

Experiment 29

THE MÖSSBAUER EFFECT – HYPERFINE SPLITTING (Experiment 28 is a prerequisite)

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A- INTRODUCTION.

1- Hyperfine Splitting.

Consider a magnetic dipole with dipole moment μ in the presence of a magnetic field

B. The potential energy for this dipole is given by

$$W = -\vec{\mu} \cdot \mathbf{B} \quad (1)$$

The magnetic moment is related to the nuclear spin I by

$$\vec{\mu} = g \mu_n \mathbf{I} \quad (2)$$

Where g is the gyromagnetic ratio which is, in general, different for all nuclei and for their excited states. μ_n is the nuclear magneton

$$\mu_n = e\hbar/2M_p = 3.152 \times 10^{-18} \text{ MeV / gauss}$$

Inserting Eq.(2) in Eq.(1) we get,

$$W = -g \mu_n \mathbf{I} \cdot \mathbf{B} \quad (3)$$

Now let the z axis point along B. Then Eq.(3) can be written as

$$W_z = -g \mu_n I_z B \quad (4)$$

Quantum mechanically I_z can only assume certain discrete values, these are given by

$$I_z = I, I-1, I-2, \dots, -I \quad (5)$$

The splitting given by Eq.(4) is different for the ground state and the excited state because their gyromagnetic ratios are different, we will denote these ratios as g and g^* for the ground state and the excited state respectively. Since the spin of the ground state is 1/2, from Eq.(5) we see that this state splits into two states, while the excited state with spin 3/2 splits into four states.

We will denote these splitting by

$$W_z = -g \mu_n B I_z \quad W_z^* = -g^* \mu_n B I_z^* \quad (6)$$

The energy of the radiated photon is given by

$$k_{rad} = E_\gamma + \Delta E_{isomeric} \quad (7)$$

while the energy of the absorbed photon is given by

$$k_{abs} = E_\gamma + W_z^* - W_z \quad (8)$$

The absorber you will use is metallic iron that contains 2.25% of Fe⁵⁷ and by definition the isomeric shift is zero. For this reason this shift is not included in Eq.(8). The energy difference between k_{rad} and k_{abs} is given by Eqs.(3), (4) and (5),

$$\Delta E = k_{rad} - k_{abs} = \Delta E_{iso} + g \mu_n B I_z - g^* \mu_n B I_z^* \quad (9)$$

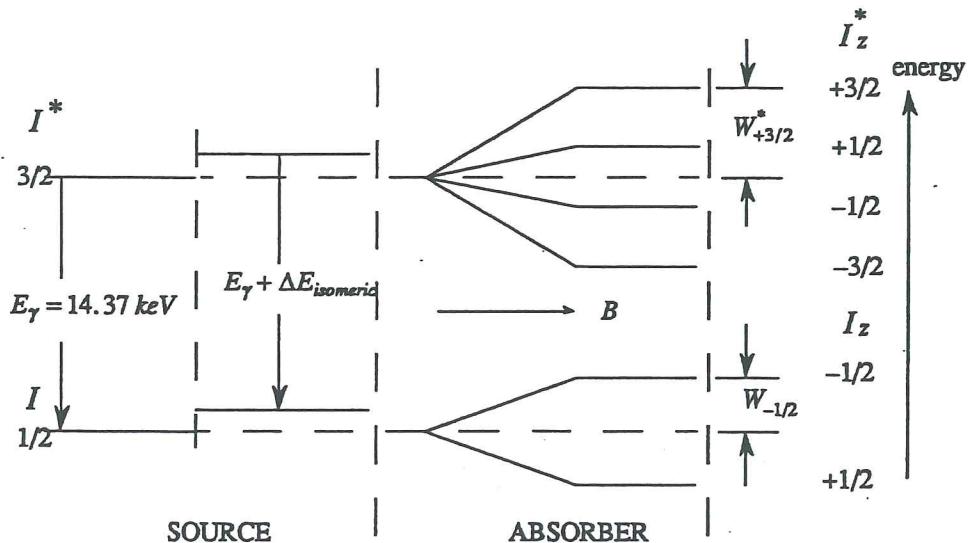


Figure 1

The hyperfine splitting due to a magnetic field. Notice that the energy scale for the difference between the excited state and the ground state energies is around 10^{11} larger than the hyperfine splitting energies.

These splittings are shown for the ground and excited states in Fig. 1. Please realize the sensitivity of this experiment: if in this figure we were to plot E_γ in the same scale as the hyperfine splittings its separation would be around one million km! (around 3 times the distance between the Earth and the Moon). The ordering of the substates for

the excited state are reversed because g^* is negative, the splitting of the ground state sublevels is larger than the splitting of the excited state sublevels because

$$g^* = -\frac{1}{1.75}g$$

Not all transitions from sublevel to sublevel are allowed. Since the photon carries away one unit of angular momentum the change, ΔI_z can only be ± 1 or 0. The allowed transitions are shown in Fig 2.

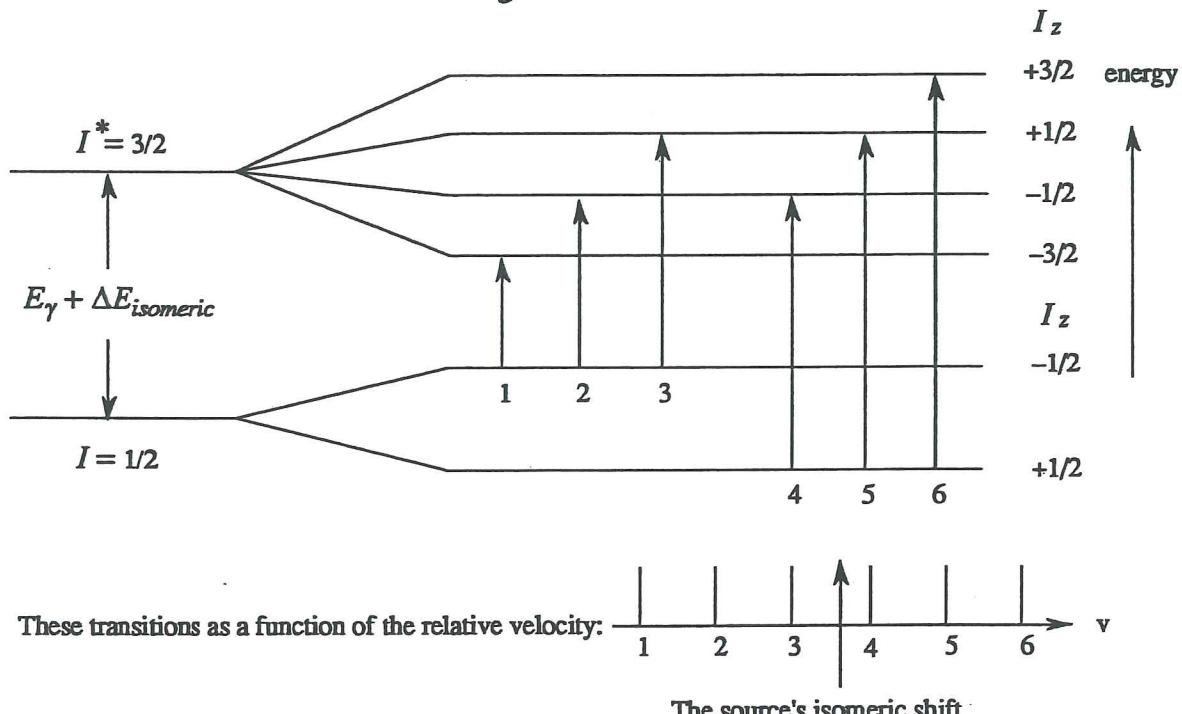


Figure 2
The allowed transitions.

As mentioned above, in this experiment you will use a natural iron absorber (the abundance of ^{57}Fe in natural iron is $\sim 2\%$). Inside the iron there are strong magnetic fields (even if the iron is not magnetized). From a fit to Eq.(9) (see Sec. C) you can determine B and g^* but the value of g is required, which can not be determined in this experiment. Using nuclear magnetic resonance, g has been measured to be

$$g = +0.18$$

Reference: Frauenfelder, pages 225-232, 325-326

2- Quadrupole splitting.

For completeness we will mention the quadrupole splitting. This, like the isomeric shift, is associated with the electrostatic energy between the nuclear charge distribution and the electric field due to the surrounding electron cloud. The potential energy of a finite charge distribution can be expressed in terms of the "multipole" expansion (this is a Taylor series expansion in three dimensions. See Jackson, Sec. 4.2).

$$W = q\Phi(0) - \mathbf{p} \cdot \mathbf{E}(0) + \frac{1}{6} \sum_{ij} Q_{ij} \frac{\partial^2 \Phi(0)}{\partial x_i \partial x_j}$$

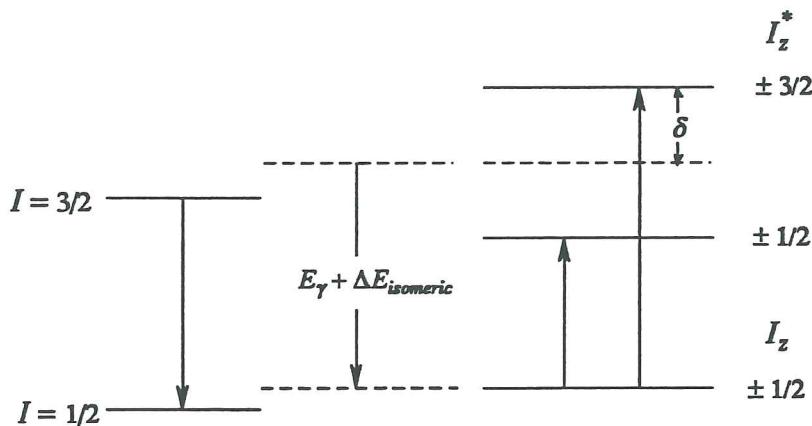


Figure 3
The quadrupole splitting.

The first term is the interaction that produces the isomeric shift. The second term vanishes because \mathbf{p} , the dipole moment, vanishes because parity is conserved in strong (nuclear) and electromagnetic interactions. The third term is the quadrupole interaction. Let's assume, as it is often the case, that the electric field has axial symmetry, and let the z axis be along this axis of symmetry. Quantum mechanically this interaction is a mess:

$$\delta = \frac{e}{4} \frac{\partial^2 \varphi_e}{\partial z^2} Q \left[\frac{3I_z^2 - I(I+1)}{I(2I-1)} \right] \quad (10)$$

where Q is the nuclear quadrupole moment, φ_e is the electric potential due to the electron cloud, and its second derivative is to be evaluated at the position of the nucleus. Because this split depends on I_z^2 , the ground state does not split, and the first excited state splits into only two sublevels, as shown in Fig. 3. This quadrupole splitting is always present but it is often very small because the second derivative of

$\varphi_e(0)$ is very small. In the $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ absorber the second derivative of φ_e is large and you can easily observe this splitting, unfortunately you can not calculate Q because there is no way for you to measure the second derivative of $\varphi_e(0)$, you will be able to measure the relative isomeric shift (see Fig. 3). In ordinary iron oxide, Fe_2O_3 , the hyperfine splitting is larger than in metallic iron, and the quadrupole splitting is detectable. See Sec. C, part 2.

References :

- H. Frauenfelder, The Mössbauer Effect, (W.A. Benjamin, Inc., N.Y., 1963)*
Mössbauer Effect- Selected Reprints
Mössbauer Effect- Data Index
G. Wertheim- The Mössbauer Effect
*All of the above are available in the laboratory.

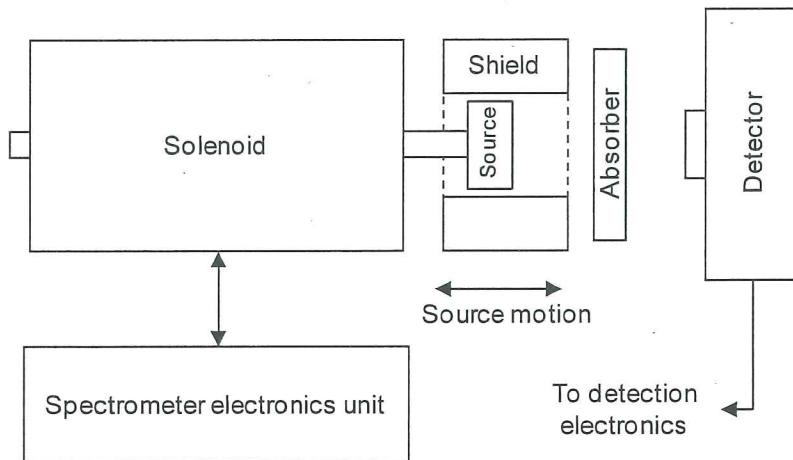


Figure 4: General arrangement of the Mössbauer hardware. The solenoid drives the motion of the source; its design is similar to that of the voice-coil in a loudspeaker.

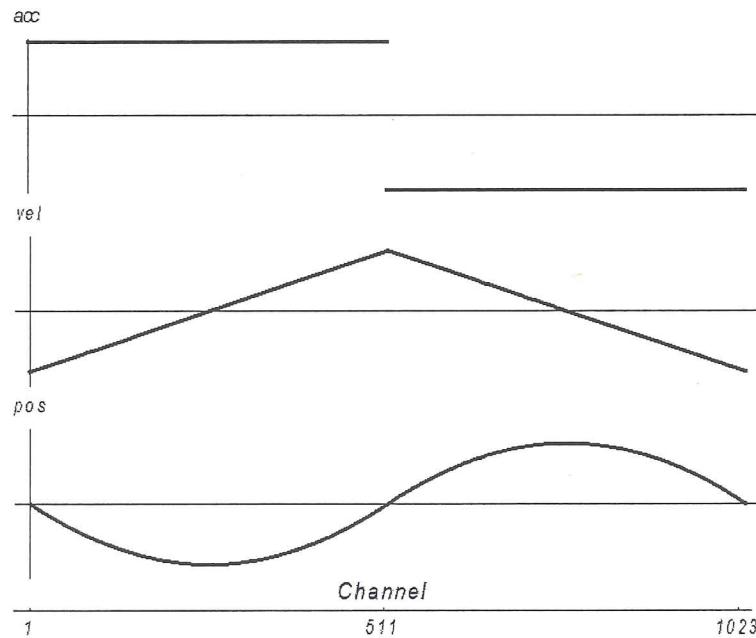


Figure 5: The relation between acceleration, velocity, position, and channel number. Channel 0 is used to record the spectrum acquisition time. Velocity is + for motion of the source toward the absorber; position is + when the source is closer to the absorber.

EXPERIMENTAL APPARATUS

The MS900A Spectrometer. The heart of the apparatus is a commercial Mössbauer spectrometer, the Ranger Scientific MS900A. Unlike the apparatus in Experiment 28, the ^{57}Co source moves while the absorber remains stationary. As diagrammed in Figure 4, the source is attached to a solenoid controlled by an electronic feedback and control unit, which oscillates the source toward and away from the absorber and detector. As we will use the system, the source will be

given a constant acceleration for $\frac{1}{2}$ of each cycle; the direction of the acceleration changes half way through the cycle. Because the acceleration of the source is constant for half of each cycle, the velocity of the source increases and decreases linearly, as shown in Figure 5. Each velocity is sampled twice during a cycle: as the velocity increases (bins 1-511) and again as the velocity decreases (bins 512-1023). Unfortunately, this apparatus does not provide a direct velocity or position readout, so you will use a natural iron spectrum you obtain to calibrate the velocities of the channels.

Control and Acquisition Electronics. As with experiment 28, the detector is a gas-proportional counter with a preamp mounted close to it. The high voltage is controlled by a large power supply mounted to the equipment rack. The output of the preamp is further amplified and fed to a *single channel analyzer* (SCA), which will generate a digital output pulse whenever an input pulse has an amplitude that falls within its adjustable discriminator window. You will set the SCA window to respond to detections of the 14.4 KeV gamma ray we use for Mössbauer spectroscopy. By using a digital oscilloscope connected to the amplifier output but triggered by the SCA output, you can see the amplified pulses that fall within the discriminator settings of the single channel analyzer. You will use the oscilloscope to adjust the SCA discriminator window to accept only the 14.4 KeV gammas. Figure 6 is a block diagram of the setup.

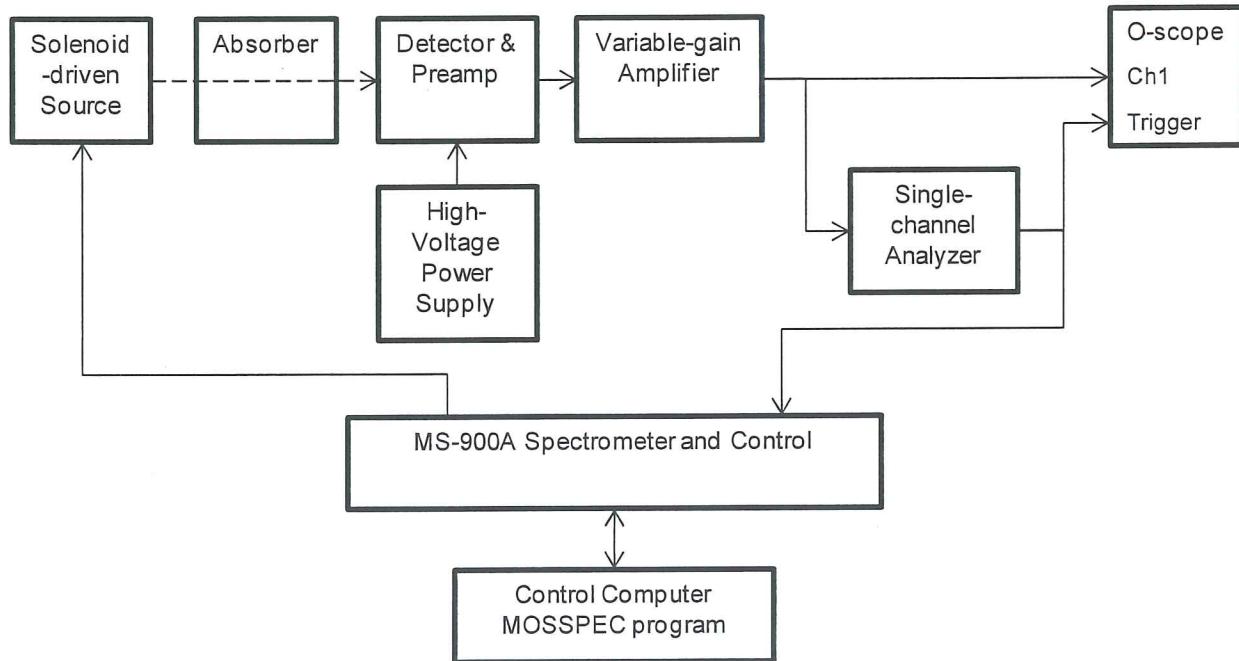
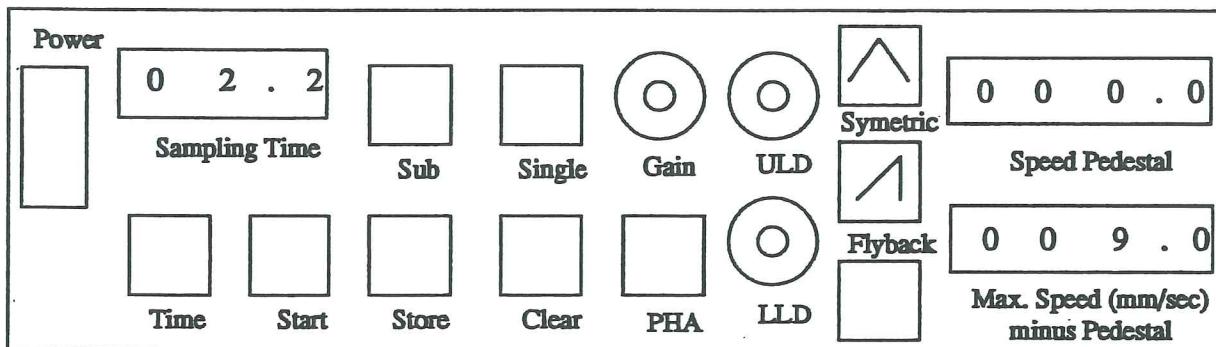


Figure 6: Block diagram of the control and acquisition electronics. The computer is a very old model running MsDos! The control program is MOSSPEC. A floppy disk is used to transfer the data to one of the more modern lab computers.

Spectrometer Front-Panel Controls and MOSSPEC Software

The front panel of the MS-900A is shown in Fig. 8. In general you only have to adjust the discriminator's levels, however, we will describe the function of those controls that are relevant for your measurements.



The front pannel of the MS-900A spectrometer.

Figure 8

Sampling Time: this is the dwell time per bin. 2.2, which means $2 \times 10^2 \mu\text{sec}$, is the setting that you should use, if this setting is changed the calibration provided by your T.A. is not valid.

Time: If this button is OFF bin zero counts the number of sweeps, while if it is ON bin zero measure the run time in msec. Keep this button ON, the data is cleaner in the first 26 bins (?).

Start: ON.

Store: Must be ON to store the spectrum.

Clear: Clears the internal memory. Your spectrum is stored in the internal memory of the MS-900A and not in the computer's memory. The MS-900A does not need the computer to acquire data, only to display the data, therefore, you can use the computer for anything you wish while you are taking data. The only way to loose your spectrum is by pushing this button, so only push it at the beginning of a run.

PHA: make sure that this button is OFF.

Symmetric: This button must be ON. It sets the mode of the spectrometer to be as shown in Fig. 5.

Flyback: This button must be OFF.

Speed Pedestal: This sets the minimum absolute speed to be analyzed in mm/sec. It should always be set at zero.

Max. Speed: When the pedestal is set at zero this setting gives the maximum absolute velocity in mm/sec (otherwise the maximum velocity is given by the sum of the pedestal and this setting). For the calibration given to you to be valid this max. velocity must be set at 9.00 mm/sec (this means that the velocity will cover the range from -9 to +9 mm/sec).

Sub and Single: We do not know what these buttons do. Keep them OFF.

3. The software.

The program to display and save the data on disk is named MOSSPEC. This is a very rudimentary program written in interpretive Basic. The only commands that you will need are:

G: This command gets the data stored in the MS-900A. The up arrow (\uparrow) and the down arrow (\downarrow) rescale the display.

S: Save the data in disk. The format is the following: bin number followed by the contents of the following eight bins, etc. The G command of FFIT has the option (3) RANGER MOSS that converts the MS-900A format into the FFIT format.

L: Loads a file saved in the disk (in the MS-900A format), and displays it.

EXPERIMENTAL PROCEDURE AND ANALYSIS

1. Setup

Change the computer to the C:/USERS directory and start MOSSPEC if it isn't already running. Make sure you have a floppy disk available to transfer files (ask the TA to find you one). **Don't keep the lab floppy disk. Leave it near the computer.**

Typical settings for the equipment:

1. High voltage: 1800V, + polarity
2. Amplifier: Coarse Gain: 200, Fine Gain 13, Polarity +
3. Single Channel Analyzer (SCA): Upper Level: 1.9-3, Lower Level: .5-1.2
4. MS-900: Sampling time: 20.1 or 02.2 (200 μ s); Vel. Pedestal: 0.0; Max Vel.: 9.5

Remove any absorbers or lead shielding between the source and the detector. Turn on the high voltage to the detector. Use the oscilloscope and the X-ray filter to identify the 6 KeV and 14.4 KeV pulses from the amplifier. Use the oscilloscope voltage cursors to bracket the 14.4 KeV pulses to help you set the SCA upper and lower levels. Trigger the oscilloscope on the SCA output pulses, and then adjust the upper and lower levels until only the 14.4 KeV pulses are triggering the SCA output. **Check with your TA to make sure you've got the SCA set properly.**

2. Stainless Steel Absorber

Insert the stainless steel absorber first. You may use the X-ray filter to help secure the absorber to the sample shelf. Start the MS-900 symmetric velocity sweep, turn on STORE, and push CLEAR.

MOSSPEC Ms-Dos program: turn on grabbing (G) and use the up and down arrows to set the vertical scale to 512 counts. You should see the spectrum starting to build up from the bottom of the graph. Use the window command (W) to look at only the first 512 channels.

As the spectrum builds into the top half of the graph, a single absorption line should be discernable near the middle channels (220-280). When you can clearly identify this absorption line, turn off grabbing (O) and save the spectrum (S). Accumulating enough data to see the line should only take about 10 minutes; don't waste a lot of time collecting this spectrum once you can identify the absorption line. Use the floppy (the A: drive) to transfer the file to another computer and save the file to the network drive.

If the absorption line doesn't appear, you probably don't have the SCA window set properly or you've set up the MS-900 incorrectly.

3. Natural Iron Absorber

Once you have obtained a useable Stainless Steel spectrum replace the absorber with a natural iron sample and CLEAR the MS-900. Collect this spectrum for at least an hour because you want a fairly high-quality spectrum of the iron. The line positions of this spectrum will be used to calibrate your channel velocities.

4. Iron Oxide or Iron Sulfate

Iron oxide (Fe_2O_3) exhibits hyperfine splitting with quadrupole shifts, whereas iron sulfate (FeSO_4) exhibits only quadrupole splitting. Use the remaining lab time to collect a spectrum of either or both of the iron oxide and iron sulfate samples Note: the iron oxide sample will take at least 90 minutes to acquire a useable spectrum.

5. Securing the Apparatus

If the equipment is not needed for another lab section right away, you may be able to continue to collect a spectrum overnight and then save it the following day. Check with your TA.

Otherwise, stop grabbing (O), turn the high voltage to standby, remove any sample, and turn off the sweep of the source solenoid.

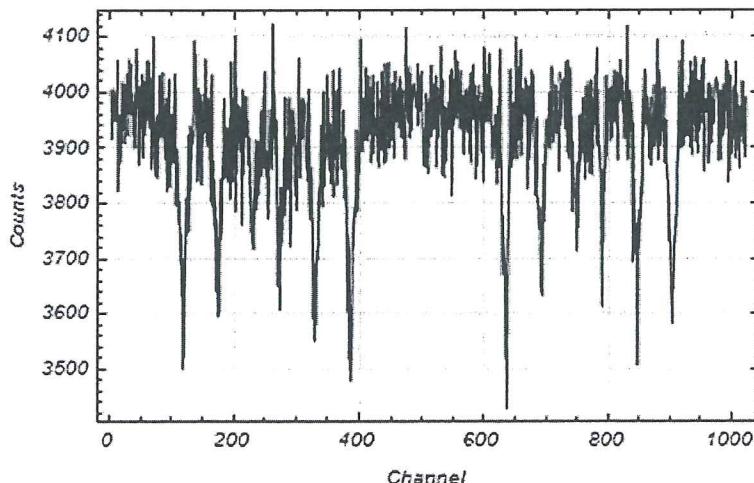
Make sure the floppy disk is left somewhere near the setup.

Make sure you've copied your data files to the lab network drive.

6. Data Analysis

The primary tools you will need for your data analysis are CurveFit, the *Mosspec.nb* notebook (on the lab drive in “*\documents\Mathematica Data Analysis\Mosspec Exp 29*”), and your brain.

Each complete data set contains two independent images of the spectrum, because during each cycle of the motion, the source experiences a given velocity twice. The image at right shows an example of a complete natural iron data set showing the two spectrum images. The velocity goes from maximally negative at channel 1, to maximally positive near channel 511, then back to maximally negative at channel 1023. The source passes



through 0-velocity near channels 256 and 768. It is farthest from the detector near channel 256 and closest near channel 768. Consequently, the 6 hyperfine absorption lines are visible in each half of the data set.

The count data in each channel has uncertainties determined by Poisson count statistics, naturally, so you will assign the appropriate uncertainties to the count data. *CurveFit* and the *Mosspec.nb* notebook have functions to assign these uncertainties for you.

Velocity calibration

Use the natural iron spectrum to calibrate both the upper and lower halves of a channel spectrum. Calibration consists of using the known natural Fe line velocities (-5.3285 , -3.0835 , -0.8335 , 0.8335 , 3.0835 , and 5.3285 mm/sec) to determine the 0-velocity channel and the velocity increment per channel. Each half (channels 1–511 and 512–1023) must be calibrated separately. *Mosspec.nb* provides a palette interface which makes this process straightforward. The steps to a full calibration are:

1. Load *Mosspec.nb* using *Mathematica*®. Make sure you execute the notebook's initialization cells. *CurveFit* should start and an additional *Mosspec* palette should appear on the left side of the display.
2. Load the natural Fe data set (**Load Mosspec File** palette button).
3. Assign Poisson uncertainties to the Y data (**Set to Poisson count data** button).
4. Select a data subset which include only the lower half of the channels (**Keep an X-range** button).
5. Determine the velocity calibration using the known natural Fe line velocities (**Calibrate** button). Check the χ^2 and the fit results plot to make sure the calibration located the 6 iron lines and is accurate. If not, try rebinning the data (**Rebin Data** button) and attempt to calibrate again.
6. Restore the full spectrum (result following step 3) by using the **Undo** palette button.
7. Select the other half of the channel spectrum and calibrate it (steps 4 and 5).

Mosspec maintains two independent channel calibrations, one for each half of the spectrum. You can see what the calibration coefficients are with its *VelocityParameters* [] and *VelocitySigma* [] functions. Use the **Help** button to see a notebook with a list of the available functions. Clicking on a function gives its description.

Fitting spectra

Once you have calibrated using natural Fe, load another spectrum and window the data to look at one half of it (as in steps 2–4 of the velocity calibration). Convert the X scale to velocity (**Convert to Velocity** button). *Mosspec* uses the results of the velocity calibration to perform the conversion. Now you can fit the lines using the appropriate *Mosspec* button.

Make sure you carefully examine the results (including a plot of the fit results) to make sure the lines were identified correctly by the program. Rebinning the data may be necessary if the lines are weak.

Analyzing the peaks and their positions

The quadrupole shift (equation 10) depends on I and I_z as $\frac{3I_z^2 - I(I+1)}{I(2I-1)}$.

For the ground state: $I = \frac{1}{2}$ and $I_z = \pm \frac{1}{2}$, so this shift is zero. For the excited state, however, $I^* = \frac{3}{2}$, so this term is $(I_z^*)^2 - \frac{5}{4}$ with $I_z^* = \pm \frac{1}{2}, \pm \frac{3}{2}$.

Since you are measuring velocities for line positions rather than energy shifts, use the relation:

$$\frac{v}{c} = \frac{\Delta E}{E_0} \text{ , where } E_0 = 14.4129 \text{ KeV}$$

Equations 9 and 10 may then be written as:

$$v_{I_z, I_z^*} = v_{\text{isomeric}} + v_B \left[I_z - \frac{g^*}{g} I_z^* \right] + v_Q \left[(I_z^*)^2 - \frac{5}{4} \right] \quad (11)$$

If the spectrum contains only one line (stainless steel), then v_B and v_Q are both too small to lead to observable line splitting. If two lines are visible, then v_Q is clearly nonzero (FeSO_4). A 6-line spectrum implies that v_B and (g^* / g) may be measured from the line velocities, and a nonzero v_Q may be measurable as well. Of course, any spectrum should provide a measurement of v_{isomeric} .

Mosspec.nb provides a function to fit the line velocities of a 6-line spectrum to the theoretical model given in equation 11. Once you have fit the lines of your Fe_2O_3 spectrum (and even your Fe spectrum), you may use the **Model 6 Lines** palette button to perform the analysis. Carefully examine the results of the model fits, including the χ^2 as well as the uncertainties in the model parameters. Note also the differences between the model's predicted line velocities and the line velocities determined from the data. You should model both the lower and upper halves of the spectrum. Are the model fit results consistent with each other given the χ^2 values and the uncertainties?

What may you conclude about the value of (g^* / g) ? Are the isomeric shifts you obtain consistent with published values? What about the line widths (γ)? How do they compare to the natural line width you calculated from the excited state's half-life (experiment 28 prelab problems)?

PRELAB PROBLEMS

1. What is the expression for v_B (equation 11 on the previous page) in terms of $g \mu_N$, B , and E_0 ? Given that $g = +0.1809$ and $E_0 = 14.4129$ KeV, calculate the value of v_B / B in (mm/sec)/Tesla.
2. Find *Mosspec.nb* on the lab network drive and copy it to your computer. Open it using *Mathematica®* and ensure that the initialization cells are executed. Use the command:

```
ModelPeaks[FeLineV[]]
```

to determine the velocity parameters (equation 11) from a fit of equation 11 to a list of the standard natural iron line velocities (executing `FeLineV[]` alone returns a list of these velocities).

- a. What is the average line velocity uncertainty according to the fit results?
- b. From the fit's value for v_B , what must be the ambient magnetic flux density B (in Tesla) at the location of an iron nucleus? What may be the source of this field?
- c. How does the fit's calculation of (g^* / g) compare to the value given at the top of page 29-4?

