A MOSSBAUER STUDY OF LATTICE DYNAMICS IN IRON AND IRON SALTS

A Dissertation

Presented to

the Faculty of the Department of Physics

University of Houston

In Partial Fulfillment

of the Requirements for the Degree

Doctor of Philosophy

---

by

Louis Dwynn Lafleur

August 1969

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ABSTRACT

Mossbauer spectra have been measured in metallic iron, sodium nitroprusside, sodium ferrocyanide, and potassium ferrocyanide absorbers at several temperatures between 78°K and 293°K. The Mossbauer fraction f_a and resonant velocity V_o in each spectrum were determined. The observed temperature dependences of f_a and V_o in each absorber were fitted to both Einstein and Debye lattice vibration models. The characteristic temperatures of the models fitted to f_a are consistently lower than those fitted to V_o, showing the sensitivity of the Mossbauer fraction to low-frequency modes of vibration. The characteristic temperatures obtained from V_o are higher for the salts than for the metal, indicating the presence of higher-frequency modes of vibration in the salts. This interpretation is verified semi-quantitatively by comparing the thermal-shift Debye temperatures of the salts to their infrared absorption frequencies.

The Mossbauer fraction of potassium ferrocyanide shows a weaker temperature dependence than expected for a harmonic solid. This suggests that potassium ferrocyanide is anharmonic in the temperature range studied.

The magnetic field at the Fe^{57} nucleus in metallic Fe and the quadrupole splitting in sodium nitroprusside were

each measured as a function of temperature. These measurements compare well with results of previous studies.

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CHAPTER I

INTRODUCTION

In the usual Mossbauer effect experiment, one observes the emission of a gamma-ray photon by a nucleus and the subsequent absorption of the photon by another nucleus of the same isotope.[1,2] In the process the source nucleus decays from an excited state to the ground state and the absorbing nucleus undergoes the reverse transition. If the energies of the excited states in the source nuclei and in the absorbing nuclei are not identical, the difference in energy ΔE is supplied to the photon through the Doppler effect. One nucleus is moved toward or away from the other at the proper velocity V_0 to restore resonance between the photon and the absorbing nucleus. If E_0 is the transition energy of the source nucleus, then

$$\frac{V_o}{c} = \frac{\Delta E}{E_o} ,$$

where c is the speed of light. At this velocity, the transmission of the absorber is minimum. A plot of the transmission versus the velocity of the source (or absorber) is called a Mossbauer spectrum.

The source and absorbing nuclei involved are usually each bound in separate macroscopic solids. Energy con-

servation therefore requires that the nuclear transition energy E_0 involved in the emission of the photon satisfy the expression

$$E_o = E_\gamma + E_R + \Delta E_I \,;$$

where E_γ is the energy of the photon, E_R is the kinetic energy of recoil of the center of mass of the solid containing the source nucleus, and ΔE_I is the change in the internal energy of the solid induced by the emission process. If a ground state nucleus is to resonantly absorb the emitted photon, it is necessary that the photon carry essentially all the energy E_0 from the emitting nucleus. For an excited level of energy width Γ, it is necessary that

$$|E_o - E_\gamma| \lesssim \Gamma \,,$$

where typically $\Gamma \sim 10^{-12} E_0$. Thus we must have

$$|E_R + \Delta E_I| \lesssim \Gamma \,,$$

i. e., the recoil energy and change in internal energy of the solid resulting from the emission process must be smaller than the width of the excited level. Emissions which satisfy this condition are said to be "recoilless".

Compared to E_γ, the rest-mass energy of the solid is essentially infinite, so that E_R is vanishingly small and can be neglected. The existence of the Mossbauer effect

then depends on whether $|\Delta E_I|$ is smaller than Γ. In other words, resonant absorption of the photon can occur only if the photon is emitted without inducing a change in the internal energy of the solid containing the source nucleus.

The internal energy of a solid can be considered to be divided among three classes of systems in the solid: (a) the nuclear systems (NS) which involve nucleon-nucleon interactions within the individual nuclei in the solid, (b) the atomic systems (AS) involving nucleus-electron and electron-electron interactions, and (c) the lattice system (LS) which involves the inter-atomic interactions forming the solid itself. The internal energy of a solid is changed if the perturbation caused by the emission of a gamma ray results in a change in energy of one or more of these three systems.

The most probable inelastic interactions between the photon and the NS and AS are internal resonant absorption, photoelectric absorption, and Compton scattering. These interactions can be minimized by proper choices of isotopic and atomic content and/or geometric shape of the solid containing the source nuclei. Furthermore, the characteristic energies of the NS and AS are sufficiently large that when these processes cannot be reduced to a negligible level, suitable detection methods can be used to discriminate

between photons which have or have not interacted inelastically with these systems.

The lattice system, on the other hand, involves much lower characteristic energies, i.e., thermal magnitude ($\sim 10^{-2}$eV). This energy takes the form of vibrations of the centers of mass of the atoms (i.e., the nuclei) about their equilibruim sites in the lattice. The magnitude of this vibrational energy is still much greater than the widths (Γ) of the nuclear states usually involved, but is much lower than the resolution of gamma ray detection systems. Thus a gamma emission process inducing a change in the lattice energy results in a photon which can neither be resonantly absorbed nor be distinguished in the detection system from a "recoilless" photon. These photons form a major part of the background in an experiment and decrease the "signal-to-noise" ratio of the Mossbauer spectrum.

The arguments in the above discussion can also be applied to the gamma ray absorption process, so that the necessary conditions for resonant absorption are that both the emission and absorption processes occur in a "recoilless" manner. A simple expression can be derived[1] for the fraction f of photons emitted (or absorbed) by a nucleus without a change in vibrational energy of the solid in which the nucleus is bound:

$$f = \left|\langle n | e^{i\vec{k}\cdot\vec{r}} | n \rangle\right|^2 \qquad (1)$$

where $|n\rangle$ is the lattice vibrational quantum state before emission (or absorption) of the photon, $\vec{k}$ is the wave vector of the photon, and $\vec{r}$ is the position of the nucleus. In the harmonic approximation, the interatomic force on each atom in a solid is assumed to be linearly dependent on the displacement of all atoms from their equilibrum sites. This is expressed as

$$F_{ij} = \sum_{k=1}^{3} \sum_{\ell=1}^{N} K_{ijk\ell}\, r_{k\ell} \ , \qquad (2)$$

where F_{ij} is the i^{th} Cartesian component of force on the j^{th} atom, K_{ijkl} is a "spring constant", r_{kl} is the k^{th} component of displacement of the l^{th} atom, and N is the number of atoms in the solid. In this case, equation (1) becomes[1,3]

$$f = e^{-k^2\langle x^2\rangle} \qquad (3)$$

where $\langle x^2 \rangle$, usually referred to as the <u>mean-square displacement</u>, is the expectation value of the square of the displacement of the Mossbauer nucleus along the direction of $\vec{k}$. An experimental determination of the Mossbauer fraction f is therefore a measure of the amplitude of the thermal

vibration of the atom containing the Mossbauer nucleus.

In addition to determining the intensity of the Mossbauer effect, the lattice dynamical motion of the Mossbauer nucleus also causes an apparent shift in the resonant energy of the nuclear transition. If thermal vibration results in an expectation value $\langle v^2 \rangle$ for the square of the velocity of the Mossbauer nucleus in the laboratory frame, the apparent resonant energy E of the nuclear transition in the laboratory frame is

$$E = E_o\left(1 - \frac{\langle v^2 \rangle}{2c^2}\right) \tag{4}$$

where E_o is the energy in the rest frame of the nucleus.[2] This follows from the relativistic expression for the Doppler effect. Because of the additional change in resonant energy due to the isomer shift*, the above expression cannot be used alone to determine $\langle v^2 \rangle$, the <u>mean-square velocity</u>. However, if the isomer shift is essentially temperature independent, a study of the variation of E with temperature, the <u>thermal shift</u>, can yield information concerning the temperature dependence of the vibrational

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*The isomer shift[1,2] is the difference in resonant energies in a source nucleus and an absorbing nucleus due to differing electrostatic interactions between the atomic electrons and the finite-sized nuclei. This occurs when the atomic electron densities at the source and absorbing nuclei are different.

velocity of the Mossbauer nucleus. It should be emphasized that the quantity $\langle x^2 \rangle$ in equation (3) is the mean-square of the component of displacement along the direction of the gamma ray, while $\langle v^2 \rangle$ in equation (4) is the sum of the mean-squares of the three components of velocity,

$$\langle v^2 \rangle = \langle v_x^2 \rangle + \langle v_y^2 \rangle + \langle v_z^2 \rangle \quad .$$

The measure of the Mossbauer fraction and thermal shift in the Mossbauer effect can be used in many cases to study thermal vibrations of dilute impurity atoms in a solid as well as atoms which are a major constituent of a solid. In a Mossbauer experiment, the source consists of the parent isotope of the Mossbauer nucleus implanted in a solid. The choice of the host material for the source nuclei depends on the desired source properties; i. e., large Mossbauer fraction, narrow emission line, etc. Quite often the host material does not contain the same element as the Mossbauer isotope studied. A typical source might consist of $\sim 10^{16}$ Mossbauer nuclei per cubic centimeter, so that the Mossbauer fraction f and thermal shift of the source will often be determined by the thermal vibration characteristics of a dilute impurity rather than by the lattice dynamics of a pure solid.

On the other hand, when gamma ray photons from the

source are in resonance with nuclei in the absorber solid, it is necessary that the resonant absorption be at least comparable to other absorption processes if the Mossbauer effect is to be observable. This requires that an appreciable fraction of the atoms in the solid contain ground-state nuclei of the source isotope, which is most easily accomplished by choosing an absorbing material in which the source element is a basic part of the chemical or metallurgical structure. In such a case, the Mossbauer fraction and thermal shift in the absorber depend on the lattice dynamical motion of an atom which is a major constituent rather than an impurity.

Several investigators have used f measurements and thermal shift measurements to study thermal lattice vibrations of Mossbauer nuclei in solids. Because the 14.4-keV gamma ray transition of Fe^{57} exhibits a strong Mossbauer effect in many materials even at room temperature, most studies have used this isotope. Of course, the relation between lattice dynamics and the Mossbauer effect discussed above apply equally to all isotopes exhibiting the effect.

The parent isotope of Fe^{57} is Co^{57}, which decays through electron capture and gamma decay[4] to the 14.4-keV excited state of Fe^{57}. Fe^{57} has a natural isotopic abundance of 2.19% in iron and a resonant photon absorption

cross section of 2.38 X 10^{-18} cm^2.[4] These two values are large enough so that an iron mineral, alloy, or compound containing an appeciable amount of natural iron can usually be used as a Mossbauer absorber without the necessity of isotopic enrichment of Fe^{57}. Therefore, studies of Co^{57} Mossbauer sources can yield information about the lattice dynamics of a dilute iron impurity in a solid; whereas studies of iron-containing solid absorbers yield information about the dynamics of a lattice in which the iron atom is a major constituent.

For example, Steyert and Taylor[5] studied sources consisting of Co^{57} diffused into several elemental metal lattices. They were able to fit f measurements with Debye models for the lattice except at high temperatures ($\gtrsim$ 600°K) where diffusion and anharmonicity were significant. Thermal shift measurements were also fit with Debye models and showed consistently lower Debye temperatures than those obtained from the f measurements. Better agreement was obtained when the f measurements and thermal shift were each fit to Einstein models, indicating perhaps the presence of a localized mode of vibration of the Fe^{57} source nucleus.

Housley and Nussbaum[6] used a single crystal of zinc as a host material for the Co^{57} and showed from f measurements that $\langle x^2 \rangle$ for the Fe^{57} impurity is at least twice as

large along the crystalline c-axis as it is perpendicular to the axis. This agrees with theoretical calculations based on measured phonon dispersion curves of zinc.

Very few f measurements in absorbers have been fit to lattice dynamical models. Herber and Wertheim[7] have measured relative f values in powdered ferrocene absorbers at temperatures from 20°K to 295°K. The results are interpreted as indicating contributions to f from both optical and acoustic modes of vibration, but no fits to models are given. Kerler[8] measured f values in metallic iron and several iron compounds at temperatures from 153°K to 353°K. Within the accuracy of his data, all temperature dependences were linear, indicating a temperature range near the classical Dulong-Petit limit. Debye temperatures were calculated for the iron metal and the salts.

Preston et al.[9] studied the Mossbauer spectrum of metallic iron absorbers from 4°K to 1300°K. Measurements of the thermal shift were fit to a Debye model in the low-temperature region. At high temperatures, there was a definite deviation from the classical Dulong-Petit limit which they interpreted as a temperature dependent isomer shift. (Their thermal shift data have recently been re-examined by Housley and Hess[10].)

More recently, Johnson and Dash[11] measured f values and

thermal shifts in powdered absorbers of anhydrous ferrous chloride at temperatures between 10°K and 300°K. By applying a general harmonic model[12] to the thermal shift data, they were able to calculate the average component of the force constant on an iron ion due to its own displacement. Both the f measurements and thermal shift measurements were fit to Einstein models at high temperatures. The experimental f values at low temperatures were larger than predicted by the Einstein fit, leading the authors to postulate a low-temperature anharmonicity.

The present paper describes measurements of the Mossbauer fraction and thermal shift in the spectra of three powdered absorbers (sodium nitroprusside, sodium ferrocyanide, and potassium ferrocyanide) and a metallic iron absorber over the temperature range 78°K to 293°K. A comparison to the predictions of a general harmonic theory[12] is made, and the data are fit numerically to simple lattice models (Einstein and Debye models).

Several factors were considered in the choice of absorbers for this study. Mossbauer spectra of the iron salts have been measured previously, showing them to be quite efficient Mossbauer absorbers even with natural isotopic abundance of Fe^{57}. It is believed, however, that no detailed Mossbauer study of the lattice dynamics of the

salts exists. Furthermore, infrared absorption spectra of these salts in powdered form have been measured in the frequency range 300-4000 cm^{-1} for sodium ferrocyanide and potassium ferrocyanide and 300-880 cm^{-1} for sodium nitroprusside.[13,14] These spectra show absorption lines which are interpreted[15] as due to interatomic vibrations involving the iron ions in the solid. It seems desirable to compare the temperature dependence of the Mossbauer fraction and resonant energy in these salts displaying optical modes of vibration to that in metallic iron which has no optical modes.

CHAPTER II

THEORY

A. Expressions for $\langle x^2 \rangle$ and $\langle v^2 \rangle$ in Harmonic Lattice Models

As seen in equations (3) and (4) of the preceding chapter, the variation with temperature of the Mossbauer fraction and resonant energy of a source or absorber depends on the thermal behavior of $\langle x^2 \rangle$ and $\langle v^2 \rangle$ of the Mossbauer nucleus. Using models for the interatomic forces, it is possible to derive expressions for $\langle x^2 \rangle$ and $\langle v^2 \rangle$ for a nucleus in a solid. Three such models are discussed here: (a) the Einstein model, (b) the Debye model, and (c) the general harmonic model. The Einstein and Debye models are special cases of the harmonic approximation, so equation (3) holds for all three models.

1. The Einstein Model

In the Einstein model, the Mossbauer nucleus is assumed to vibrate about its equilibrium position in the lattice as an isotropic three-dimensional harmonic oscillator with mass m and angular frequency ω_E. For each of the three Cartesian coordinates of such an oscillator, the quantum mechanical energy of vibration in the n^{th} level is

$$E_n = (n + \tfrac{1}{2})\hbar\omega_E \,,$$

where $\hbar$ is Planck's constant divided by 2π. When a collection of such oscillators is in thermal equilibrium at temperature T, the average energy of each oscillator is[16]

$$\langle E\rangle_T = \left(\frac{1}{2} + \frac{1}{e^{\hbar\omega_E/k_BT} - 1}\right)\hbar\omega_E , \tag{5}$$

where k_B is the Boltzmann constant. One property of the harmonic oscillator is that the energy is shared equally between the potential energy and the kinetic energy. Thus, the square of the x-component of displacement satisfies the relation

$$\tfrac{1}{2}\, m\,\omega_E^2\langle x^2\rangle = \tfrac{1}{2}\langle E\rangle_T ,$$

which, when combined with equation (5), yields

$$\langle x^2\rangle = \frac{\hbar}{m\omega_E}\left(\frac{1}{2} + \frac{1}{e^{\hbar\omega_E/k_BT} - 1}\right) . \tag{6}$$

Similarly, the square of the <u>total</u> velocity satisfies the relation

$$\tfrac{1}{2}\, m\langle v^2\rangle = 3\left(\tfrac{1}{2}\langle E\rangle_T\right).$$

We then have

$$\langle v^2\rangle_T = \frac{3\hbar\omega_E}{m}\left(\frac{1}{2} + \frac{1}{e^{\hbar\omega_E/k_BT} - 1}\right). \tag{7}$$

It is convenient to define the <u>Einstein temperature</u> Θ_E for the solid, where

$$k_B \theta_E \equiv \hbar \omega_E .$$

With this definition, equation (6) and (7) take the form

$$\langle x^2 \rangle = \frac{\hbar^2}{m k_B \theta_E} \left(\frac{1}{2} + \frac{1}{e^{\theta_E/T} - 1} \right), \tag{8}$$

and

$$\langle v^2 \rangle_T = \frac{3 k_B \theta_E}{m} \left(\frac{1}{2} + \frac{1}{e^{\theta_E/T} - 1} \right). \tag{9}$$

2. The Debye Model

In the Debye model, the motion of each nucleus is assumed to be due to a number of isotropic harmonic oscillators rather than an oscillator of a single frequency as in the Einstein model. These oscillators are the normal modes of the solid which, in this approximation, is assumed to be an isotropic elastic continuum. Since the solid actually consists of N atoms, the total number of oscillators is 3N, one for each degree of freedom. The frequency distribution of these 3N oscillators is usually given in terms of a spectral distribution function $g(\omega)$, such that $g(\omega)d\omega$ is the number of oscillators with angular frequencies between ω and $\omega + d\omega$. In the Debye approximation, $g(\omega)$ is that appropriate for an isotropic elastic

continuum, which can be shown[16] to have the property

$$g(\omega) \propto \omega^2 \tag{10}$$

In addition, $g(\omega)$ must satisfy the requirement

$$\int_0^\infty g(\omega)\, d\omega = 3N . \tag{11}$$

This is done by defining a maximum frequency ω_D for the oscillators. Thus, $g(\omega)$ can be made to satisfy equations (10) and (11) if we choose

$$g(\omega) \equiv \begin{cases} 9N\omega^2/\omega_D^3 & [\omega \leq \omega_D] \\ 0 & [\omega > \omega_D] \end{cases} \tag{12}$$

All the oscillators with frequencies between ω and $\omega + d\omega$ contribute to $\langle x^2 \rangle$, $\langle y^2 \rangle$, and $\langle z^2 \rangle$ for all N nuclei. The amount $d\langle x^2 \rangle$ contributed to a single nucleus is therefore

$$d\langle x^2 \rangle_T = \frac{1}{3N}\left[g(\omega)\, d\omega\right]\left[\frac{\hbar}{m\omega}\left(\frac{1}{2} + \frac{1}{e^{\hbar\omega/k_B T} - 1}\right)\right] ,$$

where equation (6) gives the contribution for each oscillator. The total $\langle x^2 \rangle$ for a single nucleus is found by integrating the above expression over all possible frequencies:

$$\langle x^2 \rangle_T = \int_0^\infty \frac{g(\omega)}{3N}\left[\frac{\hbar}{m\omega}\left(\frac{1}{2} + \frac{1}{e^{\hbar\omega/k_B T} - 1}\right)\right] d\omega .$$

When equation (12) is substituted into the above, one obtains

$$\langle x^2 \rangle_T = \frac{3\hbar}{4m\omega_D}\left(1 + \frac{4}{\omega_D^2}\int_0^{\omega_D} \frac{\omega\, d\omega}{e^{\hbar\omega/k_BT} - 1}\right). \tag{13}$$

In a similar manner, one obtains $\langle v^2 \rangle$ for a nucleus:

$$\langle v^2 \rangle_T = \frac{9\hbar\omega_D}{8m}\left(1 + \frac{8}{\omega_D^4}\int_0^{\omega_D} \frac{\omega^3\, d\omega}{e^{\hbar\omega/k_BT} - 1}\right). \tag{14}$$

When the Debye temperature θ_D is defined by the relation

$$k_B\theta_D \equiv \hbar\omega_D ,$$

equations (13) and (14) take the form

$$\langle x^2 \rangle_T = \frac{3\hbar^2}{4mk_B\theta_D}\left(1 + \frac{4T^2}{\theta_D^2}\int_0^{\theta_D/T} \frac{u\, du}{e^u - 1}\right), \tag{15}$$

and

$$\langle v^2 \rangle_T = \frac{9k_B\theta_D}{8m}\left(1 + \frac{8T^4}{\theta_D^4}\int_0^{\theta_D/T} \frac{u^3 du}{e^u - 1}\right). \tag{16}$$

3. The General Harmonic Model

Housley and Hess[12] have recently derived expressions for $\langle x^2 \rangle$ and $\langle v^2 \rangle$ for a nucleus in a general harmonic lattice.

The results of their work are presented here with some discussion.

In the general harmonic lattice, the solid is treated as a collection of interacting point masses of arbitrary configuration. No periodicity in the lattice is required; the solid is essentially considered to be a large, arbitrarily complex molecule. The only simplifying assumption is that the interatomic forces are of the form shown in equation (2).

In this model, $\langle x^2 \rangle$ for the j^{th} nucleus is

$$\langle x_j^2 \rangle_T = \frac{\hbar}{m_j} \sum_{i=1}^{3N} \left(\frac{1}{2} + \frac{1}{e^{\hbar\omega_i/k_B T} - 1} \right) \frac{b_{jxi}^2}{\omega_i} \quad , \tag{17}$$

where ω_i is the angular frequency of the i^{th} normal mode of the lattice. The constants b_{jxi} are elements of the matrix transforming the normal coordinates of the lattice to the Cartesian coordinates (x_j, y_j, z_j) of the nuclei. These have the properties

$$\sum_{j=1}^{N} \left(b_{jxi}^2 + b_{jyi}^2 + b_{jzi}^2 \right) = 1 \quad ,$$

and

$$\sum_{i=1}^{3N} b_{jxi}^2 = \sum_{i=1}^{3N} b_{jyi}^2 = \sum_{i=1}^{3N} b_{jzi}^2 = 1 \, .$$

The mean-square velocity is

$$\langle v^2 \rangle_T = \frac{\hbar}{m_j} \sum_{i=1}^{3N} \left(\frac{1}{2} + \frac{1}{e^{\hbar\omega_i / k_B T} - 1} \right) \left(b_{jxi}^2 + b_{jyi}^2 + b_{jzi}^2 \right) \omega_i . \quad (18)$$

Since this model is rather general, it should describe well the temperature dependence of $\langle x^2 \rangle$ and $\langle v^2 \rangle$ for most solids, as long as they are not at such high temperatures that anharmonic effects become important. Thus, the mathematical behavior of equations (17) and (18) are of interest. Some of their properties are:

(a) At T=0, $\langle x^2 \rangle$ and $\langle v^2 \rangle$ are at minimum, non-zero values. They both increase as T increases.

(b) The slope of $\langle x^2 \rangle$ and $\langle v^2 \rangle$ versus T is zero at T=0. As T increases, the slope increases and is always positive.

(c) As T becomes very large (i.e., $k_B T \gg \hbar\omega_{max}$, where ω_{max} is the largest value of ω_i), the curves of $\langle x^2 \rangle$ and $\langle v^2 \rangle$ versus T each approach straight-line asymptotes which go through the origin; i.e.,

$$\langle x^2 \rangle_T \xrightarrow[T \to \infty]{} \xi T ,$$

and

$$\langle v^2 \rangle_T \xrightarrow[T \to \infty]{} \eta T ,$$

where ξ and η are constants. This is in agreement with the classical principle of equipartition of energy. Notice in particular that

$$\langle v^2 \rangle_T \xrightarrow[T \to \infty]{} \frac{3k_B T}{m}$$

so that at high temperatures, $\langle v^2 \rangle$ does not depend on the properties of the lattice.

The above conclusions apply equally to the Einstein and Debye models since they are special cases of the general harmonic model.

B. Relation of $\langle x^2 \rangle$ and $\langle v^2 \rangle$ to the Observed Mossbauer Spectrum.

In the following discussion, it is assumed that the Mossbauer spectrum of a source-absorber combination is measured by recording the gamma-ray intensity transmitted by the absorber as a function of source velocity. The source, absorber, and detector are assumed to be in a co-linear geometry such that all radiation going from the source to the detector must travel through the absorber. The spectrum obtained is represented as N(V), where N is the detector counting rate and V is the source velocity (conventionally chosen to be positive when the source is moving toward the absorber).

It is desirable to find the relation between N(V) and

the Mossbauer fraction f_a of the absorber so that the lattice dynamical information contained in equation (3) can be extracted from the spectrum and models can be fit to that information. To do so, we apply a treatment based on works by Lang[17] and Housley et al.[18]

Let us assume the source emits I_0 photons per second from the Mossbauer transition into the solid angle subtended by the detector. These photons have an energy spectrum J(E) such that J(E)dE is the number with energy between E and E+dE. Thus,

$$I_o = \int_o^\infty J(E)\,dE .$$

The spectrum J(E) consists of two parts: (a) the "recoilless" radiation $J_M(E)$, which has a peak intensity at some energy E_0 and an energy width Γ ($\sim 10^{-12}E_0$), and (b) the "recoil" radiation $J_M(E)$ which has a peak intensity very much lower than $J_M(E)$, but is spread over an energy band of thermal magnitude.[19] Thus,

$$J(E) = J_M(E) + J_R(E),$$

and

$$I_o = \int_o^\infty \left[J_M(E) + J_R(E)\right]dE. \qquad (19)$$

The absorber attenuates this beam by nuclear resonant absorption and by atomic (photoelectric, etc.) absorption, the former acting only on $J_M(E)$ for all practical purposes. We denote the energy-dependent cross-sections for these processes as $\sigma_M(E)$ and $\sigma_A(E)$ respectively. Here, σ_A is averaged over all atoms in the absorber. The Mossbauer absorption cross-section $\sigma_M(E)$ is essentially zero for all energies except for a width Γ about the nuclear resonant energy in the absorber.

Finally, the detector window is represented by a function D(E) which is nearly unity for photon energies near the Mossbauer transtion energy and zero elsewhere.

The detector will then show a net counting rate

$$N = N_B + \int_0^\infty \left\{ J_M(E) e^{-[n_M \sigma_M(E) + n\sigma_A(E)]} + J_R(E)\, e^{-n\sigma_A(E)} \right\} D(E)\, dE \,. \quad (20)$$

Here, n_M is the area density of Mossbauer nuclei in the absorber, n is the area density of atoms in the absorber, and N_B is the background counting rate due to all radiation other than the Mossbauer transition of interest.

Equation (20) can be simplified by observing that in the extremely narrow energy range where J_M and J_R are non-zero, $\sigma_A(E)$ and D(E) are essentially constant and equal to $\sigma_A(E_0)$ and $D(E_0)$ respectively, so that

$$N = N_B + D(E_o)e^{-n\sigma_A(E_o)} \int_o^\infty [J_M(E)e^{-n_M\sigma_M(E)} + J_R(E)]\, dE. \qquad (21)$$

If the source moves with velocity V, a photon of energy E in the rest frame of the source has energy

$$E' = E + \frac{VE}{c}$$

in the rest frame of the absorber. Equation (21) then becomes

$$N(V) = N_B + D(E_o)e^{-n\sigma_A(E_o)} \int_o^\infty [J_M(E)\, e^{-n_M\sigma_M(E+VE/c)} + J_R(E)]\, dE, \qquad (22)$$

which is the expression for the Mossbauer spectrum. At a sufficiently large velocity, resonance is completely destroyed; i.e., E' and E are so different that either $J_M(E)$ or $\sigma_M(E+VE/c)$ is zero at all values of E. At such a velocity, the counting rate $N(\infty)$ is given by

$$N(\infty) = N_B + D(E_o)\, e^{-n\sigma_A(E_o)} \int_o^\infty [J_M(E) + J_R(E)]\, dE. \qquad (23)$$

It is convenient at this point to define the normalized, background-corrected absorption curve $\epsilon(V)$ as

$$\epsilon(V) \equiv \frac{N(\infty) - N(V)}{N(\infty) - N_B}, \qquad (24)$$

which is maximum when the absorption is maximum. Equations (19), (22), (23), and (24) yield

$$\epsilon(V)=\frac{1}{I_o}\int_o^\infty J_M(E)\left[1-e^{-n_M\sigma_M(E+VE/c)}\right]dE. \qquad (25)$$

If the sub-levels of the excited and ground states of the absorbing nuclei are not split by internal fields[2] in the absorber, the absorption cross-section $\sigma_M(E)$ can be represented by a Lorentzian function

$$\sigma_M(E)=\frac{f_a\,\sigma_o}{1+4(E-E_a)^2/\Gamma^2}\,, \qquad (26)$$

where f_a is the Mossbauer fraction of the absorber and E_a is the resonant energy in the absorber. The quantity σ_o is the resonance cross-section of a nucleus fixed rigidly in space, and is given by

$$\sigma_o=\frac{2\pi}{k^2}\times\frac{1+2I_e}{1+2I_g}\times\frac{1}{1+\alpha_T}$$

where I_e and I_g are the spin of the excited and ground states respectively, and α_T is the total internal conversion coeffecient. Similarly, the recoilless emission spectrum of a single-line source can be represented by

$$J_M(E)=\frac{2}{\pi\Gamma}\cdot\frac{f_s\,I_o}{1+4(E-E_o)^2/\Gamma^2}\,. \qquad (27)$$

It can be shown[20,21] that when equations (26) and (27) are substituted into equation (25), the resulting curve $\epsilon(V)$ can be represented to within about 0.5% by a Lorentzian function

$$\epsilon(V) \approx \frac{\alpha}{1+4(V-V_o)^2/W^2} , \qquad (28)$$

where

$$\alpha \equiv f_s \left[1 - e^{-t/2} J_o(\tfrac{1}{2} i t)\right]$$

is the fractional absorption at resonance, and

$$V_o \equiv \left(\frac{E_a - E_o}{E_o}\right) c .$$

In the above, J_0 is the zero-order Bessel function and $t \equiv n_M \sigma_o f_a$. The apparent width W of the absorption line is given by[21]

$$W = \begin{cases} 2\Gamma(1.00 + 0.135\,t) & [0 \leq t \leq 5] , \\ 2\Gamma(1.01 + 0.145\,t - 0.0025\,t^2) & [4 \leq t \leq 10] . \end{cases}$$

Recently, Heberle[22] has shown that equation (28) is accurate to better than 0.15% for $0 \leq t \leq 12$ if W is defined by

$$W = 2\Gamma(1 + 0.1288\,t + 4.733\times10^{-3}t^2 - 9.21\times10^{-4}t^3 + 3.63\times10^{-5}t^4) .$$

The area A under the absorption curve $\epsilon(V)$ from equation (25) is

$$A = \int_{-\infty}^{\infty} \epsilon(V)\,dV = \frac{1}{I_o} \int_{E=0}^{\infty} \int_{V=-\infty}^{\infty} J_M(E) \left[1 - e^{-n_M \sigma_M (E + VE/c)} \right] dV\, dE \,,$$

which can be written

$$A = \frac{c}{I_o} \left\{ \int_0^{\infty} \frac{J_M(E)\,dE}{E} \right\} \cdot \left\{ \int_{-\infty}^{\infty} \left[1 - e^{-n_M \sigma_M (E')} \right] dE' \right\} \,.$$

In the first integral, E^{-1} varies slowly over the small range where $J_M(E) \neq 0$, so that it can be replaced by E_0^{-1}. We then obtain

$$A = \frac{c}{I_o E_o} \left\{ \int_0^{\infty} J_M(E)\,dE \right\} \cdot \left\{ \int_{-\infty}^{\infty} \left[1 - e^{-n_M \sigma_M (E')} \right] dE' \right\} .$$

The first integral is recognized as the total recoilless radiation from the source. But the Mossbauer fraction f_s of the source is defined as the ratio of the recoilless radiation to the total radiation I_0 from the transition. Therefore,

$$A = \frac{c f_s}{E_o} \int_{-\infty}^{\infty} \left[1 - e^{-n_M \sigma_M (E)} \right] dE \qquad (29)$$

This expression is independent of the spectrum of the recoilless radiation from the source. If equation (26)

is substituted into the above, we have

$$A = \frac{f_s}{2} \frac{c\Gamma}{E_o} \int_{-\infty}^{\infty} \left[1 - e^{-\frac{t}{1+u^2}}\right] du ,$$

where t is defined as before. This can be expanded and integrated term-by-term to give[17]

$$A = \frac{\pi}{2} \frac{f_s \Gamma_c}{E_o} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n!} \frac{(2n-3)!!}{(2n-2)!!} t^n , \qquad (30)$$

which converges for all values of t.

If internal fields in the absorber split the nuclear levels, producing ν Mossbauer absorption lines in the spectrum, then each absorption transition has a cross-section similar to equation (26). The i^{th} transition cross-section is given by

$$\sigma_i(E) = \frac{f_a \sigma_{io}}{1 + 4(E-E_i)^2/\Gamma^2} \qquad (31)$$

where E_i is the resonant energy of the i^{th} transition. In such a case, we must have

$$\sum_{i=1}^{\nu} \sigma_{io} = \sigma_o = \frac{2\pi}{k^2} \times \frac{1 + 2I_e}{1 + 2I_g} \times \frac{1}{1+\alpha_T} . \qquad (32)$$

The area of the i^{th} line becomes

$$A_i = \frac{\pi}{2} \frac{f_s \Gamma_c}{E_o} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n!} \frac{(2n-3)!!}{(2n-2)!!} t_i^n \quad , \tag{33}$$

where $t_i \equiv n_M \sigma_{io} f_a$. Thus, when the area A_i of an absorption line is measured, t_i can be found by solving equation (33) graphically, assuming f_s is known from other measurements. Once t_i is found for each line, we can evaluate the total effective thickness t by summing over all lines and using equation (32):

$$t = \sum_{i=1}^{\nu} t_i = n_M f_a \sum_{i=1}^{\nu} \sigma_{io} = n_M f_a \sigma_o \quad .$$

If σ_o and n_M are known, f_a can be calculated. Even if σ_o and n_M are unknown, however, we know that

$$f_a = e^{-k^2 \langle x^2 \rangle}$$

so that

$$\ell n\ t = \tau - k^2 \langle x^2 \rangle \quad . \tag{34}$$

Thus, the quantity ln t obtained from the area of the absorption curve $\in (V)$ is equal to $-k^2 \langle x^2 \rangle$ to within an additive constant $\tau = \ln(n_M \sigma_o)$. Furthermore, the constant is independent of temperature, so that a change in $\langle x^2 \rangle$

with temperature is reflected directly by a change in ln t.

The relation between $\langle v^2 \rangle_T$ and the Mossbauer spectrum is rather obvious from equation (28). We see that the absorption is maximum when

$$V = V_o = \left(\frac{E_a - E_o}{E_o} \right) c \quad . \tag{35}$$

As stated previously, the isomer shift contributes partially to the difference $(E_a - E_o)$. Defining the isomer shift energy as $\Delta E(I.S.)$, we have from equations (35) and (4)

$$V_o = \left(\frac{\Delta E(I.S.) - E_o \langle v^2 \rangle_T / 2c^2}{E_o} \right) c$$

or,

$$V_o = \delta_o - \frac{\langle v^2 \rangle_T}{2c} \tag{36}$$

where

$$\delta_o \equiv \frac{\Delta E(I.S.)}{E_o} c \quad .$$

If δ_o is constant over the temperature range studied, as usually is the case in the absence of phase changes[23], an increase in $\langle v^2 \rangle$ with T causes a direct decrease in the source velocity at resonance.

Equations (34) and (36) can be used directly with the lattice models discussed in the previous section. Specifically, equations (8), (9), (15), and (16), when substituted into (34) and (36), yield

$$\ln t(T) = \tau - \frac{\hbar^2}{m k_B \theta_E}\left(\frac{1}{2} + \frac{1}{e^{\theta_E/T}-1}\right), \tag{37}$$

$$V_o(T) = \delta_o - \frac{3k_B\theta_E}{m}\left(\frac{1}{2} + \frac{1}{e^{\theta_E/T}-1}\right) \tag{38}$$

for the Einstein model, and

$$\ln t(T) = \tau - \frac{3\hbar^2}{4mk_B\theta_D}\left(1 + \frac{4T^2}{\theta_D^2}\int_0^{\theta_D/T}\frac{u\,du}{e^u-1}\right), \tag{39}$$

$$V_o(T) = \delta_o - \frac{9k_B\theta_D}{8m}\left(1 + \frac{8T^4}{\theta_D^4}\int_0^{\theta_D/T}\frac{u^3\,du}{e^u-1}\right) \tag{40}$$

for the Debye model.

Furthermore, the thermal behavior of $\langle x^2\rangle$ and $\langle v^2\rangle$ in the general harmonic model discussed in the previous section results in the behavior of ln t(T) and $V_0(T)$ qualitatively shown in Fig. 1.

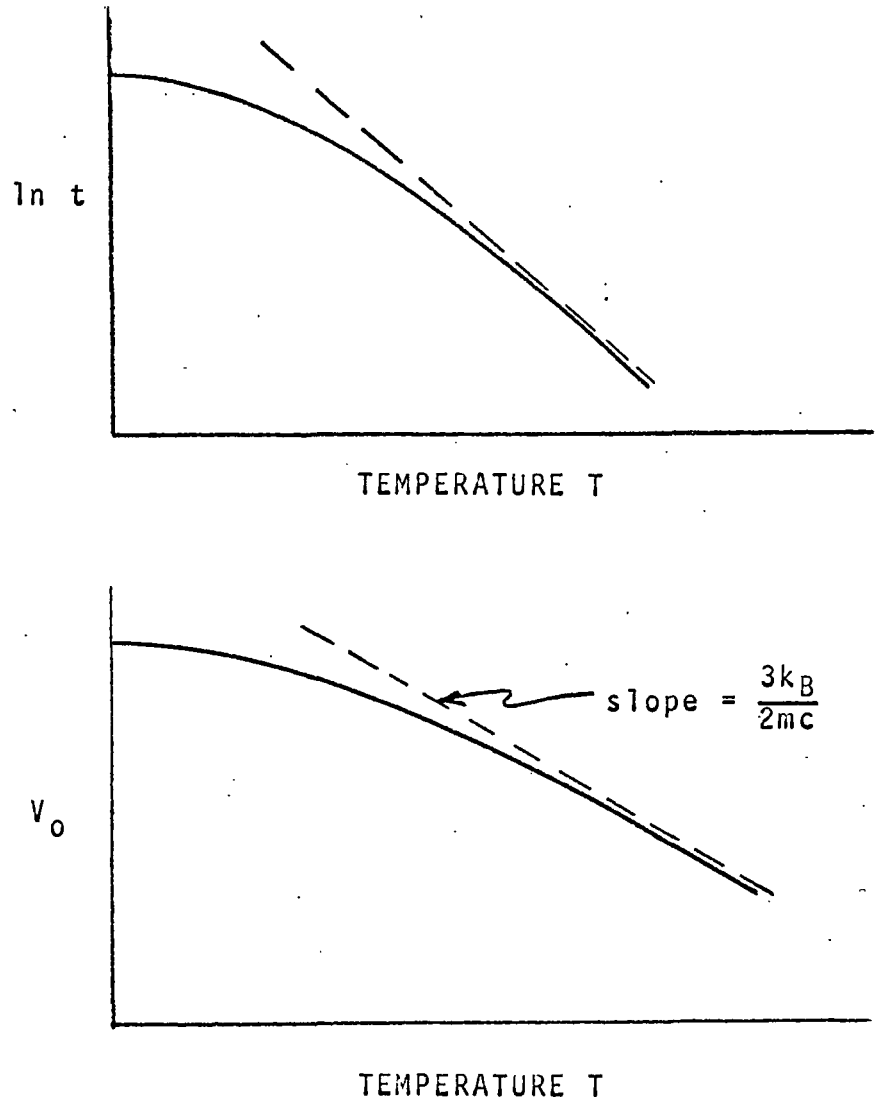


Fig. 1. The behavior of ln t(T) and $V_o(T)$ for a Mossbauer nucleus in a general harmonic lattice. (These parameters are deduced from the Mossbauer spectra described later.) Both ln t and V_o have maxima at T=0. They decrease slowly at low values of T and the slope increases as T increases. As T becomes very large, the curves become linear.

In the general harmonic model, the ln t(T) curve approaches an asymptote whose slope is a complicated function of the force constants of the solid. In the Einstein and Debye models, the slope is inversely proportional to the square of the characteristic temperature. The asymptotic slope of the $V_o(T)$ curve is independent of the properties of the solid and is equal to $3k_B/2mc$.

CHAPTER III

EXPERIMENTAL TECHNIQUE

A. Apparatus

The apparatus used in the experiment can be divided into three systems: (1) the Mossbauer spectrometer, (2) the source temperature-control system, and (3) the absorber temperature-control system.

1. The Mossbauer Spectrometer

A block diagram of the spectrometer is shown in Fig. 2. A crystal-controlled pulser (a) sends a pulse every 100 microseconds to the address advance input of the multichannel analyzer (MCA) (b). The MCA is operated in the multiscaling mode, in which only one of the 400 channels in memory is open at any instant. The pulser increases the address of the open channel by one every 100 microseconds, so that the 400 channels of memory are sequentially opened at a rate of 25 cycles per second.

The "200 FF" terminal of the MCA is the output of a flip-flop circuit which maintains a positive voltage when the open channel of the MCA is in the first half of memory, and zero voltage when in the second half. This square wave is sent into the transducer drive unit (c), where it is biased and integrated to form a symmetric triangular wave.

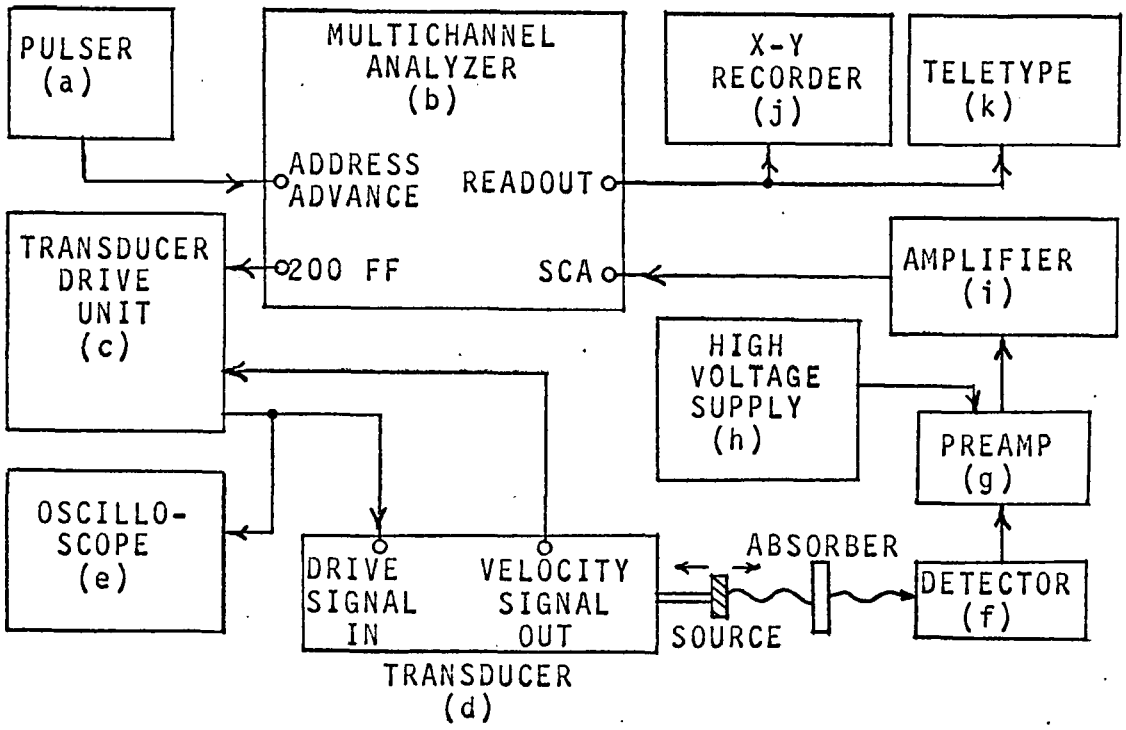


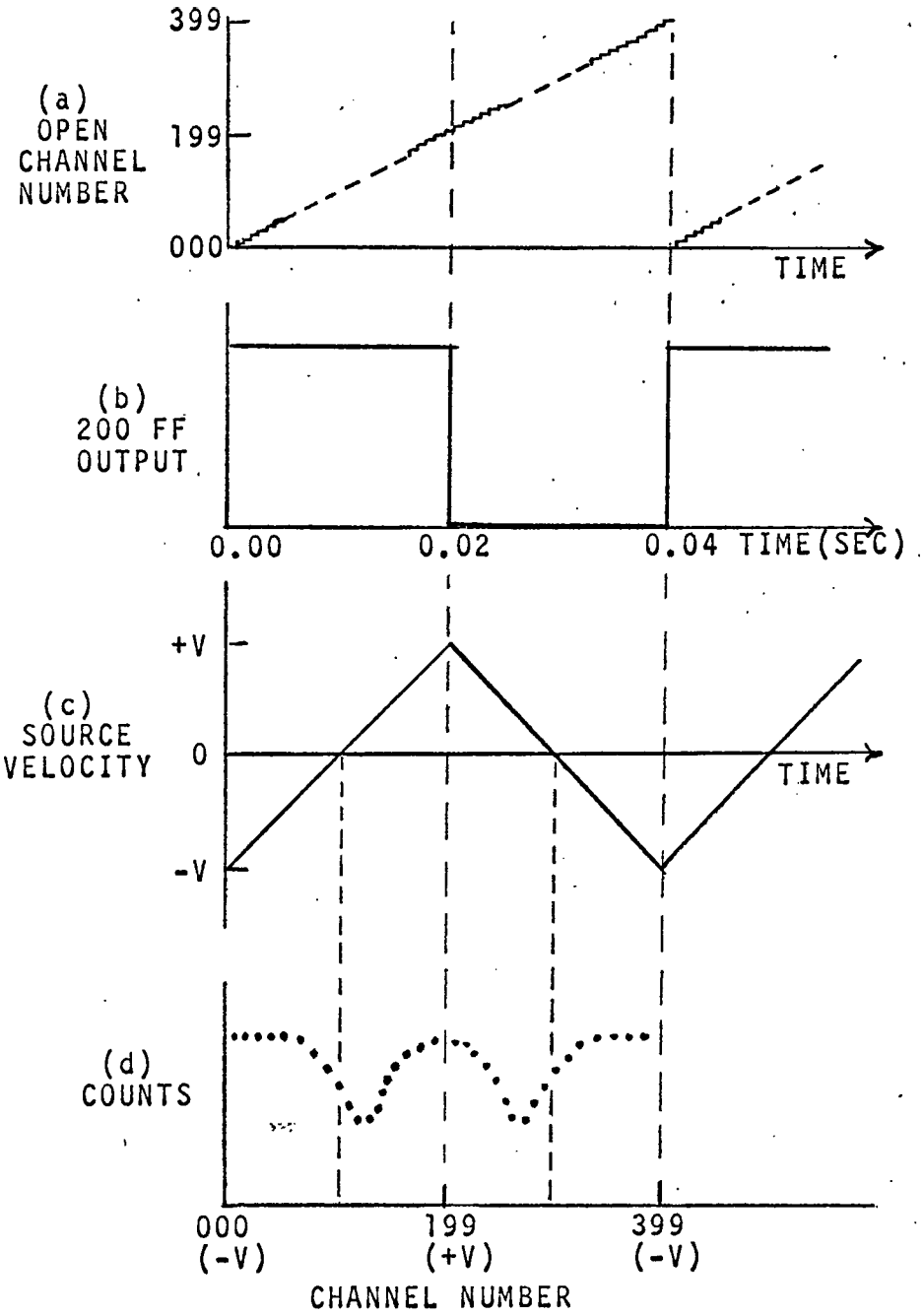
Fig. 2. The Mossbauer spectrometer. Electronic instruments used are (a) Austin Science Associates (ASA) TU-100AEC Timing Unit, (b) Victoreen PIP-400A Pulse Height Analyzer, (c) ASA S3 Mossbauer Spectrometer Drive, (d) ASA K3 Linear Motor, (e) Tektronix Type 321 Oscilloscope, (f) Reuter-Stokes RSG-61 Proportional Counter, (g) Hammer NB-19 Preamplifier, (h) Fluke 408B High Voltage Power Supply, (i) Hammer NA-12 DDL Amplifier, (j) Moseley 7035A X-Y Recorder, and (k) Teletype Model 33(P).

The signal from the velocity sensing coil of the electromagnetic transducer (d) is also sent into the drive unit, where it is compared to the triangular wave. The difference between these two signals is amplified and used as a correction signal to drive the transducer armature, to which the source is attached. Thus, the source velocity is forced by this servo loop to have a symmetric triangular wave form. The oscilloscope (e) monitors the drive signal for adjustment purposes.

Fig. 3 shows how the source velocity varies with time and open channel address in the MCA. As the first 200 channels are being scanned, the source moves from a maximum negative velocity to a maximum positive velocity, the values of which are determined by drive unit controls. The source velocity is reversed as the second 200 channels are being scanned. In this way, there is always a fixed velocity-to-channel correlation while a spectrum is measured.

The gamma-ray detection system in Fig. 2 uses a 97% Kr-3% CO_2 proportional counter (f) filled to a pressure of one atmosphere. Krypton was chosen for its strong absorption edge at 14.35 keV[24], just below the 14.41 keV Fe^{57} Mossbauer radiation. This absorption edge is helpful in minimizing background in the 14.4 keV window of the detection system

Fig. 3. Correlation between source velocity and channel number in the Mossbauer spectrometer. (a) the 100-microsecond pulser sequentially gates the 400 channels of the MCA so that the open channel number varies linearly with time. (b) The output of the "200's flip-flop", which is based on the MCA channel number that is open, is the master signal to the transducer drive unit. (c) The resulting source velocity curve is a linear function of time and, therefore, of channel number. (d) Two Mossbauer spectra, which are nearly mirror images, are collected; one with increasing velocity and the other with decreasing velocity.


399
199
000
(a)
OPEN
CHANNEL
NUMBER
TIME
(b)
200 FF
OUTPUT
0.00
0.02
0.04 TIME(SEC)
+V
0
-V
(c)
SOURCE
VELOCITY
TIME
(d)
COUNTS
000
(-V)
199
(+V)
399
(-V)
CHANNEL NUMBER

due to low-energy radiation, especially the 6.4 keV Fe X-ray following internal conversion in the source.

After being amplified and shaped, the pulses from the detector are sent to the single-channel analyzer (SCA) input of the MCA. When the amplitude of the detected pulse is between the upper and lower discriminator levels of the SCA (set to form a window for the 14.4 keV radiation), the SCA stores a count in the open channel in the MCA memory. Each detected pulse corresponding to a 14.4 keV photon is therefore stored in the channel corresponding to the instantaneous source velocity at the time of detection. Since the source executes the velocity range twice (once in each half of the memory), two Mossbauer spectra are stored in memory. Theoretically, these should be mirror images, but instrumental imperfections usually introduce a slight asymmetry.

The spectra stored in the MCA memory are read out in two modes. An X-Y recorder (j) gives an analog plot of counts versus channel number, and a teletype (k) prints the numerical contents of each channel.

Several steps were taken to minimize undesirable relative motion between the source and absorber. The transducer and the absorber mount were firmly bolted to a common one-inch aluminum plate. This aluminum plate and the

detector were placed on a "lead table" consisting of a lead slab weighing over 200 pounds supported by three stout legs, each weighing over 50 pounds. Other apparatus that had to be near the source or absorber during the experimental runs was suspended from separate supports to eliminate contact with the lead table, source, and absorber.

2. The Source Temperature-Control System

In order to study the thermal properties of the Mossbauer effect in an absorber, it is necessary to maintain a constant source temperature. This temperature must be reproduced for each spectrum taken with a given absorber, so that the temperature dependence of the Mossbauer fraction and resonant energy of the source do not have to be considered.

Fig. 4 is a drawing of the chamber placed over the source to keep it at a constant, reproducible temperature. When in use, the chamber is suspended from above, out of contact with the source and transducer. The electrical circuit used for temperature control is shown in Fig. 5. By occasionally re-adjusting the thermoregulator, the temperature of the source (assumed to be in thermal equilibrum with the nearby air) was kept within 0.1°C of 25.0°C for all experimental runs.

3. The Absorber Temperature-Control System

The absorber temperature-control system is a gas-flow

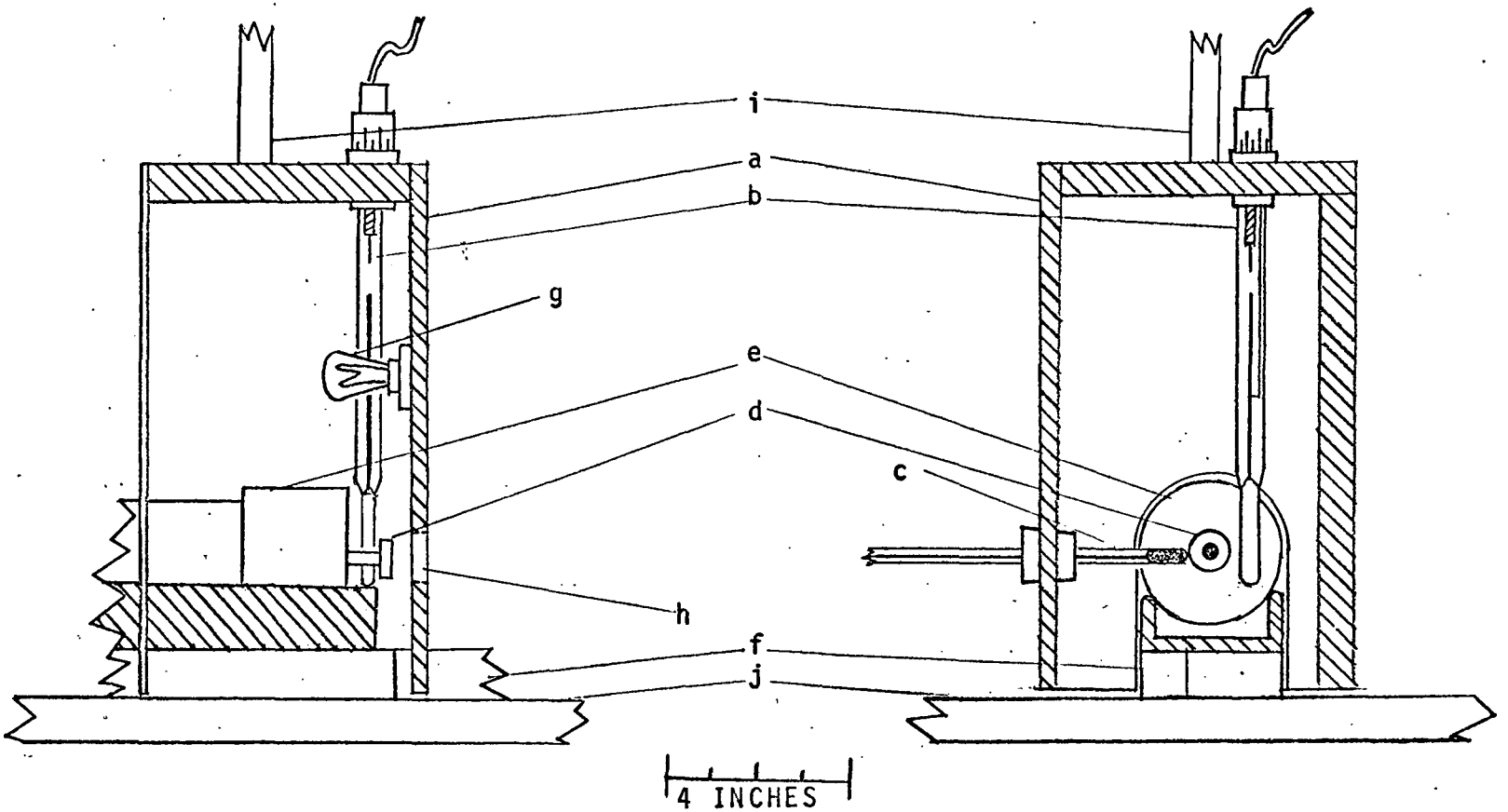


Fig. 4. Source chamber. (a) Plywood box with aluminum foil inner lining, (b) Princo Magna-Set Thermoregulator, (c) -1°C to 51°C mercury thermometer measuring air temperature near source, (d) source, (e) transducer, (f) aluminum baseplate, (g) 113-volt, 15-watt electric light bulb used as chamber heater, (h) double-walled Saran window, (i) support rod, and (j) lead table.

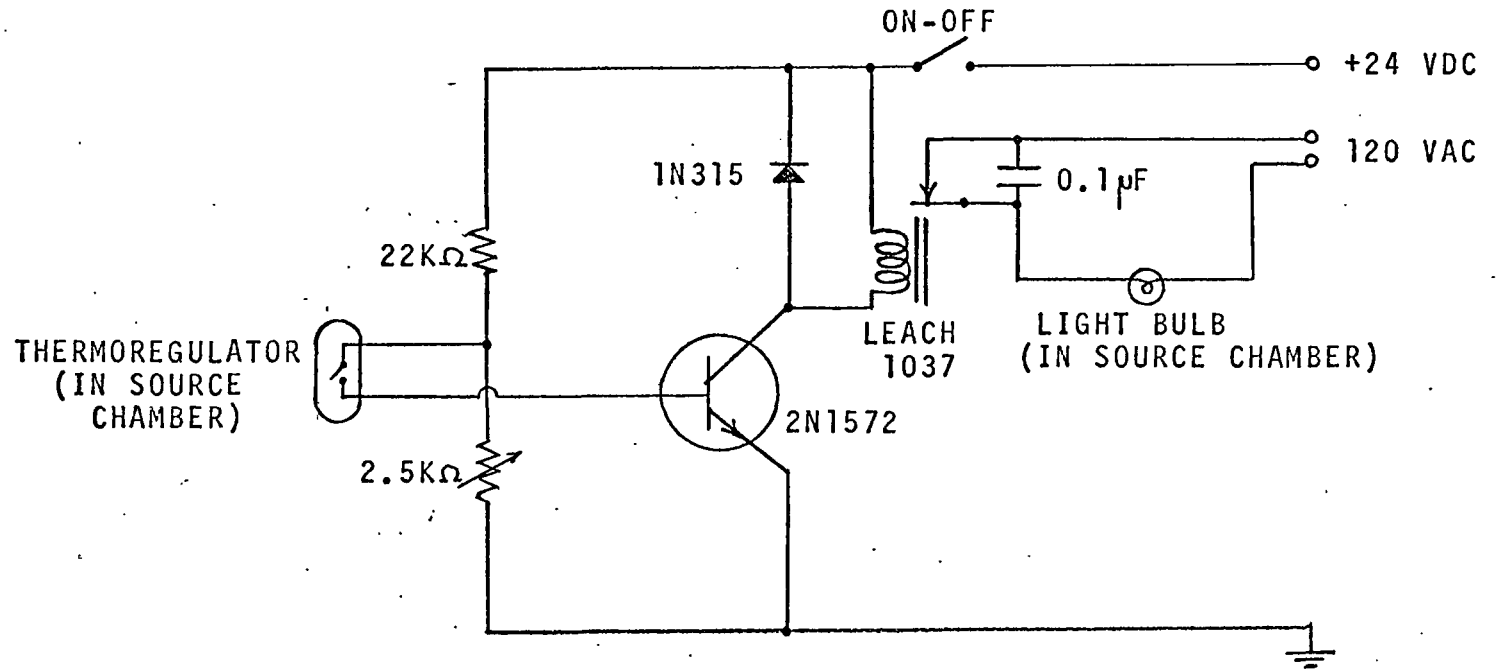


Fig. 5. Source temperature-control circuit. When the source temperature is below the desired value, the thermoregulator contacts are open. The transistor base is not forward biased, and the emitter-collector resistance is large, leaving the relay contacts closed. Power is then sent to the light bulb which raises the temperature in the source chamber to the desired value. At that point, the thermoregulator contacts close. If the potentiometer has been properly set, the transistor is then biased to saturation. The relay actuates, breaking the light-bulb circuit. The source chamber then cools until the process is repeated.

The purpose of the diode is to minimize the inductive buildup of large voltages across the transistor. The capacitor prevents excessive sparking across the relay contacts.

cryostat using the vapors from liquid nitrogen as a coolant. Fig. 6 is a schematic diagram of the system. The vacuum pump (a) draws vapor from the surface of the liquid nitrogen (f) through the absorber holder (e), shown in detail in Fig. 7. The flow rate is determined by the main flow valve (d) and, when the solenoid valve (c) is open, by the bypass valve (b). The sensor junction of the thermocouple (g) is cemented to the absorber, and its emf is measured with a potentimeter (i). The reference junctions of the thermocouple are tied to the bulb of a mercury thermometer and kept in an ice-water bath (h). This thermometer read within 0.05°C of 0.00°C during all experimental runs.

The electronic galvanometer (j) used with the potentiometer has a DC output which is proportional to the input voltage (i.e., the off-balance signal from the potentiometer). This output has a range of -1 volt to +1 volt and is sent into the solenoid control circuit (k), shown in detail in Fig. 8.

The potentiometer is set at the thermocouple emf corresponding to the desired absorber temperature. If the absorber temperature is higher than that value, the galvanometer output voltage actuates the solenoid control circuit. This opens the solenoid valve and increases the flow of coolant through the absorber holder. The absorber then cools until the potentiometer is balanced and the galvanometer reading crosses the null point and reverses

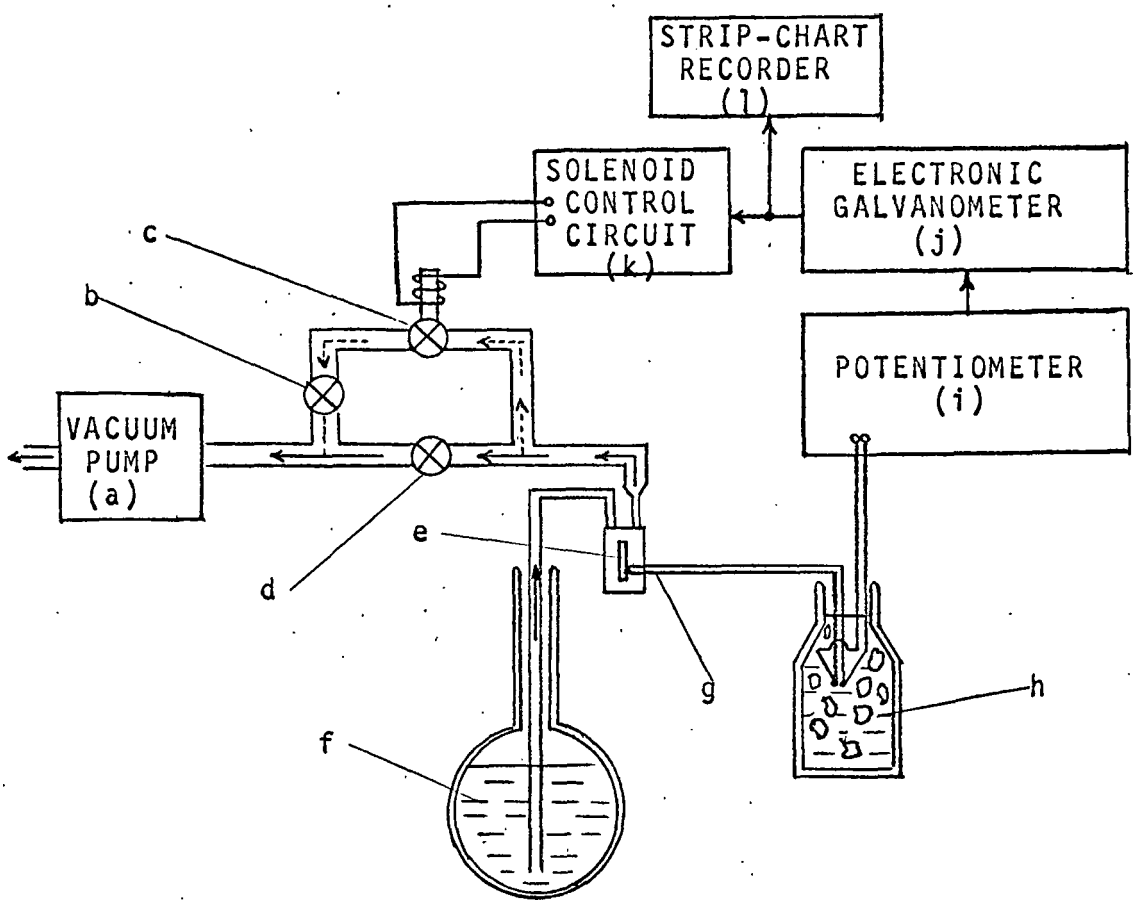


Fig. 6. Schematic diagram of the absorber temperature-control system. (a) Welch Vacuum Pump No. 1140, (b) bypass flow valve, (c) 24-volt DC solenoid valve, (d) main flow valve, (e) absorber in holder (Fig. 7), (f) liquid nitrogen, (g) chromel-constantan thermocouple, (h) ice-water bath for reference junction, (i) Leeds & Northrup No. 7552 Potentiometer, (j) Kintel Electronic Galvanometer, Model 204A, (k) solenoid circuit (Fig. 8), and (l) Esterline-Angus Graphic Ammeter (Model AW, 0-1 mA).

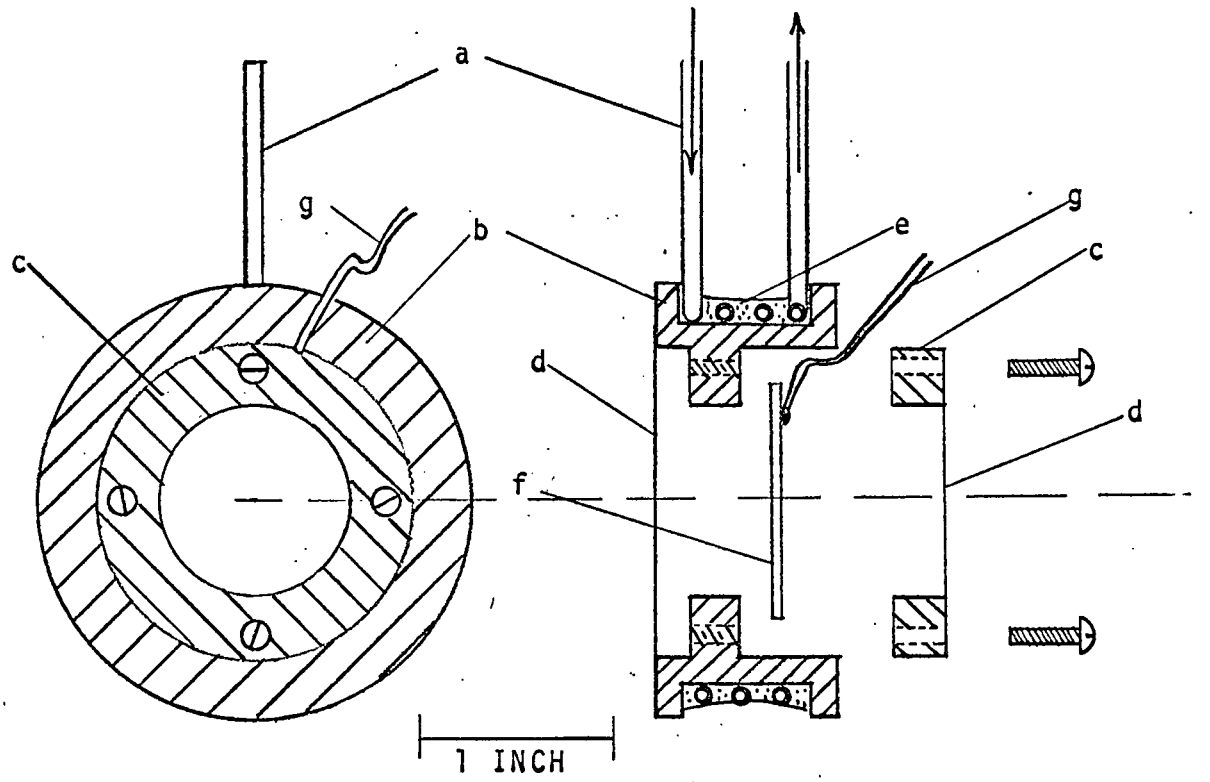


Fig. 7. Absorber holder. (a) Copper tubing (1/8-inch O. D., 1/16-inch I. D.), (b) copper housing, (c) copper retaining ring, (d) aluminum foil thermal shield, and (e) solder filling. The absorber (f), in the form of a disk, is clamped between the housing and the retaining ring. The gas coolant flows through the tubing coils around the housing; cooling the absorber by conduction. The thermocouple (g) is cemented to the absorber and clamped between the absorber and retaining ring.

The whole assembly fits snugly in a styrofoam box of ½-inch minimum thickness for thermal insulation (not shown).

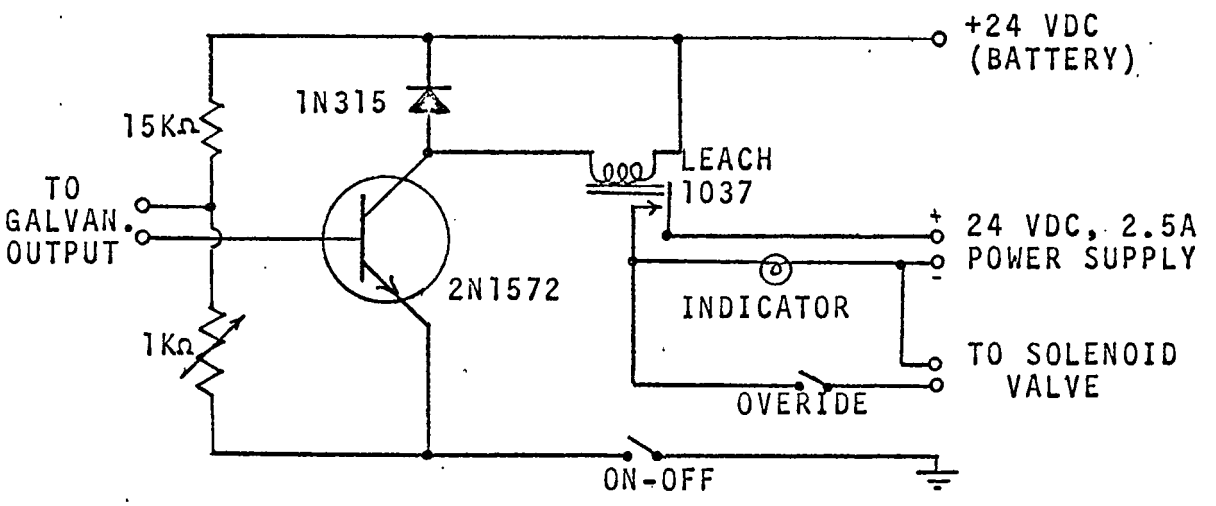


Fig. 8. Solenoid control circuit. The potentiometer biases the transistor near saturation when the galvanometer output is zero. When the galvanometer voltage is positive, the transistor goes to saturation, actuating the relay and sending 24-volt power to the solenoid. When the galvanometer output is negative, the transistor is reverse-biased, opening the relay and breaking the solenoid circuit. The SPST switch in the solenoid circuit disables the solenoid valve when it is desirable to overide the control circuit.

polarity. The solenoid circuit is then disabled and the solenoid valve closes, decreasing the vapor flow rate. The absorber then begins to warm up, repeating the cycle. A strip-chart recorder (1) continuously measures the thermal oscillations of the absorber, insuring that the absorber temperature is kept to within tolerance during a run.

This system was used successfully to limit absorber temperature variations to less than ±0.15°K at temperatures between 78°K and 293°K. Conversions from chromel-constantan emf readings to temperatures were based on a National Bureau of Standards Reference Table[25] and a correction (proportional to emf) using measurements of the boiling point of nitrogen. Absorber temperatures stated in this paper are accurate to the nearest degree Kelvin, which is sufficient resolution for the phenomena studied.

Figs. 9-12 are photographs showing several views of the apparatus described above.

B. Mossbauer Source and Absorbers

1. Source

The source used in all Mossbauer spectral measurements was 10 mCi (3-14-69) of Co^{57} in a copper host lattice, prepared by New England Nuclear Corporation. The Co^{57} was electroplated onto a 6-mm diameter area of a 12.5-mm diameter Cu foil 0.001-inch thick. This was annealed for

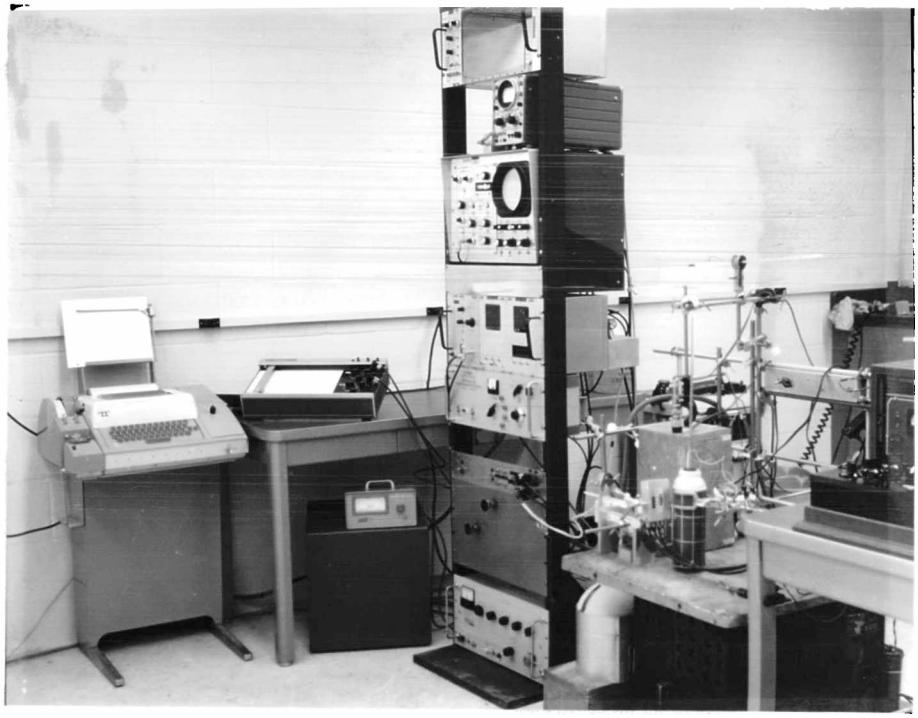


Fig. 9. View of electronic equipment in Fig. 2. The relay rack contains (starting near the top) the oscilloscope, the MCA, a modular bin containing the amplifier and pulser, the transducer drive unit, and (at the bottom) the high voltage supply. To the left of the rack are the X-Y recorder and the teletype; to the right of the rack is the lead table, upon which the source chamber, detector, and thermocouple reference bath can be seen. (See Fig. 10.)

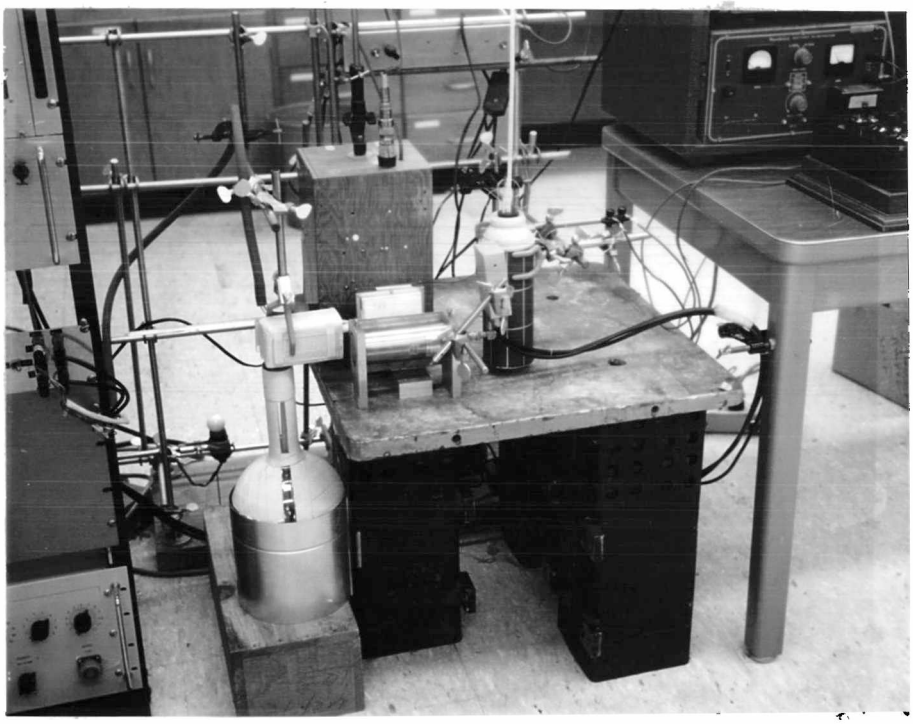


Fig. 10. View of apparatus on lead table. The wooden box to the rear is the source chamber, described in Fig. 4. In front of the chamber is the styrofoam box enclosing the absorber holder. The cylindrical detector and the preamplifier are also shown. To the left of the table is the liquid nitrogen dewar, with a styrofoam-insulated tube leading from the surface of the nitrogen to the absorber holder. To the right of the absorber is the vacuum bottle containing the ice-water bath and the thermocouple reference junctions.

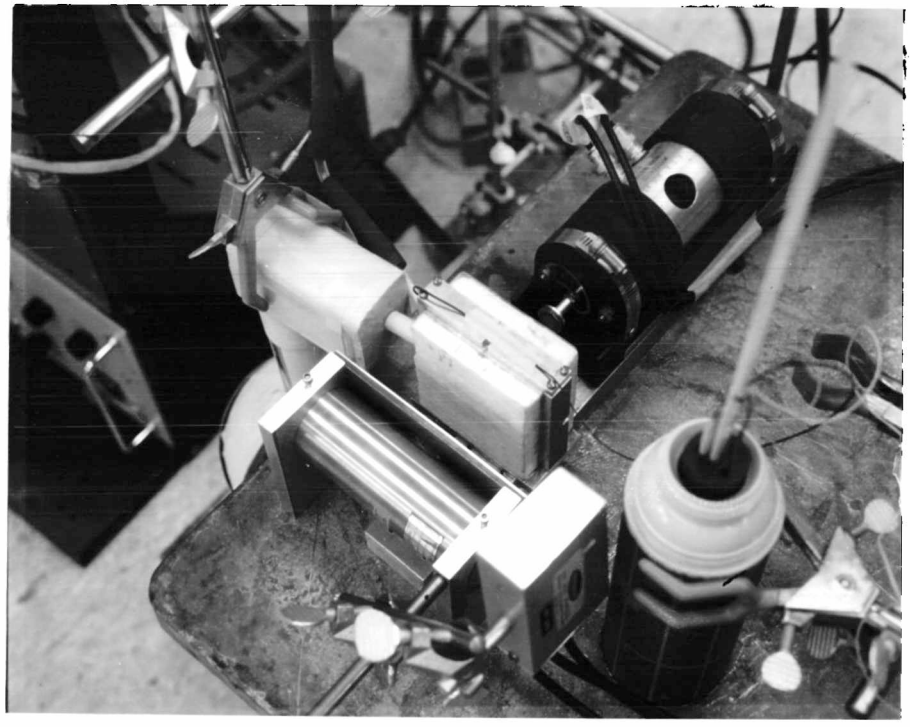


Fig. 11. Close-up view of source-absorber-detector geometry. The source chamber has been removed, exposing the transducer at the upper right and the aluminum source holder attached to the transducer armature. The absorber is at the geometric center of the styrofoam box and the detector and preamplifier are in front of the box. The source, absorber and detector window are lined on a common axis. The source-absorber distance is 5.8 cm and the absorber-detector distance is 6.1 cm. This geometry was used in every measurement.

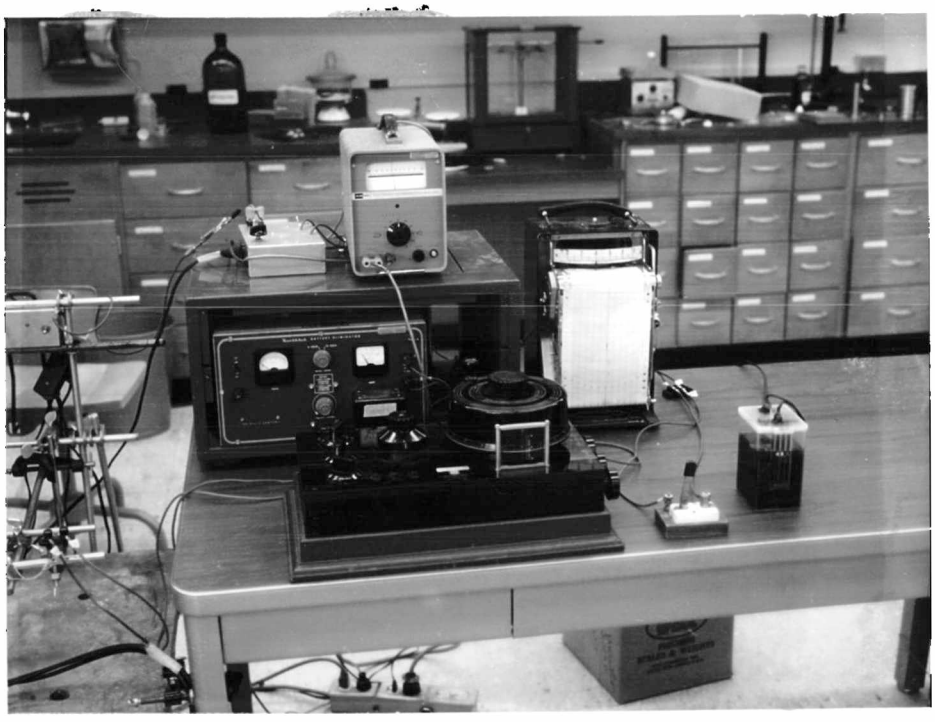


Fig. 12. Electrical apparatus for absorber temperature control. From top to bottom, the equipment shown are the electronic galvanometer, the solenoid control circuit, the strip-chart recorder, the 24-volt DC, 2.5-ampere power supply, and the potentiometer.

3 hours at 1000°C in hydrogen gas and then quenched.

In addition to being a single-line Mossbauer source, the copper source has the additional advantage of a well-measured Mossbauer fraction f_s. Several authors[5,11,26,27] have measured f_s for copper sources and their values agree within the uncertainty of their measurements. Housley et al.[26] studied copper sources using several preparation techniques. They used different grades of purity of Cu and $Co^{57}Cl_2$ in the sources and cold rolled one source between successive f_s measurements. No differences in the value of f_s could be measured in these sources. They conclude that a copper source at room temperature ($297\pm1°K$) can be used as a standard ($f_s=0.710\pm0.014$) in Mossbauer fraction measurements.

2. Absorbers

Table I is a list of the absorbers used in this experiment. Absorbers Fe, SN1, SN2, and SF were obtained from New England Nuclear Corporation. The Fe absorber is a 0.0010-inch rolled foil of natural iron. The SN1, SN2, and SF absorbers were each prepared by mixing the powdered salt with acrylic plastic and heating in a metallurgical press to form a disk-shaped absorber. Mossbauer spectra of the salts taken before and after preparation showed that no dehydration is produced by the heating.[28]

The PF absorber was prepared by mixing reagent potassium

TABLE I. Absorbers

Designation	Compound	Formula	Thickness[a] (mg Fe^{57}/cm^2)
Fe	Metallic Iron	Fe	0.46 ±0.02
SN1	Sodium Nitroprusside	$Na_2Fe(CN)_5NO \cdot 2H_2O$	0.100±0.005
SN2	Sodium Nitroprusside	$Na_2Fe(CN)_5NO \cdot 2H_2O$	0.25 ±0.01
SF	Sodium Ferrocyanide	$Na_4Fe(CN)_6 \cdot 10H_2O$	0.100±0.005
PF	Potassium Ferrocyanide	$K_4Fe(CN)_6 \cdot 3H_2O$	0.102±0.003

[a]Uncertainties shown are approximate values based on estimates of errors in mass and area measurements and on estimated sample loss during preparation.

ferrocyanide with Lucite powder. This mixture was poured into a press and acetone was added to dissolve the Lucite. (Previous efforts to detect solubility of potassium ferrocyanide in acetone gave negative results.) The acetone was then evaporated by pumping on the cylinder of the press with a mechanical vacuum pump for approximately one hour while forcing the piston of the press against the mixture. The disk-shaped absorber was then removed and allowed to dry completely.

C. Experimental Procedure

Table II is a summary of the 31 experimental runs made with the five absorbers. For each run, two spectra were obtained (one in each half of the MCA memory), resulting in a total of 62 spectra.

Because the Fe six-line spectrum covers such a large range in source velocity, it was necessary to use two velocity ranges at each temperature. The ± 7.6 mm/sec range gave the full six-line pattern used in determining ln t (see Chapter II), while the ± 1.9 mm/sec range was used to determine precisely the centroid of the spectrum from the two inner lines, giving the resonant velocity of Fe. Since Fe exhibits magnetic hyperfine splitting without a quadrupole interaction, the centroid of the two inner lines is the centroid of the spectrum.[2] The source velocity range

TABLE II. Summary of Experimental Runs

Designation	Absorber	Temperature (°K)	Source Velocity Range (mm/sec)
Fe(79)6	Fe	79[a]	±7.6
Fe(129)6	Fe	129[a]	±7.6
Fe(179)6	Fe	179[a]	±7.6
Fe(228)6	Fe	228[a]	±7.6
Fe(276)6	Fe	276[a]	±7.6
Fe(293)6	Fe	293[a,c]	±7.6
Fe(79)2	Fe	79[b]	±1.9
Fe(129)2	Fe	129[b]	±1.9
Fe(179)2	Fe	179[b]	±1.9
Fe(228)2	Fe	228[b]	±1.9
Fe(276)2	Fe	276[b]	±1.9
Fe(293)2	Fe	293[b,c]	±1.9
SN1(79)	SN1	79	±1.9
SN1(155)	SN1	155	±1.9
SN1(179)	SN1	179	±1.9
SN1(228)	SN1	228	±1.9
SN1(276)	SN1	276	±1.9
SN1(293)	SN1	293[c]	±1.9
SN2(293)	SN2	293[d]	±1.9
SF(80)	SF	80	±1.9
SF(129)	SF	129	±1.9
SF(179)	SF	179	±1.9
SF(228)	SF	228	±1.9
SF(276)	SF	276	±1.9
SF(293)	SF	293	±1.9
PF(78)	PF	78	±1.9
PF(130)	PF	130	±1.9
PF(179)	PF	179	±1.9
PF(228)	PF	228	±1.9
PF(276)	PF	276	±1.9
PF(293)	PF	293	±1.9

[a]Full six-line Fe spectrum.

[b]Two inner lines of Fe spectrum.

[c]Used for velocity calibration and for lattice dynamical calculations.

[d]Used only for velocity calibration.

of ±1.9 mm/sec was used to obtain all other spectra.

The procedure used with each absorber was:

(a) The thermoucouple junction was cemented to the absorber and it was placed in the cryostat.

(b) The source temperature was adjusted to 25.0°C (298.2°K), and the absorber temperature, to 293°K.

(c) While the temperatures of the source and absorber were being held constant, a pulse height spectrum was taken for SCA window adjustment and background measurements.

(d) A Mossbauer spectrum was then accumulated until at least 40,000 counts were recorded in each channel of the MCA. (In the case of SN1 and SN2 at 293°K, at least 80,000 counts were recorded, since these spectra were used for velocity calibration of the thermal shift measurements.) Counting rates ranged approximately from 6 to 12 counts per second per channel at maximum absorption. This depended, of course, on the absorber and temperature.

(e) Step (d) was then repeated for each absorber temperature.

CHAPTER IV

DATA ANALYSIS

The data obtained in the 31 Mossbauer spectrum runs are listed in Appendix C. These consist of the accumulated number of counts n(C) as a function of channel number C in each run. Typical spectra are shown in Figs. 13 and 14.

The analysis of these data consisted of (1) calculation of the spectrum parameters (depth, width, and position of each line, and the number of counts at "infinite" velocity) in each of the 62 spectra, (2) velocity calibration of the spectra (conversion of the parameters in units of "channels" into parameters in units of velocity), (3) calculation of ln t(T) and $V_0(T)$ for each absorber at each temperature T (using the relations derived in Chapter II), and (4) fitting the ln t(T) and $V_0(T)$ values to Einstein and Debye models.

In addition to the above analysis, information unrelated to lattice dynamical studies was extracted from the data; i.e., the temperature dependence of the magnetic field at the Fe^{57} nucleus in metallic iron and of the quadrupole splitting in sodium nitroprusside.

Throughout the analysis, the two spectra obtained in the two halves of the MCA memory were treated independently.

A. Calculation of Spectrum Parameters

In Chapter II, theoretical analysis was based on the

Fig. 13. Spectra obtained in the first half of the MCA memory in runs (a) SN1(293), (b) PF(293), and (c) SF(293) and SF(80). (Experimental run designations are listed in Table II.) In (c), the temperature dependence of the Mossbauer fraction and of the resonant energy are clearly seen. As the temperature decreases, the "strength" of resonant absorption (which is proportional to the product of the depth and width of the line) increases and the line shifts toward higher energy (higher channel number).

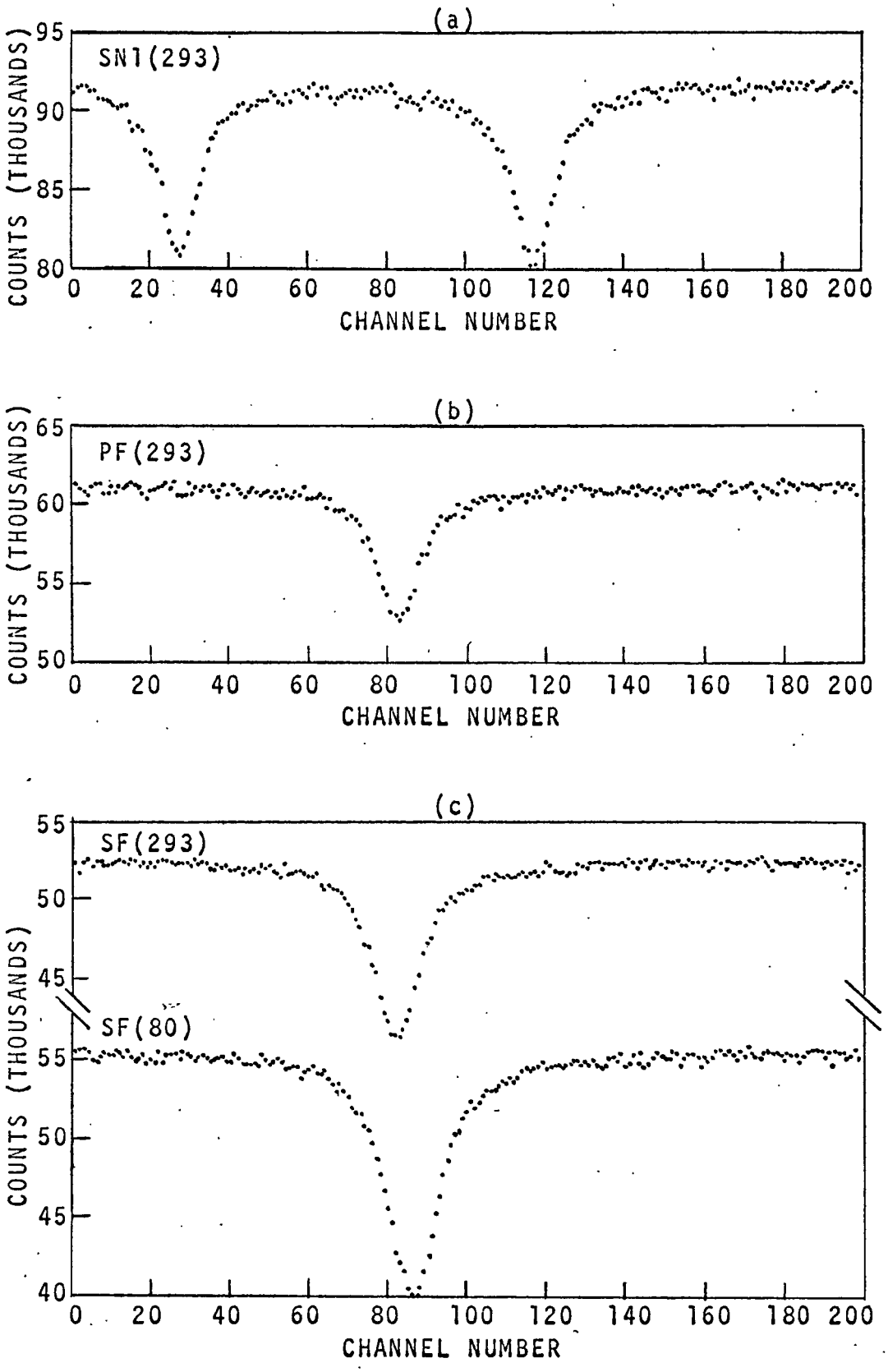
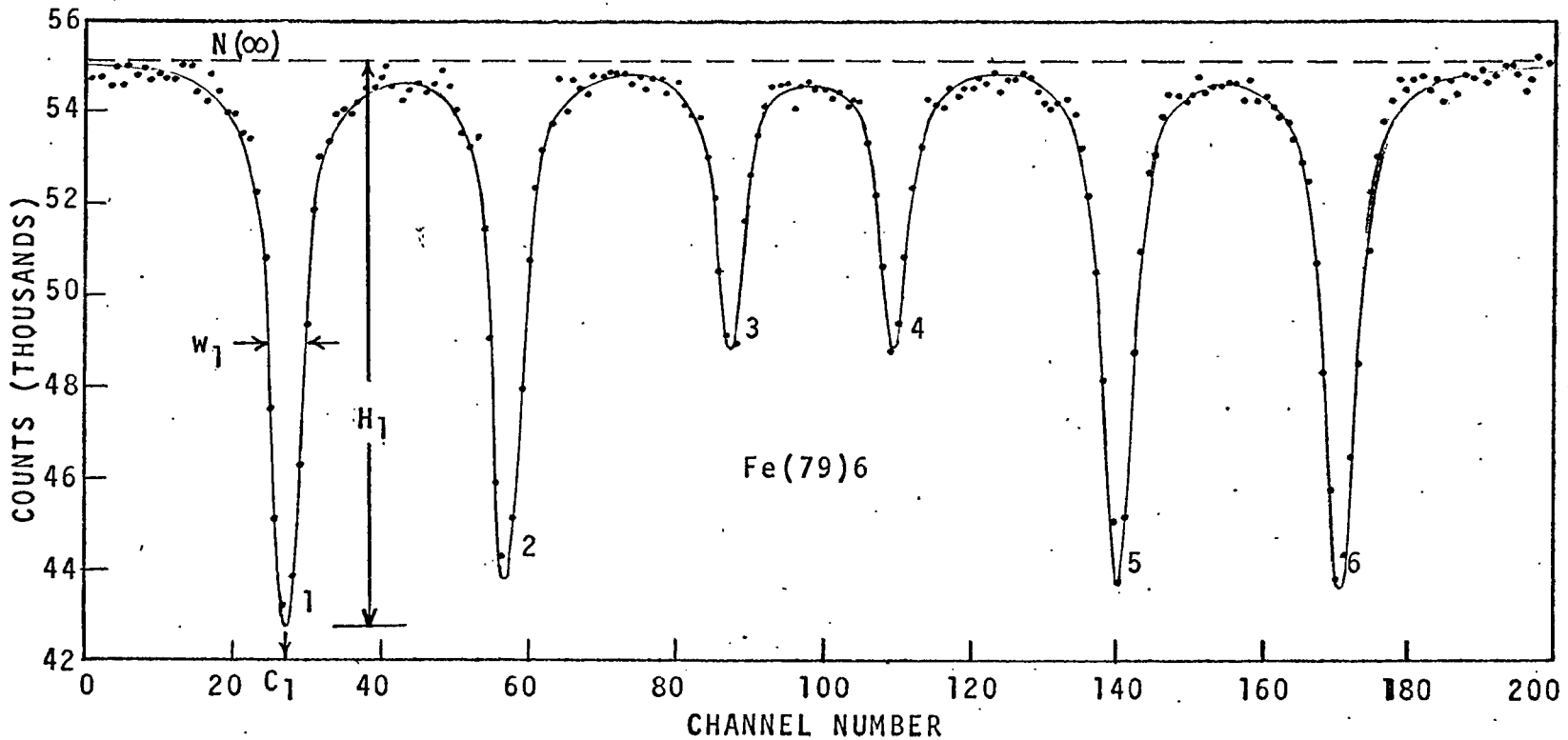

(a)
SN1(293)
COUNTS (THOUSANDS)
95
90
85
80
0
20
40
60
80
100
120
140
160
180
200
CHANNEL NUMBER
(b)
PF(293)
COUNTS (THOUSANDS)
65
60
55
50
0
20
40
60
80
100
120
140
160
180
200
CHANNEL NUMBER
(c)
SF(293)
SF(80)
COUNTS (THOUSANDS)
55
50
45
55
50
45
40
0
20
40
60
80
100
120
140
160
180
200
CHANNEL NUMBER

Fig. 14. Spectrum obtained in channels 000-199 of the MCA memory in run Fe(79)6 and the results of the least-squares fit. The solid curve is equation (47) with the spectrum parameters $N(\infty)=55,086\pm77$ counts, $a=(6.2\pm7.6)\times10^{-5}$ channel^{-1}, $b=(-3.3\pm4.0)\times10^{-7}$ channel^{-2}, and

Line No. (i)	H_i (counts)	w_i (channels)	C_i (channel no.)
1	12,450±200	4.88±0.13	27.244±0.039
2	11,280±210	4.46±0.13	57.187±0.041
3	6,260±210	4.37±0.23	87.276±0.074
4	6,320±210	4.49±0.24	109.427±0.074
5	11,680±210	4.52±0.13	139.931±0.040
6	11,670±190	5.30±0.14	170.397±0.044


56
54
52
50
48
46
44
42
COUNTS (THOUSANDS)
N(∞)
W1
H1
C1
1
2
3
4
5
6
Fe(79)6
0
20
40
60
80
100
120
140
160
180
200
CHANNEL NUMBER

absorption curve $\epsilon(V)$ defined in equation (24) as

$$\epsilon(V) \equiv \frac{N(\infty)-N(V)}{N(\infty)-N_B} \quad . \tag{24}$$

It was stated that this function can be represented accurately for a single line absorber by equation (28),

$$\epsilon(V) = \frac{\alpha}{1+4(V-V_0)^2/W^2} \quad . \tag{28}$$

By combining equations (24) and (28), we see that the expected relation between the counts N observed as a function of source velocity V in a Mossbauer spectrum is

$$N(V) = N(\infty) - \frac{H}{1+4(V-V_0)^2/W^2} \tag{41}$$

where $H=\alpha[N(\infty)-N_B]$ is the depth of the absorption line at resonance. If there are ν absorption lines in the spectrum, equation (41) is generalized to the form

$$N(V) = N(\infty) - \sum_{i=1}^{\nu} \frac{H_i}{1+4(V-V_i)^2/W_i^2} \quad , \tag{42}$$

where H_i, V_i, and W_i are the absorption depth, resonant velocity, and apparent width respectively of the i^{th} line.

The actual observed spectrum, however, may have a velocity-dependent modulation of intensity due to instrumental

effects. If this modulation is represented by a function g(V), one would observe a spectrum n(V) given by

$$n(V) = N(V) \cdot g(V) \, . \tag{43}$$

In a perfect spectrometer, g(V)=1. We define unity modulation to occur at V=0 and approximate g(V) by a Taylor expansion about g(0)≡1,

$$g(V) \approx 1 + AV + BV^2 \, . \tag{44}$$

Combining equations (42)-(44), we have

$$n(V) = \left[N(\infty) - \sum_{i=1}^{\nu} \frac{H_i}{1 + 4(V - V_i)^2 / W_i^2} \right] \cdot (1 + AV + BV^2) \, , \tag{45}$$

where we expect A and B to be sufficiently small so that the modulation factor in paranthesis is close to unity.

Finally, the actual data consists of counts as a function of channel number C rather than a function of source velocity V. Assuming C and V to be linearly related by an equation of the form

$$V = mC + Y \, , \tag{46}$$

where m and Y are constants determined by the transducer-drive controls, it is easily shown that equation (45) is transformed into the form

$$n(C)=\left[N(\infty)-\sum_{i=1}^{\nu}\frac{H_i}{1+4(C-C_i)^2/w_i^2}\right]\cdot(1+aC+bC^2), \qquad (47)$$

where C_i is the channel in which resonance occurs for the i^{th} line and w_i is the apparent width (in number of channels) of the i^{th} line. To allow for the possibility of an instrumental modulation, equation (47) was the mathematical model used in fitting the data n(C) in each of the 62 spectra. The $3\nu+3$ model parameters $N(\infty)$, H_i, C_i, w_i ($i=1, 2,\ldots,\nu$), a, and b were adjusted to minimize the variance by a least-squares procedure in each spectrum.

For any model which is non-linear in the adjustable parameters, such an equation (47), it can be shown that the standard least-squares procedure leads to a set of non-linear normal equations which are often impossible to solve analytically. To circumvent this difficulty, the data n(C) were fitted to the model by using an iterative technique described in Appendix A.

To perform the computation in the least-squares fit, a program was written in FORTRAN IV-H for use with the SDS Sigma 7 digital computer at the University of Houston. This program accepts the data n(C) on punched cards and calculates the model parameters and their standard deviations (based on the statistical scatter of the data). Fig. 14

shows an example of the results of the least-squares fit to the spectrum in channels 000-199 in the Fe(79)6 run.

The fitting of the spectra to equation (47) showed that in most cases instrumental modulation was insignificant; i.e., a and b in equation (47) were zero within the uncertainties in their values. (See, for example, Fig. 14.) In all cases, the modulation was sufficiently small that

$$0.99 < (1 + aC + bC^2) < 1.01 \quad .$$

B. Velocity Calibration

The National Bureau of Standards (NBS) has recommended the use of the sodium nitroprusside spectrum as a velocity calibration standard for Fe^{57} Mossbauer spectroscopy.[29,30] The spectrum is a two-line spectrum resulting from a quadrupole interaction*. (See Fig. 13(a).) The difference in resonant velocity between the two lines is extremely insensitive to temperature near room temperature,[8] a desirable characteristic for a velocity standard. This difference in velocity was first measured by NBS[29] to

---

*The interaction between an electric field gradient and a nucleus with an electric quadrupole moment splits the levels of nuclear states of spin greater than 1/2. In the case of Fe^{57}, the excited state splits into two levels while the ground state is unsplit, resulting in a two-line spectrum.[2]

be 1.712±0.004 mm/sec, but a later NBS measurement[30] gives 1.726±0.002 mm/sec at 25.0°C. Grant et al.[31] have recently made extremely precise measurements of the sodium nitroprusside spectrum at 23±1°C. They obtained a splitting of 1.7048±0.0025 mm/sec, in better agreement with the first NBS value.

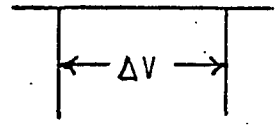
For velocity calibration of the spectra in this experiment, a weighted average of the above values was calculated. This value and its standard deviation are shown in Fig. 15 (a). In addition to sodium nitroprusside, metallic Fe is often used as a standard, expecially in spectra covering a velocity range much larger than the splitting in sodium nitroprusside. The differences is resonant velocities between the three symmetric pairs of lines in the Fe spectrum at 294°K are shown in Fig. 15 (b).[4] This six-line spectrum is due to magnetic hyperfine interaction in metallic Fe.*

As stated before, the six-line Fe spectra were obtained with the same velocity range settings on the spectrometer (±7.6 mm/sec). Velocity calibration of these spectra was therefore achieved by defining the splittings observed in the Fe(293)6 run to have the values shown in Fig. 15 (b).

---

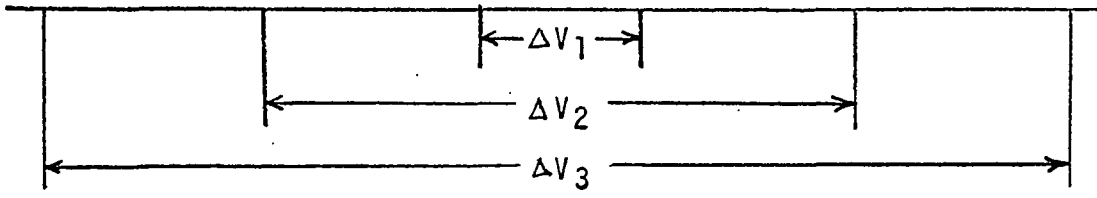
*The interaction of the magnetic moment of a nucleus with a magnetic field splits each nuclear state into sub-levels (the nuclear Zeeman effect). This results in a splitting of the Mossbauer spectrum of Fe^{57} into six lines.[2] In metallic Fe, the magnetic field at the nucleus is due to the unpaired atomic electron spins.

(a) Sodium Nitroprusside:



$\Delta V = 1.719 \pm 0.007$ mm/sec

(b) Metallic Fe:



$\Delta V_1 = 1.677 \pm 0.025$ mm/sec
$\Delta V_2 = 6.167 \pm 0.025$ mm/sec
$\Delta V_3 = 10.657 \pm 0.025$ mm/sec

Fig. 15. Values used for velocity calibration of spectra. (a) The splitting in sodium nitroprusside, showing a weighted average of three values[29,30,31]. (b) The splitting in metallic Fe, showing values for the three symmetric pairs of lines.[4] The same scale is used in each diagram.

This was done separately for each half of the MCA memory, and the results are given in Table III.

The remaining spectra were obtained at a lower velocity range setting (1.9 mm/sec). These runs were calibrated by defining the splitting of the two lines in each of the runs SN1(293), SN2(293), and Fe(293)2 to have the values in Fig. 15 and taking a weighted average of the results (Table III).

In comparing resonant velocities in several absorbers, it is conventional to define the centroid of the sodium nitroprusside spectrum at room temperature as zero velocity. In this way, all energies are measured relative to the average resonant energy of the two sodium nitroprusside transitions rather than to the energy of the photons emitted by the source. In the case of the low-velocity spectra, which were used to determine thermal shifts, this convention was followed by defining channels at the centroid of the SN1(293) and SN2(293) spectra as corresponding to zero velocity. The weighted averages are shown in Table III. Since energy shifts were not calculated using the Fe six-line spectra, a zero-velocity calibration was not made.

For each spectrum, Table III was used to convert the line positions C_i and widths w_i (in units of "channels") into parameters V_i and W_i (in units of mm/sec). These parameters, along with $N(\infty)$ and H_i, define the spectrum that would be observed in absence of instrumental modulation.

TABLE III. Velocity Calibration

Spectra	Channels in Memory	Conversion Factor (mm/sec per channel)	Zero Velocity Channel
Fe Six-Line	000-199	0.07633±0.00019	-----
(±7.6 mm/sec)	200-399	0.07636±0.00017	-----
Low-Velocity	000-199	0.019089±0.000093	72.334±0.062
(±1.9 mm/sec)	200-399	0.018676±0.000052	323.789±0.094

(See equation (42).)

C. Calculation of ln t(T) and $V_0(T)$

In Chapter II, it was shown that ln t for a given spectrum is determined by the integral of the absorption curve $\epsilon(V)$ over all velocities. If equation (42) represents the spectrum, the absorption curve for the spectrum is obtained by use of equation (24). The result is

$$\epsilon(V) = \frac{1}{N(\infty) - N_B} \sum_{i=1}^{\nu} \frac{H_i}{1+4(V-V_i)^2/W^2} \, dV \quad . \tag{48}$$

The area A_i due to the i^{th} absorption line is given by

$$A_i = \int_{-\infty}^{\infty} \frac{1}{N(\infty)-N_B} \cdot \frac{H_i}{1+4(V-V_i)^2/W^2} \, dV .$$

The result of this integration is

$$A_i = \frac{\pi}{2} \cdot \frac{H_i W_i}{N(\infty)-N_B} \quad , \tag{49}$$

which is calculated directly from the spectral parameters H_i, W_i, and $N(\infty)$, and the number of background counts N_B.

The background N_B was determined for each absorber by use of the pulse-height spectrum of the radiation transmitted by the absorber with the source at rest. Fig. 16 shows part of a typical pulse-height spectrum and the SCA window used in obtaining the Mossbauer spectrum. The amount

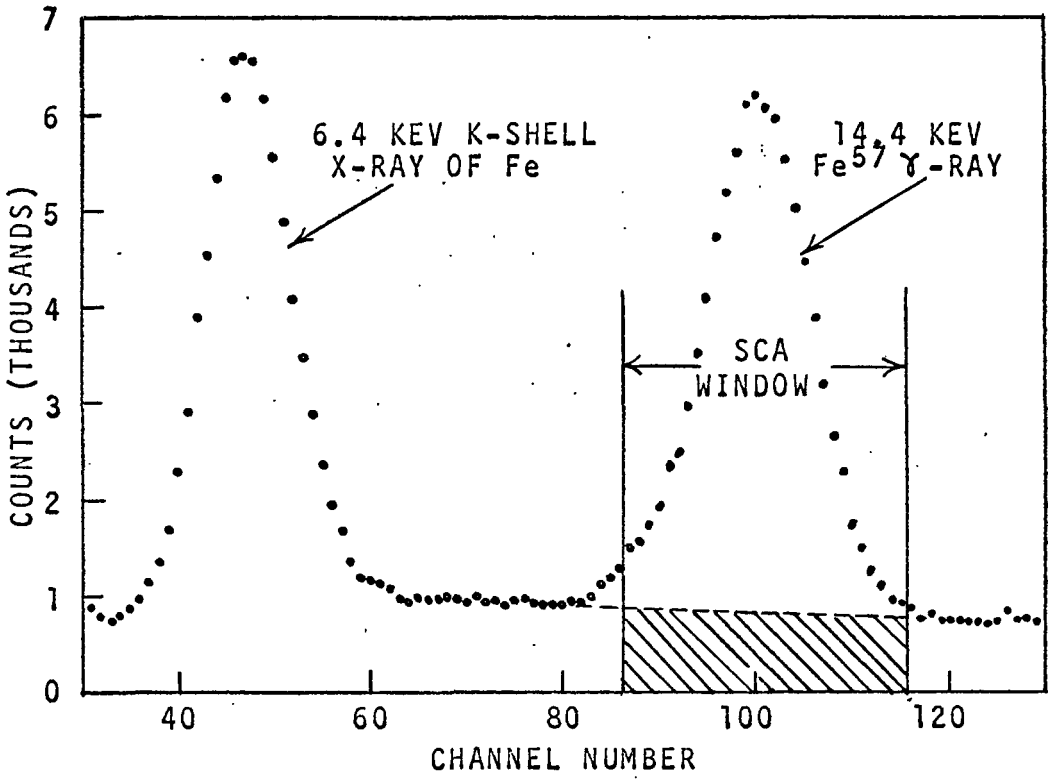


Fig. 16. Pulse-height spectrum of radiation transmitted by Fe absorber at 293°K. The vertical lines show the SCA window used in taking the Mossbauer spectrum. The shaded area is assumed to be background counts, i.e., those due to radiation not directly from the 14.4 keV transition in the source.

of background radiation (i.e., radiation not directly from the 14.4 keV transition in the source) is determined by extrapolation of a line from the background level on each side of the window. The ratio ρ of the area under this line to the total area in the window spectrum is equal to the ratio of the background intensity to the total intensity transmitted by the absorber at zero source velocity. Thus, N_B in a Mossbauer spectrum is given by

$$N_B = \rho N_o$$

where N_o is the number of counts in the Mossbauer spectrum at zero source velocity. Channels 100 and 300 should correspond to zero source velocity in a perfectly symmetric spectrometer. By use of published values[4] of velocity shifts of Fe, sodium nitroprusside, and potassium ferrocyanide relative to a Cu source, it was determined that in the low-velocity spectra, zero source velocity corresponds to channels 99 and 298, while in the six-line Fe spectra, to channels 100 and 300. Thus, in each spectrum, N_o is the contents of one of the above channels.

Using the values of N_B, H_i, W_i, and $N(\infty)$, and equation (49), the areas of each absorption line in the six-line Fe spectra and the SN1, SF, and PF spectra were calculated. There areas were used to find the value of t for each spectrum, using the method described in Chapter II. (See

the discussion following equation (33).)

Since $t=n_M\sigma_0 f_a$, the Mossbauer fraction f_a can be determined from t if n_M and σ_0 are known. It is seen from equation (32) that σ_0, and thus f_a, depends on α_T, the total internal conversion coefficient. The value of α_T for Fe^{57}, however, has not been well-established; it has ranged from an early value[3] of 15 to a recent careful measurement[32] of 8.17. (For the past few years, a value of 9.00 has been commonly used.[4])

The value $\alpha_T=8.17$ was used in equation (32) to obtain $\sigma_0=2.569 \times 10^{-18}$ cm^2, and Table I was used to obtain values of n_M. The resulting f_a values are shown in Fig. 17. The right-hand scale shows $\langle x^2 \rangle$ as determined by equation (3).

Equation (34) shows that if ln t rather than f_a is used for lattice dynamical calculations, the value of σ_0 enters only in the additive constant $\tau = \ln(n_M\sigma_0)$. This parameter τ can be treated as an adjustable parameter in least-squares fits to lattice models. In this way, the large uncertainty in σ_0 does not affect the accuracy of the model calculations. Fig. 18 shows the temperature dependence of ln t in each absorber.

To obtain the resonant velocity V_0 in each of the two-line Fe and SN1 spectra, the resonant velocities V_i of the two lines were averaged. (Since the Fe^{57} nucleus in metallic Fe has no quadrupole interaction[33], the six-line

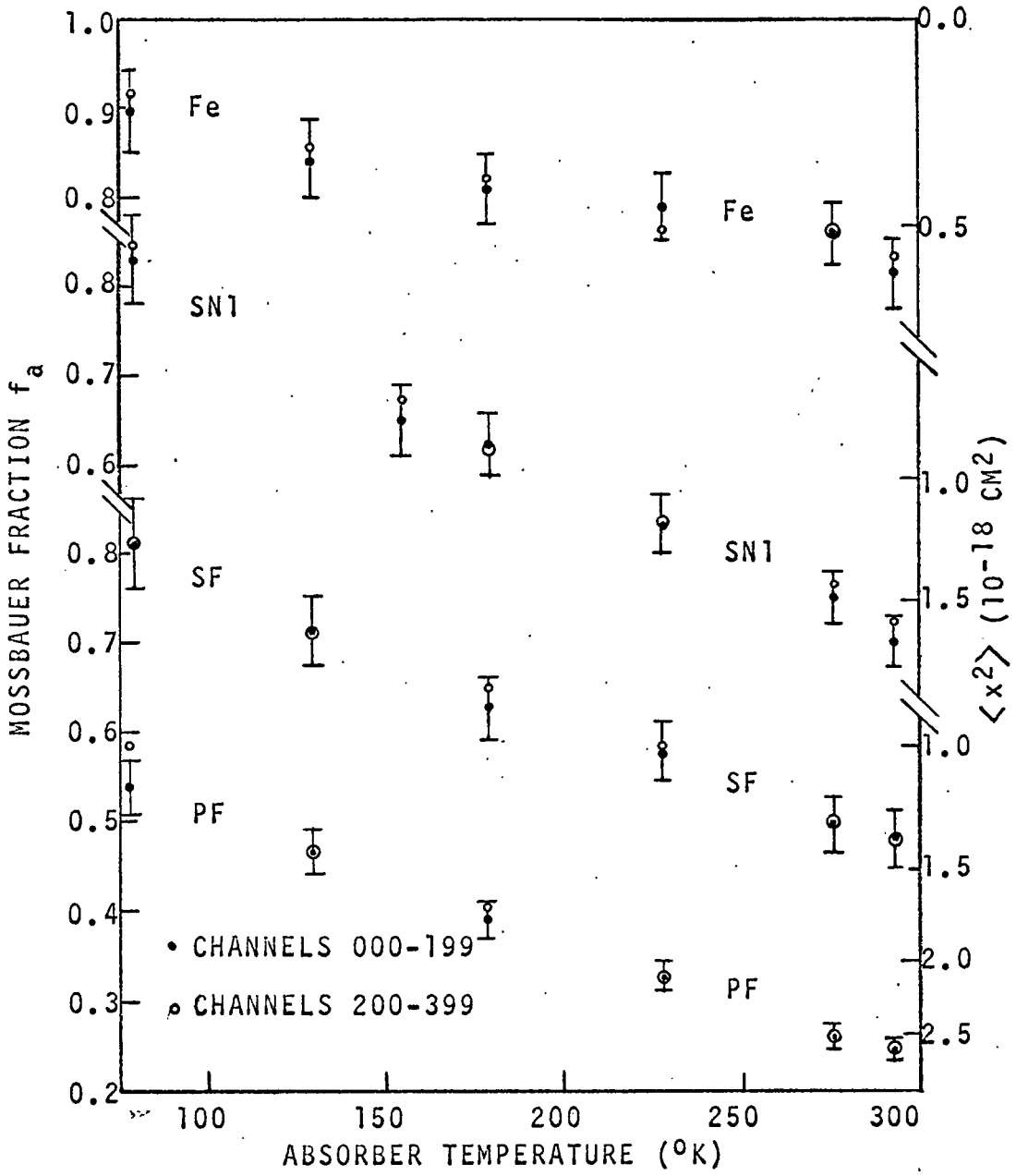


Fig. 17. Mossbauer fraction f_a in each absorber as a function of temperature. A value α_T=8.17 has been assumed. The right-hand scale shows $\langle x^2 \rangle$ as obtained from equation

$$f_a = e^{-k^2 \langle x^2 \rangle},$$

with k^2=5.335 X 10^{17} cm^{-2}. The error bars (shown only for channels 000-199) are ± one standard deviation. These are based on the standard deviations of the spectrum parameters obtained in the least-squared fit of the data to equation (47).

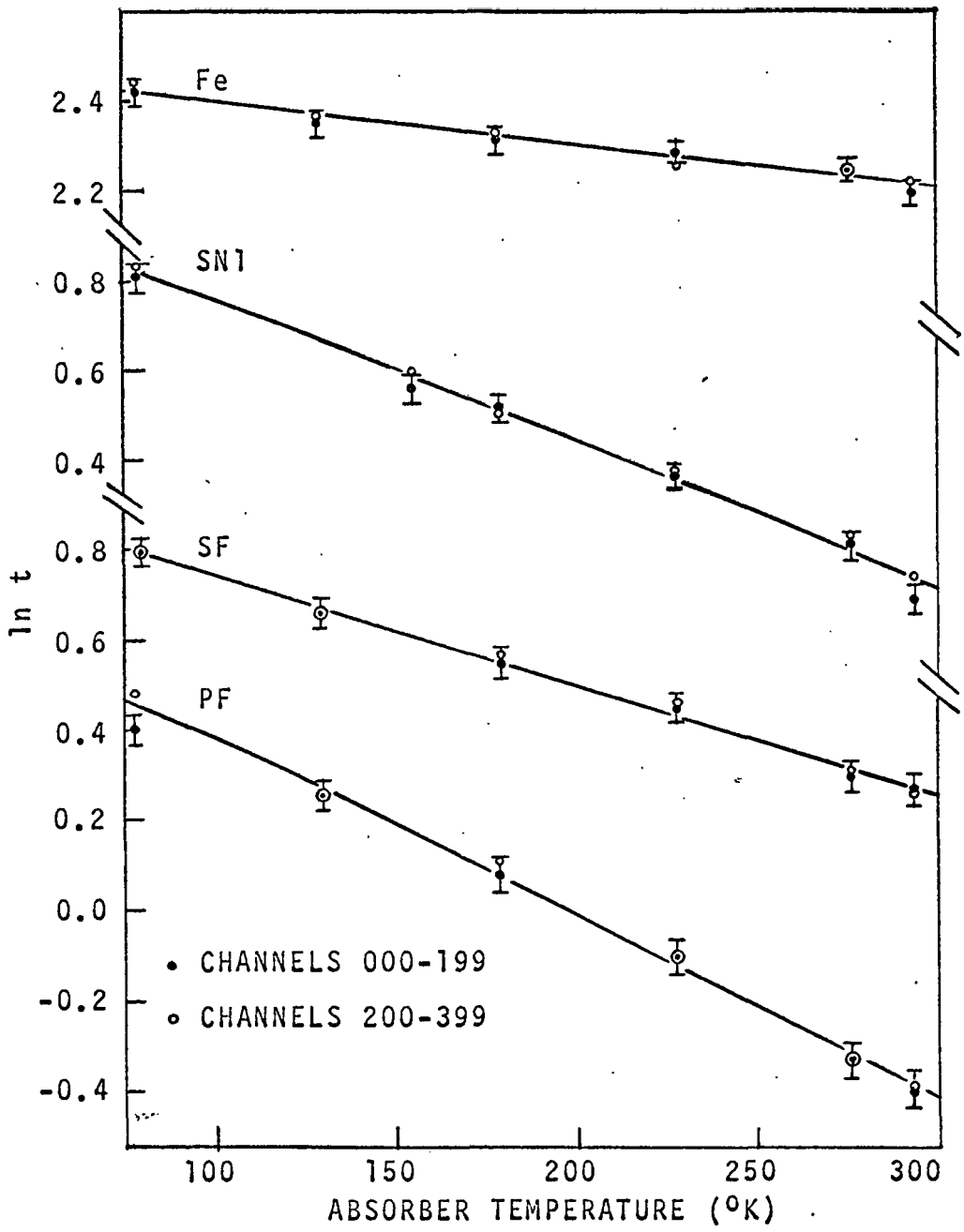


Fig. 18. Temperature dependence of ln t for each absorber, where $t=n_M \sigma_o f_a(T)$. The solid curves are the "average" Einstein models listed in Table IV.

Mossbauer spectrum is symmetric[2]. Thus, the centroid of the two inner lines is the centroid of the complete spectrum.) In the case of the single-line SF and PF spectra, the parameter V_1 obtained in the least-squares fit of the spectra is the resonant velocity V_0. Fig. 19 shows V_0 as a function of temperature for each absorber

D. Calculations of Einstein and Debye Models

The values of ln t(T) and $V_0(T)$ shown in Figs. 18 and 19 were fit to Einstein and Debye lattice models (equations (37)-(40)). Since these models are non-linear in the parameters Θ_E and Θ_D, it was necessary to use the technique described in Appendix A to perform the least-squares fit. Computer programs were written for this purpose and are shown in Appendix B. The results of the calculations for ln t(T) are shown in Table IV, and those for $V_0(T)$ are given in Table V. The solid curves in Figs. 18 and 19 represent the "average" Einstein Models in Tables IV and V respectively.

E. Temperature Dependence of Hyperfine Splittings in Metallic Fe and Sodium Nitroprusside

The total splitting in the six-line Fe spectrum (i.e., the separation between the first and last line) is proportional to the magnetic field H at the nucleus.[2] The temperature dependence of H observed in this experiment is shown in Fig. 20. The scale on the left gives the field

Fig. 19. Temperature dependence of V_0 in each absorber. V_0 is measured relative to sodium nitroprusside at 293°K. The error bars show the standard deviations calculated by fitting the spectra in the two halves of the MCA memory separately to equation (47). The actual data spread is greater than that suggested by these error bars, indicating a small systematic instrumental error, especially in the case of PF and SF. The source of the error has not yet been determined. The solid curves are the "average" Einstein models listed in Table V.

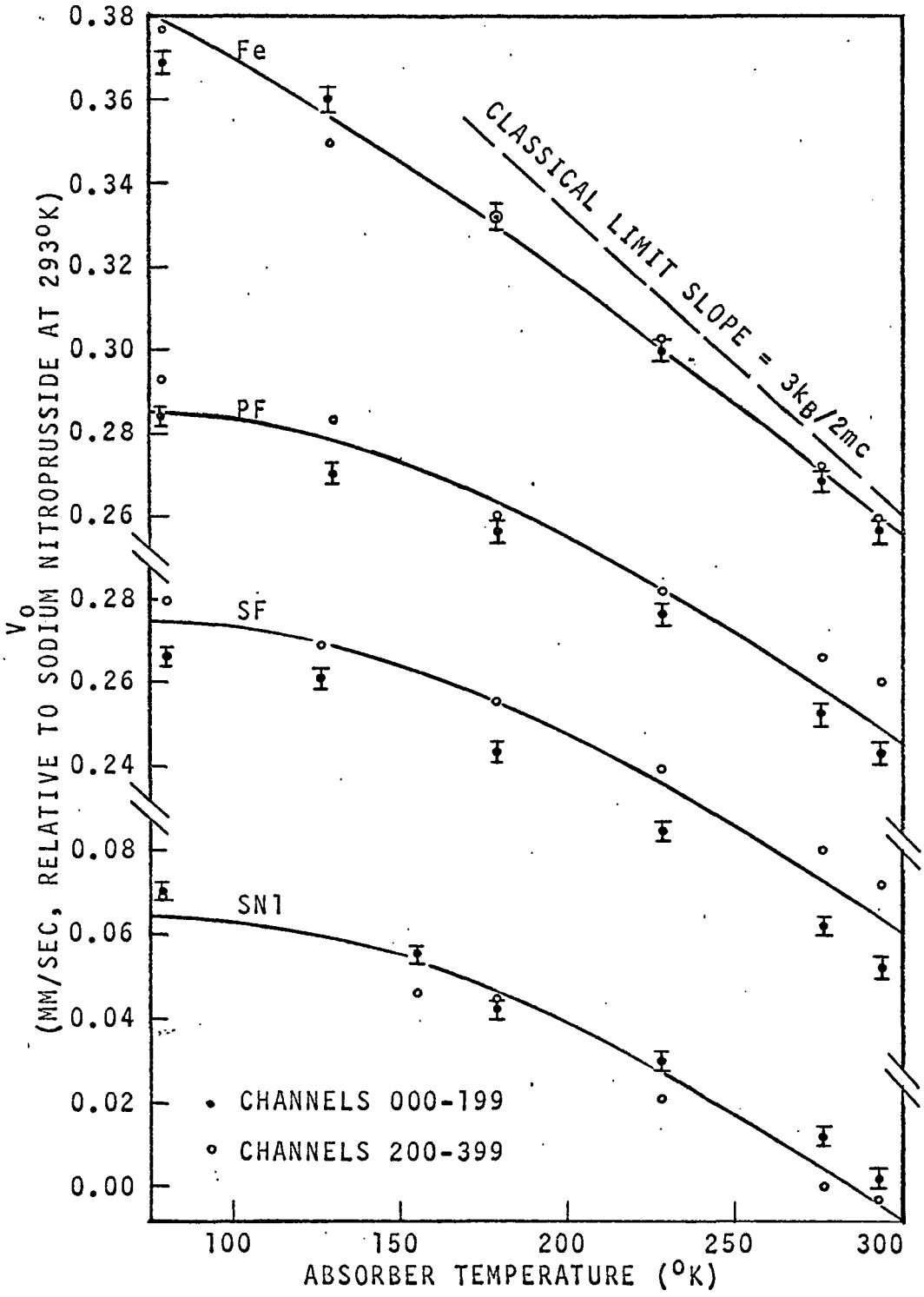

0.38
0.36
0.34
0.32
0.30
0.28
0.26
0.28
0.26
0.24
0.08
0.06
0.04
0.02
0.00
Fe
PF
SF
SN1
CLASSICAL LIMIT SLOPE = 3kB/2mc
• CHANNELS 000-199
○ CHANNELS 200-399
100
150
200
250
300
ABSORBER TEMPERATURE (°K)
V_o
(MM/SEC, RELATIVE TO SODIUM NITROPRUSSIDE AT 293°K)

TABLE IV. Einstein and Debye Models for ln t(T). Since ln t(T) is more sensitive to low-frequency vibrational modes than $V_o(T)$, the characteristic temperatures is the models below are lower than those in Table V. (See Discussion in Chapter V.)

Absorber	Channels	Einstein $\tau = \ln(n_M \sigma_o)$	Einstein θ_E(°K)	Debye $\tau = \ln(n_M \sigma_o)$	Debye θ_D(°K)
Fe	000-199	2.53±0.02	210±10	2.53±0.02	365±18
Fe	200-399	2.55±0.02	202±10	2.55±0.02	352±17
Fe	Average	2.54±0.02	206±10	2.54±0.02	358±18
SN1	000-199	1.13±0.04	116± 3	1.13±0.04	201± 5
SN1	200-399	1.13±0.02	118± 1	1.13±0.02	204± 3
SN1	Average	1.13±0.03	117± 2	1.13±0.03	203± 4
SF	000-199	1.03±0.01	133± 2	1.03±0.01	231± 3
SF	200-399	1.04±0.02	133± 3	1.04±0.02	230± 5
SF	Average	1.03±0.02	133± 3	1.03±0.02	231± 4
PF	000-199	0.78±0.03	108± 2	0.78±0.03	187± 3
PF	200-399	0.85±0.02	104± 1	0.85±0.02	181± 2
PF	Average	0.82±0.03	106± 2	0.82±0.03	184± 3

TABLE V. Einstein and Debye Models for $V_0(T)$. The higher characteristic temperatures in the salts are a result of the high-frequency (optical) vibrational modes in those substances. (See Chapter V.)

Absorber	Channels	Einstein		Debye	
		δ_0(mm/sec)	θ_E(°K)	δ_0(mm/sec)	θ_D(°K)
Fe	000-199	0.493±0.004	317±20	0.494±0.005	418±29
Fe	200-399	0.495±0.005	320±24	0.496±0.005	425±32
Fe	Average	0.494±0.003	318±22	0.495±0.005	421±30
SN1	000-199	0.285±0.011	602±40	0.294±0.011	828±52
SN1	200-399	0.264±0.011	547±40	0.271±0.011	747±53
SN1	Average	0.274±0.015	574±40	0.282±0.016	788±58
SF	000-199	0.463±0.003	538±11	0.469±0.003	732±15
SF	200-399	0.495±0.007	602±25	0.503±0.006	826±29
SF	Average	0.479±0.023	560±46	0.485±0.023	779±67
PF	000-199	0.469±0.005	514±20	0.474±0.005	698±23
PF	200-399	0.485±0.012	538±43	0.492±0.012	735±58
PF	Average	0.477±0.011	526±31	0.483±0.013	716±40

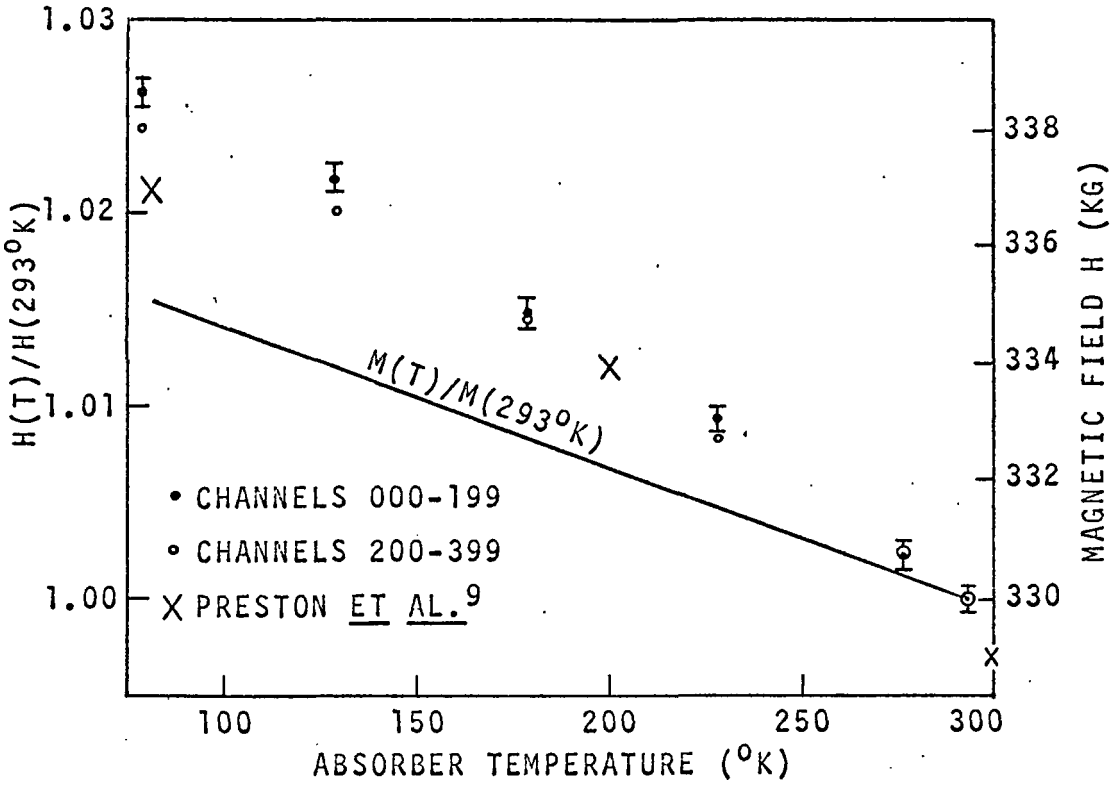


Fig. 20. Temperature dependence of magnetic field H at the Fe^{57} nucleus in metallic Fe. Also shown are the results obtained by Preston et al.[9] The solid curve gives the saturation magnetization M(T) in Fe according to the Bloch $T^{3/2}$ law

$$\frac{M(0)-M(T)}{M(0)} = CT^{3/2}$$

where $C=3.4 \times 10^{-6}$ $(°K)^{-3/2}$ for Fe.[42] See Chapter V for further discussion.

at each temperature relative to the field at 293°K. H(293°K) has been measured[9] to be 330±3kOe. This value converts the relative field values of the left-hand scale of Fig. 19 to absolute field values shown in the right-hand scale.

Fig. 21 shows the temperature dependence of the quadrupole splitting ΔE_Q in sodium nitroprusside, which at 293°K is 1.719±0.007 mm/sec. (See Fig. 15.)

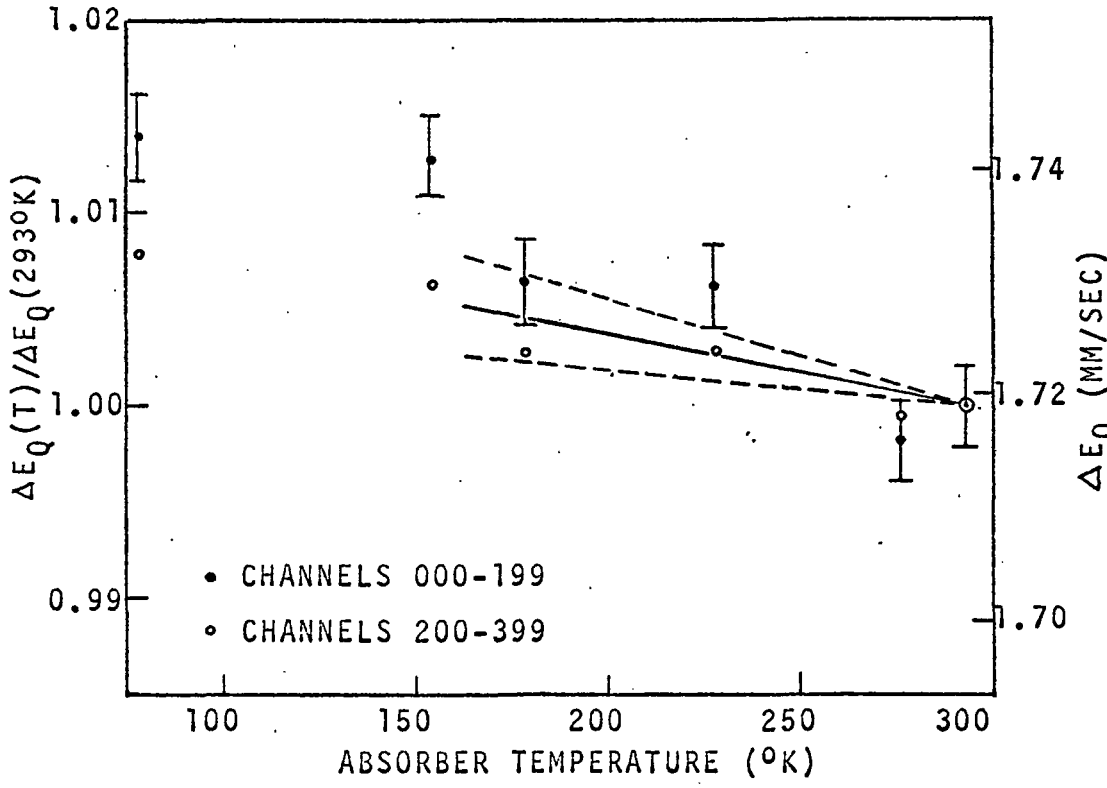


Fig. 21. Temperature dependence of the quadrupole splitting ΔE_Q in sodium nitroprusside. The solid line shows the temperature dependence observed by Kerler[8] in measurements down to 166°K. The dashed lines indicate the uncertainty in the slope of Kerler's results.

CHAPTER V

DISCUSSION OF RESULTS

A. Comparison of f_a and V_0 Values to Previous Mossbauer Studies

Margulies et al.[34] have measured the Mossbauer fraction in a metallic Fe absorber at room temperature and obtain f_a=1.44±0.15, where an internal conversion coefficient α_T=15 is used. The authors suggest that this physically impossible value can be reduced to a reasonable value if α_T is approximately 8. Using α_T=8.17, as in this work, Margulies' value is reduced to f_a=0.83±0.09 which is slightly above the value f_a=0.73±0.04 obtained in Fig. 17 for Fe at 293°K.

O'Connor and Longworth[35] have measured f_a in several metallic Fe absorbers at room temperature, obtaining f_a=0.76±0.06. The value of α_T used in their calculations is an average of 9.94±0.60 and 9.51±0.50. If one uses α_T=8.17, their result is reduced to f_a=0.65±0.05. Thus, the 293°K value f_a=0.73±0.04 given in Fig. 17 falls between Margulies' value and O'Connor's value when the same α_T is used.

Grant et al.[31] have measured f_a in single crystal absorbers of sodium nitroprusside at 296°K as a function of crystal orientation. Using α_T=8.17, they obtain f_a= 0.3674±0.0024, 0.3320±0.0035, and 0.3773±0.0037 for incident photon beams along the a, b, and c crystalline

axes respectively. These values are somewhat lower than the result $f_a=0.48\pm0.03$ in Fig. 17 for SN1 at 293°K. No explanation of this difference has been found.

Kerler[8] has measured f_a in metallic Fe, sodium nitroprusside, and potassium ferrocyanide absorbers at temperatures from 153°K to 353°K. In Chapter II it was stated that for a harmonic solid at high temperature, the $\langle x^2 \rangle$ versus T curve approaches a straight-line asymptote which goes through $\langle x^2 \rangle = 0$ at T=0. Since $f_a = e^{-k^2 \langle x^2 \rangle}$, for harmonic solid, ln f_a is proportional to $\langle x^2 \rangle$ and has a similar asymptotic behavior. Kerler calculates $t = n_M \sigma_o f_a$ as a function of T from each spectrum and fits a straight line to a plot of $\ln(t/n_M \sigma_o)$ vs T for each absorber, arbitrarily adjusting $n_M \sigma_o$ until the line goes through $\ln(t/n_M \sigma_o)=0$ at T=0. Since $f_a = t/n_M \sigma_o$, the value of f_a at each temperature is thus determined.

Fig. 22 shows the curves (solid lines) obtained by Kerler for f_a in metallic Fe, sodium nitroprusside, and potassium ferrocyanide using the method described above. When the data in Fig. 17 are re-adjusted using Kerler's method, the dashed lines in Fig 22 are obtained. The results of this work are consistently lower than Kerler's, which merely indicates that the f_a values in Fig 17 are more temperature dependent than Kerler's. One possible explanation may lie in the two different methods used to determine t from the spectra. Kerler uses only the fractional

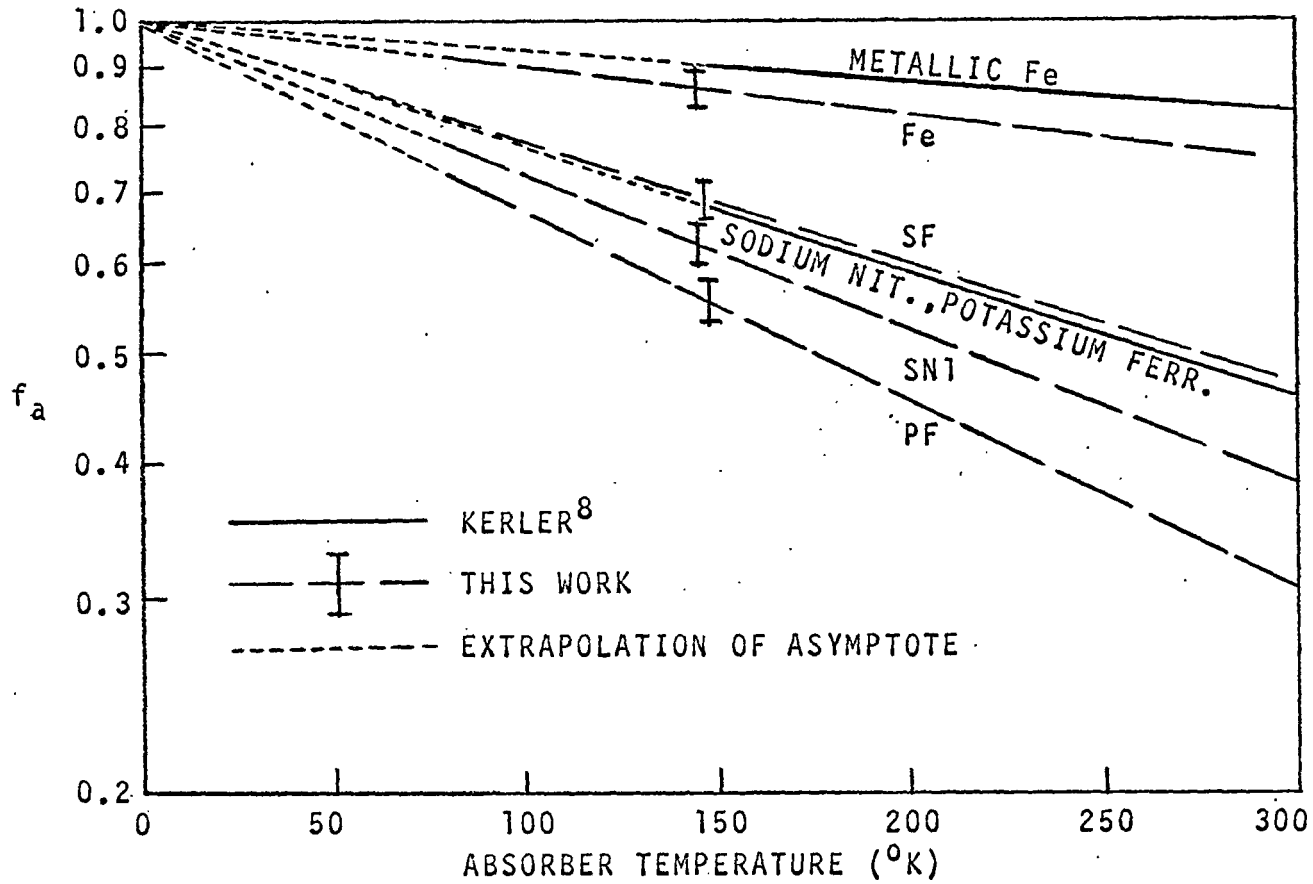


Fig. 22. Comparison of temperature dependence of f_a in metallic Fe, sodium nitroprusside, and potassium ferrocyanide. The solid lines are due to Kerler[8] and are based on data taken above 153°K. Kerler has arbitrarily shifted the curves vertically to give intercepts of $f_a=1$ at T=0. (See discussion in text.) The dashed lines are the results of the application of Kerler's method to the f_a values in Fig. 17. These lines are consistently lower than Kerler's because of a greater temperature dependence of f_a observed in this work.

absorption α at resonance, which increases with increasing t (see equation (28).), whereas the f_a values in Fig. 17 are calculated using the area A of the absorption line, which is proportional to the product of the fractional absorption α and the width of the line, both of which increase with increasing t. It can be shown[36] that A is mathematically more sensitive to an increase in t than is α. Thus, as the temperature of an absorber is lowered, the increase in t (and thus f_a) causes a greater change in A than in α. For this reason, it is preferable to use A rather than α to determine f_a.[36]

The shifts in ln f_a to obtain f_a=1 at T=0°K in Fig. 22 were small except for PF. In this case, the curve had to be shifted upward by about 0.3, which is almost a factor of 10 greater than the uncertaintity in the values of f_a. This suggests that potassium ferrocyanide may be anharmonic in the temperature range studied. A harmonic solid with f_a values as low as those of PF would exhibit a greater asymptotic temperature dependence than that shown by PF in Fig. 17.

Furthermore, the values for τ in Table IV and the absorber thicknesses can be used to determine values of σ_0 in each absorber. The results are shown in Table VI. PF gives a σ_0 considerably different from the value σ_0= 2.569×10^{-18} cm^2 based on α_T=8.17. This is another

TABLE VI. Values of σ_0 Determined from Table IV.

Absorber	τ	n_M (10^{18} cm^{-2})	σ_0 (10^{-18} cm^2)
Fe	2.54+0.02	4.9 +0.2	2.6+0.1
SN1	1.13+0.03	1.06+0.05	2.9+0.2
SF	1.03+0.02	1.06+0.05	2.6+0.1
PF	0.82+0.03	1.08+0.03	2.1+0.1

indication of an anomalously low value for f_a and suggests anharmonicity.

A similar effect has been observed in $FeCl_2$ by Johnson and Dash.[11] They observed that f_a in $FeCl_2$ is less sensitive to temperature than can be expected from a general harmonic solid. They attribute this to low-temperature anharmonicity.

Table VII compares the values of V_o at 293°K shown in Fig. 19 to those in previous studies at nearby temperatures. These differences in V_o at room temperature are often referred to as isomer shifts, even though they result partially from the lattice dynamical motion in the solids. Close agreement is obtained in all cases.

Table VIII is a comparison of previously observed shifts in V_o at various temperatures to shifts measured in this work (Fig. 19). No previous measurements of thermal shifts in sodium ferrocyanide have been found.

B. Characteristic Temperatures θ_E and θ_D

In Tables IV and V, one notes certain trends in the behavior of the characteristic temperatures θ_E and θ_D. First, θ_E and θ_D are always lower for the ln t(T) data (Table IV) than for the $V_o(T)$ data (Table V). This relationship results from the fact that ln t(T) is related to $\langle x^2 \rangle_T$ of the Mossbauer nucleus, while $V_o(T)$ is deter-

TABLE VII. Comparison of Values for V_0 near 293 °K.

Absorber	V_0[a] (mm/sec)	Temperature (°K)	Reference
Fe	0.258±0.003	293	Present Work
	0.257±0.006	298	8
	0.26 ±0.01	"room"	4
PF	0.21 ±0.01	293	Present Work
	0.219±0.006	298	38
	0.212±0.01	"room"	4
SF	0.20 ±0.01	293	Present Work
	0.25 ±0.05	"room"	37

[a] V_0 is stated relative to sodium nitroprusside at room temperature, for which V_0=0. In references where V_0 is given as an actual source velocity, and no sodium nitroprusside measurement is given, a conversion is made using known isomer shifts of sources[4].

TABLE VIII. Comparison of Thermal Shifts.

Absorber	T_1 (°K)	T_2 (°K)	$V_o(T_2)-V(T_1)$ (mm/sec)	Reference
Fe	293	79	0.115±0.004	Present Work
	298	82	0.113±0.003	9
	290	78	0.11 ±0.04	39
PF	293	130	0.065±0.003	Present Work
	295	123	0.062±0.004	40
SN1	293	155	0.050±0.003	Present Work
	298	166	0.040±0.004	38
	293	179	0.044±0.006	Present Work

mined by $\langle v^2 \rangle_T$. Recall for a harmonic solid, $\langle x^2 \rangle_T$ and $\langle v^2 \rangle_T$ are given by equations (17) and (18):

$$\langle x_j^2 \rangle_T = \frac{\hbar}{m_j} \sum_{i=1}^{3N} \left(\frac{1}{2} + \frac{1}{e^{\hbar\omega_i/k_B T} - 1} \right) \frac{b_{jxi}^2}{\omega_i} \tag{17}$$

and

$$\langle v_j^2 \rangle_T = \frac{\hbar}{m_j} \sum_{i=1}^{3N} \left(\frac{1}{2} + \frac{1}{e^{\hbar\omega_i/k_B T} - 1} \right) (b_{jxi}^2 + b_{jyi}^2 + b_{jzi}^2)\, \omega_i . \tag{18}$$

Because of the weighting factors ω_i^{-1} and ω_i for each term in equations (17) and (18) respectively, $\langle x^2 \rangle_T$ is weighted toward lower frequencies than is $\langle v^2 \rangle_T$. Thus, the characteristic temperatures calculated from ln t(T) are lower than those from $V_0(T)$.

This effect is much greater in the salts than in metallic Fe because of the existence of high-frequency (optical) modes of vibration in the former. These modes are responsible for the infrared absorption lines exhibited by these salts as discussed below. These optical modes involve intra-molecular vibrations in which ion-ion (short-range) interations are involved. Because these interactions are generally stronger than metallic bonds, they usually involve higher frequencies. Thus, θ_E and θ_D based on $V_0(T)$ measurements are larger for the salts than for the metallic Fe.

On the other hand, the ln t(T) data yield information about the low-frequency modes of vibration. These are the

acoustic modes, in which long-wavelength elastic vibrations are excited in the solid. Since the characteristic temperatures in Table IV are lower for the salts than for Fe, it can be concluded that the acoustic modes in these salts are of lower frequency than those in metallic Fe.

There is a relatively small difference in the values of θ_D for Fe in the two tables. This indicates both the Mossbauer fraction and the thermal shift in Fe can be described quite well by a single Debye model of $\theta_D \approx 390°K$.

It is of interest to compare the values of θ_D obtained for Fe in this work to those values obtained in other studies. Thermal shift studies by Preston et al.[9] resulted in $\theta_D = 400 \pm 30°K$, which agrees closely with the value in Table V. Using neutron diffraction data, Housley and Hess[10] performed theoretical calculations, predicting that the thermal shift in metallic Fe above $\sim 200°K$ should be characteristic of an Einstein solid of $\theta_D = 422 \pm 3°K$, in excellent agreement with the value of $\theta_D = 421 \pm 30°K$ in Table V. Finally, de Launay[41] gives a value $\theta_D = 420°K$ based on specific heat data for Fe at temperatures where the specific heat is about half the Dulong-Petit value. This also agrees with our results.

Hazony[40] has calculated an Einstein temperature $\theta_E = 700 \pm 50°K$ from thermal shift measurements in potassium ferrocyanide. However, he treats the oscillator mass and

frequency as variable parameters, using m=78 amu in the thermal shift data. If a value m=57 amu were used (as in the models used in this work), Hazony's value for θ_E would be reduced almost proportionally and would be much closer to that given in Table V. No other determinations of θ_E or θ_D in the salts studied in the present work have been found.

Infrared absorption lines have been measured in powdered absorbers of sodium nitroprusside, sodium ferrocyanide, and potassium ferrocyanide.[13,14] The strongest lines that are interpreted as vibrational modes involving the Fe atom are given in Table IX. The higher-frequency line is associated with the Fe-C-N bending mode, and the lower frequency, with Fe-C stretching.[15] The frequencies of absorption are given in terms of $\bar{\nu}$ in cm^{-1} as well as a characteristic temperature θ defined by $k_B\theta = \hbar\omega$, where ω is obtained from the relation $\omega = 2\pi c\bar{\nu}$. Also shown in Table IX are the thermal-shift Debye temperatures θ_D for the salts (taken from Table V). Note the relative closeness of the θ_D values to the average θ values, especially in SF and PF. This agreement is not unreasonable; in the Debye model of a solid, θ_D corresponds to the maximum vibrational frequency, while in the real solid, the infrared frequencies are the highest frequencies in the true vibrational spectrum.

TABLE IX. Infrared absorption lines involving vibrations of iron atoms in sodium nitroprusside, sodium ferrocyanide, and potassium ferrocyanide.

Absorber	$\bar{\nu}$ [a] (cm^{-1})	θ (^oK)	θ_D [b] (^oK)
SN1	425 (stretching) 500 (bending)	612 720	788±58
SF	430 (stretching) 588 (bending)	619 846	779±67
PF	419 (stretching) 588 (bending)	603 846	716±40

[a] Reference 14.

[b] From Table V.

C. Temperature Dependence of Hyperfine Splitting in Fe and SN1

In Fig. 20, the observed temperature dependence of the magnetic field H at the Fe^{57} nucleus in metallic Fe is compared to the Bloch $T^{3/2}$ law for the magnetization M(T) in a ferromagnet[42],

$$\frac{M(0) - M(T)}{M(0)} = C T^{3/2} \quad .$$

This relation is valid for $T \ll T_c$, where T_c is the Curie temperature of the solid. (T_c=1043°K for Fe.) The above equation has been experimentally verified for Fe as discussed by Kittel[42], with the result that $C=(0.34\pm0.2) \times 10^{-6} °K^{-3/2}$. As seen in Fig. 20, M(T) in Fe decreases more slowly than does H as the temperature increases. This has also been observed by Preston et al.[9]

The quadrupole splitting in SN1, shown in Fig. 21, appears to be slightly more temperature sensitive than that observed by Kerler.[8] The increase in splitting with decreasing temperature is quite common in iron compounds. Kerler has measured the temperature dependence of the quadrupole splitting in eight compounds and obtains a negative slope in splitting versus temperature in all cases. The values range from -0.01×10^{-3} mm/sec°K to -4.31×10^{-3} mm/sec°K. Danon[33] has presented data showing that the quadrupole splitting in several iron compounds becomes relatively insensitive to temperature below 100°K.

CHAPTER VI

SUMMARY AND CONCLUSIONS

Mossbauer absorption spectra of metallic iron, sodium ferrocyanide, and potassium ferrocyanide absorbers have been measured at several temperatures between 78°K and 293°K. The temperature dependence of the Mossbauer fraction $f_a(T)$ and resonant velocity $V_0(T)$ of each absorber have been explained in terms of simple harmonic (Einstein and Debye) lattice models.

For a given absorber, the characteristic temperatures of the lattice models representing $f_a(T)$ are considerably lower than in the models representing $V_0(T)$. This is explained by the greater sensitivity of $f_a(T)$ to low-frequency modes of vibration. The characteristic temperatures of the models representing $V_0(T)$ are greater in the salts than in the iron metal. This is interpreted as due to the presence of infrared vibration modes in the salts.

The value of f_a is lower in potassium ferrocyanide than in the other absorbers studied. The temperature dependence of f_a in that substance is weaker than expected for a harmonic solid with the same low value of f_a. This suggests that potassium ferrocyanide may be anharmonic in the temperature range studied.

Finally, the temperature dependence of the hyperfine splitting in metallic iron and sodium nitroprusside observed in this work agree with the results of previous studies. The magnetic field at the Fe^{57} nucleus in metallic iron is shown to be more temperature sensitive than the saturation magnetization, verifying a result of earlier work. The quadrupole splitting in sodium nitroprusside varies by less than 2% from 79°K to 293°K. Thus, when the sodium nitroprusside splitting is used for velocity calibration over a temperature range of a few degrees, temperature corrections in its splitting are relatively unimportant.

The present work suggests several possible areas of future study:

(a) The fairly close agreement between the infrared absorption frequencies and thermal-shift Debye frequencies of the salts studied in this work is an interesting, though perhaps accidental, result. Similar studies should be made using iron salts with infrared frequencies much different from those of the salts studied here to determine the significance of this result.

(b) The apparent anharmonicity of potassium ferrocyanide should be studied in more detail. An extension of the present work to temperatures below the

Dulong-Petit range for potassium ferrocyanide would furnish more detailed information concerning the lattice dynamics of that substance.

(c) A detailed study should be made concerning the value of the internal conversion coefficient α_T for the 14.4 kev decay of Fe^{57}. Specifically, the question of whether α_T is a constant independent of the absorber should be investigated. Since the transition probability for internal conversion depends on the strength of the electromagnetic interactions of the Fe^{57} nucleus with its atomic electrons, there may exist a relation between α_T and the isomer shift of an absorber.

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APPENDIX A

LEAST SQUARES FIT TO A NONLINEAR MODEL

In a least squares fit, one attempts to fit a theoretical function

$$y = f(\{A_j\}, x) \tag{1}$$

to the N data points (Y_i, X_i), i=1, 2,...,N, by choosing values of the model parameters A_j, j=1, 2,...,n ($n \leq N$) such that the sum S of the squares of the errors is minimized. Thus, if

$$S = \sum_{i=1}^{N} [Y_i - y(\{A_j\}, X_i)]^2 \quad , \tag{2}$$

then we require that

$$\frac{\partial S}{\partial A_j} = 0 \qquad [j = 1, 2, \ldots, n]. \tag{3}$$

The values of the A_j which minimize the squares of the errors are those which satisfy the n simultaneous equations (3).

If the A_j appear in equation (1) in non-linear powers, equations (3) are nonlinear and difficult (if not impossible) to solve in closed form. We may circumvent this diffulty by linearzing the model, equation (1), and applying an iterative procedure.

We estimate the values of A_j by initial guesses a_j. Expanding equation (1) in a Taylor series about these estimates, we have

$$y(\{A_j\},x) \approx y(\{a_j\},x) + \sum_{k=1}^{n} (A_k - a_k) \left.\frac{\partial y}{\partial A_k}\right|_{A_k = a_k} . \qquad (4)$$

We then fit the data (Y_i, X_i) to the approximate model, equation (6), and obtain values for A_k which are improvements over the initial guesses a_k (if these initial guesses are sufficiently accurate). These improved values can then be used as new extimates, and the process repeated until the desired accuracy is obtained.

Combining equations (2) and (3), we have

$$\sum_{i=1}^{N} [Y_i - y(\{A_j\},X_i)] \frac{\partial}{\partial A_\ell} y(\{A_j\},X_i) = 0 \qquad [\ell = 1,\ldots,n] .$$

Substituting equation (4) into the above, we obtain

$$\sum_{k=1}^{n} A_k \left(\sum_{i=1}^{N} \left.\frac{\partial y}{\partial A_k}\right|_{a_k} \left.\frac{\partial y}{\partial A_\ell}\right|_{a_\ell, X_i} \right) = \sum_{i=1}^{N} \left.\frac{\partial y}{\partial A_\ell}\right|_{a_\ell, X_i} \left[Y_i - y(\{a_j\},X_i) + \sum_{m=1}^{n} a_m \left.\frac{\partial y}{\partial A_m}\right|_{a_m, X_i} \right]$$

$$[\ell = 1,\ldots,n]$$

This equation is a matrix equation of the form

$$\overleftrightarrow{F} \cdot \vec{A} = \vec{G} \qquad (5)$$

where

$$(\overleftrightarrow{F})_{kl} \equiv \sum_{i=1}^{N} \frac{\partial Y}{\partial A_k} \frac{\partial Y}{\partial A_l}\bigg|_{a_k, a_l, X_i} \quad ; \tag{6}$$

$$(\vec{A})_k = A_k \quad ; \tag{7}$$

$$(\vec{G})_l = \sum_{i=1}^{N} \frac{\partial Y}{\partial A_l}\bigg|_{a_l, X_i} \cdot \left[Y_i - y(\{a_j\}, X_i) + \sum_{m=1}^{n} a_m \frac{\partial Y}{\partial A_m}\bigg|_{a_m, X_i} \right]. \tag{8}$$

The solutions A_k of the matrix equation (5) are the desired improved values for a_k.

The solutions to (5) are functions of experimentally measured quantities X_i and Y_i, and uncertaintities in X_i and Y_i result in uncertaintities in the values of the A_k. Assuming errors in X_i are negligible, we differentiate equation (5) with respect to Y_j to obtain

$$\overleftrightarrow{F} \cdot \frac{\partial \vec{A}}{\partial Y_j} = \vec{H}_j \qquad [j = 1, \ldots, N], \tag{9}$$

where

$$\left(\frac{\partial \vec{A}}{\partial Y_j}\right)_k \equiv \frac{\partial A_k}{\partial Y_j} \tag{10}$$

and

$$(\vec{H}_j)_\ell \equiv \frac{\partial Y}{\partial A_\ell}\Big|_{a_\ell, X_i} \quad . \tag{11}$$

Equation (9) may then be solved for the n values of $\partial A_k / \partial Y_j$. This must be done for each of the N values of Y_j, so that n X N values are obtained. The standard deviation α_k of the resulting value A_k is given by

$$\alpha_k^2 = \sum_{j=1}^{N} \left(\frac{\partial A_k}{\partial Y_j}\right)^2 \sigma_j^2 \quad ,$$

where the σ_j are the standard deviations of the measurements Y_j.

APPENDIX B

COMPUTER PROGRAMS FOR LEAST SQUARES FITS

In the following pages are the listings of three computer programs, and their subprograms, that were used in this work. Each employs the technique described in Appendix A to perform a least squares fit to a non-linear model. The programs listed are: (1) a program to fit the Mossbauer spectra collected in the MCA memory (Appendix C) to equation (47); (2) a program to fit Mossbauer fraction data, ln t *versus* temperature, to an Einstein model (equation (37)) and/or a Debye model (equation (39)); and (3) a program to fit thermal shift data, V_0 *versus* temperature, to an Einstein model (equation (38)) and/or a Debye model (equation (40)).

```
C****************** PROGRAM TO FIT M. E. DATA ******************************
      DIMENSION IDATA(200),IO(200),X(200),Y(200),ID(20),E(200),EE(200)
      DIMENSION A(33),AA(33),H(10),W(10),P(10),HH(10),WW(10),PP(10)
      DIMENSION V(200),AL(33),D(200,33),F(33,33),G(33),SIG2(200),SAL(33)
      DIMENSION SIGH(10),SIGW(10),SIGP(10),SIGA(33),FW(33,33),LL(33)
      EQUIVALENCE (AL,SAL,SIGA),(Y,SIG2),(H,HH),(W,WW),(P,PP),(E,EE)
      DATA LAST/'LAST'/
      LIMIT=2
      TOL=0.001
      TOLP=0.001
C****************** READ DATA ***********************************************
 1    READ(5,2)ID
 2    FORMAT(20A4)
      IF(IO(1).EQ.LAST)GO TO 99
      READ(5,3)NC,NO,NOV,IXO,NL
 3    FORMAT(I6,9I7)
      READ(5,3)(IDATA(I),I=1,NC)
      READ(5,3)(IO(I),I=1,NO)
      READ(5,4)(H(I),W(I),P(I),I=1,NL),BL,XO,R
 4    FORMAT(3F10.1)
C****************** WRITE DATA **********************************************
      WRITE(6,41)
 41   FORMAT(1H1)
      WRITE(6,42)ID
 42   FORMAT(/130('*')/21X,20A4/130('*'))
      WRITE(6,43)NC,NO,NOV,IXO,NL
 43   FORMAT(/'NO. CHANNELS=',I4,' -- NO. OMITTED CHANNELS=',I4,' -- NO.
     1MEMORY OVERFLOWS=',I3,' -- FIRST CHANNEL=',I4,' -- NO. LINES=',I3)
      WRITE(6,44)(IDATA(I),I=1,NC)
 44   FORMAT(/T65,'DATA'/(T31,10I7))
      WRITE(6,45)(IO(I),I=1,NO)
 45   FORMAT(/T58,'OMITTED CHANNELS'/(T31,10I7))
      WRITE(6,46)
 46   FORMAT(//T53,'***** INITIAL ESTIMATES *****'//T49,'HEIGHTS'T65,'WI
     1DTHS'T78,'POSITIONS')
```

```
      WRITE(6,47)(H(I),W(I),P(I),I=1,NL)
 47   FORMAT(/(T44,3(1X,E14.6)))
      WRITE(6,48)
 48   FORMAT(/T49,'BASELINE'T63,'PAR. PEAK',T78,'FRAC. MOD.')
      WRITE(6,47)BL,XO,R
C****************** CALCULATE DATA POINTS ***********************************
      CALL TTDATA(IDATA,NC,IO,NO,NOV,IXO,X,Y,NP)
      WRITE(6,56)NP
 56   FORMAT(/'NP=',I5)
      WRITE(6,6)(X(I),I=1,NP)
 6    FORMAT(/T66,'X'/(T16,10F10.1))
      WRITE(6,65)(Y(I),I=1,NP)
 65   FORMAT(/T66,'Y'/(T16,10F10.1))
C****************** CALCULATE ERRORS ****************************************
      NA=3*NL+3
      NTOL=0
      CALL PTOA(NL,A,H,W,P,BL,XO,R)
      WRITE(6,7)(A(I),I=1,NA)
 7    FORMAT(//T66,'A'//(9E14.6))
      IT=0
      S=0.
      DO 705 I=1,NP
      E(I)=Y(I)-YLRMOD(A,NL,X(I))
 705  S=S+E(I)**2
      WRITE(6,706)S
 706  FORMAT(/'SUM OF SQUARES OF ERRORS=',E14.6)
      DO 7111 I=1,NP
 7111 V(I)=1.
      NN=3*NL+1
      NNN=NN+1
      NNNN=NNN+1
 7112 CONTINUE
      RLAM=1.
C****************** CALCULATE D MATRIX ***************************************
      DO 712 I=1,NP
```

```
      D(I,NN)=1.+A(NNN)*X(I)+A(NNNN)*X(I)**2
      Q=A(NN)
      DO 7115 J=1,NL
      JJ=NL+J
      JJJ=2*NL+J
      B=X(I)-A(JJJ)
      C=1.+A(JJ)*B**2
      Q=Q+A(J)/C
      D(I,J)=D(I,NN)/C
      D(I,JJ)=-A(J)*B**2*D(I,J)/C
      D(I,JJJ)=2.*A(J)*A(JJ)*B*D(I,J)/C
 7115 CONTINUE
      D(I,NNN)=Q*X(I)
      D(I,NNNN)=D(I,NNN)*X(I)
 712  CONTINUE
C********************* CALCULATE F AND G MATRICES ******************************
      DO 713 J=1,NNNN
      G(J)=0.
      DO 713 K=1,NNNN
 713  F(J,K)=0.
      DO 714 I=1,NP
      DO 714 J=1,NNNN
      Z=V(I)*D(I,J)
      G(J)=G(J)+Z*E(I)
      DO 714 K=J,NNNN
      F(J,K)=F(J,K)+Z*D(I,K)
      F(K,J)=F(J,K)
 714  CONTINUE
C********************* SOLVE LINEAR NORMAL EQUATIONS ***************************
      CALL MATINV(F,FW,NNNN,33,IFLAG,LL)
      IF(IFLAG.NE.1)GO TO 7145
      WRITE(6,7144)
 7144 FORMAT(//130('*')/T52,'F MATRIX SINGULAR'/130('*'))
      GO TO 99
 7145 CONTINUE
```

```
      DO 715 I=1,NNNN
      AL(I)=0.
      DO 715 J=1,NNNN
  715 AL(I)=F(I,J)*G(J)+AL(I)
C***************** CONVERGENCE TEST ***************************************
      ALG=0.
      DO 716 J=1,NNNN
  716 ALG=ALG+AL(J)*G(J)
      IF(ALG.GE.0.)GO TO 7265
      RLAM=-RLAM
 7265 SS=0.
      DO 7266 J=1,NNNN
 7266 AA(J)=A(J)+RLAM*AL(J)
      DO 7267 I=1,NP
      EE(I)=Y(I)-YLRMOD(AA,NL,X(I))
      SS=SS+EE(I)**2
 7267 CONTINUE
      IT=IT+1
      WRITE(6,73)IT
   73 FORMAT(//40('*'),'AFTER',I3,1X,'ITERATIONS',40('*'))
      WRITE(6,74)(AA(I),I=1,NA)
   74 FORMAT(//T65,'AA'//(9E14.6))
      WRITE(6,706)SS
      IF(ICON(A,AA,NL,TOL,TOLP).EQ.1)GO TO 8
      NTOL=0
      GO TO 802
    8 NTOL=NTOL+1
      WRITE(6,801)NTOL
  801 FORMAT(/'ALL PARAMETERS WITHIN TOLERANCE, NTOL =',I2)
      IF(NTOL.EQ.LIMIT)GO TO 85
  802 CONTINUE
      DO 81 J=1,NA
   81 A(J)=AA(J)
      DO 82 I=1,NP
   82 E(I)=EE(I)
```

```
      S=SS
      GO TO 7112
C***************** CALCULATE STANDARD DEVIATIONS ***********************
 85   CONTINUE
      SIG2TH=0.
      DO 8501 I=1,NP
 8501 SIG2TH=SIG2TH+SQRT(Y(I))
      XP=NP
      SIG2TH=(SIG2TH/XP)**2
      CHISQ=SS/SIG2TH
      CHMIN=NP-SQRT(2.*XP)
      CHMAX=NP+SQRT(2.*XP)
      SIGYSQ=0.
      DO 851 J=1,NP
 851  SIGYSQ=SIGYSQ+EE(J)**2
      SIGYSQ=SIGYSQ/(NP-NA)
      DO 852 I=1,NP
 852  SIG2(I)=SIGYSQ
      DO 86 K=1,NA
      SAL2=0.
      DO 855 J=1,NP
      DAJ=0.
      DO 854 L=1,NA
 854  DAJ=DAJ+F(K,L)*V(J)*D(J,L)
 855  SAL2=SAL2+DAJ*DAJ*SIG2(J)
      SAL(K)=SQRT(SAL2)
 86   CONTINUE
      DO 87 K=1,NA
 87   SIGA(K)=SAL(K)
      DO 88 K=1,NL
      KK=NL+K
      KKK=KK+NL
      SIGH(K)=SIGA(K)
      SIGB(K)=SIGA(KK)/AA(KK)**1.5
 88   SIGP(K)=SIGA(KKK)
```

```
      SIGBL=SIGA(NN)
      T=(SIGA(NNN)/(2.*AA(NNNN)))**2
      TT=((AA(NNN)*SIGA(NNNN))/(2.*AA(NNNN)))**2
      SIGXO=SQRT(T+TT)
      T=((AA(NNN)*SIGA(NNN))/(2.*AA(NNNN)))**2
      TT=((AA(NNN)**2*SIGA(NNNN))/(4.*AA(NNNN)**2))**2
      SIGF=SQRT(T+TT)
C*****************  PRINT RESULTS  ************************************
      CALL ATOP(NL,AA,HH,WW,PP,BBL,XXO,FF)
      WRITE(6,9)
 9    FORMAT(//T24,23('*'),'  SPECTRUM PARAMETERS (STD. DEVIATIONS)  ',2
     13('*')//T32,'HEIGHTS',T64,'WIDTHS',T95,'POSITIONS')
      WRITE(6,91)(HH(I),SIGH(I),WW(I),SIGW(I),PP(I),SIGP(I),I=1,NL)
 91   FORMAT(/(T21,3(E13.6,' (',E12.6,')    ')))
      WRITE(6,92)
 92   FORMAT(/T31,'BASELINE',T63,'PAR. PEAK',T94,'FRAC. MOD.')
      WRITE(6,91)BBL,SIGBL,XXO,SIGXO,FF,SIGF
      WRITE(6,93)CHISQ,CHMIN,CHMAX
 93   FORMAT (//T24,29('*'),2X,'CHI-SQUARE=',E13.6,2X,30('*')/T41,'LOWER
     1 LIMIT=',E13.6,3X,'UPPER LIMIT=',E13.6)
      GO TO 1
 99   STOP
      END
```

```
      FUNCTION ICON(A,AA,NL,TOL,TOLP)
      DIMENSION A(33),AA(33)
      DO 2 J=1,NL
      IF(ABS(1.-A(J)/AA(J)).GE.TOL)GO TO 9
      JJ=NL+J
      IF(ABS(1.-A(JJ)/AA(JJ)).GE.TOL)GO TO 9
      JJJ=2*NL+J
      DP=(AA(JJJ)-A(JJJ))/SQRT(4./AA(JJ))
      IF(ABS(DP).GE.TOLP)GO TO 9
2     CONTINUE
      NN=3*NL+1
      NNN=NN+2
      DO 3 J=NN,NNN
3     IF(ABS(1.-A(J)/AA(J)).GE.TOL)GO TO 9
      ICON=1
      GO TO 99
9     ICON=0
99    RETURN
      END
```

```
      FUNCTION YLRMOD(A,NL,X)
      DIMENSION A(33)
      NN=3*NL+1
      NNN=NN+1
      NNNN=NNN+1
      YLRMOD=A(NN)
      DO 2 J=1,NL
      JJ=NL+J
      JJJ=2*NL+J
2     YLRMOD=YLRMOD+A(J)/(1.+A(JJ)*(X-A(JJJ))**2)
      P=1.+A(NNN)*X+A(NNNN)*X**2
      YLRMOD=YLRMOD*P
      RETURN
      END
```

```
      SUBROUTINE TTDATA(IDATA,NC,IO,NO,NOV,IXO,X,Y,NP)
      DIMENSION IDATA(NC),IO(NO),X(NC),Y(NC)
      NN=NOV*1000000
      MM=0
      DO 2 I=1,NC
      J=I+IXO-1
      IF(MM.EQ.NO)GO TO 15
      IF(J.NE.IO(MM+1))GO TO 15
      MM=MM+1
      GO TO 2
   15 II=I-MM
      X(II)=J
      Y(II)=IDATA(I)+NN
    2 CONTINUE
      NP=NC-NO
      RETURN
      END
```

```
      SUBROUTINE PTOA(N,A,H,W,P,BL,XO,F)
      DIMENSION A(33),H(N),W(N),P(N)
      NI=3*N+1
      NII=3*N+2
      NIII=3*N+3
      DO 2 J=1,N
      JJ=N+J
      JJJ=2*N+J
      A(J)=H(J)
      A(JJ)=4./W(J)**2
      A(JJJ)=P(J)
2     CONTINUE
      A(NI)=BL
      A(NII)=2.*F/XO
      A(NIII)=-F/XO**2
      RETURN
      END
```

```
      SUBROUTINE ATOP(N,A,H,W,P,BL,XO,F)
      DIMENSION A(33),H(N),W(N),P(N)
      NI=3*N+1
      NII=3*N+2
      NIII=3*N+3
      DO 2 J=1,N
      JJ=N+J
      JJJ=2*N+J
      H(J)=A(J)
      W(J)=SQRT(4./A(JJ))
      P(J)=A(JJJ)
2     CONTINUE
      BL=A(NI)
      XO=-A(NII)/(2.*A(NIII))
      F=-A(NII)**2/(4.*A(NIII))
      RETURN
      END
```

```
      SUBROUTINE MATINV(A,B,N,NDEM,IFLAG,L)
      DIMENSION A(NDEM,NDEM),B(NDEM,NDEM),L(NDEM)
C***************** INITIALIZE B MATRIX ***************************************
      DO 105 I=1,N
      DO 105 J=1,N
 105  B(I,J)=0.
      DO 106 I=1,N
 106  B(I,I)=1.
      IFLAG=0
C**** INITIALIZE L ARRAY ***********************************************************
      DO 11 I=1,N
      L(I)=0
 11   CONTINUE
      DO 60 NPASS=1,N
C**** FIND ELEMENT WITH LARGEST ABSOLUTE VALUE ***************************
 12   AMAX=0.
      DO 50 I=1,N
      DO 20 K=1,N
      IF(I.EQ.L(K))GO TO 50
 20   CONTINUE
      DO 40 J=1,N
      DO 30 M=1,N
      IF(J.EQ.L(M))GO TO 40
 30   CONTINUE
      IF(ABS(A(I,J)).LE.ABS(AMAX))GO TO 40
      AMAX=A(I,J)
      KMAX=I
      LMAX=J
 40   CONTINUE
 50   CONTINUE
      L(NPASS)=LMAX
      IF(AMAX.EQ.0.)GO TO 99
C**** INTERCHANGE ROWS KMAX AND LMAX ***************************************
      DO 55 J=1,N
      ACH=A(KMAX,J)
```

```
      A(KMAX,J)=A(LMAX,J)
      A(LMAX,J)=ACH
      BCH=B(KMAX,J)
      B(KMAX,J)=B(LMAX,J)
      B(LMAX,J)=BCH
 55   CONTINUE
C**** NORMALIZE ROW LMAX ***************************************************
      DO 56 J=1,N
      A(LMAX,J)=A(LMAX,J)/AMAX
      B(LMAX,J)=B(LMAX,J)/AMAX
 56   CONTINUE
C**** ELIMINATE OFF-DIAGONAL ELEMENTS IN COLUMN LMAX ***********************
      DO 57 I=1,N
      IF(I.EQ.LMAX)GO TO 57
      AEL=A(I,LMAX)
      DO 565 J=1,N
      A(I,J)=A(I,J)-AEL*A(LMAX,J)
      B(I,J)=B(I,J)-AEL*B(LMAX,J)
 565  CONTINUE
 57   CONTINUE
 60   CONTINUE
C**************** STORE INVERSE OF A IN A MATRIX ***************************
      DO 70 I=1,N
      DO 70 J=1,N
 70   A(I,J)=B(I,J)
      RETURN
C**** HERE IF AMAX=0. ******************************************************
 99   IFLAG=1
      RETURN
      END
```

```
C****************** PROGRAM TO FIT MOSSBAUER FRACTION DATA ******************
      DIMENSION T(20),D(20,2),E(20),F(2,2),A(2),G(2),SSA(2),S(20)
      DIMENSION ID(20),SSEX(20),DA(20,2),W(2,2)
      DATA LAST/'LAST'/
      TOL=0.001
      ICONV=2
      ITMAX=20
      ATWT=1.65981E-24
      BOLTZK=1.38041E-16
      CLIGHT=2.99792E+10
      HBAR=1.05445E-27
      WAVEK=0.73043E+09
C****************** READ DATA ***********************************************
 1    READ(5,2)ID
 2    FORMAT(20A4)
      IF(ID(1).EQ.LAST)GO TO 99
      READ(5,3)MODEL,N,THO,SS,GMW
 3    FORMAT(I2,8X,I2,8X,F10.1,F20.10,F10.1)
      READ(5,4)(T(I),I=1,N)
      READ(5,4)(S(I),I=1,N)
 4    FORMAT(8F10.1)
C****************** WRITE DATA **********************************************
      WRITE(6,5)
 5    FORMAT(1H1)
      WRITE(6,52)ID
 52   FORMAT(/130('*')/21X,20A4,/130('*'))
      WRITE(6,53)N
 53   FORMAT(/'NUMBER OF DATA PAIRS =',I4)
      IF(MODEL.GT.1)GO TO 55
      WRITE(6,54)
 54   FORMAT(/'EINSTEIN MODEL')
      GO TO 56
 55   WRITE(6,555)
 555  FORMAT(/'DEBYE MODEL')
 56   WRITE(6,561)THO,SS,GMW
```

```
 561  FORMAT(/'THETA ESTIMATE =',E14.6/'STD. DEV. SQUARED =',E14.6/'MOL.
     1 WT. =',E14.6)
      WRITE(6,57)(T(I),S(I),I=1,N)
 57   FORMAT(/('TEMPERATURE =',E14.6,3X,'NAT. LOG T =',E14.6))
C******************** FIT MODEL TO DATA ************************************
      NTOL=0
      SO=1.E20
      XM=GMW*ATWT
      AA=(HBAR**2*WAVEK**2)/(XM*BOLTZK)
      BB=0.75*AA
      IT=1
 6    CONTINUE
      IF(IT.GT.ITMAX)GO TO 1
      IF(MODEL.GT.1)GO TO 61
      CALL EINMFD(N,T,S,THO,D,E,20,AA)
      GO TO 62
 61   CALL DEBMFD(N,T,S,THO,D,E,20,BB)
 62   CALL NORMEQ(N,2,E,D,F,A,G,20,2,W)
      WRITE(6,625)IT,A(1),A(2)
 625  FORMAT(/'AFTER',I3,' ITERATIONS, SO =',E14.6,', THETA =',E14.6)
      SERR=0.
      IF(MODEL.GT.1)GO TO 6261
      DO 626 I=1,N
      ERR=S(I)-EINMF(A(1),A(2),T(I),AA)
 626  SERR=SERR+ERR**2
      GO TO 6263
 6261 CONTINUE
      DO 6262 I=1,N
      ERR=S(I)-DEBMF(A(1),A(2),T(I),BB)
 6262 SERR=SERR+ERR**2
 6263 WRITE(6,627)SERR
 627  FORMAT('SUM OF SQUARES OF ERRORS =',E14.6)
      IF(ABS(1.-SO/A(1)).GE.TOL)GO TO 628
      IF(ABS(1.-THO/A(2)).GE.TOL)GO TO 628
      GO TO 63
```

```
628   SO=A(1)
      THO=A(2)
      IT=IT+1
      GO TO 6
63    NTOL=NTOL+1
      WRITE(6,64)NTOL
64    FORMAT('TOLERANCE MET, NTOL =',I2)
      IF(NTOL.LT.ICONV)GO TO 628
      SO=A(1)
      TH=A(2)
C******************* CALCULATE STANDARD DEVIATIONS ***************************
      XN=N
      SSIG=SERR/(XN-2.)
      DO 7 I=1,N
7     SSEX(I)=SSIG
      CALL SIGASQ(N,2,F,D,SSEX,SSA,DA,20,2)
      SIGSO=SQRT(SSA(1))
      SIGTH=SQRT(SSA(2))
      CHISQ=SERR/SS
      CMIN=XN-SQRT(2.*XN)
      CMAX=XN+SQRT(2.*XN)
C******************* WRITE FINAL PARAMETERS **********************************
      WRITE(6,52)ID
      WRITE(6,71)SO,SIGSO,TH,SIGTH
71    FORMAT(/T57,'MODEL PARAMETERS'/T44,'SO =',E14.6,3X,'STD.DEV. =',E1
     14.6/T41,'THETA =',E14.6,3X,'STD.DEV. =',E14.6)
      WRITE(6,73)CHISQ,CMIN,CMAX
73    FORMAT(/T24,29('*'),2X,'CHI-SQUARE =',E13.6,2X,30('*')/T39,'LOWER
     1LIMIT =',E13.6,3X,'UPPER LIMIT =',E13.6)
      GO TO 1
99    STOP
      END
```

```
      SUBROUTINE EINMFD(N,T,S,THO,D,E,NDEM,A)
      DIMENSION T(NDEM),D(NDEM,2),E(NDEM),S(NDEM)
      DO 2 I=1,N
      D(I,1)=1.
      X=THO/T(I)
      EX=EXP(X)
      D(I,2)=(A/THO**2)*(0.5+1./(EX-1.))+(A/(THO*T(I)))*(EX/(EX-1.)**2)
      E(I)=S(I)+(A/THO)*(0.5+1./(EX-1.))+THO*D(I,2)
2     CONTINUE
      RETURN
      END
```

```
      SUBROUTINE DEBMFD(N,T,S,THO,D,E,NDEM,B)
      DIMENSION T(NDEM),D(NDEM,2),E(NDEM),S(NDEM)
      TOL=0.0001
      DO 2 I=1,N
      D(I,1)=1.
      X=THO/T(I)
      TT=12.*T(I)**2*DEBINT(1,THO,T(I),TOL)/(THO**2)
      TTT=4.*T(I)*FDEB(1,X)/THO
      D(I,2)=(B/THO**2)*(1.+TT-TTT)
      E(I)=S(I)+(B/THO)*(1.+TT/3.)+THO*D(I,2)
2     CONTINUE
      RETURN
      END
```

```
      FUNCTION EINMF(SO,TH,T,A)
      EINMF=SO-(A/TH)*(0.5+1./(EXP(TH/T)-1.))
      RETURN
      END
```

```
      FUNCTION DEBMF(SO,TH,T,B)
      TOL=0.0001
      DEBMF=SO-(B/TH)*(1.+4.*T**2*DEBINT(1,TH,T,TOL)/(TH**2))
      RETURN
      END
```

```
      FUNCTION DEBINT(N,TH,T,TOL)
      FF(X)=FDEB(N,X)
      XL=TH/T
      APP=0.
      NU=100
1     XNU=NU
      NNU=NU-1
      S=0.
      DO 2 I=1,NNU
      XI=I
      X=XI*XL/XNU
2     S=S+FF(X)
      S=2.*S
      SS=0.
      DO 3 I=1,NU
      XI=I
      X=(XI-0.5)*XL/XNU
3     SS=SS+FF(X)
      SS=4.*SS
      DEBINT=(XL/(6.*XNU))*(FF(0.)+FF(XL)+S+SS)
      DD=1.-APP/DEBINT
      IF(ABS(DD).LT.TOL)GO TO 9
      APP=DEBINT
      NU=2*NU
      GO TO 1
9     RETURN
      END
```

```
      FUNCTION FDEB(N,X)
      IF(X.GT.1.E-05)GO TO 2
      IF(N.GT.1)GO TO 1
      FDEB=1.
      RETURN
1     NN=N-1
      FDEB=X**NN
      RETURN
2     FDEB=(X**N)/(EXP(X)-1.)
      RETURN
      END
```

```
      SUBROUTINE NORMEQ(N,NA,E,D,F,A,G,NDEM,NADEM,W)
      DIMENSION F(NADEM,NADEM),A(NADEM),G(NADEM),E(NDEM),D(NDEM,NADEM)
      DIMENSION LL(20),W(NADEM)
      DO 2 L=1,NA
      G(L)=0.
      DO 15 I=1,N
   15 G(L)=G(L)+D(I,L)*E(I)
      DO 2 K=1,NA
      F(K,L)=0.
      DO 16 I=1,N
   16 F(K,L)=F(K,L)+D(I,K)*D(I,L)
    2 CONTINUE
      CALL MATINV(F,W,NA,NADEM,IFLAG,LL)
      DO 3 K=1,NA
      A(K)=0.
      DO 3 L=1,NA
    3 A(K)=A(K)+F(K,L)*G(L)
      RETURN
      END
```

```
      SUBROUTINE SIGASQ(N,NA,FINV,D,SS,SSA,DA,NDEM,NADEM)
      DIMENSION FINV(NADEM,NADEM),D(NDEM,NADEM),SS(NDEM),SSA(NADEM)
      DIMENSION DA(NDEM,NADEM)
      DO 2 J=1,N
      DO 2 K=1,NA
      DA(J,K)=0.
      DO 15 L=1,NA
15    DA(J,K)=FINV(K,L)*D(J,L)+DA(J,K)
2     CONTINUE
      DO 3 K=1,NA
      SSA(K)=0.
      DO 25 J=1,N
25    SSA(K)=SSA(K)+DA(J,K)**2*SS(J)
3     CONTINUE
      RETURN
      END
```

```
      SUBROUTINE MATINV(A,B,N,NDEM,IFLAG,L)
      DIMENSION A(NDEM,NDEM),B(NDEM,NDEM),L(NDEM)
C***************** INITIALIZE B MATRIX ***************************************
      DO 105 I=1,N
      DO 105 J=1,N
 105  B(I,J)=0.
      DO 106 I=1,N
 106  B(I,I)=1.
      IFLAG=0
C**** INITIALIZE L ARRAY ***********************************************
      DO 11 I=1,N
      L(I)=0
 11   CONTINUE
      DO 60 NPASS=1,N
C**** FIND ELEMENT WITH LARGEST ABSOLUTE VALUE *****************************
 12   AMAX=0.
      DO 50 I=1,N
      DO 20 K=1,N
      IF(I.EQ.L(K))GO TO 50
 20   CONTINUE
      DO 40 J=1,N
      DO 30 M=1,N
      IF(J.EQ.L(M))GO TO 40
 30   CONTINUE
      IF(ABS(A(I,J)).LE.ABS(AMAX))GO TO 40
      AMAX=A(I,J)
      KMAX=I
      LMAX=J
 40   CONTINUE
 50   CONTINUE
      L(NPASS)=LMAX
      IF(AMAX.EQ.0.)GO TO 99
C**** INTERCHANGE ROWS KMAX AND LMAX ***************************************
      DO 55 J=1,N
      ACH=A(KMAX,J)
```

```
      A(KMAX,J)=A(LMAX,J)
      A(LMAX,J)=ACH
      BCH=B(KMAX,J)
      B(KMAX,J)=B(LMAX,J)
      B(LMAX,J)=BCH
 55   CONTINUE
C**** NORMALIZE ROW LMAX ***************************************************
      DO 56 J=1,N
      A(LMAX,J)=A(LMAX,J)/AMAX
      B(LMAX,J)=B(LMAX,J)/AMAX
 56   CONTINUE
C**** ELIMINATE OFF-DIAGONAL ELEMENTS IN COLUMN LMAX ************************
      DO 57 I=1,N
      IF(I.EQ.LMAX)GO TO 57
      AEL=A(I,LMAX)
      DO 565 J=1,N
      A(I,J)=A(I,J)-AEL*A(LMAX,J)
      B(I,J)=B(I,J)-AEL*B(LMAX,J)
 565  CONTINUE
 57   CONTINUE
 60   CONTINUE
C****************** STORE INVERSE OF A IN A MATRIX ****************************
      DO 70 I=1,N
      DO 70 J=1,N
 70   A(I,J)=B(I,J)
      RETURN
C**** HERE IF AMAX=0. ******************************************************
 99   IFLAG=1
      RETURN
      END
```

```
C****************** PROGRAM TO FIT THERMAL SHIFT DATA **********************
      DIMENSION T(20),D(20,2),E(20),F(2,2),A(2),G(2),SSA(2),S(20)
      DIMENSION ID(20),SSEX(20),DA(20,2),W(2,2)
      DATA LAST/'LAST'/
      TOL=0.001
      ICONV=2
      ITMAX=20
      ATWT=1.65981E-24
      BOLTZK=1.38041E-16
      CLIGHT=2.99792E+10
C****************** READ DATA ***********************************************
 1    READ(5,2)ID
 2    FORMAT(20A4)
      IF(ID(1).EQ.LAST)GO TO 99
      READ(5,3)MODEL,N,THO,SS,GMW
 3    FORMAT(I2,8X,I2,8X,F10.1,F20.10,F10.1)
      READ(5,4)(T(I),I=1,N)
      READ(5,4)(S(I),I=1,N)
 4    FORMAT(8F10.1)
C****************** WRITE DATA **********************************************
      WRITE(6,5)
 5    FORMAT(1H1)
      WRITE(6,52)ID
 52   FORMAT(/130('*')/21X,20A4,/130('*'))
      WRITE(6,53)N
 53   FORMAT(/'NUMBER OF DATA PAIRS =',I4)
      IF(MODEL.GT.1)GO TO 55
      WRITE(6,54)
 54   FORMAT(/'EINSTEIN MODEL')
      GO TO 56
 55   WRITE(6,555)
 555  FORMAT(/'DEBYE MODEL')
 56   WRITE(6,561)THO,SS,GMW
 561  FORMAT(/'THETA ESTIMATE =',E14.6/'STD. DEV. SQUARED =',E14.6/'MOL.
     1 WT. =',E14.6)
```

```
      WRITE(6,57)(T(I),S(I),I=1,N)
 57   FORMAT(/('TEMPERATURE =',E14.6,3X,'VELOCITY =',E14.6))
C******************** FIT MODEL TO DATA ************************************
      NTCL=0
      SO=1.E20
      XM=GMW*ATWT
      AA=10.*3.*BOLTZK/(2.*XM*CLIGHT)
      BB=10.*9.*BOLTZK/(16.*XM*CLIGHT)
      IT=1
 6    CONTINUE
      IF(IT.GT.ITMAX)GO TO 1
      IF(MODEL.GT.1)GO TO 61
      CALL EINTSD(N,T,S,THO,D,E,20,AA)
      GO TO 62
 61   CALL DEBTSD(N,T,S,THO,D,E,20,BB)
 62   CALL NORMEQ(N,2,E,D,F,A,G,20,2,W)
      WRITE(6,625)IT,A(1),A(2)
 625  FORMAT(/'AFTER',I3,' ITERATIONS, SO =',E14.6,', THETA =',E14.6)
      SERR=0.
      IF(MODEL.GT.1)GO TO 6261
      DO 626 I=1,N
      ERR=S(I)-EINTS(A(1),A(2),T(I),AA)
 626  SERR=SERR+ERR**2
      GO TO 6263
 6261 CONTINUE
      DO 6262 I=1,N
      ERR=S(I)-DEBTS(A(1),A(2),T(I),BB)
 6262 SERR=SERR+ERR**2
 6263 WRITE(6,627)SERR
 627  FORMAT('SUM OF SQUARES OF ERRORS =',E14.6)
      IF(ABS(1.-SO/A(1)).GE.TOL)GO TO 628
      IF(ABS(1.-THO/A(2)).GE.TOL)GO TO 628
      GO TO 63
 628  SO=A(1)
      THO=A(2)
```

```
      IT=IT+1
      GO TO 6
 63   NTOL=NTOL+1
      WRITE(6,64)NTOL
 64   FORMAT('TOLERANCE MET, NTOL =',I2)
      IF(NTOL.LT.ICONV)GO TO 628
      SO=A(1)
      TH=A(2)
C****************** CALCULATE STANDARD DEVIATIONS ***************************
      XN=N
      SSIG=SERR/(XN-2.)
      DO 7 I=1,N
 7    SSEX(I)=SSIG
      CALL SIGASQ(N,2,F,D,SSEX,SSA,DA,20,2)
      SIGSO=SQRT(SSA(1))
      SIGTH=SQRT(SSA(2))
      CHISQ=SERR/SS
      CMIN=XN-SQRT(2.*XN)
      CMAX=XN+SQRT(2.*XN)
C****************** WRITE FINAL PARAMETERS **********************************
      WRITE(6,52)ID
      WRITE(6,71)SO,SIGSO,TH,SIGTH
 71   FORMAT(/T57,'MODEL PARAMETERS'/T44,'SO =',E14.6,3X,'STD.DEV. =',E1
     14.6/T41,'THETA =',E14.6,3X,'STD.DEV. =',E14.6)
      WRITE(6,73)CHISQ,CMIN,CMAX
 73   FORMAT(/T24,29('*'),2X,'CHI-SQUARE =',E13.6,2X,30('*')/T39,'LOWER
     1LIMIT =',E13.6,3X,'UPPER LIMIT =',E13.6)
      GO TO 1
 99   STOP
      END
```

```
      SUBROUTINE EINTSD(N,T,S,THO,D,E,NDEM,A)
      DIMENSION T(NDEM),D(NDEM,2),E(NDEM),S(NDEM)
      DO 2 I=1,N
      D(I,1)=1.
      X=THO/T(I)
      EX=EXP(X)
      D(I,2)=A*X*(EX/(EX-1.)**2)-A*(0.5+1./(EX-1.))
      E(I)=S(I)+A*THO*(0.5+1./(EX-1.))+THO*D(I,2)
    2 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE DEBTSD(N,T,S,THO,D,E,NDEM,B)
      DIMENSION T(NDEM),D(NDEM,2),E(NDEM),S(NDEM)
      TOL=0.0001
      DO 2 I=1,N
      D(I,1)=1.
      X=THO/T(I)
      TT=24.*T(I)**4*DEBINT(3,THO,T(I),TOL)/(THO**4)
      TTT=8.*T(I)**3*FDEB(3,X)/(THO**3)
      D(I,2)=-B*(1.-TT+TTT)
      E(I)=S(I)+B*THO*(1.+TT/3.)+THO*D(I,2)
2     CONTINUE
      RETURN
      END
```

```
      FUNCTION EINTS(SO,TH,T,A)
      EINTS=SO-A*TH*(0.5+1./(EXP(TH/T)-1.))
      RETURN
      END
```

```
      FUNCTION DEBTS(SO,TH,T,B)
      TOL=0.0001
      DEBTS=SO-B*TH*(1.+8.*T**4*DEBINT(3,TH,T,TOL)/(TH**4))
      RETURN
      END
```

```
      FUNCTION DEBINT(N,TH,T,TOL)
      FF(X)=FDEB(N,X)
      XL=TH/T
      APP=0.
      NU=100
1     XNU=NU
      NNU=NU-1
      S=0.
      DO 2 I=1,NNU
      XI=I
      X=XI*XL/XNU
2     S=S+FF(X)
      S=2.*S
      SS=0.
      DO 3 I=1,NU
      XI=I
      X=(XI-0.5)*XL/XNU
3     SS=SS+FF(X)
      SS=4.*SS
      DEBINT=(XL/(6.*XNU))*(FF(0.)+FF(XL)+S+SS)
      DD=1.-APP/DEBINT
      IF(ABS(DD).LT.TOL)GO TO 9
      APP=DEBINT
      NU=2*NU
      GO TO 1
9     RETURN
      END
```

```
      FUNCTION FDEB(N,X)
      IF(X.GT.1.E-05)GO TO 2
      IF(N.GT.1)GO TO 1
      FDEB=1.
      RETURN
1     NN=N-1
      FDEB=X**NN
      RETURN
2     FDEB=(X**N)/(EXP(X)-1.)
      RETURN
      END
```

```
      SUBROUTINE NORMEQ(N,NA,E,D,F,A,G,NDEM,NADEM,W)
      DIMENSION F(NADEM,NADEM),A(NADEM),G(NADEM),E(NDEM),D(NDEM,NADEM)
      DIMENSION LL(20),W(NADEM)
      DO 2 L=1,NA
      G(L)=0.
      DO 15 I=1,N
   15 G(L)=G(L)+D(I,L)*E(I)
      DO 2 K=1,NA
      F(K,L)=0.
      DO 16 I=1,N
   16 F(K,L)=F(K,L)+D(I,K)*D(I,L)
    2 CONTINUE
      CALL MATINV(F,W,NA,NADEM,IFLAG,LL)
      DO 3 K=1,NA
      A(K)=0.
      DO 3 L=1,NA
    3 A(K)=A(K)+F(K,L)*G(L)
      RETURN
      END
```

```
      SUBROUTINE SIGASQ(N,NA,FINV,D,SS,SSA,DA,NDEM,NADEM)
      DIMENSION FINV(NADEM,NADEM),D(NDEM,NADEM),SS(NDEM),SSA(NADEM)
      DIMENSION DA(NDEM,NADEM)
      DO 2 J=1,N
      DO 2 K=1,NA
      DA(J,K)=0.
      DO 15 L=1,NA
15    DA(J,K)=FINV(K,L)*D(J,L)+DA(J,K)
2     CONTINUE
      DO 3 K=1,NA
      SSA(K)=0.
      DO 25 J=1,N
25    SSA(K)=SSA(K)+DA(J,K)**2*SS(J)
3     CONTINUE
      RETURN
      END
```

```
      SUBROUTINE MATINV(A,B,N,NDEM,IFLAG,L)
      DIMENSION A(NDEM,NDEM),B(NDEM,NDEM),L(NDEM)
C***************** INITIALIZE B MATRIX ***************************************
      DO 105 I=1,N
      DO 105 J=1,N
 105  B(I,J)=0.
      DO 106 I=1,N
 106  B(I,I)=1.
      IFLAG=0
C**** INITIALIZE L ARRAY ***********************************************
      DO 11 I=1,N
      L(I)=0
 11   CONTINUE
      DO 60 NPASS=1,N
C**** FIND ELEMENT WITH LARGEST ABSOLUTE VALUE *****************************
 12   AMAX=0.
      DO 50 I=1,N
      DO 20 K=1,N
      IF(I.EQ.L(K))GO TO 50
 20   CONTINUE
      DO 40 J=1,N
      DO 30 M=1,N
      IF(J.EQ.L(M))GO TO 40
 30   CONTINUE
      IF(ABS(A(I,J)).LE.ABS(AMAX))GO TO 40
      AMAX=A(I,J)
      KMAX=I
      LMAX=J
 40   CONTINUE
 50   CONTINUE
      L(NPASS)=LMAX
      IF(AMAX.EQ.0.)GO TO 99
C**** INTERCHANGE ROWS KMAX AND LMAX ***************************************
      DO 55 J=1,N
      ACH=A(KMAX,J)
```

```
      A(KMAX,J)=A(LMAX,J)
      A(LMAX,J)=ACH
      BCH=B(KMAX,J)
      B(KMAX,J)=B(LMAX,J)
      B(LMAX,J)=BCH
 55   CONTINUE
C**** NORMALIZE ROW LMAX ***************************************************
      DO 56 J=1,N
      A(LMAX,J)=A(LMAX,J)/AMAX
      B(LMAX,J)=B(LMAX,J)/AMAX
 56   CONTINUE
C**** ELIMINATE OFF-DIAGONAL ELEMENTS IN COLUMN LMAX ************************
      DO 57 I=1,N
      IF(I.EQ.LMAX)GO TO 57
      AEL=A(I,LMAX)
      DO 565 J=1,N
      A(I,J)=A(I,J)-AEL*A(LMAX,J)
      B(I,J)=B(I,J)-AEL*B(LMAX,J)
 565  CONTINUE
 57   CONTINUE
 60   CONTINUE
C****************** STORE INVERSE OF A IN A MATRIX ***************************
      DO 70 I=1,N
      DO 70 J=1,N
 70   A(I,J)=B(I,J)
      RETURN
C**** HERE IF AMAX=0. ******************************************************
 99   IFLAG=1
      RETURN
      END
```

APPENDIX C

MOSSBAUER SPECTRA

The following pages contain the 62 Mossbauer spectra collected in the 31 experimental runs. The heading of each table shows the absorber, temperature, and date of the run, and the channel whose contents are listed. The upper left entry in the table is the number of counts collected in the first channel of the spectrum (either channel 000 or channel 200). The first row contains, from left to right, the contents of the first 10 channels; the second row, the second 10 channels; etc. The lower right entry is the contents of the last channel (either channel 199 or channel 399). The spectra are presented in the order shown in Table II.

METALLIC FE (6 LINES) -- 79 DEG K -- 4-18-69 -- CH 000 THRU 199

000000	054727	054652	054524	054988	054488	054985	054804	054918	054688
054761	054734	054724	055008	054986	054429	054175	054764	054423	054000
053917	053495	053442	052156	050848	047488	045082	043166	043766	046308
049278	051787	052925	053298	053902	053973	053931	054200	054509	054512
054765	055013	054532	054243	054472	054645	054357	054638	054883	054475
053969	053526	053190	053431	051352	049000	045886	044254	045095	047912
050654	052252	053160	053744	054726	053977	054725	054543	054358	054782
054836	054924	054907	054846	054551	054670	054502	054737	054677	054431
054622	054064	053895	053863	052958	052051	050455	049107	048914	051571
052603	053527	054111	054541	054491	054569	053954	054465	054577	054506
054456	054295	054422	054125	054219	054153	053259	052184	050608	048712
49323	50758	52302	53236	54182	54083	54081	54525	54325	54537
54489	54654	54571	54801	54388	54657	54703	54772	54652	54363
54217	54108	54165	54270	53886	53173	52064	50546	48136	45045
43709	45054	48655	50938	52582	53093	53924	54420	54308	54152
54364	54697	54447	54546	54463	54586	54563	54168	54677	54190
54268	54112	53905	53756	53438	52944	52423	50718	48257	45707
43717	44301	46438	48467	50932	52202	53032	53766	54168	54718
54470	54721	54798	53998	54711	54164	54675	54405	54793	54791
54944	54663	54792	55042	55036	54751	54362	54732	55197	55134

METALLIC FE (6 LINES) -- TEMP = 79 DEG K -- 4-18-69 -- CH 200 THRU 399

000000 054763 054963 054952 054836 055078 054714 055040 054661 054738
055305 055325 054629 054594 055001 055242 055026 054892 054679 054422
054839 054543 054433 053621 053866 052911 052034 050657 048248 045428
043597 043637 046710 049239 051663 052558 053605 053990 053972 054338
054227 054348 054451 054698 054254 054686 054465 054337 054666 054150
054531 054668 054327 053707 053323 053182 052586 051172 048513 045717
044123 045708 048219 050811 052105 053285 053842 054223 054478 054320
054325 054741 054466 054758 054537 054989 054953 054660 054346 054635
054411 054594 054503 054620 054320 054420 053951 053197 051987 050207
048825 049743 051058 052728 053460 054041 054615 054519 054318 054683
054340 054523 054417 054796 054353 054634 054596 054211 053830 053392
052283 050667 049277 048960 051324 052603 053135 054004 054303 054465
054677 054797 054851 054785 054832 054693 055179 053995 054679 054549
054492 055077 054782 054654 054110 054500 054363 053647 052917 051869
050180 047626 044094 043756 046390 049287 051884 053131 053623 053855
054368 054405 054791 054304 054252 054478 055005 054199 054534 054737
054284 054533 054467 054174 054403 053829 053740 053039 052772 051806
050336 047638 044841 044160 045074 047169 049191 051307 052620 053197
053871 054114 053829 054321 054713 054753 054603 054283 055057 054771
054848 054264 054867 054948 054731 054976 054288 055001 055140 055077

METALLIC FE (6 LINES) -- 129 DEG K -- 4-18-69 -- CH 000 THRU 199

00000	51143	51543	51692	51538	51820	50935	51350	51443	51287
51924	51331	51006	51271	51119	51064	50901	50775	50762	50664
50510	50475	50058	49300	47786	45321	43088	40540	40769	43804
46839	48639	49355	50064	50178	51162	51011	51167	50974	50987
51011	51453	51036	51142	51260	50923	50806	51222	50808	50881
50435	50415	50217	49901	48074	45330	42369	41325	42785	45980
48180	49183	50123	50540	50578	50335	50811	51600	51261	51464
51282	51162	51233	51184	51046	50755	51787	51340	51029	51502
51125	51069	50962	50588	49808	48206	47047	45788	46756	48298
50026	50472	50642	50750	51322	51118	51021	50716	50821	50554
50758	50802	51161	50596	50773	50567	49742	48925	46881	45586
46472	47974	49712	50275	50596	51103	51261	51147	51210	51351
51502	51205	51326	51253	51437	51322	51246	51196	51329	51382
51327	51200	50977	50525	49905	49401	48664	46875	44109	40874
41265	44465	47543	48497	49549	50272	50642	50789	51141	50925
50937	50955	51223	51055	51182	51189	51134	51433	51134	50909
50785	50931	50679	50667	50091	49719	48668	46800	43842	41370
40790	42366	44665	46936	48509	49561	50544	50592	50908	51024
51474	50901	51524	51505	51208	51165	51204	51095	51402	51210
51306	51469	51545	51531	51076	51706	51277	51349	51732	51698

METALLIC FE (6 LINES) -- TEMP = 129 DEG K -- 4-18-69 -- CH 200 THRU 399

000000 051777 051179 051486 051594 051472 051539 051538 051377 051231
051460 052073 051567 051305 051439 051469 051428 051284 051286 050855
050524 050808 051145 050742 050145 050418 049182 048454 046671 043740
040911 040029 041588 045431 048274 049132 050057 050070 050413 050740
050420 051125 051502 050811 051310 051170 051104 051245 051191 051061
051209 051295 051282 050665 050489 050161 049537 048534 046171 043509
041820 042357 044652 046869 049075 049927 050091 050271 050772 050905
051285 051094 050994 050900 051034 051509 051586 051356 051199 051770
051417 051614 051422 051103 050803 050675 050829 049963 049244 047706
046202 045800 047961 049431 050403 050864 050627 051037 050876 051093
050872 051311 051274 051269 051219 050915 050697 050752 050926 050503
049431 047710 046010 045886 047890 049177 050274 050679 050896 051380
051123 051270 051204 051341 051187 051225 051102 051466 051149 051198
051483 051153 050918 051104 050825 051025 050842 050527 049742 048907
047697 044614 041007 040492 043796 046810 048435 049962 050344 050784
050721 051243 051036 051051 051367 051107 051160 051381 051684 051177
051498 050959 050815 051106 051146 051562 050358 050353 049447 048530
047067 044349 042212 041402 042732 044889 046737 048514 049518 050063
050650 051096 051226 051032 051361 051246 051264 051377 051433 051311
051528 051343 051289 051538 051827 051621 051438 052012 051391 051378

METALLIC FE (6 LINES) -- TEMP = 179 DEG K -- 4-17-69 -- CH 000 THRU 199

00000	51252	51362	51136	51694	51500	51179	51305	51033	51737
51308	51381	51339	51090	50919	50794	51392	51361	50533	51013
50592	50565	49817	49055	48218	45924	43450	40709	40114	43275
46355	48858	48953	49803	50324	50388	50538	51149	51035	51083
51242	51058	50957	51174	51087	50956	51299	50695	50915	50676
50876	50195	49774	49211	47854	45558	42053	40341	42524	46468
47503	49076	49524	49847	50536	50802	51010	50978	51270	51206
51206	51303	51308	51044	51249	51236	51165	51224	51253	50909
50933	50756	50672	50801	49952	48218	46366	45188	46927	48914
49905	50457	50875	51022	50910	50718	50952	50817	50824	51023
50737	50518	50541	50576	50085	50311	49202	48647	45932	45434
46749	49027	49742	50795	50925	50602	50895	51051	50771	51200
51397	50918	50886	51302	51196	51128	51181	51094	51160	51185
50630	50890	50407	50500	49697	49041	47674	45242	42171	40198
42541	45846	48208	49307	49705	50006	50448	51059	50611	51210
51023	51217	50616	50899	50850	51216	51164	50968	50609	51220
50777	50986	50309	49955	49779	48734	47624	44449	41604	40273
41476	44328	46896	48524	49210	50042	50353	50774	50591	51026
50903	50945	51372	50997	51787	50936	51275	51089	50994	51109
51428	51430	51742	51195	51185	50983	51035	51232	51204	51935

METALLIC FE (6 LINES) -- TEMP = 179 DEG K -- 4-17-69 -- CH 200 THRU 399

000001 051170 051253 051293 051487 051060 051152 051594 051511 051228
051202 051146 051170 052064 051339 051340 051359 051248 050879 051003
051136 050987 050560 050701 050620 050036 050201 049248 048063 046008
043469 040493 040016 042870 046151 048230 049567 049880 050224 050477
050838 050694 050892 051166 051248 050871 051423 051034 051157 051125
050824 050758 051081 050821 050598 050183 049935 049356 048021 044965
042326 041338 042723 045907 048381 048958 050099 050598 050639 051025
050965 050949 050871 051124 051104 051149 051202 051259 051148 051332
051213 051027 051123 050930 050791 051081 050601 050509 049910 048130
046301 045955 047321 049108 049681 050395 050900 050415 050927 051032
050747 050765 050688 050927 051362 051031 050927 050893 050467 050352
049544 048400 046212 045579 046917 048713 049926 050537 050948 051064
050510 050796 051168 051134 051101 050974 051436 051062 051380 051240
051377 050969 050844 051160 050842 050844 050768 050335 049634 049246
047912 045064 041237 040276 043015 046547 049034 049309 050180 050093
050608 051103 050875 051370 051315 050981 050947 050985 051751 051166
051202 051209 050816 050823 050615 050698 050317 050212 049773 048833
046623 044198 042245 041276 042370 044665 046913 048579 049284 049828
050172 050554 050848 051096 051158 051319 051188 051396 051389 051403
051270 051645 051557 051548 051546 051137 051193 050966 051806 051339

METALLIC FE (6 LINES) -- TEMP = 228 DEG K -- 4-16-69 -- CH 000 THRU 199

00000	51913	51598	51786	51823	51120	52109	51733	51314	51862
51895	51443	52013	51906	51519	51436	51324	51474	51435	51555
51069	50744	50407	49405	48798	46619	44071	41054	40770	43797
46280	48339	49641	49564	50511	51052	50972	51118	50967	51356
51473	51327	51453	51301	51365	51367	51002	51119	51477	50803
51144	50865	50585	49071	47871	45911	42181	43140	43284	46389
48882	49728	50225	50780	50913	51266	51057	51474	51325	51461
51672	51427	51078	51100	51415	51353	51878	51648	51368	51681
51342	51320	50955	50629	49732	48367	46304	46188	48060	49875
50359	51249	50903	51171	51490	51104	51185	51141	50717	51271
51033	51426	51179	51098	50534	50518	49288	47979	46065	46502
47594	49209	50531	50644	51156	51448	51249	51639	51548	51402
51297	51581	51322	51587	51105	51378	51734	51797	51127	51059
50942	51064	51065	50227	50306	48956	47183	44328	41327	41307
44316	47298	49259	50043	50507	50935	50930	51302	51481	51044
51447	51291	51443	51384	51551	51750	51080	51265	51473	50945
51465	50621	50697	50302	49744	48249	46211	42941	40740	41739
43851	46990	48605	49458	50178	50773	51390	51341	51080	51473
51304	51784	51414	51288	51511	51750	51437	51923	51488	51733
51570	51610	51519	51747	51609	51551	51733	51617	51680	51742

METALLIC FE (6 LINES) -- TEMP = 228 DEG K -- 4-16-69 -- CH 200 THRU 399

000000	051444	052044	051665	051703	051674	051744	051768	051690	051804
051658	051445	051539	051601	051249	051768	051520	051736	051577	051848
051662	051633	051142	051388	050498	050954	050534	050539	049920	048571
046586	C43311	040200	040131	043711	047040	049043	049872	050372	051116
051228	051066	051249	051095	051091	051355	051207	051183	051431	051360
051398	051169	051362	051534	050936	050618	050855	050084	049169	047400
044662	042604	041894	044303	046645	048828	049874	050404	050274	051196
051224	051759	051318	051315	051455	051520	052062	051359	051019	051262
051346	051517	051356	051533	051389	051180	050879	050329	050038	049189
047741	045484	046364	048884	049995	050422	051247	051211	051249	051109
051095	051323	051486	051243	051053	051300	051303	051169	050892	050837
050418	049570	047529	045853	045964	048093	049618	050691	051168	051045
051210	051419	051928	051416	051595	051790	051584	051079	051900	051317
051643	051329	051262	051555	051461	051184	050981	050699	050297	049263
048447	046236	042638	040000	042764	046519	048762	049794	050824	050403
051164	051085	051417	051446	051290	051559	051337	051405	051611	051737
051337	051378	051301	051330	050761	051289	051112	050852	050054	049278
047727	045364	042340	041321	042926	044982	047770	049381	049644	050631
050799	051009	050970	051227	051316	051464	051315	051463	051610	051326
051543	051343	051641	051313	051520	051379	051266	051722	052088	051240

METALLIC FE (6 LINES) -- TEMP = 276 DEG K -- 4-16-69 -- CH 000 THRU 199

00000	51731	51268	51607	51843	51700	52202	51303	51292	51406
51948	51186	51962	51570	51601	51761	51610	51636	51044	51101
50873	51260	50454	49660	48191	46410	43897	41516	41531	43699
46788	48133	49847	49992	50110	50636	51077	51449	51400	51248
50947	51532	51398	51604	51548	51157	51615	51260	51221	51111
51100	50536	50464	49237	47451	44483	40890	41015	44182	47437
48722	49814	50704	50973	51046	51264	51373	51459	51501	51238
51593	51621	51561	51714	52019	51968	51235	51456	51507	51114
51154	51001	50887	50138	48665	46466	45667	47804	49323	50281
50685	51077	50795	51210	50800	51154	51087	51264	51333	51543
50845	51151	51323	50332	50433	50313	49156	47343	45426	46791
48378	49653	50706	50881	51464	51170	51518	51493	51853	51402
51358	51605	51387	51495	51613	51187	51211	51154	50892	51523
50952	51069	50877	49936	49522	48141	44964	41555	40492	43765
46703	49146	50009	50534	50820	50828	51257	51443	51292	50934
51084	51336	51394	51380	51339	51146	51658	51726	51120	51074
50761	50538	49919	48969	48478	46647	43309	40004	41481	44428
47360	49044	49838	50806	50631	51149	50689	51493	51264	51571
51560	51610	51438	51887	51875	51293	51443	51540	51985	51708
51556	51485	52046	51669	51934	51446	51857	51757	51762	51812

METALLIC FE (6 LINES) -- TEMP = 276 DEG K -- 4-16-69 -- CH 200 THRU 399

000000 052375 051630 051715 051530 052126 051661 051819 051876 051796
051634 051922 051382 051857 051647 051418 051378 051939 051923 051546
051544 051380 051198 051610 051069 050883 050781 050649 049823 048729
047797 044870 042699 041119 043046 045595 048071 048890 050280 050830
050995 051122 051292 051060 051317 051416 051409 051155 051447 051392
051676 051207 051589 051181 050945 051095 050317 051025 049620 048689
046524 042873 040461 042213 045726 048712 049631 049901 051327 051015
051190 050955 051546 051729 051623 051311 051780 051571 051929 051727
051401 051657 051427 051640 051724 051139 051016 050762 050264 049387
047447 046016 046639 048438 050135 050609 051163 050817 051218 050852
051159 051444 050901 051531 051597 051266 051002 051023 051209 051085
050178 049927 048782 046412 046238 048054 049589 050502 051349 051103
051577 051252 051322 051490 051183 051805 051507 051775 051410 051387
051584 051667 051010 051165 051241 051047 051267 051026 050283 049415
048340 046883 043075 040390 042298 045969 048453 049793 050217 050911
050663 051567 051452 051606 051287 051334 051438 051476 051062 051272
051139 051455 051592 051453 051185 051064 050905 049815 049654 049001
046968 044104 041047 041100 043264 046082 048208 049713 049954 050617
050695 051272 051168 051569 051506 052018 051052 051161 051652 051771
051434 051238 051884 051667 051945 051702 051645 052013 051930 051675

METALLIC FE (6 LINES) -- TEMP = 293 DEG K -- 4-15-69 -- CH 000 THRU 199

00000	50879	51118	50877	51241	51521	50821	51053	51466	51548
51003	50892	50899	50972	50777	50349	50730	50925	50797	50462
50342	50383	49919	49346	47908	45692	43284	41604	40871	43635
46802	48235	49075	49672	49822	50448	50393	50816	50367	50466
50782	50909	50931	50425	50121	50666	50473	50773	50154	50562
50237	50309	49690	48557	47313	44675	40970	40222	43665	46619
48308	49235	49558	50475	50254	50513	50620	50842	50648	50797
51264	50815	50831	51050	50494	50845	50498	50713	50151	50659
50545	50174	50270	49163	47705	45350	45690	47526	49036	49675
49907	50847	50657	50488	50556	50515	50892	50490	50460	50225
50594	50775	50332	50208	49885	49802	48507	46668	45092	46496
48105	49633	49984	50383	50538	50617	50648	50587	50584	50214
50926	50745	50564	51057	50518	50946	50539	50818	50452	50627
50573	50316	49277	49110	48610	47216	44437	40207	40542	43814
47016	47889	49170	49506	50570	50733	50926	50292	50778	50311
50927	50515	50607	50738	50519	50419	51009	50467	49979	50553
50242	49909	49781	48474	47142	44466	41136	40080	41764	44656
47801	48368	49110	49714	50123	50328	51044	50848	50175	50625
50916	50563	50718	51173	50773	50834	51113	51443	50907	51259
51326	51016	50696	50755	51065	50823	50653	51051	51459	51270

METALLIC FE (6 LINES) -- TEMP = 293 DEG K -- 4-15-69 -- CH 200 THRU 399

000000	050588	051161	051191	051294	051138	051390	051151	050993	050898
051213	051192	050824	051293	051163	050824	051106	050448	050638	051051
050876	050909	050735	050503	050746	050762	050518	050167	049749	048832
047173	045183	042555	040868	041539	044705	046991	048527	049049	050002
050211	050042	050701	050483	050550	051182	050434	050771	051106	050523
050934	050753	050199	049983	050591	050181	049977	049966	049111	048589
047157	043961	040255	040882	044111	047056	048744	049244	050108	050260
050748	050670	050979	050918	050600	051170	050970	051029	051423	050842
050742	050853	050920	050732	050588	050477	050596	050772	050024	049044
047505	044923	045727	047603	049214	049879	050203	050375	050285	050492
050930	050929	050440	050609	051067	050795	050712	050951	050789	050645
050044	049506	048355	046146	045039	047417	049155	049970	050134	050692
050706	050584	050718	051046	050625	050785	050559	051012	051079	050888
050531	051480	051002	050443	050648	050961	050441	049950	049906	049079
048412	046447	043694	040005	041129	044563	047085	048746	049750	050643
050539	050448	050707	050859	050777	050708	051158	050837	050829	050665
051075	050513	050645	050656	050086	050186	049939	049698	049374	048055
046158	043320	040803	040837	042977	045961	047947	048926	049684	050148
050468	050621	050557	050680	050847	051103	050884	050502	051037	050728
051044	051144	051102	050757	050808	051200	051251	051040	051327	051019

METALLIC FE (2 LINES) -- TEMP = 79 DEG K -- 4-18-69 -- CH 000 THRU 199

000000	034329	034428	034406	034407	034291	034329	034025	034440	034079
034169	034033	034066	034380	034374	034437	033936	034329	034173	034325
034118	033981	034252	034275	034097	034159	033614	034222	033647	033806
033562	032975	033241	033504	033087	032702	032955	032417	032316	031914
031688	031164	031081	030476	030363	030659	030773	030255	030815	031257
031531	032164	032251	032383	032905	033389	033213	033215	033290	033863
033659	033416	033779	033769	034033	033616	033993	034044	034005	034112
034131	033834	034273	034124	033884	034048	033907	034253	034057	033997
034225	033746	034029	034268	034133	034109	033972	034228	034083	034467
034159	034072	034264	034087	034218	034113	033862	034106	034049	034335
034250	034344	033871	033918	034093	034427	033978	034121	034065	034217
034143	034084	033955	033831	033913	033839	034182	033829	033832	034043
033409	033685	033718	033749	033238	033681	033565	032993	032994	033177
032624	032147	031696	031541	031495	030876	030763	030545	030562	030223
030331	030205	031101	031471	031824	032192	032443	032430	032755	032999
033445	033590	033522	033790	033845	033786	033814	033585	033754	033967
033963	034007	033866	034157	034580	034374	034167	034429	033990	034442
034387	034490	034169	034283	034314	034356	034306	034054	034156	034439
034220	034059	034186	034420	034188	034273	034289	034242	034331	034207
034541	033970	034323	034276	034432	034286	034230	034087	034271	034449

METALLIC FE (2 LINES) -- TEMP = 79 DEG K -- 4-18-69 -- CH 200 THRU 399

000000	034179	034490	034242	034045	034608	034173	034246	033980	034262
034169	034427	034613	034625	034173	034405	034250	034472	034336	033971
034102	034013	034366	034336	034219	034493	034229	034198	034229	034345
034266	034250	033901	034358	034021	034373	033961	034117	033775	033817
034037	033881	034176	033381	033537	033295	033061	032924	032778	032258
032203	031820	031216	031161	030847	030593	030184	030280	030521	030660
031255	031112	031673	031893	032155	032345	032929	032710	033139	033371
033504	033486	033866	033690	033924	033931	033766	034038	033789	034094
033936	034066	034010	034073	033923	034094	034125	034071	033566	034320
033914	033974	034118	034446	034154	033912	034059	033962	034229	034215
034180	034162	034312	034379	034269	034111	034323	034397	034404	033989
034331	034197	034301	034477	034173	034061	034231	034429	034090	034019
034336	034098	034272	034035	034282	034022	033955	034073	034355	034165
033901	033791	033894	034016	033792	033246	033409	033490	033119	033245
032870	032945	032304	032404	032254	031670	031055	030566	030559	030623
030344	030324	030150	030403	030991	031602	031827	032199	032162	032594
033155	032959	033063	033148	033309	033444	033581	033637	034092	034052
034030	033782	033971	033920	034276	034160	034317	034219	034209	034460
034212	034066	034295	034391	034157	034453	034254	034381	034272	034113
034601	034319	034184	034527	034229	034307	034375	034164	034126	034584

METALLIC FE (2 LINES -- TEMP = 129 DEG K -- 4-18-69 -- CH 000 THRU 199

000000	034677	034567	034519	034447	034589	034873	034631	034514	034413
034554	034471	034344	034494	034534	034308	034405	034671	034435	034048
034129	034391	034136	034528	034376	034122	034368	033894	033961	033750
033757	034339	033944	033362	033576	033054	033587	032782	032317	032057
031551	031349	030865	030486	030532	030002	030654	030596	031135	031346
032157	032609	032677	032779	032945	033455	033478	033419	033812	033857
034086	033989	033876	034154	034295	034021	034331	034440	034649	034394
034325	034244	034238	034331	034288	034420	034459	034120	034411	034672
034243	034460	034354	034290	034393	034582	034585	034309	034416	034386
034629	034300	034207	034328	034621	034157	034290	034296	034303	034268
034549	034216	034654	034383	034278	034452	034305	034340	034225	034408
034066	034293	033966	034317	034649	034037	034065	033925	033672	034071
033764	033720	033575	033723	033796	033727	033417	033146	033434	033206
032680	032491	032019	031642	031057	031029	030451	030223	030334	030502
030619	031003	031429	031903	032283	032549	032730	032926	033363	033565
033683	033947	033377	033859	033834	033803	034646	033908	034209	034491
034359	033858	034012	034265	034483	034560	034372	034072	034762	034203
034473	034117	034352	034614	034745	034230	034416	034463	034239	034478
034136	034607	034412	034526	034472	034322	034611	034148	034568	034662
034415	034748	034321	034214	034588	034589	034889	034491	034453	034569

METALLIC FE (2 LINES) -- TEMP = 129 DEG K -- 4-18-69 -- CH 200 THRU 399

000000	034851	034416	034667	034393	034616	034094	034729	034355	034600
034540	034604	034467	034774	034409	034575	034366	034498	034326	034859
034820	034743	034712	034603	034436	034342	034713	034509	034424	034077
034417	034778	034549	034397	034263	034543	034194	034077	034461	033981
034205	033972	033688	034069	033425	033844	033585	033713	033259	033118
032870	032340	032218	031936	031521	030982	030629	030114	030534	030254
030448	030945	031496	031705	032190	032738	032525	032690	032563	033324
033380	033209	033709	033927	033780	033757	034360	033993	033615	034279
034197	034333	034042	034635	034191	034309	034082	034617	034611	034480
034147	034160	034221	034392	034445	034532	034612	033998	034531	034195
034093	034288	034627	034655	034329	034445	034567	034352	034709	034668
034397	034110	034685	034316	034614	034497	034632	034640	034836	034427
034468	034424	034547	034189	034365	034286	034415	034104	034097	034100
034375	033936	034391	034202	034028	033882	034249	033882	033427	034032
033365	033342	033347	033450	032877	032550	032013	031709	031212	030934
030550	030242	030164	030497	030681	031065	031440	031893	031999	032605
032973	033368	033151	033077	033551	033733	033874	033966	033809	033992
033880	033821	034288	034065	033892	034303	034460	034776	034420	034337
034486	034595	034573	034654	034299	034477	034608	034528	034541	034675
034624	034533	034678	034456	034897	034364	034307	034253	034772	034565

METALLIC FE (2 LINES) -- TEMP = 179 DEG K -- 4-17-69 -- CH 000 THRU 199

000000 034564 034435 034276 034840 034924 034431 034689 034643 034471
034574 034330 034375 034440 034439 034351 033999 034377 034114 034457
034363 034046 034431 034007 034286 034123 034479 034090 034032 033970
033973 033687 033773 033083 033204 032658 032475 032024 032361 032070
030966 031037 030487 030558 030226 030399 030918 031484 031690 031860
032786 033006 033082 033215 033330 033457 033821 033791 034218 034050
033834 034000 033698 034214 033964 034271 034359 033870 034575 034283
034014 034271 034070 034233 034374 034148 034118 034373 034627 034574
034428 034201 034374 034547 034163 034547 034271 034292 034162 034366
034488 034224 034440 034448 034486 034490 034383 034460 034518 034213
034163 034522 034722 034320 034541 034350 034001 034238 034202 034515
034232 034197 034286 034185 034249 034038 034386 034198 033807 034122
033599 033908 033799 033441 033470 033603 033384 033090 032657 032411
032295 031642 031270 031210 030840 030405 030001 030352 030672 030700
031532 031604 032042 032452 033037 033011 033441 033636 033753 033749
033769 033660 033853 034081 033941 033964 034241 034055 034504 034535
034373 034547 034410 034523 034752 034666 034506 034506 034543 034182
034342 034497 034294 034460 034469 034225 034576 034332 034481 034406
034394 034545 034476 034442 034398 034779 034385 034545 035008 034262
034605 034678 034459 034703 034761 034548 034682 034422 034454 034727

METALLIC FE (2 LINES) -- TEMP = 179 DEG K -- 4-17-69 -- CH 200 THRU 399

000004	034443	034263	034516	034618	034715	034842	034721	034625	034383
034594	034516	034692	034852	034599	034527	034677	034728	034429	034694
034766	034475	034417	034498	034797	034632	034576	034627	034553	034884
034079	034335	034523	034242	034510	034173	033870	034402	034207	034359
034012	034091	034002	034063	033923	033820	033940	033495	033426	033441
033538	032645	032631	032228	031962	031389	031033	031060	030886	030413
030443	030337	030996	031159	031569	031802	032471	032866	033118	033211
033243	033379	033985	033391	033618	033899	033737	033750	034424	034075
033880	034155	034347	034367	034181	034234	034372	034532	034210	034336
034597	034550	034375	034266	034180	033975	034141	034139	034283	034144
034446	034403	034498	034432	034266	034328	034528	034393	034463	034258
034455	034277	034542	034881	034462	034399	034413	034444	034437	034378
034329	034276	034533	034321	034464	034471	034168	034169	034495	034048
033987	034175	034403	034004	034012	034430	033982	033943	033990	033883
033857	033668	033687	033246	032774	032408	032380	032000	031352	031018
030908	030700	030387	030361	030378	030797	031450	031688	031971	032001
032505	033068	033069	033486	033567	033529	033880	033620	033689	033613
034157	034305	034358	034470	034396	033976	034193	034484	034302	034675
034392	034435	034610	034350	034417	034741	034319	034635	034077	034444
034212	034263	034776	034459	034223	034291	034281	034988	034401	034282

METALLIC FE (2 LINES) -- TEMP = 228 DEG K -- 4-16-69 -- CH 000 THRU 199

000000	034582	034635	034462	034576	034358	034753	034468	034563	034269
034271	034347	034334	034039	034332	034227	034465	034350	034225	034392
034237	034300	034356	034274	033906	034163	033948	033738	033952	033520
033536	033102	033704	032894	032712	032346	032273	031760	031643	030799
030545	030304	030258	030118	030654	031065	031393	031947	032301	032839
033082	033130	033384	033410	033273	033392	033845	034040	033474	033788
034279	033502	034008	034199	034168	034242	034498	034441	034246	034011
034380	034711	034062	034155	034240	034439	034401	034035	034060	034114
034388	034294	034104	034257	034191	034385	034484	033767	034244	034508
034190	034523	034023	034492	034306	034012	034247	033969	034292	034277
034018	034254	034392	034052	034193	034068	033979	034060	034228	034429
034048	033824	033846	034184	033953	033878	033954	033762	033893	033905
033693	033332	033606	033275	033201	033188	032850	032659	032002	031870
031588	031119	030736	030464	030004	030035	030491	031034	031556	031588
031809	032327	032864	032791	033351	033380	033252	033690	034045	033810
033835	033868	033938	034045	033792	034056	034395	033934	033954	034311
034349	034123	034412	034361	034504	034096	034264	034412	034578	034449
034297	034443	034329	034662	034770	034419	034986	034391	034178	034560
034412	034370	034487	034432	034286	034404	034692	034396	034424	034563
034432	034514	034166	034644	034252	034505	034861	034633	034104	034454

METALLIC FE (2 LINES) -- TEMP = 228 DEG K -- 4-16-69 -- CH 200 THRU 399

000000	034728	034825	034496	034593	034323	034124	034380	034222	034413
034549	034245	034318	034578	034527	034365	034330	034711	034402	034025
034497	034625	034422	034183	034718	034315	034233	034243	034232	034455
034455	034447	034194	034371	034303	034174	034181	034531	034147	034474
034100	034267	033988	034149	033917	034177	033681	033766	033453	033739
033446	033394	033099	032665	032678	032131	032158	031239	031143	030442
030523	030128	030294	030588	030724	031140	031562	031907	032249	032681
033198	033468	033354	033562	033606	033468	033569	033707	034095	033860
033708	034102	034014	033924	033811	034017	033836	034020	034144	034059
033946	034115	034189	034232	034248	034293	034183	034298	034070	034340
034381	034143	034000	034051	034265	034526	034340	033885	034546	034578
034539	034232	034423	034190	034221	034726	034038	034332	034102	034662
034352	034156	034223	034264	034237	034047	034173	034281	034507	034193
034190	034065	034166	033916	034420	034286	034006	034172	033785	033742
033619	033818	033436	033416	033195	032744	032669	032527	032145	031477
031162	030988	030473	030087	030012	030126	030528	030965	031337	031919
032304	032616	032874	033310	033150	033658	033578	033543	033886	033587
033656	033989	034023	034379	034251	034134	034391	034069	034024	034341
034531	034316	034313	034331	034101	034524	034312	034252	034347	034197
034380	034545	034400	034609	034364	034458	034674	034577	034758	034302

METALLIC FE (2 LINES) -- TEMP = 276 DEG K -- 4-16-69 -- CH 000 THRU 199

000000	034328	034260	034051	034592	034410	034418	034604	034211	034220
034417	033863	034479	034329	034235	034120	034662	034273	034339	034059
034035	034134	034438	034049	033796	033677	033867	033957	033805	033563
033371	033048	033358	032737	032645	032212	031653	031138	031040	030384
030246	030150	030541	030857	031085	031640	032177	032432	032549	032987
033276	033421	033359	033771	033792	033733	033891	033501	033740	033933
033901	034331	034213	034523	034363	034345	034037	034098	034467	034036
034224	034616	033897	034153	034207	034138	034445	034076	033758	034036
034020	034498	034247	033902	034459	034040	034289	034149	034373	034058
033792	034351	034607	033967	034417	034223	034377	034275	034628	034361
034141	034105	033976	033972	033930	034254	034199	034176	033840	033771
034040	033875	033803	033833	033883	033763	034017	034060	033742	033196
033281	033403	033338	032985	032754	032562	031966	031763	031352	031142
030708	030565	030004	030161	030628	030925	031218	031770	032182	032461
032582	032937	033347	033264	033557	033580	033617	034010	033759	033743
033993	033797	033584	033809	034022	033998	033952	034402	033951	034238
033927	034144	033872	034138	034486	034317	034611	034372	034132	034200
034324	034250	034052	034328	034424	034045	034740	034300	034538	034738
034130	033986	034444	034456	034448	034282	034255	034636	034069	034462
034404	034255	034346	034461	034502	034327	034406	034608	034487	034103

METALLIC FE (2 LINES) -- TEMP = 276 DEG K -- 4-16-69 -- CH 200 THRU 399

000003 034724 034167 034508 034459 034453 034417 034174 034338 034356
034164 034466 034400 034359 034676 034315 034216 034244 034434 034551
034411 034470 034425 034539 034385 034427 034590 034264 034627 034342
034152 034050 034557 034394 034131 034059 034185 034041 033829 034186
034340 034303 034554 034240 033817 033988 033605 033745 033871 033965
033892 033713 033436 033211 032738 032861 032722 032214 031841 031277
030860 030842 030265 030406 030299 030467 031160 031584 031686 032260
032720 032968 033326 033149 033306 033370 033366 033885 033610 033771
033746 033719 033992 033829 034076 033699 033849 033823 033718 034197
034054 034267 034358 034182 034208 034127 034171 034579 034303 034663
034037 034423 034329 033943 034198 034416 034203 034345 034009 034261
034149 034256 034760 033892 034471 034441 034202 034437 034378 034453
034215 034573 033963 034170 034078 034064 034222 034099 034151 034567
034086 034182 034427 034295 034106 033981 034153 034280 033738 033899
033873 033710 033800 033691 033601 032910 033089 032562 032887 032368
032057 031439 031228 031049 030670 030585 030334 030482 030877 031384
031458 032003 032686 032573 032814 033259 033261 033467 033625 033820
034018 033921 034049 033781 034102 033874 033850 034161 034170 034204
034233 034304 034206 034509 034042 034363 034475 034234 034373 034617
034236 034697 034216 034280 034362 034189 034405 034546 034336 034102

METALLIC FE (2 LINES) -- TEMP = 293 DEG K -- 4-15-69 -- CH 000 THRU 199

000000 034246 034222 034441 034205 034141 034129 034043 034660 034660
034291 034220 034309 034206 034173 034136 034080 034361 034322 034209
030080 033861 033991 033940 033971 033526 033618 033655 033547 033147
033095 032926 033157 032441 032257 032061 031423 030987 030297 030586
010222 030159 030189 030549 031338 031627 031797 032303 032493 033172
033259 033426 033251 033344 033509 033568 033671 033736 033462 033896
030317 034203 034020 033971 034464 033902 034205 034012 034021 034305
034445 034243 034074 034305 033985 034122 034124 034190 033728 034315
030061 034253 034107 034278 033991 034019 034010 034470 033946 033943
033967 033686 034042 034081 033980 034300 034125 033759 034166 033934
033990 033797 034066 033915 033477 034248 033810 033818 034194 033687
033587 033820 033713 033793 033935 033400 033656 033498 033712 033398
030070 033103 033108 032527 032455 032434 031653 031405 030793 030615
030381 030596 030271 030530 030952 031067 031265 032088 032414 032818
000070 033034 033386 032964 033508 033418 033745 033616 033534 033735
033845 033972 033982 033967 033980 033954 034007 033737 034107 033987
030010 034285 033965 033965 034181 034520 033868 034282 034471 034158
034376 034528 034391 034110 034353 033931 034365 034187 034041 034229
030741 034292 034579 033994 034019 034427 034213 034064 034512 034248
034082 034460 034239 034497 034460 034000 034184 034323 034181 034077

METALLIC FE (2 LINES) -- TEMP = 293 DEG K -- 4-15-69 -- CH 200 THRU 399

000005 034326 034205 033955 034098 034224 034442 034069 034301 034256
034230 034144 034318 033986 034400 034518 034344 034404 034334 034426
033170 034321 034251 034240 034250 034453 034384 034210 034128 034135
034284 034137 034166 034231 034151 034342 033908 034306 033858 034139
020072 033993 034061 033595 033644 033616 034166 033932 033827 033619
033551 033310 033549 033392 033049 032668 032761 032281 031987 031952
030630 031066 030417 030476 030194 030348 030613 030700 031423 031494
032110 032331 032520 032823 033136 033432 033295 033707 033356 033357
033537 033751 033570 033902 033740 033718 033972 033920 034041 033726
033901 034476 034451 033860 034165 034208 034045 034133 033959 034196
010170 033858 034325 033930 034544 034041 034250 033793 033965 033921
034075 033937 034400 034312 034142 033877 034330 034311 034208 033971
030015 033978 034228 034196 034077 034228 034184 034022 034155 034070
034116 034271 033954 034235 033753 033749 034064 033944 033609 033846
031871 033782 033545 033702 033480 033325 032886 032793 032311 032577
032025 031582 031158 031091 030570 030002 030179 030702 030750 031326
031327 031992 032488 032402 032850 032720 033227 033022 033571 033403
033792 033358 033804 033653 033762 033845 034025 033697 033834 034473
033994 033988 034073 034308 034019 034117 034161 034203 034113 034310
034117 034249 034153 034325 034381 034000 034525 034258 034390 034161

NA N'PRUSS (0.1 MG/CM2) -- TEMP = 79 DEG K -- 3-27-69 -- CH 000 THRU 199

00000	50605	50628	50678	50251	50463	50617	50427	50462	50061
50335	50487	50061	49452	49465	49287	49322	48613	48991	48495
47902	47779	47565	46243	45955	45228	43914	43402	42464	41060
41223	40981	41435	42295	43391	43998	45096	46184	46647	47045
47592	48375	48479	48645	48837	49164	48845	50296	49677	49727
49609	49977	49858	50544	50481	50013	50411	50469	50300	50421
50441	50753	50232	50332	50763	50633	50523	50787	50581	50844
50536	50630	50594	50673	50507	49850	50452	50331	50652	50309
50171	50434	51007	50274	50511	50217	50202	50479	50425	50189
50291	50024	49954	50287	50098	50034	49937	49690	49736	49646
49947	49712	49655	49462	49349	49395	48695	49310	48848	48590
48133	47588	47195	47042	46499	45448	44483	43725	43006	42185
41192	40970	40901	41128	41582	42443	43924	44442	45284	46350
46646	47657	47783	47793	48661	48970	48883	49588	49339	49469
49628	49851	49680	50407	50032	49939	50210	50320	50378	50121
50572	50538	50793	50134	50801	50299	50500	50648	50241	50771
50865	50677	50756	50521	50832	50546	50445	50566	50781	51304
50928	50672	50900	51111	50130	51099	50855	50765	50468	50945
50696	51015	50710	50715	51181	50967	51082	51059	50960	51025
50525	50731	51131	51050	50514	51111	50555	50527	51284	51182

NA N'PRUSS (0.1 MG/CM2) -- TEMP = 79 DEG K -- 3-27-69 -- CH 200 THRU 399

000000	051306	050827	050755	051183	051000	050985	050983	050820	050771
051049	050934	051050	050865	051296	050595	051234	050435	051033	050751
050556	050770	051107	051051	051045	051138	050625	050486	050536	050985
050414	050836	051004	051034	051205	050780	050818	050918	050529	050547
050578	050518	050333	050466	050751	050288	050561	050474	C49900	049902
050375	050299	049889	050344	049580	049353	049727	049836	049362	049316
049244	048873	048567	047747	047880	047432	046290	045925	044761	044133
043190	041854	041546	040567	041097	041385	042059	042532	043982	044605
045454	046370	046496	047604	048004	048487	048162	048599	048827	049352
048970	049077	048971	049569	049429	049944	049722	049789	049737	050231
049958	050252	049690	049844	050039	050210	050130	050611	050263	050689
050496	050575	050573	050730	050276	050530	050330	050489	050731	050837
050786	050910	050858	050781	050840	050219	050716	050484	051032	050877
050456	051021	050201	050876	050428	050436	050552	050593	050733	050509
050131	050351	050295	050328	050081	050044	049753	049748	049899	049253
049003	049167	049014	048789	048580	048160	048341	047103	046695	046017
045351	044760	043720	042661	041905	041507	041002	040943	041003	042222
042840	043754	044623	045928	046320	046996	047500	047545	048373	048731
048927	049172	049191	049325	049563	050150	049808	050156	050182	050033
050026	049865	049960	050334	050425	050514	050676	050617	050473	050662

NA N'PRUSS (0.1 MG/CM2) -- TEMP = 155 DEG K -- 3-27-69 -- CH 000 THRU 199

00000	48441	48357	48194	48298	48336	48187	48005	48362	48037
48376	47798	47908	47983	47763	47551	47097	47123	46575	46482
46436	45957	45295	45186	44265	43290	42483	41786	40843	40589
40418	41007	41481	42111	42957	43923	44183	45338	45867	45906
46459	47168	46994	47449	47446	47779	47317	47599	47793	48217
47969	47554	48165	47895	47897	48018	47859	48101	48314	48605
48371	48291	48243	48438	47850	48010	48233	48408	48206	48976
48200	48387	48158	48133	48238	48122	48114	48261	48143	48627
48501	48439	48097	48624	47982	48218	48266	48678	48193	47916
47766	48080	47793	47792	47630	48032	47969	48042	47876	47941
47622	47624	47859	47304	47272	47067	46979	46618	46791	46213
46209	45752	45480	45072	44605	43900	42969	42160	41380	40951
40251	40169	40625	40940	41712	42818	43443	44076	44926	45429
45401	46037	46489	46420	47205	47244	47201	47378	47412	47561
47447	47898	47818	47996	48170	48143	48126	48349	47766	48288
48350	48135	48709	48350	48702	48788	48345	48244	48460	48296
48077	48357	48573	48381	48653	48432	47995	48422	48550	48770
48619	48545	48995	48599	48213	48766	48552	48460	48592	48851
48638	48571	48659	48735	48246	48833	48679	48433	49083	48639
48256	48078	48672	48440	48245	48654	48657	48443	48549	48683

NA N'PRUSS (0.1 MG/CM2) -- TEMP = 155 DEG K -- 3-27-69 -- CH 200 THRU 399

000000	048695	048505	048718	048758	048838	048676	048969	048614	048284
048473	048840	048493	048736	048469	048656	048694	048610	048614	048637
048202	048513	048361	048377	048524	048397	048386	048495	048176	048687
048637	048190	048878	048753	048489	048586	048619	048558	048405	048602
048568	048662	048141	048127	048532	048517	048432	048520	047849	048306
048154	047854	048457	047665	047823	047529	047937	047859	047779	047403
047541	047268	046894	046746	046585	045980	045492	045556	044976	044095
042916	042732	041874	041146	040671	040353	040552	040895	041816	042828
043376	044062	044596	045257	045852	046002	046497	046911	046882	046898
046900	046901	047436	047505	047533	047639	047506	047688	048269	047670
048070	047828	048282	048031	047953	047894	048143	048435	048266	048300
048265	048287	047922	048156	048577	048370	048560	048061	047853	048247
048584	048237	048492	048555	048792	047858	048398	048277	048487	048278
048162	048338	048643	048682	048254	048487	048213	048523	048231	048075
048046	047946	048190	048143	048155	048434	048006	047775	047966	047346
047999	047734	047356	046802	047111	046817	046345	045671	045553	045816
044822	044129	043944	043230	042214	041258	040687	040386	040359	041001
041697	041937	042490	043381	044037	044669	045542	045491	046125	046618
046716	047324	046959	047474	047289	047605	047785	047745	048028	047987
047711	048208	048308	048093	048026	047853	047971	048412	048520	048751

NA N'PRUSS (0.1 MG/CM2) -- TEMP = 179 DEG K -- 3-27-69 -- CH 000 THRU 199

00000	48013	48157	48123	48176	48105	48291	48014	48196	47770
47733	47612	47591	47067	46991	47344	46758	46372	46347	46387
46196	45623	45109	44325	44006	43066	41988	41398	40917	40698
40421	41148	41953	42459	43127	43960	44509	45549	45216	45920
46332	46568	46460	47514	46706	47063	47449	47490	47328	47762
47710	47877	47651	47646	47653	47870	48119	47784	47639	47506
48305	47725	47939	48089	47978	48223	48138	47738	47829	47997
47837	47838	47722	48030	48250	47506	48187	48208	47900	48016
48225	47892	48460	47788	47714	47779	47937	47614	47480	47795
47621	47768	47365	47770	47609	47705	47463	47259	47342	47580
47422	47050	47097	46904	47119	46942	46932	46332	46335	45946
45416	44973	44858	44351	43897	43087	42151	41735	40831	40447
40408	40278	41476	42022	42508	43109	44048	44561	45092	45310
45664	45992	46739	46749	47203	46987	47301	47287	47099	47057
47221	47520	47643	47888	47702	47866	47712	47785	47867	47765
47312	48032	47762	48289	48331	48313	47865	47871	48526	47996
48257	47965	48304	47882	48429	48230	48021	48427	48109	47782
48266	48158	48240	48170	48612	48676	47935	48350	48282	48326
48124	48452	48139	47989	48406	48229	48236	48173	47830	48324
48012	48358	47825	48308	48007	48182	48324	48397	48632	48542

NA N'PRUSS (0.1 MG/CM2) -- TEMP = 179 DEG K -- 3-27-69 -- CH 200 THRU 399

000002	048189	048178	048333	048556	048461	047855	048089	048280	048068
048572	048241	048239	048097	048103	048344	048375	047959	048307	048141
048128	048295	048315	048354	048304	048606	048271	048288	048332	047783
048116	048166	048187	047952	048098	048262	048223	048286	048182	047987
047943	047925	047942	048568	048315	047591	048012	048119	048062	047997
047877	047793	047495	047919	047952	047329	047456	047207	047017	047242
047105	046950	046578	046452	046537	046171	045750	045197	044481	044119
043501	042886	042154	041403	040888	040038	040411	041030	041831	042629
043250	043915	044568	045310	045353	045788	046001	046451	046315	046363
046751	046823	047349	047227	047366	047300	047047	047225	047551	047318
047535	047840	047556	047310	047722	048009	047769	047848	047672	047895
047807	048349	047681	048098	048137	048195	048206	047690	047923	047988
048041	047727	047978	048267	048147	048234	048317	048081	047979	048259
048171	047731	048189	048130	048250	048013	048113	048135	048275	047788
047621	048129	047945	047835	047686	047784	047674	047410	047594	047662
046635	047357	047252	047040	046662	046378	046247	046077	046002	045103
045157	044338	043808	042933	042151	041441	041071	040699	040426	041075
041650	042268	043174	043863	043987	044696	045385	046013	045839	046275
046696	046631	047080	046888	047609	047157	047378	047501	047634	047556
047850	047899	047716	048101	047719	048030	048147	048298	047893	048079

NA N'PRUSS (0.1 MG CM2) -- TEMP = 228 DEG K -- 3-26-69 -- CH 000 THRU 199

00000	47357	47258	47205	47347	47284	47220	47284	47005	46994
47344	46842	46857	46723	46576	46265	46321	46199	45502	45456
45388	45153	44651	44016	43435	42370	41824	41148	41016	40785
40872	41557	42079	42869	43834	44351	44959	45284	45900	45832
46295	46127	46165	46277	46548	46495	46706	47033	46889	46761
46821	47166	47112	47274	47335	46901	47225	47604	46943	47281
47397	47721	47331	47532	47244	47458	47938	47666	47282	47705
47594	47244	47227	47113	47488	47133	47315	47214	47342	47308
47125	47105	47170	47206	47276	46947	47364	47113	47163	46939
47323	47154	46881	47683	46559	47087	46784	47145	46547	47193
46450	46443	46594	46062	46121	46183	46126	45633	45888	45183
45375	44969	44834	43446	43061	42313	41594	41545	41023	40777
40928	40906	41798	42290	42620	43468	43974	44829	45206	45501
45688	45955	45871	46279	46512	46648	46645	46810	46760	46768
47084	47100	47362	47224	47013	47122	47400	47326	47294	47680
47122	47426	47357	47716	47120	47196	47707	47394	47303	47557
47549	47199	47127	47194	47605	47652	47457	47627	47840	47612
47455	47605	47638	47826	47296	47720	47498	47487	47377	47258
47365	47376	47503	47522	47565	47496	47919	47525	47436	47802
47633	47461	47442	47360	47505	47641	47298	47591	47427	48058

NA N'PRUSS (0.1 MG/CM2) -- TEMP = 228 DEG K -- 3-26-69 -- CH 200 THRU 399

000000	047346	047464	047177	047368	047441	047489	047442	047328	047412
047902	047636	047634	047464	047510	047509	047318	048042	047592	047891
047273	047452	047280	047622	047558	047775	047463	047724	047301	047520
047398	047593	047363	047458	047708	047761	047253	047761	047507	047401
047599	047083	047650	047892	047552	047391	047050	047453	047849	047020
046986	047353	047368	047288	047066	047201	046712	046923	046963	047082
047007	046633	046288	046183	046284	045711	045500	045569	045353	044672
044121	043548	043023	042080	041506	040724	040748	040543	041215	041611
042096	042904	043593	044324	044189	045289	045584	045426	046038	045991
045892	046193	046557	046470	046358	046749	046800	046892	046789	046648
047052	047096	046787	047081	046886	047040	046707	047418	046875	047404
047565	047120	047514	047030	046984	047074	047474	047639	047344	047425
047549	047067	047785	047315	047272	047285	047456	047380	047297	047202
047311	047445	047635	047078	047226	047722	047670	047318	047430	047299
047372	047328	047255	047080	047006	046926	047387	047247	046876	046621
046999	046514	046373	046808	046273	046121	046116	046163	045644	045738
044932	044527	044429	043484	043027	042503	041719	041138	040876	040678
041043	041300	041936	042661	043524	043569	044149	045057	045299	045794
046051	046643	046271	046531	046548	046652	046917	046971	046868	047189
047170	046999	047243	047462	047198	047363	047812	047724	047690	047419

NA N'PRUSS (0.1 MG/CM2) -- TEMP = 276 DEG K -- 3-26-69 -- CH 000 THRU 199

00000	48632	48221	48439	47561	48109	47933	47845	47981	47827
47709	47681	47231	47319	47137	47395	46846	46751	46904	45961
46180	45931	45528	44811	44080	43642	43085	42490	42482	41768
42879	43081	44286	44686	45554	45930	45695	46372	46407	46857
47154	47138	47553	47590	47370	47625	47569	47909	47728	47585
48125	48237	48245	47555	47739	48135	47950	48177	47917	47903
48392	48019	48010	48056	48177	47974	47979	47851	48416	48540
48252	48245	48080	47969	48102	48120	47856	48102	48366	47954
48053	47941	48444	47871	47977	47919	47991	47954	48042	47766
48031	47824	48022	47743	47850	47489	47531	47600	47550	47527
47703	47303	47241	47216	47039	46927	46477	46467	46462	45693
45357	45587	44802	44067	43947	43310	42783	42321	42064	42468
42601	42726	44387	44397	45038	46111	45845	46025	46130	46801
46590	46873	47174	47186	47505	47533	47389	47453	47493	48084
48183	47760	47732	48314	48356	47817	47809	48167	48266	47920
48038	47989	48046	47794	48235	48538	48290	48458	47807	48089
48404	48207	48500	48429	47998	48239	48111	48884	47856	48406
47860	48672	48222	47839	48626	48226	48149	48262	48483	48596
48473	48111	48466	48461	48090	48527	48224	48874	47933	48594
48623	48777	48390	48236	48410	48159	48074	48482	48241	48466

NA N'PRUSS (0.1 MG/CM2) -- TEMP = 276 DEG K -- 3-26-69 -- CH 200 THRU 399

000002	048146	048608	048809	048504	048321	048534	048619	048397	048258
048458	048471	048013	048751	048537	048249	048377	048279	048224	048375
048422	048282	048295	048716	048378	048379	048237	048474	048598	048114
048555	048026	048137	047632	048023	048209	048285	048044	048465	048087
048325	048487	048021	048460	048382	048195	048284	048317	048035	048314
048088	048140	047860	047657	047758	048146	048041	047870	047874	047937
047759	047268	047239	047576	047109	046986	046623	046814	046477	045585
045977	045543	044787	044235	043412	042989	042516	042482	042240	042458
042883	043443	044208	044112	045101	045424	045828	046115	046356	046464
046944	047059	047068	047085	046994	047142	047104	047314	047578	047738
047660	047381	047983	047792	047707	048041	048109	047913	048044	047835
047857	047918	047566	048093	048137	047958	048086	048007	048401	047393
047969	047671	048065	047924	048148	047856	048313	048452	048223	047839
048071	048433	048022	048372	048293	048161	048404	048179	047736	048465
048223	047930	048007	047995	047891	047650	047934	047521	047830	047615
047570	047758	047560	047554	047438	047092	047437	047043	046624	047038
046383	045917	045514	045439	044899	044431	043757	042861	042308	042527
042237	042319	042834	043230	044084	044704	044929	045208	046187	046384
046703	047108	047088	047224	047330	047249	047236	047542	047601	047412
047600	048284	047772	048127	048259	048101	047995	048007	048325	048264

NA N'PRUSS (0.1 MG/CM2) -- TEMP = 293 DEG K -- 3-26-69 -- CH 000 THRU 199

00000	91054	91283	91297	91263	91048	91134	90754	90827	90731
90621	90247	89953	90198	90211	89206	88858	88998	88790	87683
87343	86475	86213	85325	83243	82232	81597	81060	80864	81423
82223	83663	84698	85327	86293	87715	88180	88598	89212	89333
89457	89860	89894	90349	90522	89981	90429	90420	90659	90641
90686	91154	90964	90543	90396	91063	90538	91076	91149	91013
90860	91476	91790	91018	91502	91508	90912	90388	90944	90957
91091	91240	90939	91383	90947	91198	91089	91257	91244	91363
91100	91483	91156	90316	90798	90736	90912	90451	90303	90058
90899	91133	90426	90926	90243	90554	90043	90589	89757	90131
90036	89962	89232	89399	89249	88646	88890	88076	87681	87521
86433	86087	84895	83858	83126	81280	81127	80127	80103	81104
81565	82878	84074	84677	85872	86908	88199	88437	88529	88909
89075	89643	89203	90295	90015	90619	90315	90177	90060	90863
90166	90893	90626	91230	90525	91257	91328	91077	91081	90850
91522	90471	91164	91281	91822	91639	91757	91610	91682	91370
91042	91685	91489	91772	91683	91551	91479	91445	91945	91492
91139	91170	91668	90838	91568	91645	91607	91424	91166	91959
91522	91931	91297	91867	91404	91754	91360	91658	91975	91255
91441	91620	91893	91155	91401	91498	91953	91559	91977	91176

NA N'PRUSS (0.1 MG/CM2) -- TEMP = 293 DEG K -- 3-26-69 -- CH 200 THRU 399

000000	091619	091813	091844	091750	091651	091416	091510	091460	091371
091558	092439	091648	091796	092176	091770	091738	091244	092040	091647
090913	091917	091438	091513	091720	092071	091341	091020	091328	091641
091601	091637	091289	091361	090937	091971	091823	091016	091376	091297
091762	092131	091348	090800	091272	091440	090822	091318	091566	091470
091046	090795	090839	090906	090692	091093	090606	090886	090421	090121
090215	090567	090309	089513	089915	089375	088842	088824	088649	088057
087375	086616	085439	084509	083505	081968	081013	080007	080338	080110
081250	082611	083282	084525	085800	086674	087433	087768	088349	088391
089245	089466	089129	090037	089570	089844	089851	090077	090677	090515
090307	090239	090776	090473	090921	090951	090454	090235	090495	090720
090436	090879	090847	090595	091023	090887	090645	091165	090932	090858
091259	090415	091419	091298	091251	091410	091031	091303	091498	091171
090957	091273	091491	091485	091710	091071	091240	091299	091174	090998
091784	091368	091336	091319	090854	090646	091352	090780	090916	090459
090367	090061	090371	090495	089923	090077	089611	089236	088753	088825
088255	087951	087181	085989	085882	084567	083126	081881	081293	080574
080370	080678	081120	082489	083659	084281	085494	086732	087426	087935
088541	088543	089409	089132	089734	089714	089856	090686	090304	090598
090460	090508	090947	090954	091993	091007	091879	091583	090995	091456

NA N'PRUSS (0.25 MG/CM2) -- TEMP = 293 DEG K -- 3-25-69 -- CH 000 THRU 199

00000	98601	97998	98327	98195	97960	98154	97513	97558	97289
97231	96948	96663	96252	95643	94797	94818	94109	93657	93149
91495	90441	88960	87461	85302	83221	82474	81096	81811	82767
84606	86122	87599	89438	90871	91765	92647	93729	94234	95089
95876	95943	95778	95852	96282	96639	96629	97365	96657	97447
96556	97242	98153	98143	97545	97921	97713	97765	97842	98078
98657	98084	97776	98211	98532	98040	98335	98665	97805	98151
97997	98120	97850	98506	98054	97753	98271	98153	98083	98262
98203	97851	98250	97419	97815	97950	97644	97496	97354	97356
96733	97688	97547	97307	96706	96800	96993	97129	96925	96536
96042	96631	95336	95014	95241	94783	93799	92850	92584	91459
90675	89403	87600	86687	84590	83102	81800	81072	80002	82609
83325	85445	87186	88670	90162	91765	92456	92821	93564	94651
94423	95495	95823	95645	95993	97025	96785	97316	96756	97768
97300	97362	97482	97328	97706	97731	97855	98317	98436	97942
98707	98598	98537	98001	98764	98414	98822	98351	98667	98618
98352	98917	98622	98701	98384	98877	98898	98431	98287	98305
98446	98674	98851	98921	98940	98095	98657	98928	98612	98276
97888	98256	99114	98850	98867	98819	99307	98481	98844	98645
98702	98670	98344	99228	98317	98798	98843	98846	98990	98731

NA N'PRUSS (0.25 MG/CM2) -- TEMP = 293 DEG K -- 3-25-69 -- CH 200 THRU 399

000000	099174	099067	099318	099029	098788	098928	098856	098450	098759
098684	099232	098936	099037	098555	098504	098307	099272	099149	099010
098464	098762	098854	098597	098519	098432	097976	098925	098838	098645
098432	099227	098735	097558	098579	098671	098239	098750	098852	098715
098225	098117	098394	098650	098783	098114	098623	098440	098049	097939
098066	097733	097746	097436	098025	097688	097340	097021	096787	096555
096474	096477	096313	096077	095738	095324	094595	093984	093234	092002
091107	090327	089110	087020	085869	083984	082198	080665	081037	081677
082847	085081	087041	088220	089596	090663	091809	092026	093076	094560
094743	095176	095034	095966	096020	095358	096197	097401	096883	096960
097127	097068	097017	096908	097229	097172	096959	097424	097591	097622
097875	097448	097830	097176	097702	098683	098154	097970	098207	097692
097783	098048	098718	098003	097911	097872	098183	098196	098500	098411
097522	098395	098360	098138	097995	098196	098047	098340	097599	098123
097648	097800	098049	097792	097488	098158	097311	097393	097317	096625
097144	096273	096674	097027	096160	095759	094939	095378	094529	093827
093102	092122	091247	089908	088614	086850	085860	083779	082746	081558
081646	082289	083408	084696	086738	088401	090168	091029	092641	092648
094198	094220	095280	094789	095869	096055	096768	096365	097170	097268
097545	097556	097020	097461	098198	097965	097822	098302	098245	098243

NA FERROCYANIDE -- TEMP = 80 DEG K -- 3-30-69 -- CH 000 THRU 199

00000	55461	55508	55550	55383	54959	54789	55218	55284	55203
55136	55422	55173	55029	55392	55035	54908	54992	55308	54721
55035	54752	55586	54704	55249	55243	55212	54843	55403	55158
54978	54925	55083	55190	55007	54790	54854	54957	55105	54730
54812	55313	55020	54807	54750	54751	54668	54507	55168	54886
54564	54803	54981	54871	54247	54240	54260	54347	53845	54075
54154	54386	54003	54016	54111	53639	53271	52876	53356	52906
52640	51942	51739	51535	50800	50695	49595	48577	47806	46703
45531	44664	42786	42114	41633	40316	40079	40008	40691	41458
42682	43912	45058	46056	47625	48477	49664	50146	50308	51051
51539	52088	51811	52116	52622	52888	52905	52971	53156	53498
53418	53783	53582	53760	54259	54386	54244	54403	54547	54663
54349	54399	54473	54488	54468	54613	54588	54974	54850	54591
54971	54649	54983	54795	54688	54703	55056	55186	54860	55356
54712	54806	55325	54781	55619	54741	54806	55093	55422	55051
55041	54984	55466	55353	54402	54983	55264	55250	55241	54451
55136	54860	55085	55450	55592	55343	55524	55234	54996	55480
55065	55774	55427	55245	54969	55308	55333	55157	55175	55127
54858	55236	55083	55069	54847	55138	55329	55299	55543	55303
55036	55432	54690	55469	55306	55318	54993	55083	55510	54983

NA FERROCYANIDE -- TEMP = 80 DEG K -- 3-30-69 -- CH 200 THRU 399

000001 055350 055490 055354 055282 055402 055053 055166 055335 055027
055291 055129 055143 055128 055215 055285 055117 055176 055113 055401
055036 054913 055347 055455 054944 055098 055651 055691 055493 055211
055448 055250 055095 055118 054610 055122 054779 055074 055097 055303
054933 054917 055004 055504 055633 054973 054729 054707 054991 055168
055176 055188 055342 055056 054847 054895 055005 054973 054954 055009
054698 055074 054650 054877 054710 055011 055013 055012 055243 054766
054909 054420 054544 054553 054353 054708 054210 054389 053850 054402
053906 054027 054162 053763 053571 053637 053343 053621 053170 052999
053239 052213 052489 052196 051972 051744 051359 050924 050188 049627
048357 047359 046344 044782 043549 042548 041318 040946 040243 040512
040291 041153 041964 042648 043975 045740 046761 047142 048453 048958
049611 050947 051177 051735 052337 052094 052540 052818 053621 052944
053021 053957 053900 053792 054426 054249 053867 054374 054147 054467
053990 054481 054645 054603 054565 054478 055061 054908 054810 055124
055141 054426 054819 055003 054894 055195 054561 054668 055244 055325
054980 054770 054558 054932 055033 054859 055147 054811 055246 054771
054955 054988 055099 054765 055388 055490 054743 054735 054675 054804
055145 055025 055114 054786 055104 055015 055269 055449 055093 054828
055263 055185 055163 055218 055454 055215 054940 054896 055141 054811

NA FERROCYANIDE -- TEMP = 129 DEG K -- 3-29-69 -- CH 000 THRU 199

00000	54243	54271	54628	54550	53974	54409	54070	54406	54207
54320	54639	54064	54397	54541	54457	54154	54333	54093	54504
54113	54048	54186	53908	54512	54522	54221	54498	53966	54124
54245	54230	54139	54190	54163	54110	53800	53779	54329	54261
54186	54242	53947	54338	53918	54134	53983	53945	53748	53947
54087	53833	53627	54182	53955	53634	53950	53454	53374	53573
53568	53060	52878	52583	53068	52972	52281	52441	52036	52250
52009	51615	51336	50428	50264	49738	49133	48221	47577	46396
45375	44423	42828	41726	40802	40030	40020	40123	40954	41463
42968	44192	45546	46406	47451	48361	49247	49676	50144	50532
50887	51324	51380	51524	52241	51766	52571	52404	52451	53106
53151	53201	53213	53020	53127	53560	53367	53498	53495	53657
53382	53804	53544	53550	53723	53497	53450	53754	53415	54231
53674	53840	54232	54346	53910	54062	54053	54111	54069	53797
54123	54681	54216	53892	54127	54044	53584	54202	54478	54175
53793	54246	53745	53956	54154	54068	54084	54185	54004	54440
53972	53910	54272	54404	54644	54585	54140	54337	53992	53963
54449	54385	53919	54332	54147	54261	53908	54128	54187	54586
53939	54929	54272	54230	54411	54413	53920	54041	54155	54314
54167	54904	54035	54297	54165	54079	54306	54104	54426	54537

NA FERROCYANIDE -- TEMP = 129 DEG K -- 3-29-69 -- CH 200 THRU 399

000001	054173	053962	054339	054511	054329	054104	054445	054483	054757
054475	054558	053859	054184	053949	054070	054179	053788	054584	054473
054584	054559	054385	054212	054423	054314	054069	054145	054278	054172
054108	054002	053947	054373	053896	054077	053959	054058	054456	054376
054267	054038	054135	054083	054528	054131	053937	054014	053821	054287
054042	054100	054199	053384	053780	054434	053975	054339	053778	053939
054150	054170	054139	053879	054213	053592	053941	053661	054004	053741
053971	054150	053769	054070	053934	053649	053750	053753	053199	053560
053647	053746	053184	052997	052795	052644	053086	052774	052670	052208
052455	052027	051447	051484	051791	051411	051078	050317	050059	049207
048554	047769	047108	045897	044174	043130	042259	041068	040236	040451
040174	040526	041584	042355	043393	044434	046151	046972	047882	048765
049282	049847	050665	051142	051419	051639	051861	052350	052204	052042
052781	052685	052915	053049	053220	053265	053463	053107	053388	053939
053472	054064	053851	053939	053967	053978	053639	053967	054003	053928
053981	054015	053970	053589	054031	054064	054105	054437	054164	054334
054001	053713	054170	054237	054371	054525	054001	054400	053823	054388
054350	053920	053968	054493	053999	054329	054145	054228	053959	054225
054490	053626	054056	054396	053883	054389	054101	054368	053825	054098
054232	054252	054494	054366	054252	054406	054128	054100	054143	054578

NA FERROCYANIDE -- TEMP = 179 DEG K -- 3-29-69 -- CH 000 THRU 199

00000	53442	53606	53236	53484	53565	53187	53403	52965	53019
53309	53253	53351	53305	53105	53394	52935	53309	53417	53228
53163	52823	53042	53005	53058	53222	52846	52964	53048	52948
53174	53108	53268	53213	52993	53286	52885	53285	53214	52797
53030	53166	52914	52766	53305	52956	52692	53151	52812	52209
52976	53079	52527	52377	53110	52447	52613	52259	52910	52641
52150	52526	51994	52018	51851	51506	51760	51323	51033	50841
50887	50798	50397	49894	48831	48890	48301	46952	46377	45294
44080	42806	41278	41104	40204	40062	40464	40981	41778	42879
43796	45242	45893	46773	47703	48783	48969	49912	50265	50080
50554	51005	51037	50970	51316	51603	51711	52141	52177	51518
52217	52121	52226	52493	52300	52148	52991	52638	52894	52573
52813	52986	53056	52936	52643	52652	52937	53011	52888	52897
53517	53109	53075	52782	53128	53018	53440	52836	52991	53360
52982	53169	53096	53023	53046	53201	53420	53197	53344	53205
52919	53389	52961	53628	53142	53175	53033	52921	53404	53784
53174	52952	53273	53040	53132	53328	53327	53323	53117	53271
53065	53251	53544	53246	53294	53079	53286	53103	53535	53441
53358	53265	53127	53026	53313	53049	53218	53483	53113	52982
53155	53423	53208	53109	53601	54005	53100	53184	53229	53269

NA FERROCYANIDE -- TEMP = 179 DEG K -- 3-29-69 -- CH 200 THRU 399

000000	053175	053568	053107	053429	052943	053194	053522	053292	053135
053423	053325	053488	053299	053352	053150	053865	053125	052800	053339
053717	053350	052961	053696	053145	053498	053133	053502	053361	053090
053341	053320	053464	053606	052683	053221	053186	053179	053544	053309
052972	052851	052854	052821	053083	053121	053289	053396	053342	052831
053408	052682	053309	053217	052806	052590	053409	053333	052820	053519
053266	052727	053159	053424	053046	053253	052959	052946	052839	052653
053167	052898	052876	052721	052838	052888	052865	052489	052645	052435
052547	052707	052080	052197	052028	051753	051758	051919	051884	052141
051151	051539	051079	051156	050830	050578	050507	049782	049045	048893
048421	048011	047373	046422	044961	043994	042711	041758	040955	040411
040155	040572	040775	041495	042248	043611	044671	045617	047048	047846
048275	048504	049550	050321	050438	050554	050658	051264	051455	051388
052030	051624	052017	052405	052351	052366	052243	052707	052926	052467
052672	052611	052529	052782	052595	052720	053469	052741	052878	053050
053127	052718	053104	053197	052919	052730	053231	053214	052948	053000
053300	053267	053174	053298	053605	052765	053100	053042	052960	053462
052910	052689	053433	053610	052915	053366	053492	053140	053365	052935
052966	053401	053286	053163	052983	053149	052983	052990	052801	053107
053342	052960	053062	053304	053290	052992	053446	053386	052891	053184

NA FERROCYANIDE -- TEMP = 228 DEG K -- 3-28-69 -- CH 000 THRU 199

000000	052592	052479	052412	052230	052459	052C09	052766	052226	052924
052246	052384	052352	052284	052210	051896	052647	052147	052203	052318
052502	052277	052339	052413	052470	052223	051976	052114	052447	052733
052172	052011	052348	052319	052344	052305	052254	052133	051871	051851
052289	052569	052235	052157	051894	052508	052521	052113	052099	051768
051847	052081	052033	051668	052427	051746	051409	051367	051667	051310
051549	051549	051319	050957	051357	051329	050734	050620	050365	050174
049749	049406	049308	048764	048125	047430	046948	046139	045439	043985
042651	041911	041301	040646	040044	040470	041113	041783	042681	044079
044825	045661	046554	047881	048008	048531	049103	049245	049445	050477
049869	050281	049880	050353	050786	050755	050878	051008	051447	051435
051516	051794	051770	051300	051932	051701	051882	051876	051898	051998
052346	052504	051754	052086	052007	052195	051955	051928	052204	052244
052073	052164	052883	052113	052081	052612	052396	052216	052713	052405
051902	052114	052149	052325	051952	052558	052742	052307	052204	052539
052420	052401	052704	052498	052202	052408	052218	052038	052305	052687
052280	052664	052274	051915	051950	052424	052333	052519	052595	052234
052184	052584	052544	052329	052426	052467	052257	052274	052955	052394
052627	052587	052092	052588	052512	052568	052254	052552	052403	052520
052336	052480	052619	052500	052784	053134	052320	052478	052532	052297

NA FERROCYANIDE -- TEMP = 228 DEG K -- 3-28-69 -- CH 200 THRU 399

000003 052710 052137 052485 052502 052643 052806 052172 052390 052558
052985 052649 052282 052329 052713 052616 052280 052140 052261 052576
052366 052611 052684 052269 052345 052590 052432 052448 052641 052181
052298 052289 052523 052533 052123 052265 052645 052254 052549 052212
052614 052296 052180 052453 051881 052332 051918 052452 052108 052840
052316 052131 052261 052342 052285 052176 052745 052106 052191 052253
052723 052308 051926 052547 052064 052135 052167 052272 051867 051983
052302 052474 052229 052005 052229 051933 051892 051902 051677 051578
051894 051563 051241 052081 051772 051891 051560 051335 051412 050956
051232 050512 050728 050478 050596 050300 049995 049702 049344 049021
048717 048118 047288 046583 045916 044614 043768 042540 041653 040954
040442 040142 040604 040775 041817 042758 043696 044683 045635 046774
046958 048001 048686 049149 049362 049968 049996 050608 050368 050933
050997 051166 051646 050710 051261 051444 051641 051948 051747 051343
052166 051884 052054 051903 052151 051938 051788 051964 052312 052232
052394 052127 052368 052538 051914 052059 052181 052173 052301 052460
052244 052156 052312 052189 052383 052252 052082 052673 052004 052654
052244 052636 052532 052169 052264 052252 052503 052254 052573 052373
052153 052202 052042 051909 052125 052309 052382 052519 052407 051848
052134 052522 052367 052091 052601 052065 052524 052006 052136 052763

NA FERROCYANIDE -- TEMP = 276 DEG K -- 3-28-69 -- CH 000 THRU 199

000000	051441	051505	051421	051175	051627	051333	051491	050831	051365
051328	050991	051298	051560	051137	051551	051019	050967	051294	051239
051592	051392	051351	051024	051578	051503	051164	050838	051060	051574
051111	050935	051105	051597	051188	050986	051095	051176	050996	051498
051568	051193	051284	051140	050808	051266	050903	051094	051072	050965
050863	050631	050742	050663	050889	050945	050985	050929	050627	050749
050235	050520	050340	050154	050053	050112	049420	049219	048947	049261
048741	048468	047706	047509	047133	046348	045488	044855	043752	042385
041830	040828	040013	040017	040731	040866	041802	043112	043937	045011
045330	046312	047136	047627	047859	048188	048429	049168	049323	049829
049813	049685	049935	049864	049875	050201	050147	049788	050327	050495
050663	050586	050627	049956	050727	050779	050866	050732	051105	050959
050816	050963	050869	050904	051158	050919	050995	051089	051124	051217
051320	051529	050862	051184	051159	050893	051061	050974	051089	051342
051505	051567	051339	051309	051068	051149	051319	051116	051053	051044
051311	051171	051244	051202	050923	051237	051022	051553	051307	051697
051547	051381	051449	051536	051208	051357	050949	051647	050868	051334
050812	051633	051082	051611	051431	051049	051011	051144	051421	051278
051467	051212	051551	051109	051428	051704	051246	051348	051420	051023
051514	051411	051731	051404	051256	051312	050966	051167	051380	051580

NA FERROCYANIDE -- TEMP = 276 DEG K -- 3-28-69 -- CH 200 THRU 399

000000 051301 051160 051565 051130 051273 051467 051223 051731 051086
051267 051160 051379 051236 051743 051741 051366 051638 051075 051521
051582 051534 051505 051054 051093 051185 051106 051154 051607 051478
051571 051548 051162 051560 051181 051170 051135 051366 051068 051163
051057 051125 051337 051532 051410 050962 051462 051013 051184 051082
051268 051384 051877 051035 051497 051021 051239 051209 051253 051026
051177 051353 051255 050989 051099 051079 050889 050818 051068 051058
050998 050919 050689 050847 050723 051035 050854 051186 050967 050803
050826 050529 050611 050558 050411 050078 050381 050446 050156 049836
050239 050122 050080 050271 049752 049833 049580 049310 049592 049109
048416 048136 047525 046979 046323 045576 044097 043542 042028 041760
041026 040678 040229 040176 041004 041473 042183 043622 044380 045674
046361 046855 047220 047701 048095 048807 049327 049134 049449 049542
050297 050141 050044 050174 049977 050360 050073 050569 050702 050682
050755 050889 050675 050156 051157 050903 051172 050934 051176 051277
051175 050998 051257 051323 051422 051187 051465 050655 051291 051084
050890 051147 051223 051227 051224 051397 051262 050985 050923 051401
051374 051398 051492 051098 050876 051386 051170 051418 051343 051378
051467 051427 051057 051009 050883 050919 051082 051189 051011 050912
051080 051469 051495 051607 051343 051127 051192 051251 050997 051138

NA FERROCYANIDE -- TEMP = 293 DEG K -- 3-28-69 -- CH 000 THRU 199

000000 052153 051738 052186 052400 051994 052324 052306 052110 052098
052165 052260 052368 052199 052121 052437 052249 051959 052425 051857
052224 051956 052397 052448 052350 052272 052236 052218 052192 052174
052022 052466 052191 052295 052212 051865 051852 052162 051991 052079
051877 051909 052019 051615 052111 051937 051951 051716 052242 051992
052121 051848 051731 051315 052245 051540 051606 051654 051705 051618
051387 051310 051566 050882 050606 050871 050661 050510 050293 050014
049746 049255 048702 048272 047130 047031 045901 045374 043940 042884
042278 041357 041415 041284 041825 042450 043019 044509 045064 046730
047180 047525 048459 049111 049201 049840 050113 049802 050259 050212
050644 050531 050898 050920 051372 051356 051183 051540 051383 051377
051543 051288 051309 051537 051750 051433 051733 051904 051361 051750
052296 052242 051899 051819 051779 051586 051812 051795 052290 052106
052113 052335 052310 052308 051937 052301 052214 052227 052222 052314
052066 052574 052286 051919 052301 052402 052046 052060 052412 052135
052002 052404 052339 052395 052068 052142 052520 052273 052278 052149
052375 051810 051970 052385 052321 052013 052613 052391 052334 052348
052061 052403 052295 052515 052701 052287 052129 051895 052518 052321
052285 052258 052235 052101 052311 052689 052411 052455 052352 052321
052043 052538 052307 052298 052098 052393 051787 052267 052035 052070

NA FERROCYANIDE -- TEMP = 293 DEG K -- 3-28-69 -- CH 200 THRU 399

000000	052147	052407	052174	052654	052590	052425	052105	052655	052283
052581	052027	051965	052456	052619	052256	051947	052233	052383	052619
052347	052147	052462	052440	052522	052091	052144	052457	052301	052520
052089	052216	052332	052466	052159	052234	052532	052186	052050	052336
052106	052119	051925	052291	052240	052379	052332	052248	052423	051923
052185	052560	052314	051957	052238	051753	052321	052474	051731	052234
052274	051947	051838	052090	052076	051834	052108	052310	052443	051940
051902	051835	052350	051969	052099	051554	052014	051972	051594	051674
051582	051843	051480	051964	051238	051862	051699	051208	051311	051238
050699	050746	050357	050843	050268	050972	050074	050144	050077	049635
049299	049231	048536	048543	047404	046863	046137	045190	044208	043618
042072	041751	041400	041700	041901	042503	043497	044297	045261	045937
047023	047602	048510	048749	048861	049164	050111	050021	050447	050319
050420	050882	051401	051454	051486	051218	051610	051636	050803	052073
051612	051784	051670	052329	052083	051839	051281	052074	052013	051632
052153	051993	052037	052288	052055	052123	052318	052006	052396	052415
052200	052099	052288	052192	052178	052301	052179	052083	052021	052174
052418	052165	051823	051965	052344	052081	052485	051987	052386	052158
052143	052393	052249	052873	051933	052106	051993	052232	052288	052315
052241	052684	052134	051899	052279	052401	052420	052149	051969	052606

K FERROCYANIDE — TEMP = 78 DEG K -- 4-11-69 — CH 000 THRU 199

000000 059209 059067 059104 058579 058848 058844 058870 058918 058672
058751 058877 058807 058583 058846 058798 058790 058926 058942 058622
058627 059353 058798 058854 058996 059095 058519 058855 058886 058732
058677 058914 058759 058834 058847 058787 058981 058531 058500 058911
058586 058956 058757 058325 058765 058857 058363 058472 058481 058245
058733 058487 058387 058510 058437 058629 058809 058644 058107 057747
058106 058244 057933 058159 058003 057543 057822 057251 057616 057223
057089 056990 056626 056122 055827 055589 055185 054110 053408 053261
052180 051380 049792 049242 048233 046917 046443 046335 046293 047132
047640 049081 049820 051178 051587 052379 053553 053768 054838 054825
055506 055759 055929 056869 056416 056640 057312 057364 057550 057529
057901 057486 057781 057799 057515 058217 057926 058167 058551 058277
057965 058529 058383 058531 058496 058654 058646 058177 058260 058816
058579 058146 058734 058922 058540 058672 058159 058739 058422 058936
058943 058635 059036 058168 058869 058667 058862 058674 058664 058703
058759 058814 059167 059109 058745 058799 058814 059112 058694 059067
058977 058665 058848 058816 059171 058580 058806 058709 058427 058702
059214 058869 058945 059067 059020 059136 058686 058795 059006 059289
058942 058498 058717 058354 059050 058998 058950 058784 059224 059003
058857 058865 058807 059367 059213 058649 058956 058796 059113 059242

K FERROCYANIDE -- TEMP = 78 DEG K -- 4-11-69 -- CH 200 THRU 399

000000 058623 058946 058773 058805 058876 058971 058690 059228 058712
058770 059182 058926 058665 058685 059226 058867 058944 058570 058951
059015 058751 058650 058721 058712 059149 059618 058955 058955 058891
058739 059268 058941 059210 059086 058546 058600 059077 058942 058537
058946 059302 058873 059431 058744 058624 058676 058729 059240 059034
059385 058868 058506 058409 058699 058753 058865 058807 058546 058888
058861 058413 058589 059105 058891 058414 058783 058567 058925 058511
058791 058598 058344 058536 058703 058318 058613 058483 058308 058254
058230 058009 057878 057662 057447 057190 057465 057224 057377 056982
056817 057007 056766 056310 055886 055858 054940 054598 054048 053281
052602 051892 050916 050160 048759 047866 047666 046854 046630 046601
047107 047559 048813 049541 050682 051699 052285 053551 054258 054634
055365 055830 055719 056356 056726 056689 056929 056764 057337 057401
057661 057495 057739 058280 057647 058110 058061 058749 058170 058262
058402 058917 058633 058681 058698 058555 058728 058467 058887 058882
058367 058879 059080 058579 058712 058666 058471 058824 058957 058977
058587 058688 058619 059179 059131 058547 058852 058913 058745 058866
059226 059046 058898 058916 058793 058411 058912 059039 059085 058854
059097 058765 058931 058937 058889 058969 058886 058459 059007 058765
058577 058812 059098 058589 058768 058332 058973 058497 059011 058987

K FERROCYANIDE -- TEMP = 130 DEG K -- 4-11-69 -- CH 000 THRU 199

000000 059344 059357 059264 059348 058885 059188 059210 059131 058962
059034 059171 059203 059159 059149 058805 059411 059076 058872 059261
059432 058389 058820 058531 059167 059147 058784 059204 059117 059157
058965 059156 058955 059155 058806 059004 059305 059072 059216 059323
058733 058460 059007 059110 059207 058855 058513 058774 058653 058915
058712 058543 058544 058647 058845 058516 058959 058510 058996 058550
058752 057991 058101 057816 058530 057868 058202 057478 057660 057039
057183 056940 056878 056565 056195 055652 054973 054442 053833 053378
052214 051369 050206 049011 048317 047794 046869 046927 047030 047800
049293 050277 051705 052375 053303 054688 054956 055292 055405 056295
056455 056719 056676 057143 056779 056975 057426 057758 058018 057712
057677 057852 057936 058012 058560 057945 057803 058095 058277 058301
058320 058415 058565 058680 059001 058823 058639 058598 058994 058513
058736 059006 058477 058848 058901 059420 058699 059020 058728 058341
058864 058923 059041 058788 058983 058920 058787 059222 059004 058593
058945 058954 059047 058948 058782 058922 059280 059208 058852 058899
059099 058972 059300 059228 059066 059101 059048 058792 059257 058751
059186 058928 059316 059175 059205 059123 059171 059163 059468 058924
059324 059062 059118 059113 058843 059211 059131 059470 059160 058959
059457 059043 059060 058961 058640 059011 058981 059237 059110 059425

K FERROCYANIDE -- TEMP = 130 DEG K -- 4-11-69 -- CH 200 THRU 399

000001 059402 059199 059636 059451 059118 059106 059519 058997 059432
059149 059255 059246 058782 058792 059218 059198 059099 059446 059015
058766 059043 059214 059581 058793 059391 059020 058873 059173 058935
058899 059133 058751 058960 059017 058887 058942 059127 058485 059253
059088 058851 058709 059073 058607 059053 059348 058837 058857 059130
059429 058874 059431 058862 058723 059112 058829 058805 058613 059104
059031 059370 058997 058894 058768 058812 059171 059026 058823 058471
058696 058668 059170 058923 058066 058534 058515 058367 058265 058481
057748 058146 058127 057598 057684 057756 057530 057904 057293 057578
057423 057285 057250 056754 056312 056615 056529 055751 055411 054330
054250 053131 052458 051424 050582 049249 048344 047377 047204 046830
046938 048140 048996 050017 051254 052013 053127 054086 054845 055059
055470 056071 056818 056176 056738 057014 057173 056982 057187 057455
058208 058054 058367 057996 058376 058394 058733 058317 058641 058937
059063 058326 058847 058531 058767 058701 058586 058825 058612 059208
058884 058712 059113 059210 058963 058809 058945 058981 058744 059209
058969 059227 059577 059398 059323 058843 058734 059034 059303 058533
058961 059334 058955 059467 059387 059254 058982 058992 058990 058485
058721 058758 059338 059134 059009 059230 058592 058752 059119 058555
058676 059002 058914 059147 059108 058704 058762 059270 059059 058956

K FERROCYANIDE -- TEMP = 179 DEG K -- 4-11-69 -- CH 000 THRU 199

000104 061501 061421 061504 061657 061255 061633 061992 061416 061443
061632 061441 061518 061595 062030 061495 062057 062044 061468 061661
061248 061513 061727 061352 061532 061631 061635 061536 061427 061353
061679 061408 061606 061153 061507 061582 061999 062018 061422 061393
061214 061367 061141 061388 061721 061207 061260 061466 061172 061492
061312 060949 061490 061245 060720 061174 061258 060964 060784 060610
060826 060986 060636 060568 060345 060410 060609 059948 060232 059441
059965 059154 059166 059263 058575 057985 058064 057021 056915 055770
054384 053927 052580 051702 050389 050083 050160 050438 051272 052222
053531 054033 055062 055819 057131 057443 057915 058122 058979 059019
059212 059381 059867 059839 059792 059868 059666 060454 060276 060487
060615 060140 060304 060280 060592 060342 060908 060538 061055 060894
060864 061285 061018 061230 061214 061462 061393 061024 061396 061332
061368 061232 061118 061825 061542 061545 061384 061184 061207 061957
061175 061625 061541 061237 061211 061699 061531 061627 061249 061187
061287 060977 061492 061227 061979 061711 061253 061429 061163 061725
061555 061660 061294 061426 061451 061743 061515 061821 061592 061337
061619 061857 061721 061230 061827 061522 061650 061407 061776 061543
061677 061257 061809 061600 061459 061428 061488 061797 061703 062014
061541 061471 061323 061724 061187 061826 061931 061452 061367 061723

K FERROCYANIDE -- TEMP = 179 DEG K -- 4-11-69 -- CH 200 THRU 399

000000 061436 061297 061173 061779 061535 061226 061630 061530 061836
061463 061668 061311 061391 062162 061617 061811 061521 061451 062009
061770 061415 061834 061574 061330 061667 061906 061938 061567 061580
061626 061394 061709 061265 061673 061687 061627 061400 061801 061380
061575 061553 061814 061753 061414 061544 061239 061877 061190 061464
061482 061309 061331 061418 061739 061474 061793 061307 061633 060864
061179 061294 061240 061595 061313 061648 061454 061652 061337 061015
061144 060820 061048 061401 061105 061340 060875 061330 060787 060655
061120 060800 060980 061070 060321 060697 060401 060199 060109 060199
060173 059456 060228 059850 059597 059175 058783 058892 058359 058012
057565 057064 056053 055733 054636 054005 052670 051642 050779 050372
050005 050201 050763 051670 053110 053733 055234 055661 056568 057098
058106 058818 058502 058927 059199 059449 060060 059437 059914 060554
060351 060361 060905 061538 061218 060714 060875 060807 060727 061280
061166 060655 061283 061407 061249 061505 061090 061480 061504 061527
061731 061010 061238 061228 061583 061100 061562 061387 061265 061231
061174 061444 061396 061414 061487 061286 061533 061491 061509 061652
061749 061345 060934 061508 061454 062069 061537 061608 061727 061564
061549 061760 061195 061687 061608 061395 061852 061622 061818 061734
061531 061314 061200 061551 061418 061257 061664 061366 061645 061656

K FERROCYANIDE -- TEMP = 228 DEG K -- 4-11-69 -- CH 000 THRU 199

000000 060475 060010 060197 060301 060050 060256 059734 060164 060402
060138 060308 060395 060449 060161 060487 060172 059923 060275 060579
060178 060181 059942 060362 060736 060666 060327 060296 060729 060331
060440 059881 060510 060754 060449 060240 059870 059887 060203 060249
060060 060009 059651 060254 0602C1 060047 060263 060464 059998 059913
059750 059910 060100 059901 060023 060173 059633 060051 059999 059914
059731 059796 059517 059785 059757 059263 059111 058762 058606 058904
058398 058249 058419 057932 057320 057020 056740 056214 054858 054413
053787 052399 051809 051255 050697 050310 050589 051002 052518 053168
054107 055351 055699 056744 056948 057344 057378 057369 058318 058164
058578 058552 058429 059299 058785 058923 059526 058838 059253 059324
059127 059440 059490 059514 058971 059904 059639 059524 059860 060074
059918 060289 060355 060195 059965 059823 059960 059902 059903 060154
059902 060226 059749 060061 060096 059832 060239 059953 060102 060176
059990 060209 060655 059644 060133 060129 059950 060218 059928 059956
060044 060346 060532 059989 060102 060011 059978 060042 060340 060379
060298 060394 060248 060541 060768 060112 060428 060222 060225 060159
060169 060097 060037 060451 060218 060403 060449 060270 060337 060419
059971 059507 060365 060462 060304 060360 060252 059930 060035 060135
060308 059978 060119 060432 059922 060354 060303 060320 059569 060447

K FERROCYANIDE -- TEMP = 228 DEG K -- 4-11-69 -- CH 200 THRU 399

000007 060288 059631 060366 059902 059755 060456 059998 060273 060560
060434 060172 060292 060107 060237 060373 060070 060480 060276 060113
060739 060677 060111 059999 060207 060188 060612 060724 060356 060186
060067 059641 060261 059927 059992 060055 060363 060054 060216 060433
060103 060339 059969 060166 060374 059879 060086 060492 060036 060521
060554 059965 060048 060316 059891 060174 060081 060288 060009 060371
060313 060314 059774 060200 059931 059596 060150 059708 060453 060299
059901 060001 059930 060341 059550 059780 060052 060017 060031 059918
059668 059607 059876 059336 059294 059924 059546 059296 059615 059298
058864 058609 058714 058501 058356 058669 058457 058042 058302 057662
057217 056551 056589 056053 055112 054787 053415 052720 051832 051173
050658 050038 050698 051301 051620 053091 053615 054964 055606 056377
056678 057283 057890 057738 057832 058284 058968 058921 059143 059029
059048 059218 059152 059530 059297 059395 059660 060067 059701 059238
060319 060008 059741 060201 059772 059693 060025 060022 060000 060071
060103 059682 060371 060222 059859 060049 059913 060178 060066 059487
060276 060306 060450 060280 060334 060742 059985 060381 060213 060174
059877 060148 060011 060024 060224 060634 059962 059770 060064 059926
060329 060156 060540 059884 060463 059942 060140 060723 060081 060429
060111 059666 060449 060199 060304 059733 060496 060713 059756 060428

K FERROCYANIDE -- TEMP = 276 DEG K -- 4-10-69 -- CH 000 THRU 199

000000 058797 058953 058705 058891 058575 058549 058667 058704 058909
058744 058447 058572 058653 058214 058367 058620 058070 058544 058355
058344 058596 058631 058395 058192 058525 058476 058163 058740 058243
058346 058332 058526 058681 058309 058372 058428 058509 058235 058114
058504 058734 058462 058184 058277 058310 058574 058501 058740 057943
058396 058232 058210 058141 057984 058041 057850 058431 057847 058037
057737 058188 057504 057525 057849 057693 057694 057340 057508 056663
056979 056575 056724 056479 055945 055433 054970 054588 053232 052895
051539 051212 050367 050342 050081 050624 051136 052170 053018 053866
054296 054866 054937 055652 056235 055923 056652 056901 056968 057025
056960 057451 057234 057606 057053 057063 057700 057543 057754 057876
057608 057774 058206 057850 058311 057926 057860 058144 058221 058105
058218 057850 057831 058929 057944 058261 058120 058391 058541 058570
058056 057979 057951 058546 058232 058391 058630 058714 058610 058076
058033 058188 058825 058697 058735 058096 058012 058487 058905 058438
058731 058465 058592 058286 058461 058306 058777 058835 058537 058753
058226 058568 059122 058367 058674 058837 058513 058491 058705 058966
058864 058575 058682 058491 058380 058460 058401 058642 058613 058617
058739 058487 058523 058283 058745 058390 058719 058766 058976 058695
058665 058800 058604 058321 058550 058631 058619 058643 058314 058141

K FERROCYANIDE -- TEMP = 276 DEG K -- 4-10-69 -- CH 200 THRU 399

000001 058446 058607 058871 058735 058025 058869 058611 058409 058712
058216 058437 058558 058454 059037 058698 058562 059034 058271 058466
058857 058456 058153 058461 058455 058896 058748 058144 058830 058327
058293 058538 059088 058574 058814 058566 058395 058063 058566 058819
058459 058724 058294 058248 058638 058636 058842 058223 058352 058773
058504 059012 058111 058343 058060 058203 058519 058138 058336 058353
058782 058623 058338 058739 058571 058148 058221 058485 058496 058225
058113 058460 058259 057900 057968 058006 058144 058319 057826 058194
057871 058202 058081 057905 057550 057699 057821 057921 057667 057505
057622 057416 057525 057987 057595 057012 056810 057059 056589 056383
056434 056045 055906 055376 055153 054657 053404 052787 051969 051450
050622 050310 050187 050654 050934 051846 052366 052951 054102 054713
055429 055992 056184 056097 056650 057032 056819 057314 057598 057548
057322 057345 057491 057413 057564 057959 057775 057815 057570 058417
057875 058278 058189 058097 058221 058407 058158 058429 058605 058419
058097 058302 058385 057700 058209 058555 058402 058206 058511 058230
058619 058797 058865 058126 058384 058510 058502 058308 058483 058562
058373 058383 058430 058372 058596 058225 058536 058111 058248 058681
058295 058639 058572 058800 058577 058183 058618 058861 058662 058387
058934 058383 058444 058281 058753 058268 058366 058554 058729 058060

K FERROCYANIDE -- TEMP = 293 DEG K -- 4-10-69 -- CH 000 THRU 199

000000 061167 061039 060939 060662 061068 061286 061156 060841 060731
061125 060750 061173 060957 061229 061193 061228 061118 060585 060197
060970 061033 061134 061146 061397 061015 061516 060745 060696 060704
061359 060595 061090 060860 061051 061069 060945 060359 061000 061190
060563 061127 060959 060752 060535 060865 060980 060933 060651 060838
060946 060502 060827 060541 060960 060493 060387 060837 060591 061227
060404 060447 060410 060494 060413 059914 060455 059671 059818 059824
059082 059100 058963 058694 057769 057937 057087 056312 055749 054882
054334 053198 053054 052729 053092 053294 054062 054745 056179 056948
056916 057653 058250 058887 059166 059007 059103 059167 059954 059112
059766 059810 060053 060134 060345 060129 060427 060408 060163 059897
060495 060136 060436 060403 060485 060173 060740 060596 060864 060511
061055 060816 060846 060854 061133 060368 060981 060914 061175 061185
060971 061019 060679 060866 060907 060834 060872 060826 060916 061145
060852 060932 061063 060515 061139 060911 060859 061048 060689 060963
060302 060917 061049 060780 060673 061071 061227 061200 061175 060839
060789 060812 060727 060926 061105 061333 061316 061240 060878
061090 061098 061319 060771 060533 061164 060982 060890 060823 061411
061652 060936 061345 061181 061023 061250 061186 061167 061119 060962
061227 061151 061153 060874 061228 061051 061198 060973 061244 060518

K FERROCYANIDE -- TEMP = 293 DEG K -- 4-10-69 -- CH 200 THRU 399

000000	060595	061381	060694	061366	060716	061184	061057	060596	060562
060645	060982	061262	061063	061140	061347	060913	061448	061026	060686
061340	061003	061203	060886	060815	061459	061239	060930	061178	060990
060924	060958	061004	060749	061171	061242	061022	061019	060852	060702
061308	060649	060900	061277	060806	060826	060603	061149	061171	061411
061057	060726	061010	060955	061463	060742	061271	060654	060743	060906
060837	061025	060930	061208	060590	061061	060622	060901	060853	060752
060965	060822	061069	060775	060649	060485	060837	061187	060582	060479
060323	060265	061161	060645	060091	060304	060673	060428	060149	060519
060169	060189	059886	059553	060084	059522	059448	059757	059635	059118
058888	059168	058530	058169	057314	057197	056297	055927	054941	054446
053641	053316	052886	053169	053292	054164	054521	056042	056537	056903
057665	058368	058790	058770	058907	059478	060007	059531	059940	059876
059917	060118	059865	060372	060396	060342	060530	060936	060673	060958
060801	060715	060816	060912	061172	061354	060704	060495	060870	060741
061198	061010	060652	060552	061106	060879	061149	060461	060878	060542
060849	061058	060974	061070	060409	061254	060874	060833	060879	060792
060777	061036	060958	061114	060799	060700	061494	061108	060744	060730
061261	061293	060850	061073	061270	060756	060895	060863	060937	060728
061185	061168	061040	060689	061156	060842	061320	061136	060642	061160