUE
180      KS=NS2
181      48 X1=DEL(KS)
182      Y1=TJEL(KS)
183      X2=DEL(KS-1)
184      Y2=TJEL(KS-1)
185      DO 50 J=1,4
186      X=((Y2-HALF)*X1-(Y1-HALF)*X2)/(Y2-Y1)
187      X2=X1
188      Y2=Y1
189      X1=X
190      50 Y1=VALUE(DEL,TDEL,NS2,X,Q)
191      HWIDTH=((Y2-HALF)*X1-(Y1-HALF)*X2)/(Y2-Y1)
192      VALUE=SQRT(V)
193      RETURN
194      60 PRINT 908
195      908 FORMAT(' INVERSION FAILURE FINDING COVARIANCE MATRIX')
196      RETURN
197      END

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***** THEORY (TPLOT) *****

205373JULMwDRNSFACE(1),TPLOT
1      SUBROUTINE TPLOT(YMAX,BOTTOM,TOP)
2      C
3      NAME...
4      C
5      PURPOSE...
6          TO PLOT THE EXPERIMENTAL DATA AND THEORETICAL BEST-
7          FIT PROFILE.
8
9      C
10     USAGE...
11    C
12    CALL TPLOT (AMAX,BOTTOM,TOP)
13    C
14    AMAX R.O    LABEL FOR END OF Y AXIS
15    BOTTOM R.O   LABEL FOR ORIGIN OF X AXIS
16    TOP   R.O    LABEL FOR END OF X AXIS
17
18    C
19    VARIABLES IN COMMON: ALMOST EVERYTHING
20
21    C
22    SUBROUTINES USED...
23    C
24    PLOTC  STANDARD PLOT SUBROUTINE, USED TO POSITION THE PEN
25    CSCALE FINDS PLOT SCALING PARAMETERS FOR EASILY INTERPRETED
26    C
27    C
28    C
29    C
30    C
31    C
32    C
33    C
34    C
35    C
36    C
37    C
38    C
39    C
40    C
41    C
42    C
43    C
44    C
45    C
46    C
47    C
48    C
49    C
50    C
51    C
52    C
53    C
54    C
55    C
56    C

```

***** THEORY (TPLOT) *****

205373JULMwDRNSFACE(1),TPLOT

1 SUBROUTINE TPLOT(YMAX,BOTTOM,TOP)

2 C

3 NAME...

4 C

5 PURPOSE...

6 TO PLOT THE EXPERIMENTAL DATA AND THEORETICAL BEST-FIT PROFILE.

7 C

8 C

9 C

10 USAGE...

11 C

12 CALL TPLOT (AMAX,BOTTOM,TOP)

13 C

14 AMAX R.O LABEL FOR END OF Y AXIS

15 BOTTOM R.O LABEL FOR ORIGIN OF X AXIS

16 TOP R.O LABEL FOR END OF X AXIS

17 C

18 C

19 C

20 C

21 C

22 C

23 C

24 C

25 C

26 C

27 C

28 C

29 C

30 C

31 C

32 C

33 C

34 C

35 C

36 C

37 C

38 C

39 C

40 C

41 C

42 C

43 C

44 C

45 C

46 C

47 C

48 C

49 C

50 C

51 C

52 C

53 C

54 C

55 C

56 C

PLOTC STANDARD PLOT SUBROUTINE, USED TO POSITION THE PEN
NSCALE FINDS PLOT SCALING PARAMETERS FOR EASILY INTERPRETED
C
AXISN DRAWS AN AXIS
'SYMBOL' DRAWS A SYMBOL AT THE DESIRED POSITION
PAGEUP COMPLETES THE PLOT AND PREPOSITIONS THE PEN ONTO
THE NEXT PAGE

METHOD...

NOTE THAT THE AXES USED IN THIS ROUTINE ARE ROTATED 90 DEGREES CCW FROM THOSE USED BY THE SYSTEM ROUTINES. THUS, MY '+Y' DIRECTION IS THEIR '-X', AND MY '+X' IS THEIR '+Y'.

DIMENSION ARG(4),INT(4)
INCLUDE DBANK,LIST
INCLUDE GROUP,LIST
REAL L,I'T,LROUND
DATA WIDTH,HEIGHT, NY, NX
- / 8., 5.5, 5, 15/ -

BEST FIT CURVE
FIT(Z)=INT(1)*VALUE(DEL,TOEL,NS2,Z,Q)+INT(NAP6)

FIND LARGEST & SMALLEST VALUES ALONG EACH AXIS
BOTTOM=LENGTH(1)
TOP=LENGTH(NU)
YMAX=FIT(0.)
CENTER=ARG(2)+BASE
UBOUND=CENTER+10.*HWIDTH
LBOUND=CENTER-10.*HWIDTH
DO 15 KU=1,NU

DO NOT PLOT POINTS FURTHER THAN 10 MM TO EITHER SIDE
IF(LENGTH(KU).GE.LBOUND)BOTTOM=AMINI(BOTTOM,LENGTH(KU))
IF(LENGTH(KU).LE.UBOUND)TOP=AMAX1(TOP,LENGTH(KU))
N=NSHOT(KU)

```

***** THEORY (TPLOT) *****

57      DO 15 KSHOT=1,N
58      15 YMAX=AMAX1(YMAX,INTEXP(KU,KSHOT))
59      C          PLOT AT LEAST 4 MMW TO EACH SIDE
60      BOTTOM =AMIN1(BOTTOM,CENTER-4.*MMWIDTH)
61      TOP=AMAX1(TOP,CENTER+4.*MMWIDTH)
62      C
63      C          FIND SCALING PARAMETERS
64      NTICX=NX
65      CALL NSCALE(BOTTOM, TOP, NTICX, WIDTH, DX)
66      DX=1./DX
67      NTICY=NY
68      ZERO=0.
69      CALL NSCALE(ZERO, YMAX, NTICY, HEIGHT, DY)
70      DY=-1./DY
71      C
72      CALL PLOT(7.5,1.0,-3)
73      C
74      C          DRAW AXES
75      CALL AXISN(0.,0.,NTICY,HEIGHT,-.1,180.)
76      CALL AXISN(0.,0.,NTICX,WIDTH,.1,90.)
77      C
78      C          DRAW A DOTTED LINE FOR THE CONTINUUM LEVEL
79      C          (IF POSITIVE)
80      IF(INT(NARG).LT.0.)GO TO 20
81      U=DY*INT(1./NARG)
82      L=DX*(TOP-BOTTOM)
83      DL=L/69.
84      DO 18 KU=1,35
85      CALL PLOT(U,L,3)
86      CALL PLOT(U,L+DL,2)
87      18 L=L+UL+DL
88      CALL PLOT(U,L,3)
89      C
90      C          PLOT THE EXPERIMENTAL POINTS
91      20 NSYMB=4
92      DO 30 KU=1,NU
93      IF(KU.EQ.NU1)NSYMB=0
94      IF(LENGTH(KU).LT.BOTTOM .OP. LENGTH(KU).GT.TOP) GO TO 30
95      U=0.
96      N=SHOT(KU)
97      DO 25 KSHOT=1,N
98      25 U=U+II.TEXP(KU,KSHOT)
99      CALL SYMBOL(DY*U/N,DX*(LENGTH(KU)-BOTTOM),.1,NSYMB,90.,-1)
100     30 IF(KU.EQ.NU2)NSYMB=4
101     C
102     C          DRAW THE THEORETICAL CURVE
103     L=TOP
104     DL=-(TOP-BOTTOM)/250.
105     NPEN=3
106     DO 40 KU=1,251
107     U=FIT(CENTER-L)
108     CALL PLOT(DY*U/N,DX*(L-BOTTOM),NPEN)
109     NPEN=2
110     40 L=L+DL
111     CALL PAGEUP
112     RETURN
113     END

```

```

***** THEORY (AXIS) *****
205373J1M*,ORKSPACE,(1)-AXISM
1      C      SUBROUTINE AXISM (XX,YY,NTIC,ALNTH,TIC,ANGLE)
2      C
3      C      NAME...
4      C      AXIS:
5      C
6      C      PURPOSE...
7      C      TO DRAW ONE AXIS FOR A 2-DIMENSIONAL GRAPH
8      C
9      C      USAGE...
10     C
11     C      CALL AXISM (X,Y,NTIC,ALNTH,TIC,ANGLE)
12     C
13     C      X,Y    R,I    POSITION OF START OF AXIS (INCHES FROM PAPER
14     C                  ORIGIN)
15     C      NTIC   I,I    NUMBER OF LINE SEGMENTS BETWEEN TIC MARKS
16     C      ALNTH  R,I    LENGTH OF AXIS (INCHES)
17     C      TIC    R,I    LENGTH OF TIC MARKS (INCHES)
18     C
19     C      TIC.GT.0 FOR MARKS ON CLOCKWISE SIDE
20     C      TIC.LT.0 FOR MARKS ON COUNTER-CLOCKWISE SIDE
21     C
22     C      ANGLE  R,I    ANGLE OF AXIS FROM X-AXIS (DEGREES)
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
A=ALNTH/NTIC
X=XX
Y=YY
C=COS(.0174533*ANGLE)
S=SIN(.0174533*ANGLE)
AX=C*A
AY=S*A
TX=S*TIC
TY=C*TIC
CALL PLOTC(X+TX,Y+TY,3)
DO 10 I=1,NTIC
  CALL PLOTC(X,Y,2)
  X=X+AX
  Y=Y+AY
  CALL PLOTC(X,Y,2)
10  CALL PLOTC(X+TX,Y+TY,2)
  CALL PLOTC(X+TX,Y+TY,3)
  RETURN
END

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18-EJCT

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***** THEORY (NEWS) *****

205373JIMWORKSPACES(1),NEWS
1      C          SUBROUTINE NEWS(ARG,NARG)
2      C
3      C          NAME...
4      C          NFWS
5      C
6      C          PURPOSE...
7      C          TO CONVOLVE THE THEORETICAL AND THE INSTRUMENT PROFILES.
8      C
9      C          CALLING SEQUENCE...
10     C
11     C          CALL NEWS(ARG,NARG)
12     C
13     C          ARG      R,I      ARRAY OF NONLINEAR PARAMETERS
14     C          ARG(1) IS THE ELECTRON DENSITY TIMES 1.E-16 .
15     C          NARG    I,      NUMBER OF NONLINEAR PARAMETERS PRESENT
16     C
17     C          METHOD...
18     C          THE HOLTZMARK FIELD STRENGTH IS CALCULATED, AND USED TO
19     C          FIND THE AMOUNT OF BROADENING NEEDED IN (S(ALPHA),ALPHA)
20     C          SPACE. THIS IS ACCURATE IF THE FINAL ELECTRON DENSITY IS
21     C          CLOSE TO THE ORIGINAL ESTIMATE USED HERE. THE GAUSSIAN
22     C          HERMITE QUADRATURE FORMULA USED HERE IS EXACT FOR THE
23     C          INTEGRAL OF A GAUSSIAN INSTRUMENTAL PROFILE AND A FIFTH ORDER
24     C          CURVE FOR THE THEORETICAL PROFILE.
25     C
26     C          INCLUDE DBANK,LIST
27     C          DIMENSION ARG(4)
28     C          WE USE THE HOLTZMARK "NORMAL" FIELD STRENGTH
29     C          F0=2.603*2*4.8039E-10*N**{(2/3)}
30     C          F0=1.2503E-9*(1.116*ARG(1))**.6666666667
31     C          WE USE THE COORDINATE FOR THE 3 POINT GAUSSIAN
32     C          HERMITE QUADRATURE FORMULA
33     C          DELTA=(4HH/F0)*SQR((3/(2* ALOG(2))))
34     C          DELTA=1.4710685*HHH/F0
35     C          N=NS1
36     C          DO 10 KS=2,N
37     C          ALPH2(KS+1)=ALPH1(KS)
38     C          10 SALPH2(KS+1)=.1666666666*
39     C          -   (VALUE(ALPH1,SALPH1,NS1,ALPH1(KS)-DELTA,0)
40     C          -   +4.*SALPH1(KS)
41     C          -   +VALUE(ALPH1,SALPH1,NS1,ALPH1(KS)+DELTA,0))
42     C          ALPH2(1)=-ALPH2(3)
43     C          SALPH2(1)=SALPH2(3)
44     C          SALPH2(2)=.6666666666+SALPH1(1)
45     C          -   +.3333333333*VALUE(ALPH1,SALPH1,NS1,DELTA,0)
46     C          ALPH2(2)=0.
47     C          RETURN
48     C          END

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B.EJECT

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***** THEORY (NEWT) *****

205373JIM & ,ONKSCALE(1)=NEWT
1      SUBROUTINE NEWT(ARG,NARG)
2      C
3      C      NAME... .
4      C      NEWT
5      C
6      C      PURPOSE...
7      C      TO CALCULATE THE PROFILE IN WAVELENGTH SPACE, KNOWING
8      C      THE ELECTRON DENSITY AND THE PROFILE IN (S(ALPHA),ALPHA)
9      C      SPACE
10     C
11     C      CALLING SEQUENCE...
12     C
13     C      CALL NEWT (ARG,NARG)
14     C
15     C      ARG      R,I      ARRAY OF NONLINEAR ARGUMENTS
16     C                  ARG(1) IS ELECTRON DENSITY TIMES 1.E-16 .
17     C      NARG     I,I      NUMBER OF NONLINEAR ARGUMENTS
18     C
19     C      INCLUDE DBANK,LIST
20     C      DIMENSION ARG(5)
21     C
22     C      WE USE THE HOLTZMARK NORMAL FIELD STRENGTH
23     C      F0=2.603*2*4.003E-10*NE**{2/3}
24     C      IF(ARG(1).LE.0.)GO TO 90
25     C      F0=1.2503E-9*(1.E16*ARG(1))**.06006667
26     C      F0INV=1./F0
27     C      N=NS2
28     C      DO 20 KS=2,N
29     C      TDEL(KS)=T0*V*SALPH2(KS)
30     C      DEL(KS)=F0*ALPH2(KS)
31     C      TDEL(1)=TDEL(3)
32     C      DEL(1)=DEL(3)
33     C      RETURN
34     C      90 PRINT 901,ARG(1)
35     C      901 FORMAT(' NEWT: DENSITY OF',G9.3,' *1.E16 ?')
36     C      STOP
37     C      END

```

Q.EJECT

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***** THEORY (NEWU) *****

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205373w1** JRA'SPACE3(1)."t64U
1   C
2   C      NAME...
3   C          NEWU
4   C
5   C      PURPOSE...
6   C          TO SOLVE THE LINEAR PART OF THE LEAST SQUARE FIT.
7   C
8   C      USAGE...
9   C
10  C          CALL NEWU(ARG,NARG)
11  C
12  C          ARG    R,I    ARRAY OF NONLINEAR ARGUMENTS
13  C          NARG   I,I    NUMBER OF NONLINEAR ARGUMENTS
14  C
15  C          VARIABLES IN COMMON:
16  C
17  C          SUM    R,O    SUM(1,3) IS THE LINE INTENSITY
18  C          SUM(2,3) IS THE BACKGROUND INTENSITY
19  C          COVAR  R,O    COVAR(3,3), COVAR(3,4), AND COVAR(4,4) ARE
20  C          INSERTED FOR LATER USE BY PROGRAM 'FUNCT'
21  C
22  C          SUBROUTINE NEWU(ARGUM,NARGUM)
23  C          INCLUDE DBANK,LIST
24  C          INCLUDE GROUP,LIST
25  C          DIMENSION ARGUM(4)
26  C          A=ARGUM(2)+BASE
27  C          DO 15 I=1,NARGUM
28  C          DO 15 J=1,NARGUM+1
29  C          15 SUM(I,J)=0.
30  C          DO 25 K=NU1,NU2
31  C          T=VALUE(DEL,TDEL,IS2,A-LENGTH(KU),Q)
32  C          N=NSHOT(KU)
33  C          SUM(1,1)=SUM(1,1)+T*T*N
34  C          SUM(1,2)=SUM(1,2)+T*N
35  C          DO 25 KSHOT=1,N
36  C          SUM(1,3)=SUM(1,3)+INTEXP(KU,KSHOT)*T
37  C          SUM(2,3)=SUM(2,3)+INTEXP(KU,KSHOT)
38  C          25 CONTINUE
39  C          SU4(2,2)=TOTAL
40  C          SAVE ELEMENTS FOR CALCULATION OF VARIANCE-
41  C          COVARIA' CE 'ATPIX
42  C          COVAR(3,3)=SUM(1,1)
43  C          COVAR(3,4)=SUM(1,2)
44  C          COVAR(4,4)=SUM(1,2)
45  C          HAVE THIS SYMMETRIC SYSTEM SOLVED
46  C          CALL SYMSLV(SUM,SUM(1,NARGUM+1),NARGUM,4,0,$40)
47  C          RETURN
48  C          40 PRINT 908
49  C          908 FORMAT(' SINGULAR MATRIX!')
50  C          STOP
51  C          END

```

8.EJECT

```
***** THEORY (SIGMA) *****  
205373JULY4.0RKSPACES(1),SIGMA  
1      FUNCTION SIGMA(ARG)  
2      C  
3      C      PURPOSE...  
4      C          TO FIND THE MEAN SQUARE DEVIATION OF THE DATA FROM THE  
5      C          VALUES PREDICTED USING THE CURRENT PARAMETERS.  
6      C  
7      INCLUDE DBANK.LIST  
8      DIMENSION ARG(4)  
9      LOGICAL OPT  
10     SIGMA=0.  
11     A=ARG(2)+BASE  
12     DO 20 KU=1,JU1,JU2  
13     T=VALUE(DEL,TDEL,NS2,A-LENGTH(KU),0)  
14     U=SU4(1,3)*T+SUM(2,3)  
15     N=NSHOT(KU)  
16     DO 20 KSHOT=1,N  
17     SIGMA=SIGMA+(INTEXP(KU),KSHOT)-U)**2  
18     SIGMA=SIGMA/(TOTAL-4)  
19     RETURN  
20     END
```

W-EJECT

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***** THEORY (SYMSLV) *****

205373JIM@OKHSPACES(1).SYMSLV
      SUBROUTINE SYMSLV(A,B,N,NN,IT,S)
1      C
2      C      NAME...
3      C
4      C      SYMMETRIC LINEAR EQUATION SOLVER
5      C
6      C
7      C      CODE NAME...
8      C
9      C      SYMSLV
10     C
11     C      PURPOSE...
12     C
13     C      TO SOLVE A LINEAR SYSTEM AX=B WHEN THE MATRIX A IS
14     C      SYMMETRIC AND POSITIVE DEFINITE. THE ROUTINE CAN BE
15     C      CALLED SUBSEQUENTLY TO PERFORM THE SOLUTION FOR
16     C      A NEW RIGHT HAND SIDE WITHOUT DECOMPOSING AGAIN.
17     C
18     C      CALLING SEQUENCE...
19     C
20     C      CALL SYMSLV(A,B,N,NN,IT,S60)
21     C
22     C      ARGUMENTS ON ENTRY:
23     C      A      MATRIX OF COEFFICIENTS. SINCE IT IS SYMMETRIC,
24     C      ONLY ELEMENTS NEEDED ARE A(I,J), I.LE.I.LE.J.LE.N .
25     C      B      ARRAY OF ELEMENTS FROM RIGHT HAND SIDE
26     C      N      DIMENSION OF MATRIX AND B.
27     C      NN     MAXIMUM NUMBER OF ROWS IN A (FIRST DIMENSION)
28     C      IT      SWITCH...IT=1 IF MATRIX A WAS DECOMPOSED ON A
29     C      PREVIOUS CALL TO SYMSLV, AND ONLY THE ARRAY B
30     C      IS DIFFERENT THIS TIME. IT.NE.1 IF A IS NEW.
31     C      S60    CONTROL WILL BE PASSED TO THIS STATEMENT IF
32     C      A PIVOT ELEMENT IS FOUND OF ABSOLUTE VALUE
33     C      LESS THAN 1.E-10.
34     C
35     C      ARGUMENTS ON RETURN:
36     C      A      ORIGINAL MATRIX IS DESTROYED. LOWER TRIANGLE HOLDS
37     C      LOWER TRIANGLE OF MATRIX L. (DIAGONAL ELEMENTS OF L
38     C      ARE 1'S.) DIAGONAL ELEMENTS HOLD MATRIX D.
39     C      B      SOLUTION ARRAY X.
40     C
41     C      METHOD...
42     C
43     C      SYMMETRIC FACTORIZATION IS USED TO FIND A LOWER
44     C      TRIANGULAR MATRIX L AND A DIAGONAL MATRIX D SUCH
45     C      THAT A=LDU, WHERE U IS L TRANSPOSED. THE UNKNOWN
46     C      VECTOR IS CALCULATED BY BACK SOLVING THESE TRIANGULAR
47     C      SYSTEMS: UZ=B , DY=Z , LX=Y .
48     C
49     C      DIMENSION B(5),A(25) .
50     C      IF(N.GT.1)GO TO 10
51     C      B(1)=B(1)/A(1)
52     C      RETURN
53     10 IF(IT.EQ.1)GO TO 28
54     DO 25 K=1,N-1
55     IF(ABS(A(K+NN-K-N)) .LT. 1.E-10)RETURN 6
56     DO 25 J=K+1,N

```

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***** THEORY (SYNSLV) *****
57      S=A(K+NN+J-I)/A(K+NN+K-NI)
58      DO 20 I=J,N
59      20 A(J+NI,I-NN)=A(J+NI+I-1,N)-S+A(K+NI+I-JN)
60      25 A(J+NI,K-NN)=S
61      28 DO 30 J=2,N
62      30 DO 31 I=1,J-1
63      31 B(J)=B(J)-A(J+NI*I-NN)*B(I)
64      32 DO 40 J=1,N
65      40 B(J)=B(J)/A(J+NI)*J-NN)
66      41 DO 50 J=N-1,-1
67      50 DO 51 I=J+1,N
68      51 B(J)=B(J)-A(I+NI*J-NN)*B(I)
69      52 RETURN
70      END

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W-EJECT

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***** THEORY (VALUF) *****

205373JLIB0.WORKSPACE(1).VALUE
1      FUNCTION VALUE(X,Y,N,XB,P)
2      C
3      .C   NAME...
4      .C   VALUE,
5      .C
6      .C   PURPOSE...
7      .C   TO INTERPOLATE IN A TABLE TO FIND INTENSITIES FROM
8      .C   THE THEORETICAL LINE PROFILE.
9      .C
10     .C   CALLING SEQUENCE...
11     .C
12     .C   CALL VALUE(WAVE,INT,N,WANT,P)
13     .C
14     .C   WAVE  R,I   ARRAY OF WAVELENGTHS (DISPLACEMENTS FROM
15     .C           LINE CENTER)
16     .C   INT   R,I   ARRAY OF CORRESPONDING LINE INTENSITIES
17     .C   N    I,I   NUMBER OF ENTRIES IN WAVE OR INT
18     .C   WANT  R,I   WAVELENGTH AT WHICH INTENSITY IS DESIRED
19     .C   P    R,IO  WORK ARRAY OF LENGTH 4. P(1) IS USED TO STORE
20     .C           A POINTER BETWEEN CALLS, SO EACH SEARCH OF
21     .C           WAVE BEGINS WHERE THE PRECEDING SEARCH ENDED.
22     .C
23     .C   METHOD...
24     .C   BEYOND THE END OF THE TABLE, A 5/2 POWER LAW IS USED TO
25     .C   EXTRAPOLATE. WITHIN THE TABLE, AITKEN'S PROCEDURE IS
26     .C   APPLIED USING 4 POINTS. SINCE AN EVEN NUMBER OF POINTS
27     .C   IS USED, THE INTERPOLATING FUNCTION IS CONTINUOUS.
28     .C
29     .C
30     .C   DIMENSION X(N),Y(N),P(4)
31     .C   EQUIVALENCE(SAVEJ,J)
32     .C   XBAR=ABS(XB)
33     .C
34     .C   IF(XBAR.GE.X(N))GO TO 90
35     .C           RETRIEVE POINTER FROM LAST CALL
36     .C   SAVEJ=P(1)
37     .C           ENSURE J .LE. J .LE. N
38     .C   J=MAX0(MIN0(J,N)+1)
39     .C           DECIDE WHETHER TO SEARCH UP OR DOWN
40     .C   IF(XBAR-X(J)>80,20
41     .C           SEARCH DOWN
42     .C   10 IF(J.LE.1)GO TO 50
43     .C   JSTART=J
44     .C   DO 12 J=JSTART,2,-1
45     .C   IF(XBAR-X(J-1))12,75,40
46     .C   12 CONTINUE
47     .C   J=1
48     .C   GO TO 50
49     .C           SEARCH UP
50     .C   20 IF(J.GE.N)GO TO 30
51     .C   JSTART=J+1
52     .C   DO 22 J=JSTART,N+1
53     .C   IF(XBAR-X(J))40,80,22
54     .C   22 CONTINUE
55     .C   30 J=N-3
56     .C   GO TO 50

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***** THEORY (VALUE) *****

57      C      SAVE THIS POINTER
58      40 S=SAVEJ
59      C      SET J TO POINT TO FIRST OF THE 4 POINTS
60      C      IN X NEAREST XBAR
61      C      J=4INT(MAX0(J-2,1),N-3)
62      C      APPLY AITKEN'S PROCEDURE USING 4 POINTS
63      50 P(L)=Y(J)
64      C      THE GROUP OF STATEMENTS TO FOLLOW IS EQUIVALENT TO:
65      DO 60 I=2,4
66      C      P(I)=Y(J+I-1)
67      DO 60 L=2,I
68      C      P(I)=(P(L-1)*(X(J+I-1)-XBAR)-P(I)*(X(J+L-2)-XBAR))/(
69      C      - ((X(J+I-1)-XBAR)-(X(J+L-2)-XBAR)))
70      C 60 CONTINUE
71      C      ...BUT (WITHOUT LOOP CONTROL) WILL EXECUTE FASTER
72      C      P(2)=Y(J+2-1)
73      C      P(2)=(P(2-1)*(X(J+2-1)-XBAR)-P(2)*(X(J+2-2)-XBAR))/(
74      C      - ((X(J+2-1)-XBAR)-(X(J+2-2)-XBAR)))
75      C      P(3)=Y(J+3-1)
76      C      P(3)=(P(2-1)*(X(J+3-1)-XBAR)-P(3)*(X(J+2-2)-XBAR))/(
77      C      - ((X(J+3-1)-XBAR)-(X(J+2-2)-XBAR)))
78      C      P(3)=(P(3-1)*(X(J+3-1)-XBAR)-P(3)*(X(J+3-2)-XBAR))/(
79      C      - ((X(J+3-1)-XBAR)-(X(J+3-2)-XBAR)))
80      C      P(4)=Y(J+4-1)
81      C      P(4)=(P(2-1)*(X(J+4-1)-XBAR)-P(4)*(X(J+2-2)-XBAR))/(
82      C      - ((X(J+4-1)-XBAR)-(X(J+2-2)-XBAR)))
83      C      P(4)=(P(3-1)*(X(J+4-1)-XBAR)-P(4)*(X(J+3-2)-XBAR))/(
84      C      - ((X(J+4-1)-XBAR)-(X(J+3-2)-XBAR)))
85      C      P(4)=(P(4-1)*(X(J+4-1)-XBAR)-P(4)*(X(J+4-2)-XBAR))/(
86      C      - ((X(J+4-1)-XBAR)-(X(J+4-2)-XBAR)))
87      C      VALUE=P(4)
88      C      SAVF THE POINTER IN THE WORK ARRAY
89      C      P(1)=S
90      C      RETURN
91      C      XBAR APPEARS IN THE TABLE, SO WE USE THE
92      C      CORRESPONDING TABLE ENTRY
93      75 J=J-1
94      80 VALUE=Y(J)
95      C      P(1)=SAVEJ
96      C      RETURN
97      90 VALUE=Y(1)*(X(N)/XBAR)**2.5
98      C      RETURN
99      END

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B.EJECT

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