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

By

Gordon Rice Little, B.S., M.S.

The Ohio State University
1973

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CHAPTER I

INTRODUCTION

Since the development of nuclear reactors in the late 1940's as a source of thermal neutrons, neutron scattering has become a valuable tool in the study of magnetic materials. Early experiments concentrated on measuring the magnetic moments of ions and the determination of simple magnetic structures. By studying the angular dependence of magnetic scattering, information on the distribution of magnetic electrons in ions was obtained. The development of techniques for producing polarized neutron beams has led to more sophisticated measurements in magnetic systems. Recent theoretical work has shown how elastic neutron scattering from magnetic systems at low temperatures can be used to measure other quantities when the nucleus of the magnetic ion has a nonzero nuclear spin. The first such experimental study was performed by D. A. Goer on CoO. In this dissertation a similar study of metallic Holmium is presented.

The scattering of neutrons (spin $\frac{1}{2}$) from a nucleus having spin $I$ is characterized by two scattering lengths $b_+\text{ and } b_-$ belonging to the two compound nucleus-
neutron spin states $I + \frac{1}{2}$ and $I - \frac{1}{2}$. For such a nucleus in a magnetic ion, the scattering can be described by an operator of the form

$$b_{\text{coh}} = b_{\text{coh}} + b_{\text{inc}} \hat{I} \cdot \hat{\sigma} + \rho \hat{\eta} \cdot \hat{\sigma} \quad (1)$$

where

$$b_{\text{coh}} = \frac{I + 1}{2I + 1} b_+ + \frac{I - 1}{2I + 1} b_- \quad (2)$$

and

$$b_{\text{inc}} = \frac{2}{2I + 1} (b_+ - b_-) \quad (3)$$

Here the neutron spin operator is denoted by $\hat{s}$ and the nuclear spin operator by $\hat{I}$. The parameters $\rho$ and $\hat{\eta}$ describe the interaction of the neutron with the magnetic electrons in the ion.

At high temperatures, when the ion magnetic moments and the nuclear spins are not aligned, only the $b_{\text{coh}}$ term contributes to the coherent scattering and hence only $b_{\text{coh}}^2$ is measured in a study of diffraction peaks. The other terms contribute only to the incoherent background scattering. If the temperature is lowered below the magnetic transition temperature, the alignment of magnetic moments produces coherent magnetic scattering. Intensities of diffraction peaks then have terms which depend on $\rho^2$ as well as terms which depend on $b_{\text{coh}}^2$.

It is in this region that most neutron diffraction
studies on magnetic materials have been carried out.

If the temperature is lowered far enough, the hyperfine interaction between the nuclear spin and the ionic moment becomes large enough compared with the thermal energy to produce a partial polarization of the nuclear spins. This results in further contributions to the coherent scattering. In this case diffraction intensities have terms dependent separately on $b_{\text{inc}}^2$ and on $b_{\text{inc}}x p$ as well as the higher temperature terms. These new terms depend quadratically and linearly on the nuclear polarization which in turn depends on temperature. Therefore, as the temperature is lowered diffraction intensities change, either decreasing or increasing depending on the signs of the parameters involved. By studying the temperature dependence of diffraction intensities one can deduce information about the sign and magnitude of $b_{\text{inc}}$ as well as information about the hyperfine interaction. In addition, the presence of the cross term allows a study of the ionic magnetic properties to be made from a different perspective than that traditionally used.

The determination of the sign of $b_{\text{inc}}$ is of particular interest since it would allow the unambiguous
determination of \( b_+ \) and \( b_- \). That these parameters cannot be determined from traditional experiments can be seen as follows. The two quantities measured in neutron nucleus scattering experiments are the total scattering cross section \( \sigma_x \) and the coherent scattering cross section \( \sigma_c \) where

\[
\sigma_x = 4 \pi (\omega_+ b_+^2 + \omega_- b_-^2) \tag{4}
\]

and

\[
\sigma_c = 4 \pi (\omega_+ b_+^2 + \omega_- b_-^2)^2 \tag{5}
\]

Here \( \omega_+ \) and \( \omega_- \) are statistical weights for the formation of the two compound scattering states and

\[
\omega_+ = \frac{\Gamma + 1}{2 \Gamma + 1} \tag{7}
\]

\[
\omega_- = \frac{\Gamma}{2 \Gamma + 1} \tag{8}
\]

\[
\omega_+ + \omega_- = 1. \tag{9}
\]

The difference between the total cross section and the coherent cross section is called the incoherent cross section and is given by

\[
\sigma_x = 4 \pi \omega_+ \omega_- (b_+ - b_-)^2 \tag{10}
\]

or

\[
\sigma_x = 4 \pi \frac{\Gamma (\Gamma + 1)}{4} b_-^2 \tag{11}
\]
The solution of these equations for $b_+$ and $b_-$ yields

$$b_+ = b_{co} \eta \frac{\sin \omega t}{\sqrt{4\pi \omega \omega_0}} \tag{12}$$

$$b_- = b_{co} \eta \frac{\sin \omega t}{\sqrt{4\pi \omega \omega_0}}. \tag{13}$$

Thus two pairs of $b_+$ and $b_-$ are obtained from traditional measurements. However, by determining the sign of $b_{inc}$ a single pair is determined. It is one of the primary aims of this experiment to make this determination.

In Chapter II a brief description of the diffraction facility and cryostat is presented. In Chapter III the theory of elastic magnetic scattering of neutrons is discussed and application of that theory is made to metallic Holmium. The experiment is described and the data presented in Chapter IV. The data is analyzed and results are discussed in Chapter V.
II. 1. The Neutron Diffraction Facility

The experiments described in this dissertation were carried out at the OSU Neutron Diffraction Laboratory located at the Battelle Memorial Institute Research Reactor near West Jefferson, Ohio. This reactor is of the swimming pool type and operates at a power of two megawatts producing a thermal neutron flux of $2 \times 10^{13}$ n/cm$^2$-s at the reactor core. A tube, two inches in diameter and eight feet long, extends through the reactor wall defining a white neutron beam. The beam is monochromatized by reflection from the (111) planes of a lead crystal which is tuned to reflect neutrons with a wavelength of 1.097 Å with a Bragg angle of ~10 degrees. The lead crystal is set to reflect in the transmission mode. After monochromatization, the beam is collimated by passage through a rectangular slot $3/4'' \times 1-3/4''$ in a five foot long tube. The neutron flux available for diffraction purposes is roughly $3 \times 10^4$ n/cm$^2$-s. A discussion of the neutron beam is given in Appendix A. The geometry of the facility is shown in Fig. 1.

The diffractometer consists of a crystal
Figure 1
Geometry of the Diffraction Facility
table and a counter arm which are mounted for independent rotation about a common vertical axis. The diffractometer is positioned so that the vertical axis intersects the neutron beam about two feet from the aperture of the beam tube. Separate motor drive systems are provided for the crystal table and counter arm.

Two thermal neutron detectors are used in the diffraction experiments, one which monitors the neutron beam incident to the crystal (the monitor) and one which counts the neutrons scattered by the crystal (the counter). The monitor is a tube one inch in diameter which is filled with BF$_3$ gas ($11\%$ B$_{10}$ at a pressure of 20 cm Hg). The tube is inserted in the final collimating beam tube with its axis perpendicular to the beam tube axis and has a counting efficiency of 1-2%. This detector serves to monitor the incident neutron beam and is used to scale intensity measurements taken over different time periods.

The counter is a tube two inches in diameter and ten inches long which is filled with BF$_3$ gas ($96\%$ B$_{10}$ at a pressure of 60 cm Hg). This detector has an efficiency of 80% for thermal neutrons passing parallel to the cylinder axis. It is placed in a three inch diameter aluminum tube with the annular space filled with boron carbide powder. The powder serves to shield
the counter from stray neutrons present in the room. The counter is mounted on the diffractometer counter arm with its axis along the direction of the diffracted beam. The counter aperture is defined by a cadmium covered aluminum tube and is of angular width 3.60. One unique feature of this counter is that no attempt is made to shield against fast neutrons or gamma rays, thereby reducing greatly the massiveness usually found in neutron counters. Tests have been made which show that only a small number of extraneous counts are recorded over the normal background level coming through the aperture. The relative smallness of the counter allows significantly improved freedom in orienting the counter to study, for example, non-equatorial reflections.

Both detectors are alpha proportional counters which detect the 2.3 Mev alpha particles emitted in the high cross section \((n,\alpha)\) reaction of \(^{10}\text{B}\). Each captured neutron produces an electrical pulse which is amplified and then counted by a scaler (one for each detector). In operation, neutrons are counted by both detectors until the monitor scaler reaches a preset value.

Measurements of neutron scattering can be made either manually or automatically. Under manual operation the crystal and counter are first set at the desired positions. The neutron counter circuits are
then manually activated and neutrons are counted by both
detectors until a preset value on the monitor scaler is
reached. Then the data is recorded, the positions are
manually reset, and the counting circuits are manually
reactivated. This mode of operation is useful when
peak heights or single background measurements are
needed. When scanning diffraction peaks, the automatic
mode is usually preferred.

Under the automatic mode of operation, the
procedure is the same until the first preset monitor
count is reached. At this point the diffraction scaler
count and the angular positions of the crystal and
counter are automatically recorded. Then the motor
drives are initiated and the crystal and/or counter
positions are advanced by a preset amount and the
counting circuits are reactivated. This operation
continues automatically until it is stopped by the
experimentor?

II.2. The Cryostat and Thermometry

In order to obtain the temperatures necessary
for nuclear spin polarization in most materials, a He$^3$
cryostat was constructed. Since most details of this
unit have been described elsewhere$^8$, only a brief
description is presented here. One principle feature
of this cryostat is its small size. The entire unit is
only two feet long and has a diameter of three inches with a weight of less than ten pounds. The cryostat can therefore be easily oriented, eliminating the need for either an internal goniometer or a complex system of external supports.

The cryostat consists of four cooling stages (Fig. 2). A two stage nitrogen-hydrogen liquefier (Air Products Co. Cryo-Tip Model AC 2-112) maintains 80 K and 20 K flanges to which aluminum heat shields are attached. These shields provide thermal isolation of the colder stages. Stage III is a pot which contains a liquid $^4\text{He}$ reservoir and a charcoal adsorption pump. Stage IV is a container into which liquid $^3\text{He}$ is admitted. The crystal is attached to the bottom of Stage IV.

Stage III can be cooled to 1.4 K by lowering the vapor pressure over the $^4\text{He}$ reservoir with an external pump. $^3\text{He}$ gas is condensed in a tube inside the $^4\text{He}$ bath and drips down into Stage IV. The adsorption pump removes the $^3\text{He}$ vapor and cools Stage IV to about 0.32 K. A crystal temperature of 4.2 K can be maintained indefinitely by refilling the Stage III $^4\text{He}$ reservoir. One fill of 60 cc liquid lasts about 30 hours. By regulating the amount of $^3\text{He}$ used, crystal temperatures below 0.4 K can be held for about 8 hours. At these temperatures,
Figure 2

Drawing of the He³ Cryostat
when Stage III is at $1.4 \, \text{K}$, the heat leak into Stage IV is about 5 microwatts. The total amount of $\text{He}^3$ available in the cryostat storage tank is 0.04 moles. In most refrigeration cycles only one-third of the total amount is normally used.

Stage IV is suspended $1\frac{1}{8}''$ below Stage III on a $\frac{1}{8}''$ diameter, 5 mil wall stainless steel tube. This tube serves as a large pump line for the $\text{He}^3$ system and also provides good thermal isolation of Stage IV. In order to facilitate the cooling of Stage IV from room temperature to $1.4 \, \text{K}$, a "primer" system was installed. The primer system consists of a continuous tube running from an external $\text{He}^4$ gas reservoir through each cryostat stage down to Stage IV and back out. Heat exchangers are provided at each stage on the input side. A flow of $\text{He}^4$ gas is used to "prime" Stage IV. The primer is also used as a vapor pressure bulb for calibration of the Stage IV thermometers between $1.4 \, \text{K}$ and $2.1 \, \text{K}$.

Attached to Stage IV, in addition to the crystal, are five cylinders of holmium metal (0.085 moles). Due to alignment of nuclear spins near 0.3 K, holmium possesses an abnormally large specific heat$^9$ (about 7 joules/mole-K at 0.3 K). This property is used to provide a thermal ballast for Stage IV and to aid in the calibration of thermometers. With the holmium as a ballast,
the warming rate of Stage IV is only about $2 \times 10^{-3}$ K/min.

The thermometers used in this cryostat are Speers grade 1002 carbon radio resistors. There are four $\frac{1}{4}$ watt, 300 ohm resistors and one $\frac{1}{2}$ watt, 220 ohm resistor which is the type more commonly used in low temperature work. Two $\frac{1}{4}$ watt resistors are located on Stage III, one on the top and one on the bottom. They are calibrated against the vapor pressure of the $\text{He}^4$ in Stage III. The thermometer on the bottom is used for calculating a heat leak into Stage IV and also to monitor the charcoal adsorption pump. The thermometer on the top of Stage III is used primarily as an indicator when filling the $\text{He}^4$ reservoir.

The $\frac{1}{4}$ watt resistors, $R_6$ and $R_5$, and the $\frac{1}{2}$ watt resistor, $R_9$, are attached to Stage IV. The manganin lead wires are thermally shorted to Stage IV and 0.001 microfarad capacitors are soldered across resistor leads to reduce extraneous thermometer heating from radio frequency sources. By using the primer as a $\text{He}^4$ vapor pressure bulb, these thermometers are calibrated in the temperature region between 4.2 K and 1.4 K. Calibration from 1.4 K to 0.32 K is accomplished using the internal energy of Stage IV as the thermometric standard.

The first step in the calibration procedure is to operate the $\text{He}^3$ refrigeration system, bringing
Stage IV to about 0.32 K. After the He$^3$ is gone and a normal warming drift has started, a measured amount of heat is put into Stage IV using $R_0$ as a heater (typically 0.05 joules in two minutes). After an equilibrium warming drift has again been achieved (about two minutes), the thermometers are read. This cycle is repeated until a temperature within the vapor pressure calibration region has been reached. The temperature of this point is assigned using the vapor pressure work.

The calibration warm-up yields the internal energy of Stage IV as a function of thermometer reading. The internal energy of Stage IV as a function of temperature is readily calculated using the known thermodynamic properties of the constituent materials in Stage IV. A comparison of the two functions yields the temperature calibration of the thermometers. The calibration process is depicted in Fig. 3. The details of this procedure are to be published elsewhere$^{10}$. It was found that the thermometer calibration could be expressed as

$$ R = A + B/T + C/T^2 $$

(14)

to within 1% in AT/T. The values obtained for A, B, and C in the calibration used in this experiment are presented in Table 1.

This calibration technique has the feature that it can be carried out in situ with the thermometers in the
Figure 3
Graphical Depiction of the Thermometer Calibration Procedure
## TABLE 1
Thermometer Calibration Constants

<table>
<thead>
<tr>
<th>Resistor</th>
<th>$\Lambda(\Omega)$</th>
<th>$B(\Omega-K)$</th>
<th>$C(\Omega-K^2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>R5</td>
<td>441.11</td>
<td>551.52</td>
<td>21.29</td>
</tr>
<tr>
<td>R6</td>
<td>413.58</td>
<td>549.59</td>
<td>12.54</td>
</tr>
<tr>
<td>R9</td>
<td>297.54</td>
<td>406.16</td>
<td>6.33</td>
</tr>
</tbody>
</table>
position in which they are to be used. This means that problems due to questionable reproducibility of thermometers from calibration to usage can be eliminated. Further, the calibration is made over the entire temperature range accessible to the cryostat and hence no extrapolation is necessary. The accuracy of this technique is thought to be quite good since the internal energy of holmium is well known and is large enough to overwhelm any uncertainties in the internal energy of the other components of Stage IV.

The cryostat is clamped in an aluminum cradle which in turn is mounted on the diffraction table. Adjustments in the cradle are provided to center the crystal in the neutron beam. The diffractometer table has full $360^\circ$ rotation freedom about the vertical axis. The cradle is constructed to allow rotations of $\pm 40^\circ$ about a horizontal axis passing through the crystal. Therefore, a wide range of crystal orientability is possible. A photograph of the cryostat and the diffractometer is shown in Fig. 1.

II.3. The Crystal and Crystal Mount

The holmium single crystal used in this study was kindly supplied by Dr. W. C. Koehler of the Oak Ridge National Laboratory and is the one referred to as Ho(B) in his work. A drawing of the crystal is shown in
Figure 4

Photograph of the Cryostat and Diffraction Facility
Fig. 5. The crystal approximates a cylinder of diameter 0.490 cm and thickness 0.175 cm. The crystal is thinnest near the edges (0.170 cm) and thickest in the center (0.180 cm). There are two slices cut out of the general cylindrical shape as shown in the drawing. The cylinder axis coincides with the (001) crystallographic axis. A chemical analysis was reported by Koehler et al. yielding the following limits on impurities: less than 0.01% Lu, Yb, and Y; less than 0.05% Er, Tm, Tb, Gd, Eu, and La; and less than 0.1% Ce, Pr, Nd, Sm, and Dy. A further comment on impurities is made in Chapter IV.

The crystal was mounted in a pure (99.99%) aluminum holder as shown in Fig. 6. The holder consists of two aluminum slabs between which the crystal is sandwiched. Two 0-80 brass screws are used to clamp the crystal firmly in place. Because of the non-planar nature of the crystal faces, pieces of 0.002" lead shim were placed between the crystal and the aluminum slabs. A thin coating of Apiezon grade T vacuum grease was applied to the crystal to further insure a good thermal contact. These precautions were needed because of the relatively large amount of energy removal required to cool holmium to 0.3 K. Tests indicated that no noticeable reduction in neutron transmission resulted from the lead and grease.
Figure 5

Drawing of the Holmium Crystal
Figure 6

Drawing of the Crystal Holder
The crystal was mounted with the $(h00)$ and $(00l)$ reciprocal lattice directions in the horizontal plane with the $(o0l)$ axis along the tilt axis of the cryostat cradle. Thus, the reflections available for study in the equatorial plane without cryostat tilt were the $(h0l)$ reflections.
CHAPTER III
THE ELASTIC SCATTERING OF NEUTRONS FROM HOLMIUM

III.1. The Neutron-Atom Interaction

The scattering of neutrons from magnetically ordered solids has been treated extensively by many authors;\(^{12,13,14}\) the original definitive work being that of Halpern and Johnson\(^ {12}\) in 1939. The approach taken is to first formulate the interaction potential and then to use the first Born approximation to calculate the scattering cross section. There are four interactions involved:

1) the neutron-nucleus interaction through the strong nuclear force;

ii) the electromagnetic interaction of the neutron magnetic field with the electric currents of the atomic electrons;

iii) the direct neutron-electron interaction through the weak nuclear force; and

iv) the electromagnetic interaction of the neutron magnetic field with the nuclear magnetic moment.

The relative strengths of these interactions can be seen by comparing their scattering amplitudes. The strong nuclear force (1) yields scattering amplitudes of \(\sim 10^{-12}\) cm (\(b_{\text{coh}}=0.85 \times 10^{-12}\) for holmium\(^ {39}\)). The scattering amplitude for the direct neutron-electron interaction (iii) has been measured to be \(b_e=1.4 \times 10^{-16}\) cm\(^4\) and can be neglected even for heavy atoms (for holmium, \(z=67\) and \(30\).
For atoms with magnetic moments, the scattering amplitude in the forward direction due to the neutron-ion electromagnetic interaction (i) is $\sim 10^{-12}\text{cm}$ ($2.6 \times 10^{-12}\text{cm}$ for holmium). The neutron-nuclear electromagnetic interaction (iv) is smaller than the neutron-ion electromagnetic interaction by the ratio of nuclear to ionic moments and hence has scattering amplitudes of $\sim 10^{-15}\text{cm}$. We can then see that only (i) and (ii) need be considered.

The neutron interacts directly with the nucleus through the strong nuclear force. This interaction is not well understood and it is not yet possible to construct the true interaction potential. It is known, however, that this interaction extends over distances of the order of $10^{-12}\text{cm}$, much smaller than the thermal neutron wavelength of $10^{-8}\text{cm}$. This implies that only neutrons with zero angular momentum can be scattered and that the scattered wave must have zero angular momentum. In the partial wave analysis of scattering, there is only s-wave scattering which can be described by a single parameter, the scattering amplitude $b$. The scattering cross section can be written $\sigma = 4\pi b^2$.

This result is a consequence of the short range nature of the neutron-nucleus interaction and does not depend on the actual nature of the interaction except as that nature
affects b. Since we desire to describe the scattering and not to describe the interaction, it is sufficient for our purposes to replace the true neutron-nucleus potential with a fictitious potential which produces the same cross section. The potential used is the Fermi pseudo-potential and is written

\[ V_n(\hat{r}) = \frac{\mu \hbar^2}{m_n} b \xi(\hat{r} - \hat{R}) \tag{16} \]

where \(m_n\) is the neutron mass, \(\hat{r}\) is the neutron position, and \(\hat{R}\) is the position of the nucleus. The parameter \(b\) is adjusted to fit the scattering data. This potential, unlike the true potential, is weak enough to be used in the Born approximation.

When the nucleus has a spin \(I\), the neutron-nucleus interaction has two strengths depending on the orientation of the neutron spin \(\frac{1}{2}\) with respect to the nuclear spin. If the neutron and nucleus form a compound state of total angular momentum \(I + \frac{1}{2}\), one scattering amplitude \(b^+\) results and, if they combine with total angular momentum \(I - \frac{1}{2}\), another scattering amplitude results. This spin dependence can be inserted into the Fermi pseudo-potential by replacing \(b\) in equation (16) with \(b_{\sigma \rho}\) where

\[ b_{\sigma \rho} = \frac{I + 1}{2} b_+ + \frac{I}{2} b_- + \frac{2}{2I + 1} (b_+ - b_-) \tag{17} \]

Here \(\hat{I}\) and \(\hat{S}\) are the nucleus and neutron spin operators. It is easily shown that

\[ b_{\sigma \rho} |I + \frac{1}{2}\rangle = b_+ |I + \frac{1}{2}\rangle \tag{18} \]

and

\[ b_{\sigma \rho} |I - \frac{1}{2}\rangle = b_- |I - \frac{1}{2}\rangle \tag{19} \]
where $|\tilde{\mathbb{I}} \cdot \frac{1}{2}\rangle$ represents the compound neutron-nucleus spin state of total spin $\tilde{\mathbb{I}} \cdot \frac{1}{2}$. This operator does not contain the true spin dependence of the interaction; it only serves as a mechanism for inserting a spin dependence into the scattering. To simplify notation, we write

$$b_{cp} = b_{coh} + b_{inc} \mathbb{I} \cdot \mathbb{S}$$

(20)

where

$$b_{coh} = \frac{I_{11}^r}{2I_{11}^t} b_+ + \frac{I_{11}^r}{2I_{11}^t} b_-$$

(21)

and

$$b_{inc} = \frac{2}{2I_{11}^t} (b_+ - b_-)$$

(22)

Here $b_{coh}$ is called the coherent scattering amplitude and $b_{inc}$ is called the incoherent scattering amplitude. The terms coherent and incoherent are applied because, when unpolarized neutrons scatter from a crystal at high temperatures, only $b_{coh}$ contributes to Bragg reflection while $b_{inc}$ contributes only to isotropic background scattering. In scattering from a single isolated atom, both amplitudes yield isotropic scattering.

The interaction of the neutron magnetic moment with the electric currents of the atomic electrons is not short range. In fact, the interaction extends over distances comparable with the neutron wavelength. The scattering is therefore highly anisotropic having a maximum in the forward direction and decreasing rapidly.
with increasing scattering angle. The interaction is weak enough that the Born approximation can be applied. The interaction of a neutron with a single atom can be written

$$V_n(r) = \frac{i}{\epsilon} \sum_{\ell} \frac{\vec{m}_n \times (\vec{r} - \vec{r}_\ell)}{|\vec{r} - \vec{r}_\ell|^3} \cdot j'_\ell(\vec{r}_\ell)$$

where $\vec{m}_n$ is the magnetic moment of the neutron at position $\vec{r}$. The current due to the $\ell$th electron at position $\vec{r}_\ell$ is given by $j'_\ell(\vec{r}_\ell)$. The summation is over all electrons in the atom although those electrons in closed shells do not contribute.

The interaction potential for the scattering of neutrons from a crystal is the summation of the interactions of each atom in the crystal

$$V(r) = \sum_j \frac{2e_i e_j}{m_n} \left[ V_{\text{core}} + b_{\text{inc}} \cdot \vec{J}_i \cdot \vec{s} \right] S(\vec{r} - \vec{R}_j) + \sum_{\ell} \frac{i}{\epsilon} \frac{\vec{m}_n \times (\vec{r} - \vec{r}_\ell)}{|\vec{r} - \vec{r}_\ell|^3} \cdot j'_\ell(\vec{r}_\ell).$$

### III. 2. Scattering of Neutrons in the Born Approximation

In the first Born approximation the scattering cross section is given by

$$\frac{d\sigma}{d\Omega dE} = \frac{k'}{k} \left( \frac{m_n}{2\pi \hbar^2} \right)^2 \sum_{q'q} \rho_{q'} \cdot U_{q'q}(\hat{k}) \cdot U_{q'q}(\hat{k'}) \rho \cdot S\left( \frac{k}{2m_n}(k'^2 - k^2) + E_{q'} - E_q \right)$$

where $\hat{k}$ and $\hat{k}'$ are the initial and final wave vectors of the neutron and $\hat{k} = \hat{k}' - \hat{k}$ is the scattering vector. The initial and final states of the scattering system are denoted by $q$ and $q'$ with associated energies $E_q$ and $E_{q'}$. The probability of the initial state $q$ being occupied is given by $\rho_q$. The averaging over initial neutron spin...
states is contained in the trace where $\rho$ is the density matrix describing the neutron beam polarization and

$$\rho = \frac{1}{2} \hat{1} + \hat{P} \cdot \hat{s}$$  \hspace{1cm} (26)$$

where $\hat{1}$ is the 2x2 identity matrix, $\hat{P}$ is the neutron beam polarization vector, and $\hat{s}$ is the neutron spin operator. Here $\mathcal{U}(\hat{k})$ is the Fourier transform of the interaction potential $V(\hat{r})$,

$$\mathcal{U}(\hat{k}) = \int e^{i \cdot \hat{k} \cdot \hat{r}} V(\hat{r}) d\hat{r}.$$  \hspace{1cm} (27)$$

This form of the cross section is sufficiently general to describe both elastic and inelastic scattering using either polarized or unpolarized beams. In evaluating it we follow the procedure outlined by Schermer and Blume obtaining a general formula which will then simplify to a form suitable for the applications desired in this study.

The Fourier transform of the nuclear potential is easily evaluated to be;

$$\mathcal{U}_{n}(\hat{k}) = \frac{z_{n}^{2}}{m_{n}} \sum_{j} \left( b_{i}^{j} + b_{i}^{j} \hat{1} \cdot \hat{s} \right) e^{i \hat{k} \cdot \hat{r}_{i}}.$$  \hspace{1cm} (28)$$

The Fourier transform of the magnetic interaction has been given by Halpern and Johnson as

$$\mathcal{U}_{m}(\hat{k}) = \frac{z_{n}^{2}}{m_{n}} \sum_{j} \sum_{\alpha} \left[ \hat{r}_{i} \cdot \hat{s}_{i} \right] \hat{k} \cdot (\hat{s}_{j} \times \hat{k}) \cdot \frac{1}{2} \mathcal{U}_{n}(\hat{k}) \cdot (\hat{r}_{i} \cdot \hat{s}_{j})^2$$  \hspace{1cm} (29)$$

where $m$, $\hat{s}_{i}$, $\hat{r}_{i}$, and $\hat{k}$; are the mass, spin, position and momentum of the $\ell$th electron in the $j$th atom and $\gamma = 1.913$ is the neutron magnetic moment in nuclear magnetons. We can write
\[ U_m (\mathbf{r}) = \frac{2 \pi \hbar^2}{m_n} \mathbf{z} \cdot \mathbf{s} \]  

and

\[ U_n (\mathbf{r}) = \frac{2 \pi \hbar^2}{m_n} \left[ T_0 + \mathbf{\bar{T}}_1 \cdot \mathbf{s} \right] \]  

so that

\[ U_{\nu' \nu} (\mathbf{r}) = \frac{2 \pi \hbar^2}{m_n} \left[ T_{\nu' \nu} + (\mathbf{\bar{T}}_{\nu' \nu} \cdot \mathbf{z}) \cdot \mathbf{s} \right] \]  

The matrix elements of \( U (\kappa) \) are then given by

\[ U_{\nu' \nu} (\mathbf{r}) = \frac{2 \pi \hbar^2}{m_n} \left[ T_{\nu' \nu} + (\mathbf{\bar{T}}_{\nu' \nu} + 2 \mathbf{\bar{Q}}_{\nu' \nu}) \cdot \mathbf{s} \right] \]  

where we have used the fact that \( \varsigma \) and \( \varsigma' \) refer only to states of the target to bring \( \mathbf{s} \) out of the matrix element. The trace in equation (25) is easily evaluated using the properties of the Pauli spin matrices. One obtains

\[ \frac{d\sigma}{d\omega dE} = \frac{\hbar^4}{\pi^2} \sum_{\nu' \nu} \rho_0 \left\{ T_{\nu' \nu} T_{\nu' \nu} + \frac{1}{2} \mathbf{\bar{T}}_{\nu' \nu} \cdot \mathbf{\bar{T}}_{\nu' \nu} + \mathbf{\bar{Q}}_{\nu' \nu} \cdot \mathbf{\bar{Q}}_{\nu' \nu} \right\} 
+ \frac{1}{2} \left[ \mathbf{\bar{T}}_{\nu' \nu} \cdot \mathbf{\bar{Q}}_{\nu' \nu} + \mathbf{\bar{Q}}_{\nu' \nu} \cdot \mathbf{\bar{T}}_{\nu' \nu} \right] 
+ \frac{i}{\hbar} \left[ \mathbf{\bar{P}} \cdot \mathbf{\bar{T}}_{\nu' \nu} \times \mathbf{\bar{Q}}_{\nu' \nu} \right] + \frac{1}{2} \left| \mathbf{\bar{T}}_{\nu' \nu} \times \mathbf{\bar{Q}}_{\nu' \nu} \right| 
+ \frac{1}{2} \left[ \mathbf{\bar{T}}_{\nu' \nu} \cdot \mathbf{\bar{Q}}_{\nu' \nu} + \mathbf{\bar{Q}}_{\nu' \nu} \cdot \mathbf{\bar{T}}_{\nu' \nu} \right] \right\} \times \left[ \frac{k^4}{\hbar^2 m_n^2} (\hbar^2 - r^2) + E_{\nu'} - E_{\nu} \right] \]  

In evaluating equation (34) for the scattering of unpolarized neutrons we may drop all terms involving \( \mathbf{\bar{P}} \). We then have

\[ \frac{d\sigma}{d\omega dE} = \frac{\hbar^4}{\pi^2} \sum_{\nu' \nu} \rho_0 \left\{ T_{\nu' \nu} T_{\nu' \nu} + \frac{1}{2} \mathbf{\bar{T}}_{\nu' \nu} \cdot \mathbf{\bar{T}}_{\nu' \nu} + \mathbf{\bar{Q}}_{\nu' \nu} \cdot \mathbf{\bar{Q}}_{\nu' \nu} \right\} 
+ \frac{1}{2} \left[ \mathbf{\bar{T}}_{\nu' \nu} \cdot \mathbf{\bar{Q}}_{\nu' \nu} + \mathbf{\bar{Q}}_{\nu' \nu} \cdot \mathbf{\bar{T}}_{\nu' \nu} \right] \right\} \times \left[ \frac{k^4}{\hbar^2 m_n^2} (\hbar^2 - r^2) + E_{\nu'} - E_{\nu} \right] \]
In calculating the elastic cross section, we make the approximations of Schermer and Blume who assume that phonon states are not excited and that the electron spins are rigidly fixed in the lattice, and who further assume that the nuclear spins can change $z$ component of spin in order to allow for the spin flip of the neutron produced by the $I\cdot\xi$ term in $V_n(\vec{r})$. The states $\psi$ and $\psi'$ then differ only in their nuclear spin parts. We take $E_{\psi'} = E_{\psi}$ and $\hbar' = \hbar$. The matrix elements are then

$$\hat{\mathbf{Q}}_{\psi\psi'} = \delta_{\psi\psi'} <\psi'|\hat{\mathbf{Q}}|\psi>,$$  \hspace{1cm} (36) $$T_0 \psi' = \delta_{\psi\psi'} T_0$$ \hspace{1cm} (37) and

$$\hat{T}_1 \psi' = <\psi'|\hat{T}_1|\psi>. \hspace{1cm} (38)$$

In the matrix elements of $\hat{T}_1$, only the nuclear spin parts of $\psi$ and $\psi'$ are different. The diagonal matrix element of the magnetic operator $\hat{\mathbf{Q}}$ has been given by Halpern and Johnson for ions where the orbital angular momentum is zero. They obtain

$$\langle \psi | \hat{\mathbf{Q}} | \psi \rangle = \sum_{i,j} e^{i \cdot \vec{r} \cdot \vec{r}_i} \rho_i(\vec{r}) \vec{Q}_i \psi \rangle,$$ \hspace{1cm} (39)

where

$$\vec{Q}_i = \vec{Q}_i - (\vec{Q}_i \cdot \vec{r}) \vec{r}$$ \hspace{1cm} (40) and

$$\rho_i(\vec{r}) = \frac{\chi}{2m c^3} z \hat{s}_i(\vec{r})$$ \hspace{1cm} (41)

and $\vec{Q}_i$ is the unit vector along the direction of the ion spin $\vec{S}_i$. 


The magnetic scattering of neutrons from ions with non-zero orbital angular momentum has been theoretically studied by Trammell and Odiot and St. James. Using their results, we can still use equation (39) with the modification that
\[ f_j(\vec{r}) = \frac{\gamma_g}{2m_e} A_j f_j(\vec{r}) \] where, for \( \frac{\gamma}{m_e} < 0.6 \ h^{-1} \), \( f_j(\vec{r}) \) is given to 5% accuracy by
\[ f_j(\vec{r}) = \frac{\vec{L}_j \cdot \vec{J}_j}{(\vec{L}_j + 2\vec{S}_j) \cdot \vec{J}_j} f_{LJ}(\vec{r}) + 2\vec{S}_j \cdot \vec{J}_j f_{SJ}(\vec{r}) \] The quantity \( f_j(\vec{r}) \) is called the magnetic scattering amplitude of the \( j \)th ion and \( f_j(\vec{r}) \)is its magnetic form factor. \( S_j, L_j, \) and \( J_j \) are the spin, orbital, and total angular momenta of the \( j \)th ion. With these matrix elements, we obtain
\[ \frac{d\sigma}{d\Omega} = T_0^k T_0 + \frac{1}{4} \sum_q r_q \langle q|\vec{r}_1,\vec{r}_2\rangle \cdot \langle q|\vec{r}_1,\vec{r}_2\rangle + \hat{\alpha}^{+} \cdot \hat{\alpha} \] where
\[ \hat{\alpha} \equiv \langle \mu|\hat{Q}|\nu\rangle. \] Writing out \( \hat{T} \), explicitly, the remaining terms can be evaluated,
\[ \sum_q r_q \langle q|\vec{r}_1,\vec{r}_2\rangle = \sum_q r_q \langle q|\vec{r}_1,\vec{r}_2\rangle \sum_j e^{i\vec{r}_1 \cdot \vec{J}_j} \frac{\chi_{linc}}{\vec{m}_{inc} \cdot \vec{J}_j} l_j \] and
\[ \frac{1}{4} \sum_q r_q \langle q|\vec{r}_1,\vec{r}_2\rangle \cdot \langle q|\vec{r}_1,\vec{r}_2\rangle = \frac{1}{4} \sum_q r_q \langle q|\vec{r}_1,\vec{r}_2\rangle \sum_j e^{i\vec{k} \cdot \vec{J}_j} h_{inc} \frac{\chi_{linc}}{\vec{m}_{inc} \cdot \vec{J}_j} l_j \]
If we define
\[ \langle \tilde{r}_{ij} \rangle = I_{ij} \hat{f}_{ni} \hat{f}_{ni}^* \]  
(48)
the total elastic scattering cross section for unpolarized neutrons is

\[
\frac{d\sigma}{d\Omega} = \frac{1}{4} \sum_{ij} b_{inc}^2 [ I_{ij} (I_{ij} + 1) - I_{ij}^2 f_{ni}^2 ]
\]
+ \[
| \sum_{ij} e^{i \tilde{r}_{ij} \cdot \vec{q}_{ij}} |^2
\]
= \[
| \sum_{ij} e^{i \tilde{r}_{ij} \cdot \vec{q}_{ij}} [ \rho_i (\vec{q}_{ij}) \phi_{ij} + \frac{1}{2} b_{inc} I_{ij} \hat{f}_{ni} \hat{f}_{ni}^*] |^2.
\]

Equation (49) is a general expression for the total elastic cross section for the scattering of unpolarized neutrons from a crystal. We see that there are two types of scattering described. In the first line, the intensities of the waves scattered from each atom are added to obtain the total intensity. The scattering described therein is therefore called incoherent scattering. In the remaining terms, the amplitudes of the scattered waves are added and this scattering is called coherent scattering. The nomenclature applied earlier to \( b_{coh} \) and \( b_{inc} \) now becomes clear because when \( f_n \) is zero, \( b_{coh} \) appears only in the coherent scattering and \( b_{inc} \) only in the incoherent scattering. It
should be noted that in the evaluation of the cross section formula, we have omitted the peak broadening effect produced by the thermal vibrations. To accurately describe the coherent scattering we need to insert the Debye Waller factor in the cross section formula.

### III.3. The Crystallographic and Magnetic Properties of Holmium

Holmium is found to exhibit the hexagonal close packed (hcp) crystal structure at all temperatures below 1800 K. In the hcp structure, two dimensional hexagonal nets are stacked on each other in the pattern ABABAB..., i.e. with the third layer directly above the first and the fourth directly above the second. There are two equivalent positions for the second layer relative to the first giving rise to a ACACAC... sequence as well.

The unit cell is defined by the three lattice basis vectors $\hat{a}$, $\hat{b}$, and $\hat{c}$. The vectors $\hat{a}$ and $\hat{b}$ lie in the plane of the hexagonal net (the basal plane) and are 120 degrees apart. The vector $\hat{c}$ is taken perpendicular to $\hat{a}$ and $\hat{b}$ along the stacking direction of the crystal. The hcp structure including the two second layer positions and the lattice vectors is shown in Fig. 7. Defining a cartesian coordinate system $\hat{e}_1$, $\hat{e}_2$, and $\hat{e}_3$ with $\hat{e}_1 = \frac{\hat{a}}{|\hat{a}|}$, $\hat{e}_2 = \frac{\hat{b}}{|\hat{b}|}$, and $\hat{e}_3 = \hat{c}$, we can write
The Unit Cell of the hcp Crystal Structure

The sites denoted by dots (•) represent the ABAB.... stacking sequence. The sites denoted by crosses (x) represent the equivalent C layer in the ACAC.... stacking sequence.
There are two atoms in the unit cell, one at \((0,0,0)\) and the other at either \((\frac{1}{2}, \frac{3}{2}, \frac{1}{2})\) or \((\frac{5}{2}, \frac{1}{2}, \frac{3}{2})\) depending on which stacking sequence is present. The notation here is that \((\alpha, \beta, \gamma)\) corresponds to \(\mathbf{r} = \alpha \hat{a} + \beta \hat{b} + \gamma \hat{c}\).

The reciprocal lattice is defined by the reciprocal lattice basis vectors \(\mathbf{\hat{a}}, \mathbf{\hat{b}},\) and \(\mathbf{\hat{c}}\) where

\[
\mathbf{\hat{a}} = \frac{2\pi}{\mathbf{a}} \frac{\mathbf{\hat{b}} \times \mathbf{\hat{c}}}{\mathbf{a} \cdot \mathbf{\hat{b}} \times \mathbf{\hat{c}}},
\]

\[
\mathbf{\hat{b}} = \frac{2\pi}{\mathbf{b}} \frac{\mathbf{\hat{c}} \times \mathbf{\hat{a}}}{\mathbf{c} \cdot \mathbf{\hat{b}} \times \mathbf{\hat{c}}},
\]

\[
\mathbf{\hat{c}} = \frac{2\pi}{\mathbf{c}} \frac{\mathbf{\hat{a}} \times \mathbf{\hat{b}}}{\mathbf{a} \cdot \mathbf{\hat{b}} \times \mathbf{\hat{c}}}.
\]

In the cartesian coordinate system we have

\[
\mathbf{\hat{a}} = \frac{2\pi}{\mathbf{a}} \left( \frac{\sqrt{3}}{2} \mathbf{\hat{e}}_{1} + \frac{1}{2} \mathbf{\hat{e}}_{2}\right),
\]

\[
\mathbf{\hat{b}} = \frac{2\pi}{\mathbf{b}} \mathbf{\hat{e}}_{2},
\]

\[
\mathbf{\hat{c}} = \frac{2\pi}{\mathbf{c}} \mathbf{\hat{e}}_{3}.
\]

It is easily verified that

\[
\mathbf{\hat{a}} \cdot \mathbf{\hat{a}} = \mathbf{\hat{b}} \cdot \mathbf{\hat{b}} = \mathbf{\hat{c}} \cdot \mathbf{\hat{c}} = 2\pi,
\]

\[
\mathbf{\hat{a}} \cdot \mathbf{\hat{b}} = \mathbf{\hat{b}} \cdot \mathbf{\hat{c}} = \mathbf{\hat{c}} \cdot \mathbf{\hat{a}} = \mathbf{\hat{c}} \cdot \mathbf{\hat{b}} = 0.
\]

A reciprocal lattice vector \(\mathbf{\hat{r}}\) is defined to be

\[
\mathbf{\hat{r}} = h \mathbf{\hat{a}} + k \mathbf{\hat{b}} + l \mathbf{\hat{c}}.
\]
where \( n \), \( k \), and \( l \) are integers.

The magnetic structure of holmium has been extensively studied by Koehler et al. They find two ordered phases, an antiferromagnetic helix with Neel point \( T_N = 133 \ \text{K} \) and a ferromagnetic helix with Curie temperature \( T_C = 20 \ \text{K} \). In the antiferromagnetic region the ion moments are described by \( \vec{\mu}_j = -\gamma_j \vec{\eta}_j \) where

\[
\begin{align*}
\vec{\eta}_j \cdot \vec{r}_j &= \cos \phi \cos (\vec{c} \cdot \vec{R}_j + \alpha) \\
\vec{\eta}_j \cdot \vec{c}_z &= \sin \phi \sin (\vec{c} \cdot \vec{R}_j + \alpha) \\
\vec{\eta}_j \cdot \vec{c}_z &= 0.
\end{align*}
\]

Here \( \vec{R}_j \) is the position of the \( j \)th ion and \( \alpha \) is an arbitrary phase. The vector \( \vec{c} \) is called the wave vector of the helix and is parallel to the \( c \) axis in the crystal. We then see that the moments are ordered ferromagnetically within a given hexagonal layer with a rotation of \( \frac{2\pi}{3} \) radians between one layer and the next. This rotation is called the interlayer turn angle. Koehler determined that the turn angle decreases from \( 50^\circ \) at \( T_N \) to \( 30^\circ \) at \( T_C \). Below \( T_C \), the moments are tilted out of the basal plane by an amount \( \gamma \) such that

\[
\begin{align*}
\vec{\eta}_j \cdot \vec{r}_j &= \cos \phi \cos (\vec{c} \cdot \vec{R}_j + \alpha) \\
\vec{\eta}_j \cdot \vec{c}_z &= \cos \phi \sin (\vec{c} \cdot \vec{R}_j + \alpha) \\
\vec{\eta}_j \cdot \vec{c}_z &= \sin \phi.
\end{align*}
\]

It was found that \( \gamma \) increases from zero at \( T_C \) to \( 10^\circ \) at 10 K. The interlayer turn angle was found to remain
constant at 30° below $T_C$, a value which is commensurate with the lattice.

A detailed study of the (001) reflections\textsuperscript{11} indicated the presence of a perturbation in the helical structures. The explanation proposed was that the large magnetic anisotropy in the basal plane\textsuperscript{19} causes the moments to be shifted away from hard directions toward easy directions. In the ferromagnetic phase where the helix wave vector is commensurate with the lattice, the ion moments were found to be grouped or bunched about the easy directions. It was found that the $i$th moment in the $\nu$th unit cell was directed along $-\hat{n}_{i\nu}$, where

\[ \hat{n}_{i\nu} \cdot \vec{e}_1 = \cos \gamma \cos (\hat{e} \cdot \hat{A}_\nu + \xi \gamma) \]
\[ \hat{n}_{i\nu} \cdot \vec{e}_2 = \cos \delta \sin (\hat{e} \cdot \hat{A}_\nu + \xi \gamma) \]
\[ \hat{n}_{i\nu} \cdot \vec{e}_3 = \sin \gamma \]

Here, $\hat{A}_\nu$ is the position vector of the $\nu$th unit cell and $\delta$ is the bunching angle, a parameter describing the bunching of moments about the easy directions. For no bunching, $\delta = 15^\circ$, and for complete bunching, $\delta = 0^\circ$. Kochler et al.\textsuperscript{11} reported the value $\delta = 5.8^\circ$.

Other magnetic measurements on holmium\textsuperscript{20,21} show that the atoms behave to good approximation as tripositive ions with atomic magnetic moments close to the 10.6 $\mu_B$ value expected from the Ho$^{+++}$ $^5I_8$ spectroscopic state. In computing the magnetic form factor for holmium,
we will use the values $I=6$, $S=2$ and $J=8$ appropriate for the $^5I_8$ state.

A summary of the crystallographic, magnetic and nuclear parameters for holmium is shown in Table 2.

III.4. Application of the Scattering Formula to Holmium

We can write the scattering cross section for holmium as

$$\frac{d\sigma}{d\Omega} = \frac{1}{4} b_{1nc} \left[ I(I+1) - I^2 f_N^2 \right]$$

$$\times \left[ |\sum_j e^{i\vec{R}_j \cdot \vec{R}_i} b_{coh}|^2 + |\sum_j e^{i\vec{R}_j \cdot \vec{R}_i} (\rho \delta_{j,i} + \frac{1}{2} \delta_i)|^2 \right]$$

where we have used the fact that there is only one type of ion present to drop the subscripts on $I$, $f_N$, $b_{1nc}$, $b_{coh}$, and $p$. We have defined the quantity $\vec{d}_i$ where

$$\vec{d}_i = b_{1nc} f_N \hat{P}_{Ni}.$$  

The incoherent scattering is trivially evaluated and is given by

$$\frac{d\sigma_i}{d\Omega} = 2N \frac{1}{4} b_{1nc} \left[ I(I+1) - I^2 f_N^2 \right]$$

where $N$ is the total number of unit cells in the crystal. The calculation of the $b_{coh}$ contribution to the coherent is also easily accomplished. The coherent scattering amplitude is factored out of the sum and the sum is divided into two parts, a sum over the unit cells in the crystal, and a sum over the atoms in one unit cell. We write

$$\vec{R}_j = \vec{R}_v + \vec{r}_j$$

where $\vec{R}_v$ is the position of the $v$th unit cell and $\vec{r}_j$ is
<table>
<thead>
<tr>
<th>Parameter</th>
<th>300K</th>
<th>80K</th>
<th>4.2K</th>
</tr>
</thead>
<tbody>
<tr>
<td>a(Å)</td>
<td>3.5763(^a)</td>
<td>3.5605(^a)</td>
<td>3.56(^b)</td>
</tr>
<tr>
<td>c(Å)</td>
<td>5.6135(^a)</td>
<td>5.6197(^a)</td>
<td>5.63(^b)</td>
</tr>
<tr>
<td>2B(Å(^2))</td>
<td>1.30(^c)</td>
<td>.38(^c)</td>
<td>.20(^c)</td>
</tr>
</tbody>
</table>

**Magnetic Structure**
- Paramagnetic
- Antiferromagnetic Helix
- Ferromagnetic Helix

<table>
<thead>
<tr>
<th></th>
<th>300K</th>
<th>80K</th>
<th>4.2K</th>
</tr>
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<tbody>
<tr>
<td>(\xi)</td>
<td>--</td>
<td>.23(^d)</td>
<td>(\frac{1}{6})(^d)</td>
</tr>
<tr>
<td>(\delta)</td>
<td>--</td>
<td>--</td>
<td>5.8(^d)</td>
</tr>
<tr>
<td>(b_{coh}) (x10(^{-12})cm)</td>
<td>.85(^e)</td>
<td>.85(^e)</td>
<td>.85(^e)</td>
</tr>
<tr>
<td>(b_{inc}) (x10(^{-12})cm)</td>
<td>.23(^f)</td>
<td>.23(^f)</td>
<td>.28(^f)</td>
</tr>
</tbody>
</table>

\(^a\)Ref. 18  
\(^b\)Extrapolation of values in ref. 18  
\(^c\)Calculated from \(\Theta\) ref. 38  
\(^d\)Ref. 11  
\(^e\)Ref. 39  
\(^f\)Calculated from \(\sigma_{cut}\) and \(\alpha_{coh}\) in ref. 39
the location of the \(i\)th atom in the unit cell. We have
\[
|\sum_j e^{\imath \vec{r}_j \cdot \vec{r}_i} b_{\text{coh}}|^2 = b_{\text{coh}}^2 \left| \sum_{\nu} e^{\imath \vec{r}_\nu \cdot \vec{r}_i} \right|^2
\]
\[
= N^2 b_{\text{coh}}^2 \left| \sum_{\nu} e^{\imath \vec{r}_\nu \cdot \vec{r}_i} \right|^2
text{ (61)}
\]
where we have used the well known result\(^{22}\) that
\[
\sum_{\nu} e^{\imath \vec{r}_\nu \cdot \vec{r}_i} = N \delta (\vec{\nu} - \vec{r}_i)
\]
\text{ (62)}
where \(\vec{\gamma}\) is a reciprocal lattice vector. The evaluation of the summation over the unit cell is accomplished straightforwardly with the result
\[
|\sum_j e^{\imath \vec{r}_j \cdot \vec{r}_i} b_{\text{coh}}|^2 = 4 b_{\text{coh}}^2 \cos^2 \frac{\vec{\gamma} \cdot \vec{r}_i}{2} N^2 \delta (\vec{\gamma} - \vec{\gamma}_i)
\]
\text{ (63)}
The second term is more difficult to evaluate due to the vector nature of the summation argument. We make the assumption that the nuclear polarization is colinear with the ionic moment so that
\[
\vec{d}_{i\nu} = \vec{d} \cdot \vec{\gamma}_{i\nu}
\]
\text{ (64)}
with
\[
\vec{d} = b_{\text{coh}} I \delta_N.
\]
\text{ (65)}
Using equation (40) for \(\vec{\gamma}_i\), we can write the summation argument as
\[
\rho \vec{d}_{i\nu} \frac{1}{2} \vec{d}_{i\nu} = (\rho + \frac{d}{2}) \vec{\gamma}_{i\nu} - \rho (\vec{\gamma}_{i\nu} \cdot \vec{\gamma}) \vec{\gamma}
\]
\text{ (66)}
Following Schermer and Blume\(^5\) we write \(\vec{\gamma}_{i\nu}\) and \(\vec{\gamma}\) in terms of \(\vec{e}_3, \vec{e}_2, \text{ and } \vec{e}\), where
\[ \hat{e}_z = \hat{e}_z - i \hat{e}_x \]
\[ \hat{e}_+ = \hat{e}_1 + i \hat{e}_2 . \] (67)

We have
\[ \hat{H}_{i\nu} = \eta_{ii} \hat{e}_3 + \frac{\eta_{\perp}}{2} \left[ \hat{e}_- e^{i(\hat{e}_- \cdot \hat{n}_r + (\nu)^{\perp} \hat{s})} + \hat{e}_+ e^{-i(\hat{e}_+ \cdot \hat{n}_r + (-\nu)^{\perp} \hat{s})} \right] \quad (68) \]
and
\[ \hat{K} = K_{ii} \hat{e}_3 + \frac{K_{\perp}}{2} \left[ \hat{e}_- e^{i\nu} + \hat{e}_+ e^{-i\nu} \right] \quad (69) \]

where
\[ \eta_{ii} = \sin \gamma \]
\[ \eta_{\perp} = \cos \gamma . \] (70)

It is assumed that there is no difficulty in distinguishing the summation index \( \nu \) from \( \nu' \) in the exponentials. We calculate \( \hat{H}_{i\nu} \hat{K} \) as
\[ \hat{H}_{i\nu} \hat{K} = \eta_{ii} K_{ii} + \frac{\eta_{\perp} K_{\perp}}{2} \left[ \hat{e}_- e^{i(\hat{e}_- \cdot \hat{n}_r + (\nu)^{\perp} \hat{s})} + \hat{e}_+ e^{-i(\hat{e}_+ \cdot \hat{n}_r + (-\nu)^{\perp} \hat{s})} \right] \]
and the argument of the summation is
\[ (\nu + \frac{d}{2}) \eta_{ii} \nu - \nu (\hat{H}_{i\nu} \hat{K}) \]
\[ \left( \hat{e}_3 \left[ (\nu + \frac{d}{2}) \eta_{ii} - \nu \eta_{ii} K_{ii} \right] - \nu \eta_{\perp} K_{\perp} \frac{K_{\perp}}{2} \left[ \hat{e}_- e^{i(\hat{e}_- \cdot \hat{n}_r + (\nu)^{\perp} \hat{s})} + \hat{e}_+ e^{-i(\hat{e}_+ \cdot \hat{n}_r + (-\nu)^{\perp} \hat{s})} \right] \right) \]
\[ + \hat{e}_3 \left[ (\nu + \frac{d}{2}) \eta_{ii} e^{i(\hat{e}_- \cdot \hat{n}_r + (-\nu)^{\perp} \hat{s})} - \nu \eta_{\perp} K_{\perp} \frac{K_{\perp}}{2} e^{i\nu} \right] \]
\[ + \hat{e}_- \left[ (\nu + \frac{d}{2}) \eta_{ii} e^{i(\hat{e}_- \cdot \hat{n}_r + (\nu)^{\perp} \hat{s})} - \nu \eta_{\perp} K_{\perp} \frac{K_{\perp}}{2} e^{-i\nu} \right] \]
\[ + \hat{e}_+ \left[ (\nu + \frac{d}{2}) \eta_{ii} e^{-i(\hat{e}_+ \cdot \hat{n}_r + (-\nu)^{\perp} \hat{s})} - \nu \eta_{\perp} K_{\perp} \frac{K_{\perp}}{2} e^{i\nu} \right] \]
\[ \quad + \hat{e}_3 \left[ (\nu + \frac{d}{2}) \eta_{ii} e^{i(\hat{e}_- \cdot \hat{n}_r + (\nu)^{\perp} \hat{s})} - \nu \eta_{\perp} K_{\perp} \frac{K_{\perp}}{2} e^{-i\nu} \right] \]
\[ + \hat{e}_- \left[ (\nu + \frac{d}{2}) \eta_{ii} e^{i(\hat{e}_- \cdot \hat{n}_r + (\nu)^{\perp} \hat{s})} - \nu \eta_{\perp} K_{\perp} \frac{K_{\perp}}{2} e^{-i\nu} \right] \]
\[ + \hat{e}_+ \left[ (\nu + \frac{d}{2}) \eta_{ii} e^{-i(\hat{e}_+ \cdot \hat{n}_r + (-\nu)^{\perp} \hat{s})} - \nu \eta_{\perp} K_{\perp} \frac{K_{\perp}}{2} e^{i\nu} \right] \]
\[ + \hat{e}_3 \left[ (\nu + \frac{d}{2}) \eta_{ii} e^{-i(\hat{e}_+ \cdot \hat{n}_r + (\nu)^{\perp} \hat{s})} - \nu \eta_{\perp} K_{\perp} \frac{K_{\perp}}{2} e^{i\nu} \right] \]
\[ + \hat{e}_- \left[ (\nu + \frac{d}{2}) \eta_{ii} e^{-i(\hat{e}_+ \cdot \hat{n}_r + (\nu)^{\perp} \hat{s})} - \nu \eta_{\perp} K_{\perp} \frac{K_{\perp}}{2} e^{i\nu} \right] \]
\[ + \hat{e}_+ \left[ (\nu + \frac{d}{2}) \eta_{ii} e^{i(\hat{e}_+ \cdot \hat{n}_r + (-\nu)^{\perp} \hat{s})} - \nu \eta_{\perp} K_{\perp} \frac{K_{\perp}}{2} e^{-i\nu} \right] \]
\[ + \hat{e}_3 \left[ (\nu + \frac{d}{2}) \eta_{ii} e^{i(\hat{e}_- \cdot \hat{n}_r + (-\nu)^{\perp} \hat{s})} - \nu \eta_{\perp} K_{\perp} \frac{K_{\perp}}{2} e^{-i\nu} \right] \]

We define the vector sum \( \vec{S} \) as
\[ \vec{S} = \sum_{\alpha} e^{i \vec{k} \cdot \vec{R}_{\alpha}} \left[ (p_{\parallel \alpha} d \eta_{\alpha} - p (\vec{\eta}_{\alpha} \cdot \vec{R}) \vec{R}_{\alpha} \right] \]

\[ = S_3 \vec{e}_3 + S_- \vec{e}_- + S_+ \vec{e}_+ \]

and evaluate the components \( S_3, S_-, \) and \( S_+ \) separately.

Using
\[ \vec{R}_{\alpha} = \vec{A}_{\alpha} + \vec{r}_{\alpha} \]

and separating each sum as before, we proceed.

\[ S_3 \sum_{\alpha} e^{i \vec{k} \cdot \vec{A}_{\alpha}} e^{i \vec{r}_{\alpha} \cdot \vec{R}_{\alpha}} \left[ (p_{\parallel \alpha} d \eta_{\alpha} - p \eta_{\parallel \alpha} k^2_{\alpha} \right] \]

\[ = \left[ (p_{\parallel \alpha} d \eta_{\alpha} - p \eta_{\parallel \alpha} k^2_{\alpha} \right] \sum_{\alpha} e^{i \vec{k} \cdot \vec{r}_{\alpha}} \sum_{\alpha} e^{i \vec{r}_{\alpha} \cdot \vec{A}_{\alpha}} \frac{-p \eta_{\parallel \alpha} k^2_{\alpha} e^{-i \phi}}{2} \sum_{\alpha} e^{i \vec{r}_{\alpha} \cdot \vec{A}_{\alpha}} e^{-i \vec{r}_{\alpha} \cdot \vec{e}} - \frac{p \eta_{\parallel \alpha} k^2_{\alpha} e^{-i \phi}}{2} \sum_{\alpha} e^{i \vec{r}_{\alpha} \cdot \vec{A}_{\alpha}} e^{-i \vec{r}_{\alpha} \cdot \vec{e}} + \frac{p \eta_{\parallel \alpha} k^2_{\alpha} e^{-i \phi}}{2} \sum_{\alpha} e^{i \vec{r}_{\alpha} \cdot \vec{A}_{\alpha}} e^{-i \vec{r}_{\alpha} \cdot \vec{e}} \]
or

\[ S_3 = \left[ (p + \frac{ie}{2}) \eta_{ii} - \rho \eta_{ii} k_{ii}^2 \right] e^{i \frac{\vec{k} \cdot \vec{r_i}}{2}} 2 \cos \frac{k_{\perp} r_i}{2} N S(i \vec{r} - \vec{i}) \]  

\[ - \frac{\rho \eta_{ii} k_{ii}^2}{2} e^{-i \phi} e^{i \frac{\vec{k} \cdot \vec{r_i}}{2}} z \cos \left( \frac{\vec{k} \cdot \vec{r_i}}{2} \right) NS(i \vec{r} + \vec{i} - \vec{z}) \]

\[ - \frac{\rho \eta_{ii} k_{ii}^2}{2} e^{i \phi} e^{i \frac{\vec{k} \cdot \vec{r_i}}{2}} z \cos \left( \frac{\vec{k} \cdot \vec{r_i} - \vec{s}}{2} \right) NS(i \vec{r} - \vec{z} - \vec{s}) \]

Similarly

\[ S_- = \sum \frac{e^{i \vec{k} \cdot \vec{A}_r} e^{i \vec{k} \cdot \vec{r_i}}}{z} \left[ - \frac{\rho \eta_{ii} k_{ii} k_{il}}{2} e^{i \phi} \right. \]

\[ + \left[ (p + \frac{ie}{2}) \eta_{ii} - \rho \eta_{il} k_{il}^2 \right] e^{i \frac{\vec{k} \cdot \vec{r_i}}{2}} z \cos \left( \frac{\vec{k} \cdot \vec{r_i}}{2} \right) NS(i \vec{r} + \vec{s}) \]

\[ + \frac{\rho \eta_{il} k_{il}^2}{4} e^{2i \phi} e^{i \frac{\vec{k} \cdot \vec{r_i}}{2}} z \cos \left( \frac{\vec{k} \cdot \vec{r_i} - \vec{s}}{2} \right) NS(i \vec{r} - \vec{s}) \]

\[ S_- = - \frac{\rho \eta_{il} k_{il} k_{il}}{2} e^{i \phi} e^{i \frac{\vec{k} \cdot \vec{r_i}}{2}} z \cos \frac{k_{\perp} r_i}{2} N S(i \vec{r} - \vec{i}) \]

\[ + \left[ (p + \frac{ie}{2}) \eta_{il} - \rho \eta_{il} k_{il}^2 \right] e^{i \frac{\vec{k} \cdot \vec{r_i}}{2}} z \cos \left( \frac{\vec{k} \cdot \vec{r_i}}{2} + \vec{s} \right) NS(i \vec{r} + \vec{i} - \vec{s}) \]

\[ + \frac{\rho \eta_{il} k_{il}^2}{4} e^{2i \phi} e^{i \frac{\vec{k} \cdot \vec{r_i}}{2}} z \cos \left( \frac{\vec{k} \cdot \vec{r_i} - \vec{s}}{2} \right) NS(i \vec{r} - \vec{s}) \]
and
\[
S_+ = \sum e^{i \mathbf{\hat{k}} \cdot \mathbf{A}_v} e^{i \mathbf{\hat{\nu}} \cdot \mathbf{r}_i} \left[ -\rho \frac{\eta_{uv} \mathbf{K}_u \mathbf{K}_v}{2} e^{-i \phi} \right.
\]
\[
+ \left. -\rho \frac{\eta_{uv} \mathbf{K}_v^2}{4} e^{-2i \phi} e^{i \mathbf{\hat{\nu}} \cdot \mathbf{A}_v} e^{-i(-\mathbf{\hat{\nu}} \cdot \mathbf{r}_i)} \right]
\]
\[
+ \left[ (\rho_{uv} \mathbf{v}) \frac{m}{2} - \rho \frac{\eta_{uv} \mathbf{K}_v^2}{4} \right] e^{i \mathbf{\hat{\nu}} \cdot \mathbf{A}_v} e^{-i \mathbf{\hat{\nu}} \cdot \mathbf{r}_i}\]
\]
\[
S_+ = -\rho \eta_{uv} \mathbf{K}_u \mathbf{K}_v \frac{m}{2} e^{-i \phi} e^{i \mathbf{\hat{\nu}} \cdot \mathbf{r}_i} 2 \cos \frac{u \mathbf{\hat{\nu}} \cdot \mathbf{K}_v}{2} N \mathbf{S}(\mathbf{\hat{\nu}} - \mathbf{r}_i) \tag{80}
\]
\[
- \rho \frac{\eta_{uv} \mathbf{K}_v^2}{4} e^{-2i \phi} e^{i \mathbf{\hat{\nu}} \cdot \mathbf{r}_i} 2 \cos \left( \frac{u \mathbf{\hat{\nu}} \cdot \mathbf{K}_v}{2} + \frac{u \mathbf{\hat{\nu}} \cdot \mathbf{K}_v}{4} \right) N \mathbf{S}(\mathbf{\hat{\nu}} + \mathbf{r}_i - \mathbf{r}_i)
\]
\[
+ \left[ (\rho_{uv} \mathbf{v}) \frac{m}{2} - \rho \frac{\eta_{uv} \mathbf{K}_v^2}{4} \right] e^{i \mathbf{\hat{\nu}} \cdot \mathbf{A}_v} e^{-i \mathbf{\hat{\nu}} \cdot \mathbf{r}_i} 2 \cos \left( \frac{u \mathbf{\hat{\nu}} \cdot \mathbf{K}_v}{2} - \frac{u \mathbf{\hat{\nu}} \cdot \mathbf{K}_v}{4} \right) N \mathbf{S}(\mathbf{\hat{\nu}} - \mathbf{r}_i - \mathbf{r}_i).
\]

Here we have again used the result that
\[
\sum e^{i \mathbf{\hat{\nu}} \cdot \mathbf{A}_v} = N \mathbf{S}(\mathbf{\hat{\nu}} - \mathbf{r}_i). \tag{81}
\]

Our vector summation \( \mathbf{\hat{S}} \) then takes the form
\[
\mathbf{\hat{S}} = \left[ S_{13} \mathbf{S}(\mathbf{\hat{\nu}} - \mathbf{r}_i) + S_{23} \mathbf{S}(\mathbf{\hat{\nu}} + \mathbf{r}_i - \mathbf{r}_i) + S_{33} \mathbf{S}(\mathbf{\hat{\nu}} - \mathbf{r}_i - \mathbf{r}_i) \right] \mathbf{\hat{S}}_3 \tag{82}
\]
\[
+ \left[ S_{13} \mathbf{S}(\mathbf{\hat{\nu}} - \mathbf{r}_i) + S_{23} \mathbf{S}(\mathbf{\hat{\nu}} + \mathbf{r}_i - \mathbf{r}_i) + S_{33} \mathbf{S}(\mathbf{\hat{\nu}} - \mathbf{r}_i - \mathbf{r}_i) \right] \mathbf{\hat{S}}_2
\]
\[
+ \left[ S_{13} \mathbf{S}(\mathbf{\hat{\nu}} - \mathbf{r}_i) + S_{23} \mathbf{S}(\mathbf{\hat{\nu}} + \mathbf{r}_i - \mathbf{r}_i) + S_{33} \mathbf{S}(\mathbf{\hat{\nu}} - \mathbf{r}_i - \mathbf{r}_i) \right] \mathbf{\hat{S}}_1
\]

and \( \mathbf{\hat{S}} \cdot \mathbf{\hat{S}} \) is given by
\[
\mathbf{\hat{S}} \cdot \mathbf{\hat{S}} = \left[ S_{13} \mathbf{S}_{13} + 2 S_{13} \mathbf{S}_{11} + 2 S_{13} \mathbf{S}_{14} \right] \mathbf{S}(\mathbf{\hat{\nu}} - \mathbf{r}_i) \tag{83}
\]
\[
+ \left[ S_{23} \mathbf{S}_{23} + 2 S_{23} \mathbf{S}_{22} + 2 S_{23} \mathbf{S}_{24} \right] \mathbf{S}(\mathbf{\hat{\nu}} + \mathbf{r}_i - \mathbf{r}_i)
\]
\[
+ \left[ S_{33} \mathbf{S}_{33} + 2 S_{33} \mathbf{S}_{32} + 2 S_{33} \mathbf{S}_{34} \right] \mathbf{S}(\mathbf{\hat{\nu}} - \mathbf{r}_i - \mathbf{r}_i).
Using equations (76), (78), and (80) we have

\[ S_x S_y = \left[ (p_{\text{ul}})^2 \gamma_{\text{u}} - \rho_{\text{ul}} \gamma_{\text{u}}^2 \right] + \left[ (p_{\text{ul}})^2 \gamma_{\text{u}} - \rho_{\text{ul}} \gamma_{\text{u}}^2 \right] + \left( \frac{\rho_{\text{ul}}^2 \gamma_{\text{u}}}{C} \right)^2 \]

\[ + \left[ \left( \frac{\rho_{\text{ul}}^2 \gamma_{\text{u}}}{C} \right)^2 + \left( \frac{\rho_{\text{ul}}^2 \gamma_{\text{u}}}{C} \right)^2 + \left( \frac{\rho_{\text{ul}}^2 \gamma_{\text{u}}}{C} \right)^2 \right] + \left( \frac{\rho_{\text{ul}}^2 \gamma_{\text{u}}}{C} \right)^2 \]

\[ + \left[ \left( \frac{\rho_{\text{ul}}^2 \gamma_{\text{u}}}{C} \right)^2 + \left( \frac{\rho_{\text{ul}}^2 \gamma_{\text{u}}}{C} \right)^2 + \left( \frac{\rho_{\text{ul}}^2 \gamma_{\text{u}}}{C} \right)^2 \right] \]

By straightforward manipulation, using the fact that

\[ K_1^2 + K_2^2 = 1, \]

we obtain

\[ S_x S_y = \left[ \rho^2 (1 - K_1^2) + \rho^2 (1 - K_1^2) \right] \gamma_{\text{u}}^2 \frac{4N^2 \cos^2 \frac{E_i}{2} S(\delta - \delta)}{S(\delta + \delta)} \]

\[ + \left[ \frac{\rho^2}{C} (1 + K_1^2) + \frac{\rho^2}{C} (1 + K_1^2) \right] \gamma_{\text{u}}^2 \frac{4N^2 \cos^2 \frac{E_i}{2} S(\delta - \delta)}{S(\delta + \delta)} \]

\[ + \left[ \frac{\rho^2}{C} (1 + K_1^2) + \frac{\rho^2}{C} (1 + K_1^2) \right] \gamma_{\text{u}}^2 \frac{4N^2 \cos^2 \frac{E_i}{2} S(\delta - \delta)}{S(\delta + \delta)} \]

Combining equations (59), (63), and (85), and defining

\[ q_1^2 = 1 - K_1^2, \]

the total scattering cross section becomes

\[ \frac{d\sigma}{d\Omega} = 2N \frac{b_{\text{inc}}}{4} \left[ I(I+1) - I^2 \right] \]

\[ + N^2 \left[ 4 b_{\text{inc}}^2 + 4 \rho^2 (1 - K_1^2) b_{\text{inc}}^2 \left( I_{\text{su}} \right) \left( I_{\text{su}} \right) \cos^2 \frac{E_i}{2} S(\delta - \delta) \right] \]

\[ + N^2 \left[ 4 b_{\text{inc}}^2 + 4 \rho^2 (1 - K_1^2) b_{\text{inc}}^2 \left( I_{\text{su}} \right) \left( I_{\text{su}} \right) \cos^2 \frac{E_i}{2} S(\delta - \delta) \right] \]

As mentioned previously, there are two equivalent sites for the second atom in the unit cell

\[ \vec{r}_2 = \left( \frac{1}{3}, \frac{2}{3}, \frac{1}{2} \right) \]

and

\[ \vec{r}_2' = \left( \frac{2}{3}, \frac{1}{3}, \frac{1}{2} \right). \]
Since these sites are equivalent, it is reasonable to assume that the domains associated with the sites are equally populated. The scattering formula in equation (86) is only correct for one of these domains. The observed cross section will be the average of the cross sections for the individual domains. Since \( \vec{r}_i \) appears only in terms of the form \( \cos\left(\frac{\vec{r}_i \cdot \vec{s}}{z}\right) \), we need only average these terms. We can perform all three averages at once. We write \( \vec{r} \) as

\[
\vec{r} = \vec{r}_1 + \vec{r}_2 + \vec{r}_3
\]

We note that

\[
\vec{c} = \vec{c}_3
\]

and hence

\[
\vec{c} \cdot \vec{r}_i = \vec{c} \cdot \vec{r}_2.
\]

Defining \( G^2 \) as the average of \( \cos^2\left(\frac{\vec{r}_i \cdot \vec{s}}{z}\right) \), we proceed using well known trigonometric identities.

\[
2 G^2 = \cos^2\left(\frac{\vec{r}_1 \cdot \vec{s}}{z}\right) + \cos^2\left(\frac{\vec{r}_2 \cdot \vec{s}}{z}\right)
\]

\[
= \frac{1}{2} + \frac{1}{2} \cos(\vec{r}_1 \cdot \vec{s}) + \frac{1}{2} + \frac{1}{2} \cos(\vec{r}_2 \cdot \vec{s})
\]

\[
= 1 + \frac{1}{2} \cos\left(\frac{\vec{r}_1 \cdot \vec{s}}{z} + (\vec{c} \cdot \vec{r}_2 - 2\pi)\right) + \frac{1}{2} \cos\left(\frac{\vec{r}_2 \cdot \vec{s}}{z} + (\vec{c} \cdot \vec{r}_1 - 2\pi)\right)
\]

\[
= 1 + \cos\left(\frac{\vec{r}_1 \cdot \vec{r}_2}{2}\right) \cos\left[\frac{\vec{r}_1 \cdot (\vec{r}_2 + \vec{r}_2)}{2} + (\vec{c} \cdot \vec{r}_2 - 2\pi)\right]
\]

\[
= 1 + \cos\left(\frac{\vec{r}_1 \cdot \vec{r}_2}{2}\right)\left[\cos\left(\frac{\vec{r}_1 \cdot (\vec{r}_2 + \vec{r}_2)}{2}\right) \cos(\vec{c} \cdot \vec{r}_2 - 2\pi)
\right]
\]

\[
+ \sin\left(\frac{\vec{r}_1 \cdot \vec{r}_2}{2}\right) \sin(\vec{c} \cdot \vec{r}_2 - 2\pi).
\]
At this point we note that
\[ \vec{r}_2 + \vec{r}_2' = (1, 1, 1) \] (92)
and that
\[ \sin \frac{\vec{r}_2 \cdot (\vec{r}_2 + \vec{r}_2')}{2} = 0. \] (93)

We then have
\[ Z G^2 = 1 + \cos \frac{\vec{r}_2 \cdot (\vec{r}_2 - \vec{r}_2')}{2} \cos \frac{\vec{r}_2 \cdot \vec{r}_2'}{2} \cos (\vec{e} \cdot \vec{r}_2 - 2\phi) \]
\[ = 1 + \frac{1}{2} \left[ \cos \frac{\vec{r}_2 \cdot \vec{r}_2'}{2} \cos (\vec{e} \cdot \vec{r}_2 - 2\phi) \right]. \] (94)

Using the values of \( \vec{r}_2 \) and \( \vec{r}_2' \), it can be shown that
\[ \cos \frac{\vec{r}_2 \cdot \vec{r}_2'}{2} = \cos \frac{\vec{r}_2 \cdot \vec{r}_2'}{2} \]
for all \( \vec{r}_2 \).

Hence
\[ G^2 = \frac{1}{2} + \frac{1}{2} \cos (\vec{e} \cdot \vec{r}_2 - 2\phi). \] (96)

For the second line in equation (96) there is no \( \vec{e} \) or \( \vec{e} \) appearing, so that the value of \( G^2 \) appropriate there becomes
\[ G^2 = \cos^2 \frac{\vec{r}_2 \cdot \vec{r}_2'}{2}. \] (97)
and the term is unchanged by the domain averaging.

For the third and fourth lines in equation (96), equation (96) directly applies and we write
\[ G^2 = \frac{1}{2} + \frac{1}{2} \cos (\vec{e} \cdot \vec{r}_2 - 2\phi). \] (98)

The total elastic scattering cross section is then
\[ \frac{d\sigma}{d\Omega} = 2 N \frac{1}{4} \beta \cos \left[ I (I+1) - I' I' \right] \]
\[ + N^2 \left[ 4 \beta \cos \left( \lambda \phi + \lambda \phi' \right) + 4 \rho^2 \rho^2 \beta \cos \left( \lambda \phi + \lambda \phi' \right) + 4 N \right] G^2 \frac{1}{2} \left( \vec{r}_2 \cdot \vec{r}_2' \right) \]
The first line describes the spin incoherent scattering. As can be seen there is no \( \mathbf{k} \) dependence so that this scattering is isotropic. This scattering appears as a contribution to the background counting rate and does have a temperature dependence through the nuclear polarization. It should be noted, however, that the other contributions to the background tend to mask this effect.

The coherent scattering is described by the last three lines. We see that this scattering occurs only when the neutron scattering vector \( \mathbf{k} \) satisfies

\[
\mathbf{k} = \mathbf{n}
\]

or

\[
\mathbf{k} = \mathbf{n} \pm \mathbf{c}
\]

where \( \mathbf{n} \) is a reciprocal lattice vector, and \( \mathbf{c} \) is the helix wave vector. Therefore, there are three diffraction peaks associated with each reciprocal lattice vector, a central peak at \( \mathbf{k} = \mathbf{n} \), and two satellites, one at \( \mathbf{k} = \mathbf{n} \pm \mathbf{c} \), and the other at \( \mathbf{k} = \mathbf{n} - \mathbf{c} \). We will use the standard convention of labeling diffraction peaks with the Miller indices. The central peak corresponding to

\[
\mathbf{n} = h\mathbf{a} + n\mathbf{b} + l\mathbf{c}
\]

will be denoted by \( (hnl) \). The associated satellites
will be denoted by \((h, k, l)^+\) and \((h, k, l)^-\) where the + sign goes with the satellite at \(\hat{r} = \hat{r}_1 + \hat{r}_c\) and the - sign goes with the satellite at \(\hat{r} = \hat{r}_1 - \hat{r}_c\).

The central peak is given by line two in equation (99). It contains the high temperature coherent nuclear scattering \(4b^{z}_{\text{coh}}\) and the ferromagnetic component of the magnetic scattering \(4\rho^{z}_{\text{f}} s^{z}_{\text{h}}\). In addition, there are contributions proportional to \(f_N\) and \(f_N^2\). However, \(b_{\text{coh}}\) is fairly large for holmium and \(b_{\text{inc}}\) and \(s^{z}_{\text{h}}\) are small with the result that there is only a slight temperature dependence in the central peaks.

The satellite peaks contain most of the magnetic scattering \(2\rho^{z}_{\text{f}} (1 - \frac{s^{z}_{\text{h}}}{s^{z}_{\text{h}}}) \cos^{z}_{\text{h}}\). These reflections also contain terms dependent on \(f_N\) and \(f_N^2\), and it is in these peaks that the temperature dependence is most evident. It is seen that the location of the satellites is determined by the helix wave vector, but that \(\hat{r}_c\) does not effect the strength of the reflection. The bunching parameter \(\xi\) occurs in \(G^{z}\) and it affects the intensity of these reflections. The effect is generally small except that \(G^{z}\) is non-zero for all \(\hat{r}_c\), including those \(\hat{r}_c\) for which \(G^{z}\) is zero. It was the presence of satellites for the forbidden \((001)\) reflection that led Koehler\(^{11}\) to the bunched spin model for holmium.
In evaluating the terms dependent on $\vec{K}$ in the cross section formula, we note that the $30^\circ$ turn angle implies that

$$\vec{p} = \frac{1}{3} \vec{C}$$

so that

$$\frac{\vec{p}}{3} + \vec{C} = n \hat{A} + k \hat{B} + \left( l \hat{v} + \frac{1}{3} \vec{C} \right) \hat{C}.$$

(103)

It is a simple matter to show that the conditions in equation (100) directly imply the familiar Bragg law of diffraction. One obtains

$$\frac{\sin \theta}{\lambda} = \frac{1}{4\pi} |p \cdot \hat{C}|$$

(104)

where $\vec{e} = 0$ applies for a central reflection. Here $\theta$ is the Bragg angle and $2\theta = 4(\hat{t}, \hat{z})$. Explicit formulae for the quantities involved in evaluating the cross section of a given reflection are given in Table 3.

Before continuing, it should be noted that there are two types of magnetic domains possible: a reversal of the helix wave vector $\vec{z}' = -\vec{z}$; and a reversal of the ferromagnetic component of the helix $\gamma' = -\gamma$. The reversal of the helix wave vector directly implies a change in sign of the bunching parameter $S' = -S$ in order that the ion moments remain bunched about the easy directions. Hence there is no alteration of the cross section except to interchange the labelling of the peaks. The reversal of the ferromagnetic component of the helix also has no effect on the cross section because $\gamma$ enters
## TABLE 3

**Formulae for Evaluating the Scattering Cross Section for Holmium**

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Central Reflection</th>
<th>Satellite Reflection ((\vec{e} = e', \vec{C}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\sin \Theta)</td>
<td>(\frac{\lambda}{2} \sqrt{\frac{4}{3a^2} \left( \frac{h^2}{3} + h_k + k^2 \right) + \frac{p^2}{c^2}})</td>
<td>(\frac{\lambda}{2} \sqrt{\frac{4}{3a^2} \left( \frac{h^2}{3} + h_k + k^2 \right) + \frac{(l \pm \varepsilon')^2}{c^2}})</td>
</tr>
<tr>
<td>(q_0^2)</td>
<td>(1 - \frac{\frac{h^2}{a^2} (h^2 + h_k + l^2) + \frac{p^2}{c^2}}{\frac{4}{3a^2} (h^2 + h_k + k^2) + \frac{l^2}{c^2}})</td>
<td>(1 - \frac{\frac{h^2}{a^2} (h^2 + h_k + k^2) + \frac{(l \pm \varepsilon')^2}{c^2}}{\frac{4}{3a^2} (h^2 + h_k + k^2) + \frac{(l \pm \varepsilon')^2}{c^2}})</td>
</tr>
<tr>
<td>(G^2) ((77,\text{K}))</td>
<td>(\cos^2 \pi \left( \frac{h + 2k}{3} + \frac{l}{2} \right))</td>
<td>(\cos^2 \pi \left( \frac{h + 2k}{3} + \frac{l}{2} \right))</td>
</tr>
<tr>
<td>(G^2) ((4.2,\text{K}))</td>
<td>(\cos^2 \pi \left( \frac{h + 2k}{3} + \frac{l}{2} \right))</td>
<td>(\frac{1}{2} \left( 1 + \cos 2\pi \left( \frac{h + 2k}{3} + \frac{l}{2} \right) \cos (30^\circ - \phi) \right))</td>
</tr>
</tbody>
</table>
Equation (99) can also be used to describe the high temperature coherent scattering. In the antiferromagnetic region \( 200 ^{<} T < 133 \, \text{K} \) we let \( \xi_N \to \xi, \gamma \to \gamma, \) and \( \xi_0 \to \xi_0^* \). We let \( \xi \) and \( \gamma \) take on the values appropriate for the particular temperature in question. In the paramagnetic region we let \( \rho \to \rho \). At these temperatures it is necessary to insert the Debye-Waller correction factor in the coherent scattering portion.

In describing coherent scattering it is more common to use the quantity \( F^2 \) rather than the cross section. \( F \) is called the structure factor and \( F^2 \) is related to the cross section by

\[
F^2 = \frac{1}{N^2} \frac{d \sigma_{\text{coh}}}{d \Omega}.
\]

In traditional experiments the structure factor is interpreted as the coherent scattering amplitude for a unit cell in the crystal. In our case this interpretation is somewhat clouded by the fact that the helical structure is not contained in the unit cell.

**III.5. The Nuclear Polarization**

We have seen that the coherent scattering from holmium depends on the nuclear polarization. The nuclear polarization is defined as

\[
\xi_N = \frac{1}{2} \sum_{m_i} m_i \rho(m_i).
\]
where $P(m_i)$ is the probability that a spin $\mathbb{T}$ has component $m_i$ along the polarization axis. We can use Boltzmann statistics and write

$$P(m_i) = \frac{\exp(-E_{m_i}/k_B T)}{\sum_{m_i} \exp(-E_{m_i}/k_B T)} \tag{107}$$

where $E_{m_i}$ is the energy associated with spin state $m_i$, $k_B$ is the Boltzmann constant, and $T$ is the temperature. At high temperatures ($k_B T \gg E_{m_i}$) all probabilities are equal and $f_N$ is zero. At low temperatures only the $P(m_i)$ associated with the lowest energy state is nonzero and $f_N$ is unity.

In order to evaluate $f_N$, we need the energy levels $E_{m_i}$ which are determined by the hyperfine interaction. It has been shown that the hyperfine Hamiltonian for holmium can be expressed as

$$\frac{\mathcal{H}}{k_B} = \alpha' I_3 + \rho (I_3^2 - \frac{1}{3} I(I+1)) \tag{108}$$

where $\alpha'$ is a parameter describing the magnetic dipole interaction and $\rho$ is a parameter describing the electric quadrupole interaction. The parameters $\alpha'$ and $\rho$ have been measured or calculated by several authors using different techniques. A summary is presented in Table 4. For preliminary calculation, the parameters of Lounasmaa were chosen. The nuclear polarization calculated with these values of $\alpha'$ and $\rho$ is shown in Fig. 8.
<table>
<thead>
<tr>
<th>( a' (K) )</th>
<th>( P (K) )</th>
<th>Method Used</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>+.290</td>
<td>——</td>
<td>Polarized Neutron Transmission</td>
<td>25</td>
</tr>
<tr>
<td>+.319</td>
<td>.003</td>
<td>Calculated</td>
<td>26</td>
</tr>
<tr>
<td>.320</td>
<td>.007</td>
<td>Specific Heat Measurement</td>
<td>27</td>
</tr>
<tr>
<td>.319</td>
<td>.004</td>
<td>Specific Heat Measurement</td>
<td>28</td>
</tr>
<tr>
<td>+.307</td>
<td>.003</td>
<td>Calculated from Atomic Beam Resonance Measurement on Atomic Ho</td>
<td>29</td>
</tr>
</tbody>
</table>
Figure 8
Temperature Dependence of the Nuclear Polarization of Holmium
III.6. The Integrated Intensity

For a perfect crystal and a perfectly monochromatic, perfectly collimated neutron beam, the coherent scattering would appear as a sharp narrow beam whenever the Bragg condition is satisfied. However, crystals presently available are permeated with lattice defects such that the crystal is broken up into small perfect units called mosaic blocks. These blocks have dimensions typically of a few thousand angstroms and have orientations distributed over a few tenths of a degree. In addition, thermal neutron beams are also imperfect, having a wavelength spread of a few percent and an angular spread of a few tenths of a degree, depending largely on the degree of collimation applied and the quality of the monochromator. In order to obtain a true measure of the scattering, it is necessary to rotate the crystal in the incident beam so that all possible orientations of the mosaic blocks are brought into reflection with all components of the neutron beam. This process yields the scattered intensity as a function of the crystal orientation. This function is integrated to obtain the integrated intensity $P$. It has been shown that, for equatorial reflections, $P$ is given by the equation:

$$P = \frac{C_0 N c^2 \lambda^2}{\sin^2 \theta} F^2 \quad (109)$$
where \( N_c \) is the number of unit cells per unit volume in the crystal, \( \lambda \) is the mean wavelength of the neutron beam, and \( \theta \) is the Bragg angle. The factor \( \sin 2\theta \) is the form of the Lorentz factor applicable for measurement in the equatorial plane. The Lorentz factor adjusts for the different speeds with which the reflecting planes are tuned through the reflecting position. The factor \( C_0 \) is called the instrument constant and is given by

\[
C_0 = \alpha I_0 V
\]

(110)

where \( I_0 \) is the incident beam intensity and \( V \) is the crystal volume. The factor \( \alpha \) is a scale factor which contains the angular velocity of the crystal rotation and the time used for each measurement. In practice \( C_0 \) is determined from a study of known reflections.

It is customary to describe the strength of a diffraction peak in terms of the crystallographic \( Q \) factor given by

\[
Q = \frac{N_c^2 \lambda^3}{\sin 2\theta} F^2
\]

(111)

with the integrated intensity given by

\[
I = C Q
\]

(112)

This equation is applicable when all portions of the crystal are uniformly bathed by the neutron beam. In practice several processes alter the beam intensity as it progresses through the crystal. These processes include true absorption, incoherent scattering, primary
extinction and secondary extinction.

In true absorption, neutrons are captured by the nuclei in the crystal. When a neutron is captured it is lost completely from participation in further scattering events. The absorption process is described by a reaction probability, the capture cross section $\sigma_c$. In incoherent scattering, neutrons are scattered from the nuclei in such a way that they lose their phase relationship with those scattered coherently. The incoherent scattering is characterized by the incoherent scattering cross section $\sigma_i$. In both of these processes neutrons are lost from participation in the coherent scattering and they are therefore equivalent in their effect on the coherent scattering. If a neutron beam passes through a length of crystal $dl$, the change in beam intensity $dI$ is given by the number of reaction sites in $dl$ times the total reaction probability at each site

$$dI = -N_c dl (\sigma_c + \sigma_i)$$

or

$$\lambda = N_c (\sigma_c + \sigma_i)$$

where $\lambda$ is called the effective linear absorption coefficient. Integrating over a path of length $l$, we obtain

$$I = I_0 e^{-\lambda l}.$$
We define an absorption factor $A$ as

$$A = e^{-\mu \lambda l} \quad (116)$$

and hence we can write the intensity as

$$I = A I_0. \quad (117)$$

In Bragg reflection, each point in the crystal $\vec{r}$ has a specific path length $l(\vec{r})$ associated with it. The absorption factor for the reflection is then the average over the entire crystal

$$A = \frac{1}{V} \int_{\text{crystal}} e^{-\mu \lambda l(\vec{r})} d\vec{r} \quad (118)$$

and the integrated intensity is then given by

$$P = C_0 A Q. \quad (119)$$

The absorption factor can be directly calculated using equation (118) given the geometries of the crystal and the reflection. For geometries where equation (118) cannot be analytically evaluated, Busing and Levy have written a computer program to numerically integrate it to obtain absorption coefficients.

The extinction processes cannot be treated in the same way. Extinction occurs when the neutron beam is attenuated by coherent scattering. Primary extinction occurs when the depletion occurs over a single mosaic block and secondary extinction occurs when the depletion occurs over different mosaic blocks having the same orientation.
For typical single crystals, the mosaic block size limits the effect of primary extinction so that secondary extinction is usually dominant. We shall consider only secondary extinction here.

As mentioned above, in extinction the depletion of the neutron beam is due to coherent scattering. Neutrons, then, are not lost from coherent scattering. Neutrons which are removed from the incident beam appear in the diffracted beam and neutrons in the diffracted beam are reflected back into the incident beam. Zachariasen\textsuperscript{33} has formulated equations to describe both extinction and absorption. He writes

\begin{align}
\frac{dP_i}{dl_i} &= -(\sigma + \mu_a) P_i + \sigma P_r \\
\frac{dP_r}{dl_r} &= -(\sigma + \mu_a) P_r + \sigma P_i
\end{align}

where $P_i$ and $P_r$ are the incident and reflected beam intensities, $dl_i$ and $dl_r$ are length increments along the incident and reflected beam directions, $\mu_a$ is the effective linear absorption coefficient, and $\sigma$ is the linear reflectivity of the reflection. $\sigma$ is given by

$$\sigma = Q \, W(\Delta)$$

where $W(\Delta)$ is the function describing the distribution of mosaic blocks in the crystal. A reasonable approximation to the actual distribution is a gaussian
\[ W(\Delta) = \frac{1}{h^2} \eta_c e^{-\frac{h^2}{4 \eta_c}} \quad (123) \]

\( \eta_c \) is called the mosaic spread parameter and is of the order of ten minutes of arc for typical crystals. Analytic solutions for the differential equations have been found for simplified geometries by Hamilton. Hamilton approximates \( W(\Delta) \) as

\[ W(\Delta) = \frac{1}{\sqrt{3} \eta_c} \quad |\Delta| < \sqrt{3} \eta_c \quad (124) \]

\[ W(\Delta) = 0 \quad |\Delta| > \sqrt{3} \eta_c \]

where \( \eta_c \) has the same value as in equation (123). Hamilton has also devised a numerical technique for obtaining extinction corrections. The basic procedure is to follow the incident and diffracted beams through the crystal, modifying them according to the prescription given in the differential equations. The final diffracted beam intensity is compared with the intensity predicted by equation (112), yielding a multiplicative correction \( E\eta \) for the integrated intensity. We then have

\[ P = C_0 E\eta Q. \quad (125) \]

Computer programs using the method of Hamilton were written to obtain extinction and absorption corrections for this and other studies. A detailed description of the programs is given in Appendix B.
There is another effect which can alter the measured intensity of a given reflection. If two sets of diffraction planes simultaneously satisfy the conditions for Bragg reflection, then each reflection will alter the intensity of the other. This phenomenon is known as coincident or simultaneous reflection. Coincident reflection is easily understood if one uses the Ewald sphere description of Bragg reflection. The Ewald sphere is a sphere in reciprocal lattice space whose radius is the magnitude of the neutron wave vector \( \mathbf{\tilde{a}} \). The center of the sphere is taken to be at \( -\mathbf{\tilde{a}} \). The sphere then passes through the origin of the reciprocal lattice. The location of the sphere depends on the orientation of the crystal with respect to the incident beam. A Bragg reflection will occur if one of the reciprocal lattice points \( \mathbf{\tilde{T}} \) lies on the surface of the sphere, the diffracted beam wave vector \( \mathbf{\tilde{b}} \) being the vector from the sphere center to the lattice point with \( \mathbf{\tilde{b}} - \mathbf{\tilde{a}} = \mathbf{\tilde{T}} \). If a second reciprocal lattice point \( \mathbf{\tilde{T}}'' \) lies on the sphere, then a reflection to associated wave vector \( \mathbf{\tilde{b}}'' \) can occur. In the scattering process neutrons in the incident beam \( \mathbf{\tilde{b}} \) can be scattered to \( \mathbf{\tilde{b}}' \) or to \( \mathbf{\tilde{b}}'' \). Neutrons which have been scattered to \( \mathbf{\tilde{b}}' \) can then also scatter back to \( \mathbf{\tilde{b}} \) (as described in the extinction process), or can scatter into \( \mathbf{\tilde{b}}'' \). Neutrons scattered into \( \mathbf{\tilde{b}}'' \) can then be
scattered into \( \mathbf{h} \) or \( \mathbf{h}' \). It is clear that the calculation of the effect of a coincidence is complicated, depending critically on the strengths of the various reflections. The process \( \mathbf{h} \rightarrow \mathbf{h}' \) is called the primary reflection, the process \( \mathbf{h} \rightarrow \mathbf{h}'' \) is called the coincident reflection, and the process \( \mathbf{h}'' \rightarrow \mathbf{h} \) is called the crossover reflection. When the coincident reflection is strong and the crossover reflection is weak, the measured primary reflection is weakened. On the other hand, if the crossover reflection is strong, the measured primary reflection may be enhanced. The depletion of the primary reflection is usually small, being the same magnitude as the extinction correction. The enhancement can be quite large especially if the primary reflection is weak.

There is no completely satisfactory way of calculating coincidence corrections. The approach to the problem taken in this study is to avoid reflections and crystal orientations where coincidence may be present. The technique used is to first determine the location of the Ewald sphere for a particular reflection in question. Then each reciprocal lattice vector is examined to determine if it lies close enough to the sphere to cause coincidence. If none are close, or if those near the sphere represent weak reflections, then the reflection is taken to be free of coincidence. A computer program to carry
out this procedure was written, and a description of the program is given in Appendix C along with some general comments on the coincident reflection problem.
CHAPTER IV

THE EXPERIMENT

IV.1. Intensity Measurements

Measurements were taken in four temperature regions. At room temperature studies were made to determine the effective linear absorption coefficient, the crystal mosaic spread parameter, and the instrument constant. At both 77 K and 4.2 K a wide range of diffraction peaks were studied to verify the magnetic structures proposed by Koehler et al. and to select reflections for study in the 0.3 to 4.2 K temperature range. The selected peaks were then studied in this lowest range to determine the sign and magnitude of the incoherent scattering amplitude. These measurements are described and the results are presented in this chapter.

Integrated intensities in all temperature regions were obtained in the standard manner by rocking the crystal through the reflecting position. Points on the rocking curve were obtained at 0.1° or 0.2° intervals depending on the angular width of the peak. For the strong reflections, a monitor preset of $10^5$ counts (~31 seconds) was used, and for weak reflections, monitor
presets of $2 \times 10^5$ and $4 \times 10^5$ were used. The integrated intensity was obtained by summing the diffraction counter counts at the measured points on the rocking curve and then subtracting out the background count contribution to the sum. The background is obtained by extending the rocking curve on either side of the diffraction peak. If there are $N$ points in the peak, we have

$$P = \sum_{i=1}^{N} I_i - NI_{bg}$$

where $I_i$ is the number of counts recorded at the $i$th point on the rocking curve and $I_{bg}$ is the average background count. In reporting integrated intensities, all measurements have been scaled to $10^5$ monitor and $0.1^\circ$ angular increment.

In scanning the low scattering angle reflections, the counter was often left at the central position for the peak. This type of scan, called a $\Theta$ scan or a counter fixed scan, was possible because the counter aperture of $3.6^\circ$ was large enough to receive all neutrons scattered coherently in the reflection. For large scattering angle reflections, the counter was moved with the crystal, the counter advancing at twice the rate of the crystal. This type of scan is called $\Theta - 2\Theta$ scan or a counter moving scan.

In the temperature region accessible only with the He$^3$ refrigeration system, it was not usually possible
to maintain a constant crystal temperature for periods of
time sufficient to obtain integrated intensity measure-
ments. It was found, however, that an adequate measure
of the integrated intensity could be obtained by measur-
ing only the maximum intensity of the diffraction peak.
In order to obtain accuracy equivalent to that of an in-
tegrated measurement, monitor presets of $10^6$ and larger
were used. The validity of this approach is discussed
in section IV.5.

IV.2. Measurement at Room Temperature

The effective linear absorption coefficient
was measured before the crystal was mounted in the
cryostat. The technique used was to measure the attenu-
ation of the neutron beam in passage through the crystal.
To this end the diffraction counter was positioned to
measure the direct beam. In order to reduce the neutron
flux to an acceptable level and in order to define a beam
small enough to insure no leakage around the crystal, a
beam aperture of ~1mm was used. The crystal in its alu-
minum holder was positioned directly in front of the aper-
ture with the crystal cylinder axis coincident with the
neutron beam axis. In this position the neutron beam
passed through 0.76 cm. of aluminum and 0.18 cm. of
holmium. The beam was measured attenuated by the crystal
and holder ($\Phi_2$) and unattenuated ($\Phi_1$). Experimental
corrections \( \phi_c \) were made for the presence of non-thermal neutron components in the beam and the transmission coefficient \( T \) of the crystal and holder was obtained
\[
T = \frac{\phi_2 - \phi_c}{\phi_1 - \phi_c}. 
\] (127)

To determine the corrections, the beam was measured with the thermal neutron component eliminated by placing a 0.036" piece of cadmium over the aperture. It was found that approximately 20% of the total measured flux was due to non-thermal neutron components. The transmission of the crystal and holder was found to be
\[
T = 0.692 \pm 0.007. 
\] (128)
The aluminum transmission \( T_{al} \) was calculated using equation (113) taking the total cross section instead of the incoherent cross section obtaining
\[
T_{al} = 0.934. 
\] (129)
The transmission of the crystal is then
\[
T_{\text{NaCl}} = 0.698 \pm 0.007 \] (130)
and the linear absorption coefficient is
\[
\mu_a = 1.99 \pm 0.06 \text{ cm}^{-1}, \] (131)

Since the correction for non-thermal neutron components was large, an independent measurement of \( T \) was made. In this measurement a NaCl crystal was placed on the diffraction table with the counter and NaCl crystal
positioned to measure the (200) NaCl reflection. This reflection was measured with the direct beam and with the beam attenuated by the holmium crystal and its holder. The resulting transmission coefficient was

\[ T = 0.653 \pm 0.012 \]

in good agreement with equation (128).

As shown in Chapter III, it is possible to calculate \( \mathcal{M}_a \) based on the capture and incoherent scattering cross sections of the holmium ions. At low temperatures, where the only incoherent scattering is the spin incoherent scattering, we have

\[ \mathcal{M}_a = 1.44 \text{ cm}^{-1} \]  

using the values \( \sigma_a = 40 \text{ barns} \) and \( \sigma_c = 3.9 \text{ barns} \) as given by Bacon\(^{30} \) and the lattice parameters in Table 2. Preliminary low temperature measurements indicated a much smaller value of \( \sigma_c \approx 0.5 \text{ barns} \) giving

\[ \mathcal{M}_a = 1.32 \text{ cm}^{-1}. \]

At room temperature, the magnetic scattering is incoherent and must be included in a calculation of \( \mathcal{M}_a \).

\[ \mathcal{M}_a = 2 N_c (\sigma_a + \sigma_c + \sigma_{pm}) \]

where \( \sigma_{pm} \) is the paramagnetic scattering cross section. Using the differential cross section of Trammell\(^{13} \) we obtain

\[ \sigma_{pm} = \frac{\pi}{3} \left( \frac{y e^2}{2mc^2} \right) \mathcal{M} \frac{f^2}{f} \]
where $f^2$ is the square of the form factor averaged over all scattering directions. Using the form factor as calculated by Blume, Freeman, and Watson\textsuperscript{36} we obtain

$$\bar{f}^2 = 2.79$$

and

$$U_m = 9.6 \text{ barns}$$

(137)

and the expected value of $\mu_a$ at room temperature is

$$\mu_a = 1.67 \text{ cm}^{-1}.$$  \hspace{1cm} (138)

It is seen that there is a significant discrepancy between the measured and the calculated absorption coefficients. It is known that some of the rare earths, particularly gadolinium and samarium, have extremely large thermal neutron capture cross sections. In fact, using the values of $\sigma_a$ in Bacon\textsuperscript{30} and the limits on impurities in this holmium sample as presented in Chapter II, the discrepancy between the measurement and calculation can be explained. On the other hand, it is possible that some systematic error was present in the transmission measurement. A 6% increase in $\bar{T}$ is sufficient to bring the measurement into agreement with the calculation.

It was decided to use both the calculated and measured values of $\mu_a$ with the hope that further work could distinguish between them. The values of $\mu_a$ used at 77 K were obtained by scaling $\sigma_{pm}$ with the coherent magnetic scattering and are
After the crystal was mounted in the cryostat, attempts were made to determine the mosaic spread parameter $\gamma_c$. A technique which has been applied previously is to select a value of $\gamma_c$ which correctly predicts the intensity ratio of two peaks, one with little or no extinction, and one with a large amount of extinction. Reflections with small Bragg angles are chosen to minimize the influence of the thermal vibration factor. The reflections investigated here were the (002), (101), and (100) reflections. These all have Bragg angles of about 11° and thermal vibration factors of about 0.99. The Q values for these reflections are in the ratio $24.7: 17.8: 6.8$ respectively so that ratios of (002) and (100) and the (101) and (100) reflections should be the most accurate in determining $\gamma_c$. Unfortunately it was found that none of these peaks was severely affected by extinction and that no accurate value of $\gamma_c$ could be assigned. It appeared that

$$\gamma_c = 12' \pm 5'.$$

(141)

If these room temperature peaks represented the largest peaks studied, as is the case in many magnetic crystals,
then there would be no problem with this large uncertainty in \( \gamma_e \) because there would be little or no extinction present in any peak and a pure absorption correction would suffice to describe the intensities. In holmium, however, the satellites of the (002) reflection, for example, are approximately five times as large as the (002) itself so that they may have considerable extinction even if the (002) peak has none.

Koehler et. al.\textsuperscript{11} do in fact claim that there is little or no extinction present in this crystal. However, they find that \( f^2 \) determined at the (100)\textsuperscript{5} satellites is about 10\% higher than \( f^2 \) determined at the (002)\textsuperscript{−} peak. Since these reflections are at about the same scattering angle, they should have the same value of \( f^2 \). Such a discrepancy could have been caused by neglecting a 10\% extinction on the (002)\textsuperscript{−} reflection. In order for there to be little extinction on the (002)\textsuperscript{−} reflection, a large value of \( \gamma_e \) is necessary. As shown in Appendix 1, the mosaic parameter directly affects the observed width of diffraction peaks. For holmium, the room temperature peaks were quite narrow, approaching the limit established by the collimation and the monochromator. A rough estimate of \( \gamma_e \) based on the observed peak widths of the holmium reflections yields

\[ \gamma_e \approx 7' \] (142)
In analyzing the room temperature data, it was noted that the observed diffraction peaks were asymmetric. A plot of the (101) peak is shown in Fig. 9 where it is seen that the high angle side has a sizeable bulge in it. This was observed on all small scattering angle reflections in all temperature regions. An analysis of the (101) reflection indicated that the peak could be described as two gaussian shaped peaks separated by 0.4° with intensities in the ratio 6:1. The explanation proposed was that there is a small fraction \( \frac{1}{7} \) of the crystal which is misoriented from the bulk of the crystal by 0.4°. The splitting of the crystal into these two pieces has the effect of decreasing the extinction because no extinction can occur between the two portions of the crystal. The splitting is not reflected in equation (142) and therefore the rough value of \( \eta_c = 12' \) was adopted for preliminary use in calculating absorption coefficients.

In order to test the symmetry of the crystal, two pairs of reflections were studied at room temperature: (002) and (002); and (101) and (101). The results are presented in Table 5. It is seen that sizeable differences are present. Such differences can occur if the geometries of the reflections are different or if there is a considerable inhomogeneity in the mosaic distribution
Figure 9

Scan of the (101) Reflection at Room Temperature

The solid curve represents the observed scan. The broken curves represent the resolution of the observed scan into two gaussians as described in the text.
<table>
<thead>
<tr>
<th>Peak</th>
<th>P (10^5 Mon-1°)</th>
<th>P (10^6 Mon-1°)</th>
<th>Q (x10^-4 cm^-1)</th>
<th>EA (r=1.99 cm^-1)</th>
<th>C_o (x10^7)</th>
<th>EA (r=1.63 cm^-1)</th>
<th>C_o (x10^7)</th>
</tr>
</thead>
<tbody>
<tr>
<td>002</td>
<td>15624</td>
<td>15267</td>
<td>24.71</td>
<td>.4856</td>
<td>1.27</td>
<td>.5401</td>
<td>1.14</td>
</tr>
<tr>
<td>002</td>
<td>14911</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>5846</td>
<td>14780</td>
<td>17.87</td>
<td>.6709</td>
<td>1.23</td>
<td>.7172</td>
<td>1.15</td>
</tr>
<tr>
<td>101</td>
<td>14127</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>101</td>
<td>15432</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>7270</td>
<td></td>
<td>8.08</td>
<td>.6844</td>
<td>1.31^a</td>
<td>.7309</td>
<td>1.23^a</td>
</tr>
</tbody>
</table>

Average Value of C_o

\[ C_o = 1.24 \times 10^7 \]
\[ C_o = 1.14 \times 10^7 \]

^a The deviance on the (300) is thought to be due to an incorrect choice of 2B. An error there should not affect the other reflections.
in the crystal. As pointed out in Chapter II, the crystal is somewhat asymmetric and this may partially explain the observed differences in the equivalent reflections. Normally this problem is handled by measuring all equivalent reflections and taking the average as the best measure of the reflection. In this study, where the measurement of integrated intensities was not of primary importance, this was not done. Rather, only one of the equivalent sets was measured and the observed room temperature differences were considered in extracting information.

The instrument constant $C_5$ was determined from a study of the $(002)$, $(101)$, $(100)$, and $(300)$ reflections. The value of the Debye-Waller factor used was $2.8 = 1.3^0 \text{Å}^2$. The analysis was carried out for both $\mu = 1.99 \text{ cm}^{-1}$ and $\mu = 1.67 \text{ cm}^{-1}$. The results are shown in Table 5.

**IV.3. Measurements at 77 K**

Measurements were made at 77 K with the aims of verifying the magnetic structure deduced by Koehler et al.\textsuperscript{11} and of determining the holmium magnetic form factor. The technique for cooling the crystal to 77 K was to fill the Stage III pot with liquid nitrogen and allow Stage IV and the crystal to come into equilibrium with Stage III. A He\textsubscript{4} gas flow through the primer was used to reduce the cool-down time to about six hours. In this mode of
operation, the high pressure nitrogen and hydrogen gas systems were not operated. The cryostat can be operated indefinitely in this mode with a liquid nitrogen fill being necessary every five hours.

The square of the structure factor for this temperature region is

\[ F^2 = 4 \sum_{\text{coh}} G_c^2 e^{-\frac{\pi}{\lambda}(\frac{2\pi}{\lambda})^2} \varepsilon(\vec{r} - \vec{\tau}) \]

\[ + 2 \rho^2(\kappa) (1 - \frac{\rho^2}{2}) G_c^2 e^{-\frac{\pi}{\lambda}(\frac{2\pi}{\lambda})^2} \varepsilon(\vec{r} - (\vec{\tau} + \vec{\delta})) \]

\[ + 2 \rho^2(\kappa) (1 - \frac{\rho^2}{2}) G_c^2 e^{-\frac{\pi}{\lambda}(\frac{2\pi}{\lambda})^2} \varepsilon(\vec{r} - (\vec{\tau} - \vec{\delta})). \]

(143)

The helical spin structure is readily indicated by the presence of the two satellite reflections \( \vec{k} = \vec{\tau} \pm \vec{\delta} \) for each central reflection \( \vec{k} = \vec{\tau} \). Satellites were observed for all peaks. Scans of the (002) and the (300) sets are shown in Fig. 10. It is seen that the (300) satellites are identical while the (002) peak is considerably larger than the (002) peak. This is taken to imply that \( k_{(300)} = k_{(300)} \) and \( k_{(002)} = k_{(002)} \) which indicates that the helix wave vector is directed along the (001) direction in the crystal. Since \( k_{(300)} = k_{(300)} \), the (300) satellites have identical Bragg angles and the difference in peak location is a direct measure of the angle \( \phi_{300} \) between \( \vec{k}_{(300)} \) and \( \vec{k}_{(300)} \). This angle, with the lattice constants, allows for a determination of the magnitude of \( \vec{\delta} \).

This is true for any of the (h00) sets if the crystal is oriented with the (001) axis horizontal. If \( \phi_{h00} \) is the
Figure 10

Scans of the (002) and (300) Sets at 77 K
difference in angular position of the two satellites and if we write \( \varepsilon = \varepsilon' \vec{C} \) where \( \vec{C} \) is the reciprocal lattice basis vector, we have

\[
\tan \left( \frac{\phi_{\text{hoo}}}{2} \right) = \frac{\varepsilon'}{\frac{2}{\sqrt{3}a}}
\]

or

\[
\varepsilon' = \frac{2}{\sqrt{3}} \frac{\varepsilon}{a} \tan \left( \frac{\phi_{\text{hoo}}}{2} \right).
\]

The \((100)^*\) satellites were not accessible with the particular orientation of the crystal and cryostat cradle. The \((200)^*\) and \((300)^*\) satellites were accessible and were used to obtain \( \varepsilon' \). The results are shown in Table 6. The value of \( \varepsilon' \) obtained is

\[
\varepsilon' = 0.233 \pm 0.001
\]

in good agreement with the value \( \varepsilon' = 0.23 \) reported by Koehler et al. The turn angle corresponding to this value of \( \varepsilon' \) is 41°.

A comparison of the room temperature intensities with the 77 K central reflections verifies that there is no ferromagnetic component to the holmium moments at 77 K. An analysis of the central reflections is presented in Table 7 for both values of \( k_a \). The Debye-Waller factor \( 28 = 39.9^2 \) was used. It is seen that the instrument constant agrees with that obtained at room temperature.

It should be noted that some of the reflections were not completely resolved. In general the problem is
### TABLE 6

**Determination of the Interlayer Turn Angle at 77 K**

<table>
<thead>
<tr>
<th>Peak</th>
<th>Center Line</th>
<th>( \phi_{h00} )</th>
<th>( \varepsilon' )</th>
<th>( \varepsilon'' )</th>
</tr>
</thead>
<tbody>
<tr>
<td>((200)^-)</td>
<td>69.42°</td>
<td>7.31(5)°</td>
<td>1.476</td>
<td>.2330</td>
</tr>
<tr>
<td>((200)^+)</td>
<td>76.73(5)°</td>
<td>4.87(5)°</td>
<td>1.475</td>
<td>.2327</td>
</tr>
<tr>
<td>((300)^-)</td>
<td>81.90°</td>
<td>76.73(5)°</td>
<td>1.476</td>
<td>.2330</td>
</tr>
<tr>
<td>((300)^+)</td>
<td>86.77(5)°</td>
<td>4.87(5)°</td>
<td>1.475</td>
<td>.2327</td>
</tr>
</tbody>
</table>

### TABLE 7

**Analysis of Central Reflections at 77 K**

<table>
<thead>
<tr>
<th>Peak</th>
<th>( P ) ((x10^6) \text{ M} \text{eA} \text{ cm}^{-1})</th>
<th>( Q ) ((x10^7) \text{ cm}^{-1})</th>
<th>( EA ) ((x10^7) \text{ M} \text{ eA} \text{ cm}^{-1})</th>
<th>( C_0 ) ((x10^7) \text{ cm}^{-1})</th>
<th>( EA ) ((x10^7) \text{ cm}^{-1})</th>
<th>( C_0 ) ((x10^7) \text{ cm}^{-1})</th>
</tr>
</thead>
<tbody>
<tr>
<td>((002))</td>
<td>16802</td>
<td>25.86</td>
<td>.5103</td>
<td>1.27</td>
<td>.5722</td>
<td>1.14</td>
</tr>
<tr>
<td>((200))</td>
<td>3167</td>
<td>3.62</td>
<td>.7253</td>
<td>1.21</td>
<td>.7729</td>
<td>1.13</td>
</tr>
<tr>
<td>((300))</td>
<td>8919</td>
<td>10.15</td>
<td>.7060</td>
<td>1.25</td>
<td>.7542</td>
<td>1.16</td>
</tr>
</tbody>
</table>

**Average Value of \( C_0 \)**

\( C_0 = 1.24 \times 10^7 \)
\( C_0 = 1.14 \times 10^7 \)
worst for the (00l) reflections and best for the (h00) reflections, as may be inferred from Fig. 10 where the (002) \( \dagger \) satellites overlap the (002) central peak whereas the (300) \( \dagger \) satellites are almost completely resolved from (300) peak. The resolution becomes worse at large scattering angles where the peaks have a greater width. It was found that the resolution could be improved by strategic use of the counter. For example, by using a \( \phi \) scan, the (300) \( \dagger \) satellites can be completely resolved from the (300) peak and by using a \( \phi \) scan the (002) \( \dagger \) satellites can be resolved from the (002) peak. Even with these precautions, the integrated intensities may be somewhat in error. The problem with peak overlap becomes much worse at 4.2 K.

The analysis of the integrated intensities of the satellites is shown in Table 8. The instrument constants deduced at 77 K and at room temperature were used. Values of \( (-\frac{a}{2}) \) and \( G_c \) were calculated from the formulae in Table 3 in Chapter III. The extraction of the magnetic form factor is carried out in Chapter V.

IV.3. Measurements at 4.2 K

Analyses similar to those at 77 K were performed at 4.2 K. In cooling the crystal to 4.2 K, it was necessary to first pre-cool Stage III and Stage IV to 77 K as described earlier. Then the gas systems, Stage I
<table>
<thead>
<tr>
<th>Peak</th>
<th>( P \times 10^5 \text{ Mon.}^{-1} \text{ m}^2 )</th>
<th>( G_c^2 )</th>
<th>((1-\frac{q^2}{2}))</th>
<th>( e^{-2W} )</th>
<th>( \sin 2\theta )</th>
<th>( EA )</th>
<th>( p^2(K) )</th>
<th>( EA )</th>
<th>( p^2(K) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>((002)^-)</td>
<td>35588</td>
<td>1.00</td>
<td>1.00</td>
<td>.9906</td>
<td>.3401</td>
<td>.4532</td>
<td>3.135</td>
<td>.5084</td>
<td>3.039</td>
</tr>
<tr>
<td>((002)^+)</td>
<td>26936</td>
<td>1.00</td>
<td>1.00</td>
<td>.9852</td>
<td>.4249</td>
<td>.4875</td>
<td>2.771</td>
<td>.5441</td>
<td>2.700</td>
</tr>
<tr>
<td>((101)^-)</td>
<td>17807</td>
<td>.75</td>
<td>5757</td>
<td>.9883</td>
<td>.3790</td>
<td>.6972</td>
<td>2.637</td>
<td>.7435</td>
<td>2.690</td>
</tr>
<tr>
<td>((101)^+)</td>
<td>17349</td>
<td>.75</td>
<td>6565</td>
<td>.9856</td>
<td>.4192</td>
<td>.6808</td>
<td>2.559</td>
<td>.7289</td>
<td>2.600</td>
</tr>
<tr>
<td>((200)^-)</td>
<td>2084</td>
<td>.25</td>
<td>5020</td>
<td>.9607</td>
<td>.6661</td>
<td>.7261</td>
<td>1.844</td>
<td>.7733</td>
<td>1.883</td>
</tr>
<tr>
<td>((200)^+)</td>
<td>1962</td>
<td>.25</td>
<td>5020</td>
<td>.9607</td>
<td>.6661</td>
<td>.7267</td>
<td>1.734</td>
<td>.7738</td>
<td>1.772</td>
</tr>
<tr>
<td>((201)^-)</td>
<td>5308</td>
<td>.75</td>
<td>5214</td>
<td>.9591</td>
<td>.6775</td>
<td>.7171</td>
<td>1.555</td>
<td>.7645</td>
<td>1.580</td>
</tr>
<tr>
<td>((201)^+)</td>
<td>4937</td>
<td>.75</td>
<td>5511</td>
<td>.9565</td>
<td>.6960</td>
<td>.7093</td>
<td>1.469</td>
<td>.7578</td>
<td>1.500</td>
</tr>
<tr>
<td>((300)^-)</td>
<td>2385</td>
<td>1.00</td>
<td>5009</td>
<td>.9139</td>
<td>.9031</td>
<td>.7133</td>
<td>.767</td>
<td>.7619</td>
<td>.781</td>
</tr>
<tr>
<td>((300)^+)</td>
<td>2416</td>
<td>1.00</td>
<td>5009</td>
<td>.9139</td>
<td>.9031</td>
<td>.7128</td>
<td>.777</td>
<td>.7616</td>
<td>.791</td>
</tr>
</tbody>
</table>
and Stage II were operated, bringing the heat shields to 77 K and 20 K. Liquid helium was then transferred into the Stage III reservoir and the primer was used to bring Stage IV to 4.2 K. It took about eight hours to cool the crystal from room temperature to 4.2 K. In principle the crystal can be maintained at 4.2 K indefinitely by refilling the Stage III reservoir every thirty hours, but in practice it was found that impurities in the cylinder gasses used in Stage I and Stage II would freeze in the cryostat disrupting the experiment. Extensive external trapping was applied, but even so experiments longer than 48 hours were not generally possible.

At 4.2 K the square of the structure factor is given approximately by

\[ F^2 = (4b_{coh}^2 + 4p^2) \sin^2 \theta \sin^2 \phi \left( e^{-2\frac{G}{2\pi}} G_{e} \right) \left( \begin{array}{c} \mathbf{k} \end{array} \right) \]

\[ + 2p^2(\kappa) \left( -\frac{\alpha^2}{2} \right) \cos^2 \phi \left( e^{-2\frac{G_{v}}{2\pi}} G_{s} \right) \left( \begin{array}{c} \mathbf{k} \end{array} \right) \]

The approximation is that the nuclear polarization contributions have been omitted. In intensity analysis, corrections for this omission deduced from the low temperature work were applied. These corrections amounted to one or two percent typically.

Scans of the (002) set and the (300) set are shown in Fig. 11. It is seen that the (300)\(^{\pm}\) satellites are identical and that the (002)\(^{-}\) satellite is larger
Figure 11

Scans of the (002) and (300) Sets at 4.2 K
than the (002) satellite as observed at 77 K, indicating that $\vec{c}$ points along the (00l) direction. The magnitude of $\vec{c}$ was determined as at 77 K using the $(\bar{2}00)^\pm$ and the $(\bar{3}00)^\pm$ satellites. The results are shown in Table 9. We obtain

$$\epsilon' = 0.169 \pm 0.003$$

in good agreement with the value, $\epsilon' = 0.166$, reported by Koehler et. al.\textsuperscript{m}

As can be seen by comparing the (002) and $(\bar{3}00)$ sets at 4.2 K with those at 77 K, the resolution is much worse at 4.2 K. The magnetic satellites could sometimes be resolved by offsetting the counter from its normal position as shown in the scan of the (002) in Fig. 12. However the central peaks often could not be separated from the satellites. This made an accurate analysis of the central peaks impossible. The results of the analysis are shown in Table 10. The observed deviations of the (101) and (102) peaks were also found by Koehler et. al.\textsuperscript{11} and may indicate some further perturbation in the magnetic structure. The instrument constants deduced in the higher temperature regions and the Debye-Waller factor, $\sigma = 0.003$, were used in the analysis.

To verify the bunching of moments as described in Chapter III, the (001)$^\ddagger$ satellites were studied. The scan is shown in Fig. 13. It is seen that there is no
### TABLE 9

**Determination of the Interlayer Turn Angle at 4.2K**

<table>
<thead>
<tr>
<th>Peak</th>
<th>Center Line</th>
<th>$\phi_{h00}$</th>
<th>$\varepsilon'/\varepsilon$</th>
<th>$\varepsilon'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(200)$^-$</td>
<td>70.20°</td>
<td>5.33°</td>
<td>1.075</td>
<td>0.170</td>
</tr>
<tr>
<td>(200)$^+$</td>
<td>75.53°</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(300)$^-$</td>
<td>82.42°</td>
<td>3.51°</td>
<td>1.061</td>
<td>0.168</td>
</tr>
<tr>
<td>(300)$^+$</td>
<td>85.93°</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### TABLE 10

**Analysis of Central Reflections at 4.2 K**

<table>
<thead>
<tr>
<th>Peak</th>
<th>P ($10^5 M_{\text{at}}^{-1}$)</th>
<th>Q ($\times 10^{-3}$ cm)</th>
<th>EA $(\times 10^{-7}$ cm$^2$</th>
<th>$C_0$ $(\times 10^7)$</th>
<th>EA $\lambda_{n}=1.32$ cm$^{-1}$</th>
<th>$C_0$ $(\times 10^7)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(101)</td>
<td>16356</td>
<td>23.17</td>
<td>.7057</td>
<td>1.00</td>
<td>.7531</td>
<td>.94</td>
</tr>
<tr>
<td>(102)</td>
<td>5692</td>
<td>5.44</td>
<td>.6774</td>
<td>1.54</td>
<td>.7324</td>
<td>1.43</td>
</tr>
<tr>
<td>(200)</td>
<td>3652</td>
<td>4.39</td>
<td>.7416</td>
<td>1.12</td>
<td>.7883</td>
<td>1.06</td>
</tr>
<tr>
<td>(201)</td>
<td>9812</td>
<td>12.49</td>
<td>.7232</td>
<td>1.04</td>
<td>.7707</td>
<td>1.02</td>
</tr>
<tr>
<td>(300)</td>
<td>10166</td>
<td>11.49</td>
<td>.7230</td>
<td>1.22</td>
<td>.7694</td>
<td>1.15</td>
</tr>
<tr>
<td>(401)</td>
<td>6133</td>
<td>7.13</td>
<td>.7000</td>
<td>1.23</td>
<td>.7461</td>
<td>1.15</td>
</tr>
</tbody>
</table>
Figure 12

Resolution of the (002) Reflection at 4.2 K

The solid curve was obtained with a $\phi$ scan with the counter offset from the peak center position by $0.5^\circ$. The dashed and dotted lines represent the excess contributions due to the (002) reflection in a $\phi$ scan with the counter at peak center and a $\phi - 2\phi$ scan.
Figure 13

Scan of the (001) Set at 4.2 K

The scan is a $e^{-2\theta}$ scan. The small peak at 145° was found to be due to a coincident reflection. Located on the plot are the positions of the $\frac{1}{4}\lambda$ (002) reflections and the (001) reflection.
peak corresponding to the (001) reflection but that reflections corresponding to (001)$^+$ and (001)$^-$ do occur. The small peak to the left of the (001)$^-$ was found to be due to coincident reflection and was eliminated by a rotation of the crystal about the (001) axis. The value of the bunching parameter $\delta$ was deduced by comparing the intensities of the (002)$^+$ satellites with the intensities of the (001)$^+$ satellites. It was necessary to correct the (001)$^-$ peaks for the $\frac{1}{3}\lambda$ reflection of the (002) set which can be seen as the large bulges on the (001)$^-$ peaks. It was found that

$$\delta = 8.3 \pm 2.0^\circ. \quad (149)$$

This value disagrees with the value of $\delta = 5.3^\circ$ obtained by Koehler et al. The values of $G_s^z$ as calculated with various values of $\delta$ are shown in Table 11. It is seen that there is little effect on the reflections except for those where $G_s^z$ is zero. In further analysis, the value of $\delta$ obtained here is used.

The analysis of the magnetic satellites is shown in Table 12. The values of $(1 - \frac{\delta}{\zeta})$ are calculated from the formulae in Table 3 in Chapter III, and the instrument constants deduced in the higher temperature work are used. The magnetic form factor is extracted and discussed in Chapter V. Intensities have been corrected for the nuclear polarization contributions based on the
TABLE 11

The Geometric Structure Factor for Various Values of the Bunching Parameter

<table>
<thead>
<tr>
<th>$G_c^2$</th>
<th>$G_s^2 \delta = 0^\circ$</th>
<th>$G_s^2 \delta = 5.8^\circ$</th>
<th>$G_s^2 \delta = 8.3^\circ$</th>
<th>$G_s^2 \delta = 15^\circ$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.000</td>
<td>.933</td>
<td>.974</td>
<td>.986</td>
<td>1.000</td>
</tr>
<tr>
<td>.750</td>
<td>.716</td>
<td>.737</td>
<td>.743</td>
<td>.750</td>
</tr>
<tr>
<td>.250</td>
<td>.283</td>
<td>.263</td>
<td>.257</td>
<td>.250</td>
</tr>
<tr>
<td>0.000</td>
<td>.067</td>
<td>.026</td>
<td>.014</td>
<td>0.000</td>
</tr>
</tbody>
</table>
### TABLE 12
Analysis of Satellite Reflections at 4.2 K

<table>
<thead>
<tr>
<th>Peak</th>
<th>P$_{10^3}$ &lt;10$^{-3}$</th>
<th>G$^2$</th>
<th>1- G$^2$</th>
<th>e$^{-2W}$</th>
<th>Sin2$\theta$</th>
<th>EA</th>
<th>$p^2$kl cos$^2\gamma$</th>
<th>EA</th>
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lower temperature work.

IV.3. Measurements between 4.2 K and 0.4 K

As shown in Chapter III, the coherent scattering cross section has terms dependent on the polarization of the holmium nuclear spins. For the satellite reflections we have

\[ F_z^* = [z \rho^2(\xi) (1 - q^2) + z \rho(\xi) (1 - q^2) b_{inc} I f_N + \frac{1}{2} b_{inc} I f_N^2] x \cos^2 \gamma e^{-2 \theta(\xi)(\xi)} \gamma^2 \delta \left( \frac{\gamma}{(\xi - x \xi)} \right) \]

(150)

The integrated intensity can then be written as

\[ \mathcal{P}_2 = \mathcal{P}_0 \left[ 1 + \frac{b_{inc} I}{\rho(\xi)} f_N + \frac{b_{inc} I}{\gamma \rho(1 - q^2)} f_N^2 \right] \]

(151)

where, to first approximation, \( \mathcal{P}_0 \) is independent of the nuclear polarization. (A small polarization dependence in \( \mathcal{P}_0 \) does result through the extinction-absorption factor. This is discussed in Chapter V.) We see that, knowing \( \rho(\xi) \) and \( f_N(\gamma) \) the sign and magnitude of \( b_{inc} \) can be determined from a study of the temperature dependence of the satellite reflections. To this end, a selection of peaks was studied at temperatures from 4.2 K to 0.4 K.

Crystal temperatures from 1.5 K to 4.2 K were obtained by pumping on the \( \text{He}^4 \) liquid in Stage III and allowing Stage IV and the crystal to come into equilibrium with Stage III. Crystal temperatures below 1.5 K were obtained by operating the \( \text{He}^3 \) refrigeration system as described in Chapter II. It was possible to regulate
the crystal temperature above 1.5 K simply by controlling
the vapor pressure of the helium in Stage III but no
temperature control was possible below 1.5 K. In this
region, once the He$^3$ was gone, the crystal warmed at a
slow rate governed by the heat leak from Stage III.
Because of this feature, it was not possible to obtain
integrated intensity measurements for all reflections
below 1.5 K. As described earlier, it was found that an
adequate measure of the integrated intensity could be
obtained quickly by measuring only the maximum intensity
$I_m$ of the reflection. We have
\[ p = a (I_m - I_{bg}) \]
where $I_{bg}$ is the contribution to $I_m$ due to the background
scattering and $a$ is a proportionality constant which
depends on the width of the peak. The validity of this
relation was tested by comparing the (002)$^-$ integrated
intensity at several temperatures with the corresponding
maximum intensity. The results are shown in Table 13
where it is seen that equation (152) is valid.

In order to obtain a satisfactory measure of
$I_m$, it is necessary that the measurement be made at the
position of the maximum intensity. In preliminary mea-
surements it was found that small shifts of the peak
positions occasionally occurred due either to slippage of
the cryostat in its mount or to thermal contractions
inside the cryostat. For some of the sharp peaks, an
TABLE 13

The Maximum Intensity as a Measure of the Integrated Intensity - The (002)* Reflection

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<th>$P$ (10^5 Mon^-1°)</th>
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offset of a few hundredths of a degree can mean an error of several percent in $I_m$. It was decided that the safest way to proceed was to scan across the peak center, taking the three largest measurements as the measure of the maximum intensity. The scan of the (002) peak center is shown in Fig. 14. The background correction was obtained by measuring the scattering with the crystal detuned from the reflection. The background does have a nuclear polarization dependence as shown in Chapter III. However, the contribution of the spin incoherent scattering to the total background was so small that no temperature dependence could be detected. The use of the maximum intensity, rather than the integrated intensity, eliminates some of the problems due to poor resolution in that, even when peaks overlap, the peak centers may be separated far enough to be unaffected by overlaps. In such cases, the maximum intensity may even be a better measure of the reflection.

Based on the 4.2 K work, the (002)$^+$, (101)$^+$, (201)$^+$, (300)$^-$, and (401)$^+$ satellite peaks were selected for study below 4.2 K. In addition, the (002), (101), and (401) central reflections were also followed to look for their predicted temperature dependence. Data was taken in three separate experiments each separated by a
Figure 14

Scan of the (002) Peak Center at 80 K
week or two at room temperature. The first set of data was taken during the weekend of 4/29/73 and was restricted to measurements between 4.2 K and 1.5 K. The second and third sets were taken during the weekends of 5/5/73 and 5/20/73 respectively and included data down to 0.4 K. It was found that an overall shift in intensities of 1.3% occurred between the 5/5 run and the 5/20 run and that a similar shift of 1.1% occurred during the 5/5 run. Shifts of this type were observed by Goer in his study of Co0, and are attributed to changes in the instrument constant. The intensities were normalized to the first portion of the 5/5 run where most of the lowest temperature data was obtained. The raw data and the normalized data are presented in Table 14. All intensities have been normalized to a monitor preset of $10^6$ counts. The temperature was deduced from the calibration described in Chapter II and the nuclear polarization was calculated using the hyperfine constants as presented in Chapter III. The analysis of the data is presented in Chapter V.
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CHAPTER V

ANALYSIS OF RESULTS

V.1. The Magnetic Form Factor

In Chapter IV, the magnetic scattering amplitude has been deduced from the integrated intensity measurements. As shown in Chapter III, \( \rho(\kappa) \) is given by

\[
\rho(\kappa) = \frac{ye^2}{2mC^2} \mathcal{A} f(\kappa)
\]  

(153)

where \( \mathcal{A} \) is the effective magnetic moment of the holmium ions in Bohr magnetons. In order to extract the form factor \( f(\kappa) \) it is necessary to obtain a value for \( \mathcal{A} \). Traditionally this is done by using theoretical calculations of the form factor for low scattering angle reflections where the theories are most accurate. In our case the (002)\( ^\pm \) and (101)\( ^\pm \) satellites were used. The analysis is presented in Table 15. The theoretical form factor is taken from the calculations of Blume, Freeman, and Watson. Here the (002)\( ^\pm \) and (101)\( ^\pm \) intensities are adjusted based on the observed differences of the (002) and (00\( \bar{2} \)) and the (101) and (1\( \bar{0} \)1) reflections at room temperature. We find agreement between the two different sets of absorption coefficients, except for the presence
**TABLE 15**

Determination of the Holmium Magnetic Moment

<table>
<thead>
<tr>
<th>$\mathcal{H}_a$ (cm$^{-1}$)</th>
<th>Peak</th>
<th>$p(K)$ (10$^{-12}$ cm)</th>
<th>$p'(K)$ (10$^{-12}$ cm)</th>
<th>$f(K)$ theory</th>
<th>$\mathcal{H}$ ($\mathcal{H}_B$)</th>
<th>$\mathcal{H}_a$ (cm$^{-1}$)</th>
<th>Peak</th>
<th>$p(K)\cos\gamma$ (10$^{-12}$ cm)</th>
<th>$p'(K)\cos\gamma$ (10$^{-12}$ cm)</th>
<th>$f(K)$ theory</th>
<th>$\mathcal{H}\cos\gamma$ ($\mathcal{H}_B$)</th>
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<td>1.80</td>
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<td>1.750</td>
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<td>7.15</td>
<td>1.67</td>
<td>(002)$^-$</td>
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<td>2.360</td>
<td>.892</td>
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<td>1.645</td>
<td>.863</td>
<td>7.07</td>
<td>(002)$^+$</td>
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<td>.869</td>
<td>9.68</td>
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<tr>
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<td>(101)$^-$</td>
<td>1.624</td>
<td>1.659</td>
<td>.888</td>
<td>6.93</td>
<td>(101)$^-$</td>
<td>2.186</td>
<td>2.234</td>
<td>.886</td>
<td>9.36</td>
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<tr>
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<td>1.600</td>
<td>1.635</td>
<td>.867</td>
<td>7.00</td>
<td>(101)$^+$</td>
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<td>1.32</td>
<td>(002)$^-$</td>
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<td>2.337</td>
<td>.892</td>
<td>9.72</td>
</tr>
<tr>
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<td>(002)$^+$</td>
<td>1.643</td>
<td>1.624</td>
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<td>(002)$^+$</td>
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<tr>
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<td>1.676</td>
<td>.888</td>
<td>7.00</td>
<td>(101)$^-$</td>
<td>2.225</td>
<td>2.234</td>
<td>.886</td>
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<td>2.198</td>
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<td>9.38</td>
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Average $\mathcal{H} = 7.03 \pm 0.07 \mathcal{H}_B$

Average $\mathcal{H}\cos\gamma = 9.5 \pm 2 \mathcal{H}_B$
of somewhat larger deviations in the results obtained from the experimentally determined $M_{\alpha}$ values. At 77 K we find

$$M_{77} = 7.03 \pm 0.7$$

(154)

and at 4.2 K

$$M_{4.2} \cos \gamma = 9.54 \pm 2.$$ Using $\gamma = 10^\circ$ we obtain

$$M_{4.2} = 9.7 \pm .2$$

(155)

in good agreement with Koehler et. al.\textsuperscript{11}

The form factor is now easily calculated and is shown in Table 16. It is seen that there is good agreement again between values obtained with the two different sets of $M_{\alpha}$. There is also good agreement between the 77 K results and the 4.2 K results. This is taken to imply that the extinction has been treated adequately, and that the choice of $M_{\alpha}$ is not critical. In further analysis, only the calculated absorption coefficients are used.

It has been shown by Trammell\textsuperscript{13} that the form factor for the rare earth ions is given approximately by

$$f(L) = \frac{L \cdot J \cdot f_L(L) + Z \cdot \frac{J}{2} \cdot f_J(L)}{L \cdot J + Z \cdot \frac{J}{2}}$$

(156)

where

$$Z \cdot \frac{J}{2} \cdot L \cdot J = J(J+1) + L(L+1) - S(S+1)$$

(157)
**TABLE 16**

*Determination of the Holmium Magnetic Form Factor From Integrated Intensity Measurements*

<table>
<thead>
<tr>
<th>Peak</th>
<th>$p(K)$</th>
<th>$f(K)$</th>
<th>$p(K)$</th>
<th>$f(K)$</th>
<th>$\frac{K}{4\pi} = \frac{\sin \theta}{\lambda}$</th>
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<td>1.723</td>
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<td>1.624</td>
<td>.859</td>
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<td>.886</td>
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<td>.871</td>
<td>.1956</td>
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<th>$f(K)$</th>
<th>$p(K) \cos \theta$</th>
<th>$f(K)$</th>
<th>$\frac{K}{4\pi} = \frac{\sin \theta}{\lambda}$</th>
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<td>.907</td>
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<td>.925</td>
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and

\[ \mathcal{Z} S \cdot J = J(J+1) - L(L+1) + S(S+1). \quad (158) \]

This expression is derived neglecting crystal field effects and assuming Russell-Sanders coupling and includes only the spherical portion of the form factor. The function \( f_s(k) \) is the spin contribution to the form and is given by

\[ f_s(k) = \int_0^\infty U_{4f}^2(r) \frac{\sin kr}{kr} \, dr \quad (159) \]

where \( U_{4f}(r) \) is the 4f electron radial wave function. The function \( f_L(k) \) is the orbital contribution to the form factor and is given by

\[ f_L(k) = \int_0^\infty U_{4f}^2(r) \left[ \frac{3 \sin kr}{(kr)^3} - \frac{3 \cos kr}{(kr)^3} \right] \, dr \quad (160) \]

Blume, Freeman and Watson\(^{36}\) have evaluated \( f_s(k) \) and \( f_L(k) \) for many rare earth ions using Hartree-Fock wave functions. They do not tabulate these functions for holmium but indicate that linear interpolation in their tables is accurate to two significant figures for \( \frac{k}{4\pi} < 1.0 \, \text{Å}^{-1} \).

For holmium we have \( L=6, \, S=2, \) and \( J=8 \) and equation (156) becomes

\[ f(k) = 0.6 f_L(k) + 0.4 f_S(k). \quad (161) \]

The form factor deduced from these calculations is shown in Fig. 15. The experimentally determined points are also shown. It is seen that good agreement is found for \( \frac{k}{4\pi} < 0.5 \, \text{Å}^{-1} \), considering the problems in resolution. In
Figure 15
The Magnetic Form Factor of Holmium

The solid curve represents the form factor calculated for Ho+++ using the theory of Trammell and the wave functions of Blume, Freeman and Watson as described in the text.
fact, the only points in disagreement are those for the (401)\textsuperscript{-1} satellites measured at 4.2 K. These reflections were at or near the limits of resolution. A plot of the (401) and (401)\textsuperscript{-1} reflections against crystal position is shown in Fig. 16. It is seen that in terms of crystal position, the reflections are not resolved. However, the counter has different phases for the three scans. The proper counter positions are shown for each peak center. The difference in crystal-counter phases was thought to be sufficient to resolve the reflections. As a check, a counter scan was made with the crystal tuned to the (401)\textsuperscript{-1} peak center. This scan is shown in Fig. 17. Here we see a large peak which is due to the (401) reflection and a small peak due to the (401)\textsuperscript{-1} satellite. It is seen that at the counter position appropriate to the satellite there is no contribution due to the central reflection. To verify this, the counter position was lowered by 0.5° from its proper phase and the (401)\textsuperscript{-1} scan was repeated with no reduction in intensity. The variation of the (401)\textsuperscript{-2} form factors from the theory may be real.

V.2. The Incoherent Scattering Amplitude

As shown in Chapter IV, the integrated intensity of the magnetic satellite reflections can be written

\[ P = P_0 \left( 1 + \frac{b \text{inc} I}{P} f_N + \frac{b^2 \text{inc} I^2}{P^2 (1 - q^2)} f_N^2 \right), \]  

(162)
Figure 16

Scans of the (401) Set at 4.2 K

Each scan is an e-ze scan and each was taken separately. The counter positions at peak center for each reflection are shown on the plot.
Figure 17

Counter Scan of the (401)\(^{-}\) Reflection

The solid curve represents the observed counter scan with the crystal tuned to the (401)\(^{-}\) peak center. The dashed curves represent the resolution of the observed plot into contributions from the (401)\(^{-}\) and the (401) reflections. It is seen that there is no contribution to the (401)\(^{-}\) intensity due to the (401) reflection when the counter is below 91.4°.
The maximum intensity is then
\[ I_m = I_0 \left( 1 + \frac{b_{inc}}{p(K)} f_N + \frac{b_{inc}^2}{4p(K)} \frac{T}{1 + f_N} \right) + I_{se}, \quad (163) \]

A plot of \( I_m \) against \( |f_N| \) should then be a parabola, and, by fitting curves to the data, it should be possible to extract \( b_{inc} \), \( p(K) \) and \( (1-\frac{q}{2}) \). A plot of the data for the \((300)^-\) reflection is shown in Fig. 24. Here it is seen that no quadratic term is evident. Rough calculations based on the slope of this curve and the previously measured value of \( p(K) \) yield
\[ |b_{inc}| \sim 0.8 \times 10^{-12} \text{ cm}. \]

For such a small value of \( b_{inc} \), it is easy to verify that the quadratic term may indeed be neglected for the reflections studied here. We then have
\[ I_m = I_0 \left( 1 - \frac{b_{inc}}{p(K)} f_N \right) + I_{se}. \quad (164) \]

If extinction is present, equation (164) does not completely describe the nuclear polarization dependence of \( I_m \). This occurs because the changing strength of the reflection produces a change in the extinction for the reflection. A plot of the extinction-absorption coefficient for the \((002)^-\) reflection against \( \frac{Q}{Q_c} \) is shown in Fig. 18. It is seen that for small changes in \( Q \) we can write
\[ E_A = EA_0 (1 - \beta Q) \quad (165) \]
where \( \beta \) and \( EA_0 \) are constants.
Figure 18
The Variation of the Extinction-Absorption Factor of the (002) Reflection with Q
We write the \(Q\) factor for a reflection as

\[
Q = Q_0 \left( 1 + b \frac{\sin \theta}{\rho_{(k)}^2} f_N \right) = Q_0 \left( 1 + \alpha f_N \right)
\]

and then

\[
E A = E A_0 \left( 1 - 3 Q_0 - \alpha Q_0 f_N \right).
\]

The measured peak intensity is then

\[
I_m - I_0 = D E A_0 \left( 1 - 3 Q_0 - \alpha Q_0 f_N \right) (1 + \alpha f_N)
\]

\[
= D E A_0 \left( 1 - 3 Q_0 \right) \left( 1 + \alpha \left( \frac{1 - 2 \beta Q_0}{1 - 3 Q_0} \right) f_N \right)
\]

or

\[
I_m = I_0 \left( 1 + \alpha \chi f_N \right) + I_0^C
\]

where

\[
\chi = \frac{1 - 2 \beta Q_0}{1 - 3 Q_0}
\]

is a correction factor due to the changing extinction. It is seen that the magnitude of the observed slope is decreased by the extinction effect.

The reflections most severely affected by extinction were the \((002)^\pm\) and the \((101)^\pm\) satellites. Correction factors were deduced for these reflections from the calculated variations of \(E A\) with \(Q\). We have

\[
\chi_{002^-} = .745
\]
\[
\chi_{002^+} = .504
\]
\[
\chi_{101^-} = .940
\]
\[
\chi_{101^+} = .941
\]

The reason for the large difference between the \((002)^\pm\) corrections and the \((101)^\pm\) corrections is that the \((002)^\pm\) reflections are affected more severely by extinction than
the (101)$^\dagger$ reflections due primarily to the crystal shape. Since the remaining reflections were less than one third as strong as the (101)$^\dagger$ satellites, it was assumed that no correction was needed for them.

The data for the temperature dependence of the selected reflections are presented in Table 14 in Chapter IV. It is seen that in the experiment of 5/20/73 the maximum intensities were measured at only two temperatures for each reflection. The lowest temperature points were measured while the crystal and Stage IV were cooling toward 0.3 K and are somewhat uncertain since it is doubtful that equilibrium had been achieved. Further, as noted in Chapter IV, the high temperature points were in ~1% disagreement with previous measurements. It was therefore decided to exclude these data from analysis.

In examining the data for the (401)$^-$ peak, it is seen that a considerable discrepancy exists between the data of 4/28/73 and that of 5/5/73. By comparing the maximum intensity data with the peak height observed in the (401)$^-$ scan (Fig. 16), it is seen that the data of 5/5/73 is in disagreement. It is assumed that either the counter or the crystal was misset in the 5/5 experiment, and the excess in counts in the 5/5 experiment was taken to be due to scattering from the (401) central reflection. Since the (401) central reflection was observed to
have negligible temperature dependence, the data of 5/5 was corrected by subtracting 160 counts from each point to bring the 5/5 experiment into agreement with the data of 4/28.

Inspection of the central peak data in Table 14 shows that no clear temperature dependence is evident. The reason for this is that the polarization effect produces only a small temperature dependence in the ferromagnetic component of the peaks which is itself only a small part of the entire reflection. It was not possible to extract any information from the central reflections.

The data for the satellite reflections as presented in Chapter IV are plotted in Figs. 19 through 26. The error bars represent the statistical uncertainties in the total recorded and are normalized to $10^6$ monitor. Also shown in the plots are the least square fitted lines of the form

$$I_m = A + B |f_N|,$$

From equation (169), we see that the constants $A$ and $B$ have the interpretation

$$A = I_0 + I_{\pm\pm},$$

and

$$B = I_0 \alpha \chi$$

so that

$$\chi \alpha = \frac{B}{A - I_{\pm\pm}}.$$
Figure 19

Polarization Dependence of the (002)\textsuperscript{−} Reflection
Figure 20

Polarization Dependence of the (002)\(^+\) Reflection
Figure 21
Polarization Dependence of the (101)\textsuperscript{-} Reflection
Figure 22

Polarization Dependence of the (101)\(^+\) Reflection
Figure 23
Polarization Dependence of the (201)$^+$ Reflection
Figure 24
Polarization Dependence of the (300) reflection
Figure 25
Polarization Dependence of the (401)" Reflection
Figure 26
Polarization Dependence of the (401)$^+$ Reflection
Using the background measurements from Table 14 and the parameters $A$, $B$ and $X$ appropriate to a particular reflection, we can find $\alpha$. The results are presented in Table 17. The error limits were obtained by drawing limiting lines on the plots.

In order to determine the magnitude of the incoherent scattering length, it was decided to use the $(002)^z$ and $(101)^z$ reflections where the form factor is thought to be most accurate. The results are shown in Table 18. It is seen that the value of $|b_{inc}|$ deduced from the $(101)^+$ reflection disagrees somewhat from the others. We note at this point that, without the extinction correction, the values would be in gross disagreement with each other. We find, using all four reflections,

$$|b_{inc}| = 0.036 \pm 0.003 \times 10^{-12} \text{cm.} \quad (176)$$

Once $|b_{inc}|$ has been determined, the temperature dependence of $\text{Im}$ can be used to deduce the magnetic form factor. The results for the remaining satellite reflections are also shown in Table 19. It is seen that the form factor deduced in this way agrees within error limits with that determined using the standard technique, and that, except for the $(401)^-$ reflection, the form factor deduced here agrees with the theory.

The last piece of information to be extracted
<table>
<thead>
<tr>
<th>Peak</th>
<th>(I_{Bg}) Counts 10^6 Mon</th>
<th>A</th>
<th>B</th>
<th>(\chi)</th>
<th>(\alpha)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(002)^-</td>
<td>1514</td>
<td>91613</td>
<td>-8112</td>
<td>-.0900</td>
<td>-.1209</td>
</tr>
<tr>
<td>(002)^+</td>
<td>1434</td>
<td>74984</td>
<td>-7547</td>
<td>-.1026</td>
<td>-.1276</td>
</tr>
<tr>
<td>(101)^-</td>
<td>1522</td>
<td>52320</td>
<td>-5735</td>
<td>-.1129</td>
<td>-.1201</td>
</tr>
<tr>
<td>(101)^+</td>
<td>1701</td>
<td>48679</td>
<td>-6620</td>
<td>-.1409</td>
<td>-.1497</td>
</tr>
<tr>
<td>(201)^+</td>
<td>750</td>
<td>10971</td>
<td>-1783</td>
<td>-.1744</td>
<td>-.1744</td>
</tr>
<tr>
<td>(300)^-</td>
<td>437</td>
<td>4290</td>
<td>-994</td>
<td>-.2580</td>
<td>-.2580</td>
</tr>
<tr>
<td>(401)^-</td>
<td>368</td>
<td>1436</td>
<td>-235</td>
<td>-.2199</td>
<td>-.2199</td>
</tr>
<tr>
<td>(401)^+</td>
<td>379</td>
<td>1103</td>
<td>-274</td>
<td>-.3783</td>
<td>-.3783</td>
</tr>
</tbody>
</table>
TABLE 18

Determination of the Incoherent Scattering Amplitude

<table>
<thead>
<tr>
<th>Peak</th>
<th>$\alpha$</th>
<th>$p(K) \times 10^{-12}$ cm</th>
<th>$b_{inc} \times 10^{-12}$ cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>(002)$^-$</td>
<td>.1209</td>
<td>2.36</td>
<td>.081 ± .008</td>
</tr>
<tr>
<td>(002)$^+$</td>
<td>.1276</td>
<td>2.30</td>
<td>.084 ± .003</td>
</tr>
<tr>
<td>(101)$^-$</td>
<td>.1201</td>
<td>2.34</td>
<td>.080 ± .008</td>
</tr>
<tr>
<td>(101)$^+$</td>
<td>.1497</td>
<td>2.30</td>
<td>.098 ± .01</td>
</tr>
</tbody>
</table>
**TABLE 19**

Determination of the Holmium Magnetic Form Factor from Maximum Intensity Measurements

<table>
<thead>
<tr>
<th>Peak</th>
<th>( \alpha )</th>
<th>( f(K) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(002)(^-)</td>
<td>.1209</td>
<td>.94 ± .09</td>
</tr>
<tr>
<td>(002)(^+)</td>
<td>.1276</td>
<td>.89 ± .09</td>
</tr>
<tr>
<td>(101)(^-)</td>
<td>.1201</td>
<td>.95 ± .09</td>
</tr>
<tr>
<td>(101)(^+)</td>
<td>.1497</td>
<td>.76 ± .08</td>
</tr>
<tr>
<td>(201)(^+)</td>
<td>.1744</td>
<td>.65 ± .13</td>
</tr>
<tr>
<td>(300)(^-)</td>
<td>.2580</td>
<td>.44 ± .04</td>
</tr>
<tr>
<td>(401)(^-)</td>
<td>.2199</td>
<td>.52 ± .16</td>
</tr>
<tr>
<td>(401)(^+)</td>
<td>.3783</td>
<td>.30 ± .09</td>
</tr>
</tbody>
</table>
from this study is the sign of the incoherent scattering amplitude. We see that

\[ \frac{b_{inc}}{\rho(K)} f_N < 0 \]  

and we need only to determine the signs of \( \rho(K) \) and \( f_N \) to complete this task. The magnetic scattering amplitude \( \rho(K) \) is given by

\[ \rho(K) = \frac{\gamma e^2}{2m_0 c^2} \mathcal{H} f(K). \]  

Here all quantities are taken to be positive including the neutron gyromagnetic ratio \( \gamma \) and hence \( \rho(K) \) is positive. With this assignment of sign, the vector \( \mathbf{\hat{\gamma}} \) in equation (40) is taken to point along the angular momentum of an ion \( \mathbf{\hat{J}} \) and hence opposite to the atomic magnetic moment. The nuclear polarization was defined to be positive if \( \langle \mathbf{I} \rangle \) is parallel to \( \mathbf{\hat{\gamma}} \). Hence, \( f_N \) is positive if \( \overrightarrow{\mathbf{I}} \) tends to be parallel to \( \mathbf{\hat{J}} \) and is negative if \( \overrightarrow{\mathbf{I}} \) tends to be antiparallel to \( \mathbf{\hat{J}} \). The hyperfine Hamiltonian can be written to first approximation as

\[ \mathcal{H} = A \overrightarrow{\mathbf{I}} \cdot \mathbf{\hat{J}}. \]  

For holmium, \( A \) has been found to be positive implying that the lowest energy occurs when \( \overrightarrow{\mathbf{I}} \) and \( \mathbf{\hat{J}} \) are antiparallel. We therefore conclude that \( f_n \) is negative. Since \( \rho(K) \) is positive and \( f_N \) is negative, we find that \( b_{inc} \) is positive and

\[ b_{inc} = +0.086 \pm 0.003 \times 10^{-12} \text{ cm}. \]
The incoherent scattering cross section $\sigma_i$ can be calculated from $b_{ic}$ using equation (11) in Chapter I. We find
\[ \sigma_i = 0.371 \pm 0.06 \text{ barn}. \] (181)

The coherent scattering $\sigma_c$ of holmium has been measured by Koehler, Wollan and Wilkinson\textsuperscript{39} from powder diffraction studies of Ho$_2$O$_3$ at room temperature. They find
\[ \sigma_c = 9.1 \pm 0.5 \text{ barn}. \] (182)

Using this value of $\sigma_c$, we calculate the total nuclear scattering cross section $\sigma_s$ to be
\[ \sigma_s = 9.5 \pm 1.5 \text{ barn}. \] (183)

For most naturally occurring elements, the total nuclear scattering cross section is known. However, for holmium, the large paramagnetic scattering and absorption cross section ($\sigma_{pm}$ and $\sigma_a$) make an accurate determination of $\sigma_s$ difficult using standard techniques. There have been two attempts to deduce a value of $\sigma_s$.

Koehler et. al.\textsuperscript{39} used their measure of $\sigma_{pm} = 11$ barn at neutron energy .055 ev to deduce a value of $\sigma_{pm} \approx 1$ barn at .5 ev. They then subtracted this value from the ionic scattering cross section $\sigma_{pm} + \sigma_s = 14$ barn deduced by Bernstein et. al.\textsuperscript{40} at .5 ev to obtain $\sigma_s = 13$ barn. Bernstein's original measurement was of the total ionic cross section $\sigma_I$ including absorption. In obtaining the ionic scattering cross section of 14 barn,
Bernstein assumes that $\sigma_0 = 14$ barn and subtracts $\sigma_0 = 14$ barn from $\sigma_T = 28$ barns to obtain $\sigma_T - \sigma_0$. However, the .5 ev $\sigma_T$ measurement appears to be somewhat high (2-3 barn) relative to the smooth variation observed at lower energies and may be in question by a few barns. It seems clear that the value of $\sigma_T = 13$ barn is not to be taken as being reliable, at least in terms of obtaining $\sigma_T$.

Another estimate of $\sigma_T$ was made by Schermer who measured the transmission of polarized neutrons through holmium samples with polarized nuclei. The quantity obtained was the nuclear polarization dependent portion of the total nuclear cross section $\sigma_{pT}$ where

$$\sigma_{pT} = \frac{I}{2I+1} \left( \sigma_{T+} - \sigma_{T-} \right) \quad (184)$$

and

$$\sigma_{T+} = \sigma_{a+} + 4\pi b_+^2 \quad (185)$$

$$\sigma_{T-} = \sigma_{a-} + 4\pi b_-^2.$$  

He writes

$$\sigma_{pT} = \sigma_{ps} + \sigma_{pa} \quad (186)$$

where

$$\sigma_{ps} = 4\pi b_+^2 - 4\pi b_-^2 \quad (187)$$

is the polarization dependent portion of the nuclear scattering cross section and $\sigma_{pa}$ is the polarization dependent portion of the absorption cross section. Schermer measured $\sigma_{pT}$ at neutron energies of .064 ev, .161 ev and .789 ev for a single crystal sample of holmium, and was
therefore able to deduce the energy dependence of $\sigma_{\text{RT}}$. Then, assuming a $\frac{1}{\nu}$ dependence to $\sigma_{\text{PA}}$, Schermer was able to extract $\sigma_{\text{PA}}$. He then measured $\sigma_{\text{RT}}$ at .789 ev on a polycrystalline sample of holmium and took the difference $\sigma_{\text{RT}} - \sigma_{\text{PA}}$ to obtain

$$\sigma_{\text{PS}} \approx -1 \text{ barn.}$$

Using this result we calculate

$$b_{\text{inc}} = -0.026 \times 10^{12} \text{ cm}$$

$$\sigma_i = 0.03 \text{ barn}$$

and

$$\sigma_s = \sigma_{\text{PS}}.$$ (191)

In Schermer's measurement on the polycrystalline sample, multiplicative corrections had to be made for the neutron beam depolarization effect and for the fact that the nuclear polarization in individual crystallites does not lie along the direction of the polarizing field. The approximate nature of these corrections, in view of the small value of $\sigma_{\text{PS}}$, makes this estimate also unreliable, both in sign and magnitude.

Schermer made a further attempt to estimate $\sigma_s$ directly by measuring $\sigma_{\text{RT}}$ over a range of energies and by subtracting $\sigma_{\text{PA}}$ from $\sigma_{\text{RT}}$ to obtain $\sigma_s + \sigma_{\text{PA}}$ as a function of $\frac{1}{\nu}$. By extrapolating to $\frac{1}{\nu} = 0$, he estimated

$$\sigma_s < 10 \text{ barn}$$

which is in agreement with our result.
We see, then, that the estimates of Koehler et al. and Schermer do not provide accurate values for comparison with our data. The measurement we report is the only one which provides a direct observation of the incoherent scattering amplitude or cross section.

As discussed in Chapter I, the sign of \( b_{inc} \) can be used to select the pair of scattering amplitudes \( b_+ \) and \( b_- \) associated with the two compound neutron-nucleus scattering states. The coherent scattering amplitude is given by

\[
b_{coh} = \frac{I+\frac{1}{2}}{2I+1} b_+ + \frac{I-\frac{1}{2}}{2I+1} b_-
\]

and the incoherent scattering amplitude is given by

\[
b_{inc} = \frac{2}{2I+1} (b_+-b_-)
\]

so that

\[
b_+ = b_{coh} + \frac{I}{2} b_{inc}
\]

and

\[
b_- = b_{coh} - \frac{I}{2} b_{inc}.
\]

Using Koehler's value of \( b_{coh} = 0.85 \pm 0.02 \times 10^{-12} \text{cm} \), we find

\[
b_+ = 1.00 \pm 0.04 \times 10^{-12} \text{cm}
\]

and

\[
b_- = 0.66 \pm 0.04 \times 10^{-12} \text{cm}.
\]

We see then that the two amplitudes \( b_+ \) and \( b_- \) are nearly equal with the \( I+\frac{1}{2} \) state contributing slightly more to the scattering than the \( I-\frac{1}{2} \) state. The positive signs on \( b_+ \) and \( b_- \) imply that the scattering is potential scattering with a phase change of 180° as opposed to reso-
nance scattering.

At this point, we should discuss the affect the choice of hyperfine constants has on our results. As described in Chapter III, there is a range of hyperfine constants available in the literature, some calculated, some obtained in resonance experiments, some obtained in specific heat measurements, and some from polarized neutron transmission measurements. In Table 20 we present the nuclear polarization at several temperatures as calculated using various values for the hyperfine constants. It is seen that the differences resulting from the various choices of parameters amounts to $\sim 0.01$. Taken over the range of $f_N$ covered in this experiment ($\sim 0.6$) we have at most errors of 2%, considerably less than the experimental errors involved.

V.3. Summary and Conclusion

The results of this study can be divided into three areas: we have verified the magnetic structures for metallic holmium; we have measured the magnetic form factor, extending the measurements to higher scattering angles than previously measured; and we have determined the sign and magnitude of the holmium nuclear scattering amplitudes, $b_+ \text{ and } b_-$.

We find generally good agreement with the holmium magnetic structures proposed by Koehler et. al.
TABLE 20

The Effect of the Holmium Hyperfine Constants on the Nuclear Polarization

<table>
<thead>
<tr>
<th>T (K)</th>
<th>$f_{N, \alpha'=.290}$ P=0</th>
<th>$f_{N, \alpha'=.320}$ P=.007</th>
<th>$f_{N, \alpha'=.319}$ P=.0074</th>
<th>$f_{N, \alpha'=.300}$ P=0</th>
</tr>
</thead>
<tbody>
<tr>
<td>.3</td>
<td>.826</td>
<td>.828</td>
<td>.837</td>
<td>.834</td>
</tr>
<tr>
<td>.4</td>
<td>.739</td>
<td>.748</td>
<td>.757</td>
<td>.750</td>
</tr>
<tr>
<td>.5</td>
<td>.659</td>
<td>.674</td>
<td>.682</td>
<td>.671</td>
</tr>
<tr>
<td>.6</td>
<td>.589</td>
<td>.609</td>
<td>.615</td>
<td>.602</td>
</tr>
<tr>
<td>.7</td>
<td>.530</td>
<td>.552</td>
<td>.557</td>
<td>.543</td>
</tr>
<tr>
<td>.8</td>
<td>.479</td>
<td>.503</td>
<td>.507</td>
<td>.492</td>
</tr>
<tr>
<td>.9</td>
<td>.436</td>
<td>.460</td>
<td>.464</td>
<td>.448</td>
</tr>
<tr>
<td>1.0</td>
<td>.400</td>
<td>.424</td>
<td>.427</td>
<td>.411</td>
</tr>
<tr>
<td>1.5</td>
<td>.279</td>
<td>.300</td>
<td>.301</td>
<td>.288</td>
</tr>
<tr>
<td>2.0</td>
<td>.213</td>
<td>.231</td>
<td>.231</td>
<td>.220</td>
</tr>
<tr>
<td>2.5</td>
<td>.172</td>
<td>.187</td>
<td>.187</td>
<td>.177</td>
</tr>
<tr>
<td>3.0</td>
<td>.144</td>
<td>.157</td>
<td>.157</td>
<td>.148</td>
</tr>
<tr>
<td>3.5</td>
<td>.123</td>
<td>.135</td>
<td>.135</td>
<td>.128</td>
</tr>
<tr>
<td>4.0</td>
<td>.108</td>
<td>.118</td>
<td>.118</td>
<td>.112</td>
</tr>
</tbody>
</table>
The only point of disagreement is in the determination of the bunching parameter $\xi$ where we find

$$\xi = 8.3 \pm 2^\circ$$  \hspace{1cm} (199)

in contrast with Koehler's value of

$$\xi = 5.8^\circ.$$  \hspace{1cm} (200)

Since $\xi=0$ represents complete bunching, it is seen that our measurement suggests lesser magnetic anisotropy than does Koehler.

The metallic holmium form factor as deduced in our measurements is seen to agree quite well with the theory of the $\text{Ho}^{++}$ ion out to $\frac{K}{4\pi} = 0.5 \text{Å}^{-1}$. We find possible disagreement for $\frac{K}{4\pi} > 0.6 \text{Å}^{-1}$ but resolution problems limit the quantitative interpretation of this measurement. The total magnetic moment of the holmium ions was found to be

$$\mathcal{M} = 9.7 \pm 2 \text{M}_\beta$$  \hspace{1cm} (201)

and at 77 K, the effective moment was found to be

$$\mathcal{M} = 7.03 \pm 0.7 \text{M}_\beta.$$  \hspace{1cm} (202)

The incoherent scattering amplitude was deduced to be

$$b_{\text{inc}} = +0.026 \pm 0.008 \times 10^{-12} \text{cm}$$  \hspace{1cm} (203)

yielding a total scattering cross section for the holmium nucleus of

$$\sigma_\text{c} = 9.5 \text{ barns.}.$$  \hspace{1cm} (204)
APPENDIX A

BEAM CHARACTERISTICS AND PEAK SHAPE

It is well known that the neutron beams used in neutron diffraction are not ideal. Sizeable wavelength spreads and angular divergences exist in all experimental arrangements. These distributions, along with the mosaic block distributions in crystals, produce a broadening of diffraction peaks. Two models of this effect are presented here.

If one assumes that there is no correlation between the wavelength and the angular divergence of a neutron in the beam incident to the crystal, particularly simple relations result. We assume that the wavelength and angular distributions can be approximated by gaussians.

\[ P_\lambda = e^{-\frac{\lambda^2}{\alpha^2}} \]
\[ P_\delta = e^{-\frac{\delta^2}{\sigma^2}} \quad (A-1) \]

where

\[ \alpha = \frac{\lambda - \lambda_0}{\lambda} \]

Here \( \lambda_0 \) is the mean neutron wavelength and \( \delta \) is the angular divergence of a neutron with respect to the beam center.
line. $\lambda$ and $\eta$ are measures of the degree of divergence of $\lambda$ and $\delta$ from $\lambda$ and $\delta = 0$. We also approximate the distribution of mosaic blocks in the crystal as a gaussian

$$P_\alpha = e^{-\frac{\Delta^2}{2\eta^2}} \quad (A-2)$$

where $\Delta$ is the orientation of a mosaic block with respect to the mean position and the mosaic spread parameter $\eta$ is a measure of the width of the distribution. We assume that the counter aperture is sufficiently wide to admit all neutrons scattered from the crystal. We denote the crystal angular position as $\phi$ and the crystal position for reflecting $\lambda^*\phi_0$, $\delta = 0$ neutrons from the $\Delta = 0$ mosaic blocks as $\phi_0$. The quantity we wish to obtain is the number of neutrons scattered at each crystal position $P(\phi - \phi_0)$.

The probability that a neutron is scattered at crystal angle $\phi - \phi_0$ is the summation over all $\delta$, $\alpha$ and $\Delta$ of the product of the probability of the neutron having parameters $\delta$, $\alpha$, and $\Delta$, the probability that the crystal has a mosaic block with orientation $\Delta$ and the probability that the combination $(\alpha, \lambda, \delta, \phi - \phi_0)$ will produce a Bragg reflection. We then have

$$P(\phi - \phi_0) = \int d\alpha \int d\delta \int d\phi_0 \ e^{-\frac{\Delta^2}{2\eta^2}} e^{-\frac{\delta^2}{2\eta^2}} e^{-\frac{\phi_0^2}{2\eta^2}} P(\alpha, \lambda, \delta, \phi - \phi_0). \quad (A-3)$$

In order to determine $P(\phi, \lambda, \delta, \phi - \phi_0)$ it is useful to construct a diagram of the reflection process.
Here angles are defined to be positive if the glancing angle of the neutron on the reflecting plane is increased by increasing the magnitude of the angle. We see that

$$\gamma + \theta_0 + \phi - \phi_0 + \Delta = \theta_0$$

or

$$\theta_0 - \theta_0 = \gamma + \Delta + \phi - \phi_0$$

where $\theta_0$ is the Bragg angle for $\alpha = 0$ neutrons and $\theta_\alpha$ is the Bragg angle for neutrons with wavelength coordinate $\alpha$. Using the Bragg condition we have

$$\theta_\alpha - \theta_0 = \Delta \theta = \frac{\Delta \lambda}{\lambda \cos \theta_0} = \frac{\Delta \lambda}{\lambda} \tan \theta_0$$

or

$$\theta_\alpha - \theta_0 = a \tan \theta_0 \quad (A-4)$$

Then $P(\alpha, \gamma, \phi, \phi_0)$ can be written

$$P(\alpha, \gamma, \phi, \phi_0) = \delta \left( \alpha \tan \theta_0 - \gamma - \Delta - (\phi_0 - \phi) \right) \quad (A-5)$$

We can now evaluate $P(\phi - \phi_0)$. The integrations in equa-
tion (A-3) are straightforward and yield the result that
\[ P(\phi - \phi_0) = e^{-\frac{(\phi - \phi_0)^2}{2\sigma^2_{\phi_0}}} \]  \hspace{1cm} (A-6)

where
\[ \gamma_{\text{eff}}^2 = \gamma_c^2 + \gamma_0^2 + \Lambda^2 \tan^2 \rho_0 \]  \hspace{1cm} (A-7)

and we have neglected a constant factor in \( P(\phi - \phi_0) \). We see then that, in this model, diffraction peaks have a gaussian shape whose widths are determined by the crystal mosaic distribution and the quality of the incident neutron beam. We further see that this model predicts that the width of diffraction peaks increases with the square of the tangent of the Bragg angle. In Fig. 27 a plot of the square of experimentally measured holmium peak widths against \( \tan^2 \theta_0 \) is shown. It is seen that remarkable agreement with the prediction of equation (A-7) is found for \( \theta_0 \approx 10^\circ (\tan^2 \theta_0, 0^4) \). Similar results have been found for CoO diffraction peaks.

The major problem with this result is that it neglects the correlation between \( \alpha \) and \( \delta \) for neutrons in the incident beam. This correlation produces the so-called "focussing-defocussing effect" in which diffraction peaks are sharper for \( \theta > 0 \) than for \( \theta < 0 \). (Here \( \theta > 0 \) means the diffracted beam tends to be parallel to the beam incident to the monochromator.) The reason for the good agreement of the measurements with the first theory is that the monochromator Bragg angle was...
Figure 27

The Variation of the Peak Width with Bragg Angle
quite small ~10° for the studies involved here. This point becomes clearer after a more precise treatment of the problem.

In principle it should be possible to exactly describe the diffraction peak shape given only the dimensions of the collimating tubes and the mosaic properties of the monochromator and diffraction crystals. The essential problem is to obtain a distribution function $\rho_{\alpha \delta}$ describing the neutron beam incident to the diffraction crystal. Once that is accomplished, we can use the analysis presented above and write

$$p(\phi - \phi_0) = \int \int \int \rho_{\alpha \delta}(\alpha, \theta_0, \delta, \phi, S) \delta(\alpha \tan \theta_0 - \delta - (\phi - \phi_0)) \, \, (A-3)$$

The first step in obtaining $\rho_{\alpha \delta}$ is to describe the neutron beam incident to the monochromator. We assume that all wavelengths in the range passed by the monochromator are present with equal probability. We assume that the collimation is provided by a single tube of length $L$ and diameter $D$. The effects of such a collimator are to restrict the angular divergence $\alpha$ of neutrons striking the crystal and to restrict the area of the monochromator which is bathed in radiation. We can describe the distribution of neutrons striking the monochromator as

$$p_{\text{mon}} = p_\alpha(\alpha) \, \rho_\alpha. \, \, \, (A-9)$$

Here $p_\alpha(\alpha)$ represents the angular distribution of neutrons striking the monochromator at position $\alpha$ and $\rho_\alpha$ is the
probability that point $x$ is bathed in radiation. Here we should note that we need only consider coordinates in the plane of reflection. All geometrical coordinates are taken to be positive if increasing the magnitude of the coordinate increases the glancing angle of neutrons on the Bragg reflection plane.

Having described the neutron distribution incident to the monochromator, we now seek to describe the neutron distribution after reflection by the monochromator. For simplicity, we consider that the monochromator is a thin slab so that neutrons at a point in the reflected beam come from a single corresponding point in the incident beam. We can then describe the position of neutrons in the reflected beam by $y = y(x)$. The distribution $p_x$ then transforms to $p_y$. We write the distribution of the mosaic blocks in the monochromator as $p_{\Delta_m}$. The probability of having a neutron at position $y$ with angular coordinate $\delta$ and wavelength $\alpha$ is the summation over all $\Delta_m$ and $\alpha$ of the products of the probability that a neutron has coordinates $x$, $\alpha$ and $\delta$, the probability that the monochromator has a mosaic block at orientation $\Delta_m$, and the probability that the combination $(\alpha, \Delta_m, \delta)$ will produce a Bragg reflection. To determine the Bragg reflection restrictions, we construct a diagram of the reflection.
We see that
\[ \theta = \theta_m + \alpha \]
\[ \theta + \theta_m = \theta_m + \delta \]
or
\[ \delta_m = \delta - \alpha \tan \theta_m \]
\[ \alpha = \frac{\delta}{\tan \theta_m} \]

and we have
\[ P_{\alpha \delta}(y) = S d\alpha S d\delta_m P_{\alpha m} P_{\delta m} P_{\alpha m} P_{\alpha \delta}(y = \delta_m - \delta - \alpha \tan \theta_m) \]
\[ = P_{\alpha \delta}(y) \sum_{\alpha = \delta / \tan \theta_m} \delta_m = \delta - \alpha \tan \theta_m \]

We now seek to find the distribution of neutrons incident to the diffraction crystal. We assume that a tube of length \( \ell \) and diameter \( d \) connects the monochromator crystal with the diffraction crystal. We further assume that the diffraction crystal is small so that, even with a beam aperture, the crystal is exposed to radiation from all parts of the monochromator. Under this assumption, not all neutrons at the monochromator will strike the crystal. We let \( p_{\alpha \delta} \) represent the probability that a neutron at \((y, \delta)\) strikes the crystal. The distribution of neutrons
striking the crystal is then

\[ P_{a\delta} = \int dy \: P_{a\delta} \: P_{\odot m} \: P_{\alpha(y)} \: P_y \: \xi^{2-2\alpha\tan\theta_m} \]  \hspace{1cm} (A-12)

and

\[ P(\psi-\theta_o) = \int d\phi \: d\xi \: d\alpha \: P_{\alpha\delta} \: \xi^{2\alpha\tan\theta_o} \xi^{2}(\psi-\theta_o) \]  \hspace{1cm} (A-13)

All that remains is to insert appropriate functional forms for the various distributions in equation (A-12). For ease in analytical computation, we define \( P_{\odot m}, P_{\alpha(y)}, P_y \) and \( P_\alpha \) to be gaussian

\[ P_\alpha(x) = e^{-\frac{(x-x_0)^2}{2\sigma_\alpha^2}} \]  \hspace{1cm} (A-14)

\[ P_{\odot m} = e^{-\frac{\theta_m^2}{2\sigma_{\odot m}^2}} \]

\[ P_y = e^{-\frac{y^2}{2\sigma_y^2}} \]

\[ P_\alpha = e^{-\frac{\alpha^2}{2\sigma_\alpha^2}} \]

The quantity \( x_0(y) \) in \( P_\alpha(x) \) represents the center of the angular distribution of neutrons incident to the monochromator at point \( x \). We see that

\[ \tan x_0 \approx \theta_o = \frac{x}{L} \]  \hspace{1cm} (A-15)

For the function \( P_{\alpha(y)} \), we use a small crystal limit where only neutrons with a particular \( s=s_0 \) at each point \( y \) at the monochromator can hit the crystal. Geometrical considerations yield

\[ \tan s_0 \approx s_0 = \frac{y}{2} \]  \hspace{1cm} (A-16)

and we have

\[ P_{s_0} = s(y - e \xi) \]  \hspace{1cm} (A-17)

We need, at this point, to obtain the transformation between \( y \) and \( x \). There are two limiting cases for
a thin slab monochromator. If the monochromator is cut and oriented in the reflecting mode, then \( \gamma = -\gamma \) and if the monochromator is cut and oriented in the transmission mode, then \( \gamma = \gamma \).

We find

\[
P_{a \gamma} = e^{-\frac{\xi^2}{2 \eta^2}} e^{\frac{(\xi - a \tan \theta_m)^2}{2 \eta^2}} e^{\frac{(2 a \tan \theta_m - 5 \xi - \eta)^2}{2 \eta^2}} \tag{A-17}
\]

where

\[
\eta \equiv \eta_n \gamma \tag{A-14}
\]

and the - sign in the last term applies for a transmission monochromator and the + sign applies for a reflection monochromator. If \( \zeta = \lambda \) we find for the transmission case

\[
P_{a \gamma t} = e^{-\frac{\xi^2}{2 \eta^2}} e^{\frac{(\xi - a \tan \theta_m)^2}{2 \eta^2}} e^{\frac{(2 a \tan \theta_m - 5 \xi - \eta)^2}{2 \eta^2}} \tag{A-19}
\]

where

\[
\eta^2 = \frac{(\eta_u^2 \eta_m^2}{\eta_m^2 + (\eta_u^2 \xi^2)} \tag{A-20}
\]

For the reflection case

\[
P_{a \gamma r} = e^{-\frac{\xi^2}{2 \eta^2}} e^{\frac{(\xi - a \tan \theta_m)^2}{2 \eta^2}} e^{\frac{(2 \tan \theta_m - 5 \xi - \eta)^2}{2 \eta^2}} \tag{A-21}
\]

We note that the reflection monochromator provides a finer
beam than the transmission monochromator. The reason for this is that the reflection monochromator tends to give larger angular divergences to neutrons with large wavelength divergences so that these neutrons do not strike the crystal, while the transmission monochromator tends to focus these neutrons. The transmission monochromator then provides a more intense beam of somewhat poorer quality than the reflection monochromator.

The evaluation of the integrals in equation (A-3) can be straightforwardly carried out. Both cases yield the result that

\[ P(\phi - \phi_0) = e^{-\frac{(\phi - \phi_0)^2}{2\sigma_k^2}} \]  

(A-22)

In the course of the integration, it is useful to introduce the parameter

\[ \kappa = \frac{\tan \theta_0}{\tan \theta_m} \]  

(A-23)

With this definition, we can express \( \eta_{\text{eff}}^2 \) for both cases as

\[ \eta_{\text{eff}}^2 = A + B \kappa^2 + C(\kappa - 1)^2 \]  

(A-24)

For the transmission monochromator

\[ \eta_{\text{eff}}^2 = \eta_c^2 + \eta_t^2 \kappa^2 + \eta_s^2 (\kappa - 1)^2 \]  

(A-25)

and for the reflection monochromator

\[ \eta_{\text{eff}}^2 = \eta_c^2 + \frac{\eta_t^2 \eta_m^2}{(\kappa)^2 \eta_s^2 + \eta_s^2 (\kappa - 1)^2} \]

(A-26)

We note that for \( \eta_a \to \infty \) the two expressions become identical as required by equations (A-19) and (A-21). We also note that

\[ \eta_{\text{ess}}^2 (\kappa) \neq \eta_{\text{eff}}^2 (-\kappa) \]
and that there is a distinct asymmetry between the two crystal reflection orientations \((\pm \theta)\). This is the well known focus-defocus effect. The sharpest peaks occur when \(\eta \eta = \) is minimum. This is easily seen to be when
\[
\kappa = \frac{c}{b+c} \equiv \kappa_{\min}.
\]  

Our model then predicts \(\kappa_{\min} = \) \(\leq 1\). This is in disagreement with the result of Willis who finds \(\kappa_{\min} \geq 1\). It is thought that our analysis provides a somewhat more general treatment of the problem. No tests have been made to check the two models.

As a final note, we see that for \(\kappa \gg 1\), we have
\[
\eta \eta = A + (b+c) \kappa^2
\]

in agreement with the peak widths observed for holmium and CoO.
APPENDIX B

EXTINCTION - ABSORPTION CORRECTION FACTORS

As described in Chapter III, the numerical technique of Hamilton\textsuperscript{34} was applied to the calculation of extinction-absorption coefficients for use in this study. The basic algorithm comes from the differential equations given in Chapter III

\[
\frac{\partial \rho_i}{\partial l_i} = -(\sigma + \mu_a) \rho_i + \sigma \rho_r
\]

\[
\frac{\partial \rho_r}{\partial l_r} = -(\sigma + \mu_a) \rho_r + \sigma \rho_i
\]

where \( \rho_i \) and \( \rho_r \) are the neutron fluxes in the incident and reflected beams, \( dl_i \) and \( dl_r \) are length increments along the two beams, \( \mu_a \) is the affective linear absorption coefficient and \( \sigma \) is the linear reflectivity of the peak, is defined by

\[
\sigma = Q \ W(\Delta)
\]

where \( Q \) is the Q factor of the reflection and \( W(\Delta) \) is the distribution function of the mosaic blocks in the crystal.

The procedure in analytically solving for the observed integrated intensity would be to solve equations (B-1) for \( \rho_r(\Delta) \) at the exit side of the crystal as a function of \( \Delta \). The total integrated intensity \( \rho \) would then be
The integrated intensity in the absence of extinction and absorption would be
\[ P_0 = I_0 \mathcal{Q} V \]  
(3-4)

where \( I_0 \) is the incident beam flux and \( V \) is the crystal volume. The extinction-absorption coefficient is then
\[ \mathcal{E}A = \frac{P}{I_0 \mathcal{Q} V} \]  
(3-5)

The analytic solution for \( f_r(\hat{r},\hat{n}) \) has only been found for simplified geometries. The technique developed by Hamilton\(^{34}\) is to numerically determine \( f_r(\hat{r},\hat{n}) \) at the exit surface. In this technique, the neutron beams are followed through the crystal, each being altered according to the prescription provided by the differential equation. To this end, the crystal is subdivided into small parallelepipeds whose three edges are parallel to the incident beam \( \hat{e}_m \), the diffracted beam \( \hat{e}_n \) and the perpendicular to the beam plane \( \hat{e}_s \). The lengths of the edges of a single block are \( \delta e_i \), \( \delta e_r \) and \( \delta e_s \) respectively. We index the blocks by \((m,n,s)\) where the position of the \((m,n,s)\) block is given by
\[ \hat{r}_{mns} = m \delta e_i \hat{e}_m + n \delta e_r \hat{e}_n + s \delta e_s \hat{e}_s \]  
(3-6)

We can write the differential equations in differential form
Here we note that the quantities \( \rho_i \) and \( \rho_r \) represent neutron current densities. In following the beams through the crystal, we need to consider neutron currents rather than current densities. If \( \rho_i \) represents the current density in the incident neutron beam incident on a particular block, then we can write the corresponding neutron current as

\[
\rho_i A_i = \rho_i \Delta s \Delta \ell_i \sin \theta
\]

where \( \theta \) is the Bragg angle of the reflection and \( \omega \) is the angle between \( \hat{e}_m \) and \( \hat{e}_n \). The neutron current in the reflected beam becomes

\[
\rho_r A_i = \rho_r \Delta s \Delta \ell_i \sin \theta.
\]

At this point it becomes convenient to define quantities \( \Delta m \) and \( \Delta n \) where

\[
\Delta m = \Delta \ell_i \sin \theta
\]
\[
\Delta n = \Delta \ell_r \sin \theta
\]

We can now use the difference equations (B-7) to write the neutron currents in the diffracted and incident beams which strike a particular block \((m,n,s)\) in terms of the currents incident to earlier blocks. We have

\[
\rho_i(m,n,s) \Delta s \Delta n = \rho_i(m-1,n,s) \Delta n \Delta s (1-(\sigma+\omega)\Delta \ell_i) + \rho_r(m-1,n,s) \Delta m \Delta s \sigma \Delta \ell_r
\]
In terms of neutron fluxes we have
\[ P_r(m,n,s) \Delta s \Delta m = P_r(m,n-1,s) \Delta m \Delta s \left( 1 - (\sigma + \partial \alpha) \right) \Delta \xi_r + P_\alpha(m,n-1,s) \Delta n \Delta s \sigma \Delta \xi_\alpha. \]

Equations (13-9) are the difference equations introduced by Hamilton.\(^{34}\) We see that by starting at blocks where \( P_\alpha \) and \( P_r \) are determined by the initial conditions \( P_\alpha = \ln \) and \( P_r = \ln \) we can iterate through the crystal in a systematic way and calculate \( P_\alpha \) and \( P_r \) at all points in the crystal. In the iteration process, each layer (constant \( s \)) is treated independently. We iterate along rows of constant \( m \). The first block in the row is denoted by \( \eta_\alpha(m) \) and the last block by \( \eta_\alpha(m) \). The values of \( \eta_\alpha \) and \( \eta_\sigma \) are determined by the crystal and reflection geometries. It can be seen that one need only retain the \( P_\alpha \) and \( P_r \) values for one row. This provides for a considerable savings in computer storage. When this is done it is necessary to accumulate \( \sum P_r(\eta_\sigma) \) as each row is completed.

The accumulated \( \sum P_r(\eta_\sigma) \) is a numerical approximation to the total diffracted neutron current. There is a dependence on \( \Delta \) through \( \sigma \). The integrated intensity \( \bar{P} \) is obtained by calculating \( \sum P_r(\eta_\sigma) \) for values of \( \Delta \) and numerically integrating to obtain
\[ P = \sum_{\Delta} \left( \varepsilon \rho (n_0) \Delta \right) \]  

(3-10)

and the extinction-absorption coefficient is

\[ \varepsilon \rho = \frac{P}{\varepsilon} \Delta \sqrt{\varepsilon} \]  

(3-11)

as before.

A considerable savings in computer time is realized if \( W(\Delta) \) is approximated by

\[ W(\Delta) = \frac{1}{2} \eta \]  

\[ |\Delta| < \sqrt{3} \eta \]  

(3-12)

\[ W(\Delta) = 0 \]  

\[ |\Delta| > \sqrt{3} \eta \]  

The factors \( 2 \sqrt{3} \) are chosen so that the standard deviation of this square distribution is the same as that of a gaussian distribution

\[ W(\Delta) = \frac{1}{2 \eta} e^{-\frac{\Delta^2}{2 \eta^2}} \]  

(3-13)

With this square approximation, we write

\[ P = \sum_{\Delta} \rho (n_0) \Delta \sqrt{3} \eta \]  

(3-14)

and

\[ \bar{\rho} = \frac{P}{2 \sqrt{3} \eta} \]  

(3-15)

so

\[ \varepsilon \bar{\rho} = \frac{\varepsilon \rho (n_0)}{I_0 \sqrt{\varepsilon}} \]  

(3-16)

We have written several computer programs to calculate extinction-absorption coefficients for this and other studies. The statement listing for the program used for this study is given at the end of this appendix. In all
of these programs there are two parts: a geometrical part where $n_A(m,s)$ and $n_A(m,s)$ are determined; and a part where the iteration over the crystal is carried out. In this particular program, the geometrical analysis is carried out in a brute force manner where specific formulae for $n_A$ and $n_3$ are obtained. In this approach it is necessary to have different equations for four classes of different reflection geometries. An inspection of the statement listing shows that the geometrical portion constitutes the larger part of the program. The iterative process is contained primarily in the last 40 statements of the program. Special consideration is given to the boundary points, in that some face the incident beam and some do not and some are exit points of the diffracted beam and others are not. In the programs it was found that small errors resulting from a finite grid size could be minimized by using a grid of $N \times N \times N$ and one of $2N \times 2N \times 2N$ and extrapolating

$$E_A = E_A(2N) + (E_A(2N) - E_A(N)).$$

(β-17)

In calculating extinction-absorption coefficients for this and other studies, it was noted that the geometry of the reflection is very important in determining $E_A$. This is illustrated in Figure 28 where we have calculated $E_A$ coefficients for reflections of $\Theta = 10.3$ and $\Theta = 32.3$ as a function of the angle that the incident beam makes with the cylinder axis ($\alpha$). The Q values used were
Figure 28
The Effect of the Reflection Geometry on the Extinction Absorption Coefficient
$10^4 \times 10^4 \text{ cm}^{-1}$ and $4.22 \times 10^4 \text{ cm}^{-1}$. These values of $Q$ correspond to those of the $(002)$ and $(300)^*$ reflections at 4.2 K. In the calculations, $\chi = 1.32 \text{ cm}^{-1}$ and $\eta = 12\degree$ were used. Sharp minima in $E$ are observed for values of $\alpha = 90\degree$ and $\alpha = 90\degree + 2\theta$. At these angles, either the incident or the diffracted beam is parallel with the cylinder face. Smaller cusps are also found for $\alpha = 0\degree$ and $\alpha = 2\theta$ when either the incident or diffracted beams are parallel to the cylinder axis. If one is calculating an $E$ coefficient for a reflection near a sharp cusp, it is particularly important to have the geometries accurate.
Extinction Absorption Program
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<thead>
<tr>
<th>Page</th>
<th>Text</th>
</tr>
</thead>
<tbody>
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<td>IT = 2, PP = AL, T = 0</td>
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<tr>
<td>102</td>
<td>IT = 2, PP = AL, T = 0</td>
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<tr>
<td>104</td>
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</tr>
<tr>
<td>105</td>
<td>IT = 2, PP = AL, T = 0</td>
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</tbody>
</table>

Note: The text appears to be a programming or algorithmic code, but the specific meaning is not clear without additional context.
<table>
<thead>
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<th>Line</th>
<th>Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
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</tr>
<tr>
<td></td>
<td>j = 2</td>
<td></td>
</tr>
<tr>
<td>211</td>
<td>IF(I = 2) GOTO 221</td>
<td></td>
</tr>
<tr>
<td>211</td>
<td>IF(I = 3) GOTO 221</td>
<td></td>
</tr>
<tr>
<td>211</td>
<td>IF(I = 4) GOTO 221</td>
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<td>212</td>
<td>GOTO 213</td>
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<td>213</td>
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<td></td>
</tr>
<tr>
<td>221</td>
<td>GOTO 222</td>
<td></td>
</tr>
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<td>222</td>
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<td>GOTO 224</td>
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</tr>
<tr>
<td>224</td>
<td>GOTO 226</td>
<td></td>
</tr>
</tbody>
</table>
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APPENDIX C

THE COINCIDENT REFLECTION

We have seen in Chapter III that the observed intensity of a given reflection can be affected by the presence of a simultaneous or coincident reflection. In this appendix, a few brief comments on the problem are presented and the statement listing of the computer program used to determine the presence of coincidence is given.

In the simplest case of coincident reflection, there are three processes, the primary reflection, the coincident reflection and the crossover reflection as described in Chapter III. If the coincident reflection is strong the observed primary reflection can be reduced in intensity. In order for this to occur, it is necessary that, at a particular crystal orientation, the same neutrons (wavelength and angular coordinates) be scattered by the primary and the coincident reflection. This implies that the primary and the coincident reciprocal lattice points be within the crystal mosaic spread parameter of the Ewald sphere. If, at a given point in the primary reflection scan, the coincident reflection scatters
neutrons which cannot, at that point, scatter from the primary reflection, then there is no effect on the primary intensity.

If the primary reflection is weak and the crossover reflection strong, the observed primary reflection can be enhanced. In order for this effect to occur and not be detected as a spurious peak, it is only necessary for the coincident reflection to come in tune at some point in the primary reflection scan. In other words, an effect can be seen if the coincident reflection is as close as the primary peak width to the Ewald sphere.

The similarity of the coincidence processes to extinction processes suggest that similar techniques could be used to calculate the effect of a coincidence. In fact, we can write similar equations to equations (B-1).

\[
\frac{\partial P_k}{\partial E_k} = -(\sigma_1 + \sigma_2 + \mu_a) P_k + \sigma_1 P_r + \sigma_2 P_s
\]

\[
\frac{\partial P_r}{\partial E_r} = \sigma_1 P_k - (\sigma_1 + \sigma_3 + \mu_a) P_r + \sigma_3 P_s
\]

\[
\frac{\partial P_s}{\partial E_s} = \sigma_2 P_k + \sigma_3 P_r - (\sigma_2 + \sigma_3 + \mu_a) P_s
\]

The generalization of Hamilton's\textsuperscript{34} numerical procedure should be straightforward. A calculation of this type was not desired for this study so this thought has not been pursued.

As mentioned in Chapter III, a computer program
was written to aid in the avoidance of reflections thought to be affected by coincidence. The program is fairly straightforward. For each reflection, the first portion of the program locates the center of the Ewald sphere in reciprocal space. The program has the capability of describing crystal rotations about the \( \text{Coo} \) axis. Once the Ewald sphere center is specified, the equation of the sphere is known. At this point, an iterative routine is commenced where the distance of each reciprocal lattice point to the sphere is calculated. If this distance is less than a certain specified amount, a message is printed identifying the coincident and crossover reflections. For temperatures below \( T_N \), provision was made for including the satellite reflections in the search. The statement listing of this program follows.
Coincident Reflection Search Program

<table>
<thead>
<tr>
<th>i</th>
<th>j</th>
<th>k</th>
<th>l</th>
<th>m</th>
<th>n</th>
<th>o</th>
<th>p</th>
<th>q</th>
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</thead>
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<td></td>
<td></td>
</tr>
</tbody>
</table>

The table above represents the coincident reflection search program with variables i, j, k, l, m, n, o, p, and q.


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