IITRI

Report No. IITRI V6032-10

COMPOSITIONAL ANALYSIS OF LUNAR AND PLANETARY SURFACES USING NEUTRON CAPTURE GAMMA RAYS

to

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data points for the 6.13 Mev oxygen peak and its associated single escape peak. The reliability of this analysis can be judged by the goodness of fit parameter, χ^2/NDF, where

$$\chi^2 = \Sigma\, w_i (N_i - \overline{N}_i)^2,$$

the N_i are the experimental data points with associated weights w_i, the $\overline{N}_i$ are the calculated values, and NDF is the number of degrees of freedom. A χ^2/NDF of less than about 2.0 normally indicates that a good fit to the experimental data has been made. In this case χ^2/NDF = 0.57, indicating an excellent fit.

Figure 4 shows the calculated spectrum and the experimental data points for the 1.46 Mev potassium-40 peak. Again the fit is quite good (χ^2/NDF = 1.4). The calculated areas for the above four peaks (with errors ranging between 8 and 21 percent) together with the values of χ^2/NDF are given in Table 1. The errors in the peak areas listed in the table were determined from the inverse matrix using the equation

$$\Delta A = \left(\frac{\partial A}{\partial w}\right)^2 \text{var } \omega + 2 \left(\frac{\partial A}{\partial y}\right)\left(\frac{\partial A}{\partial w}\right) \text{ covar } (\omega, y) + \left(\frac{\partial A}{\partial y}\right)^2 \text{ var } y.$$

Here A is the area which is given by the equation

$$A = \int_{-\infty}^{+\infty} y \exp\left\{-\left[\frac{(x - x_o)}{\omega/2 \cdot \log 2}\right]^2\right\} dx,$$

FOREWORD

This is Report No. IITRI V6032-10, a quarterly report under Contract No. NASr 65(18), entitled "Compositional Analysis of Lunar and Planetary Surfaces Using Neutron Capture Gamma Rays," covering the period July 1, 1968 to September 30, 1968.

The following personnel have contributed to the work described in this report: J. H. Reed, principal investigator, and J. W. Mandler, co-investigator.

Respectfully submitted,
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ABSTRACT

During this reporting period program GAUST was successfully used for the analysis of prominent peaks in the gamma-ray spectra from the combined neutron experiment. Preliminary capture gamma-ray spectra were obtained from basalt using a recently acquired large-volume Ge(Li) detector.

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I. INTRODUCTION

The purpose of this research program is the continued development of the combined neutron experiment in three areas. These areas are conveniently described by three major tasks: (1) the development of computer techniques for the analysis of the data, (2) the experimental determination of the extent to which a large-volume high-resolution solid-state detector will add to the analytical capabilities of the combined experiment, and (3) the completion of studies aimed at detailing the final space-hardened detector probe (based on a NaI(Tl) detector).

During this reporting period the major effort has been focused on the first two tasks. Program GAUST was successfully used for the analysis of selected prominent peaks in the capture gamma-ray, cyclic activation, and inelastic scattering spectra from basalt. A large-volume Ge(Li) detector was purchased and was used to obtain preliminary capture gamma-ray spectra from basalt.

II. DATA ANALYSIS

The data from the combined experiment consist of a series of complex gamma-ray spectra which contain peaks that are characteristic of the material being inspected. In order to obtain the elemental composition of the material, these gamma-ray peaks must be identified and their areas accurately determined. Since the determination of the intensity of a given peak from the pulse height spectrum is generally not a simple problem, computer programs are used frequently. We are presently using the program GAUST (discussed briefly in Report No. IITRI-V6032-9) for the analysis of the capture gamma-ray, cyclic activation, and inelastic scattering spectra.

Program GAUST determines peak intensity and location (energy) if an initial estimate of the peak position is known. GAUST assumes that the region of the pulse height spectrum being analyzed is composed of a Gaussian shaped peak plus a quadratic background together with contributions due to the Compton edge and the first escape peak. Selected peaks in the capture and cyclic activation spectra (Figure 1) and the inelastic scattering spectrum (Figure 2) from basalt have been analyzed successfully using GAUST.

The 6.13 Mev oxygen, 2.61 Mev natural thorium chain, 1.78 Mev silicon, and 1.46 Mev potassium-40 peaks in the cyclic activation spectrum (Figure 1B) were analyzed using GAUST. Figure 3 shows the calculated spectrum and the experimental data points for the 6.13 Mev oxygen peak and its associated single escape peak. The reliability of this analysis can be judged by the goodness of fit parameter, χ^2/NDF, where

$$\chi^2 = \Sigma\, w_i(N_i - \overline{N}_i)^2,$$

the N_i are the experimental data points with associated weights w_i, the $\overline{N}_i$ are the calculated values, and NDF is the number of degrees of freedom. A χ^2/NDF of less than about 2.0 normally indicates that a good fit to the experimental data has been made. In this case χ^2/NDF = 0.57, indicating an excellent fit.

Figure 4 shows the calculated spectrum and the experimental data points for the 1.46 Mev potassium-40 peak. Again the fit is quite good (χ^2/NDF = 1.4). The calculated areas for the above four peaks (with errors ranging between 8 and 21 percent) together with the values of χ^2/NDF are given in Table 1. The errors in the peak areas listed in the table were determined from the inverse matrix using the equation

$$\Delta A = \left(\frac{\partial A}{\partial w}\right)^2 \text{var}\ \omega + 2\left(\frac{\partial A}{\partial y}\right)\left(\frac{\partial A}{\partial w}\right) \text{covar}\ (\omega, y) + \left(\frac{\partial A}{\partial y}\right)^2 \text{var}\ y.$$

Here A is the area which is given by the equation

$$A = \int_{-\infty}^{+\infty} y \exp\left\{-\left[\frac{(x - x_o)}{\omega/2\cdot\log 2}\right]^2\right\} dx,$$

y is the height of the normal distribution, ω is the width of the normal distribution at y/2, x_o is the center of the normal distribution, var ω and var y are the variances of ω and y, and covar (ω,y) is the covariance of ω and y. The variances and covariance are products of χ^2/NDF and appropriate elements of the inverse matrix.

The 7.64 Mev iron and 2.21 Mev hydrogen peaks and the 1.37 Mev titanium plus 1.46 Mev potassium-40 doublet in the combined capture plus cyclic activation spectrum (Figure 1A) also were analyzed using GAUST. Figure 5 shows the calculated spectrum and the experimental data points for the 7.64 Mev iron peak and its associated single escape peak. Figure 6 shows the calculated spectrum and the experimental data points for the 2.21 Mev hydrogen peak. Both of the fits are good. Figure 7 shows the calculated spectrum and experimental data points for the 1.37 Mev titanium plus 1.46 Mev potassium-40 doublet. This calculated spectrum was obtained by fitting a single Gaussian, a quadratic background, plus the potassium-40 peak calculated from the cyclic activation data (Figure 4) to the experimental data. The fit is good (χ^2/NDF = 2.00), although not as good as the fits for the other peaks analyzed. The areas in the above three capture gamma-ray peaks exhibit errors ranging between 11 and 20 percent.

The 6.13 Mev oxygen, 1.78 Mev silicon, 1.37 Mev magnesium, 1.27 Mev iron, and 1.01 Mev aluminum peaks in the inelastic spectrum from basalt (Figure 2) were also analyzed using GAUST. The fits were all good and, with the exception of the weak 1.27 Mev iron peak, the errors in the areas ranged between 11 and 19 percent. Table 1 contains the calculated areas and values of χ^2/NDF for these analyses.

From the above analyses of capture, inelastic, activation, and background gamma-ray peaks, it is concluded that program GAUST can be used to determine the energy and areas of the prominent peaks. Errors ranging between 10 and 20 percent can be expected in the calculated areas. Analysis of the weaker peaks has not yet been attempted. No estimate of the expected accuracy of the results for these peaks can be made at this time.

III. SPECTRUM FROM BASALT OBTAINED USING Ge(Li) DETECTOR

A 40-cm^2 Ge(Li) detector and Tennelec TC-135 preamplifier have been purchased and used to obtain preliminary capture gamma-ray spectra from basalt. The detector has a system resolution of 2.9 kev at 1332 kev and a peak to Compton ratio of 17:1 at 1332 kev.

Figures 8 and 9 show portions of the combined capture plus cyclic activation spectrum from basalt obtained using this large Ge(Li) detector. This preliminary spectrum was obtained with an 8-cm-thick polyethylene reflector located above the neutron source. The reflector was not shielded from the detector and the neutron output appears not to have been optimum.

Capture gamma rays from iron, titanium, calcium, and hydrogen are present in the low energy portion of the spectrum (Figure 8) together with activation gamma rays from sodium-24m, manganese-56, sodium-24, and silicon. The high energy portion exhibits capture gamma rays from iron and titanium and activation gamma rays from oxygen.

IV. CONCLUSIONS

Program GAUST has been successfully used for the analysis of the prominent peaks in the capture, activation, and inelastic gamma-ray spectra from basalt. Errors in the 10 to 20 percent range can be expected in the calculated areas of the prominent peaks. The success that GAUST will have in analyzing weaker peaks and the expected errors in the results are not yet known. The analysis of low intensity peaks will be studied during the next reporting period.

A large volume Ge(Li) detector has been purchased and used to obtain preliminary capture gamma-ray spectra. During the next reporting period capture, cyclic activation, and inelastic gamma-ray spectra will be obtained using this large Ge(Li) detector. Analysis of the spectra will be performed in order to evaluate the advantages and disadvantages of using a Ge(Li) detector rather than a NaI(Tl) detector.

Table 1

PEAK AREAS CALCULATED USING GAUST

Element	Energy (Mev)	Type of Spectrum	χ^2/NDF	Area
K-40	1.46	Activation	1.4	4990 ± 429
Silicon	1.78	Activation	2.2	3333 ± 297
Nat. Thorium	2.61	Activation	1.3	546 ± 117
Oxygen	6.13	Activation	0.57	524 ± 43
Titanium	1.37	Capt. + Activ.	2.0	2253 ± 435
Hydrogen	2.21	Capt. + Activ.	0.97	2073 ± 411
Iron	7.64	Capt. + Activ.	0.77	962 ± 109
Aluminum	1.01	Inelastic	0.18	2710 ± 299
Iron	1.27	Inelastic	1.1	1145 ± 440
Magnesium	1.37	Inelastic	1.1	5690 ± 900
Silicon	1.78	Inelastic	0.83	7724 ± 752
Oxygen	6.13	Inelastic	1.8	1562 ± 290

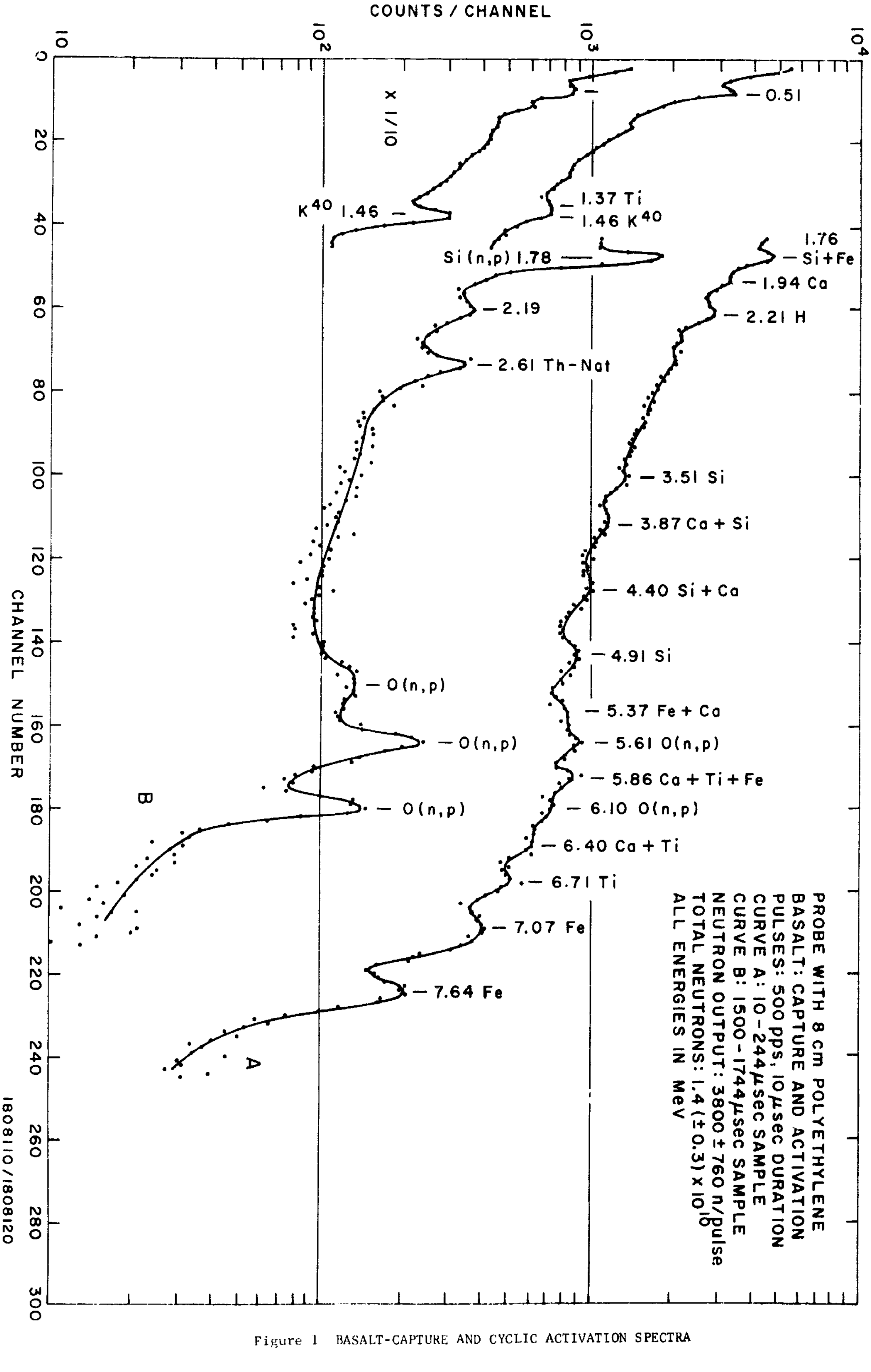

Figure 1 BASALT-CAPTURE AND CYCLIC ACTIVATION SPECTRA

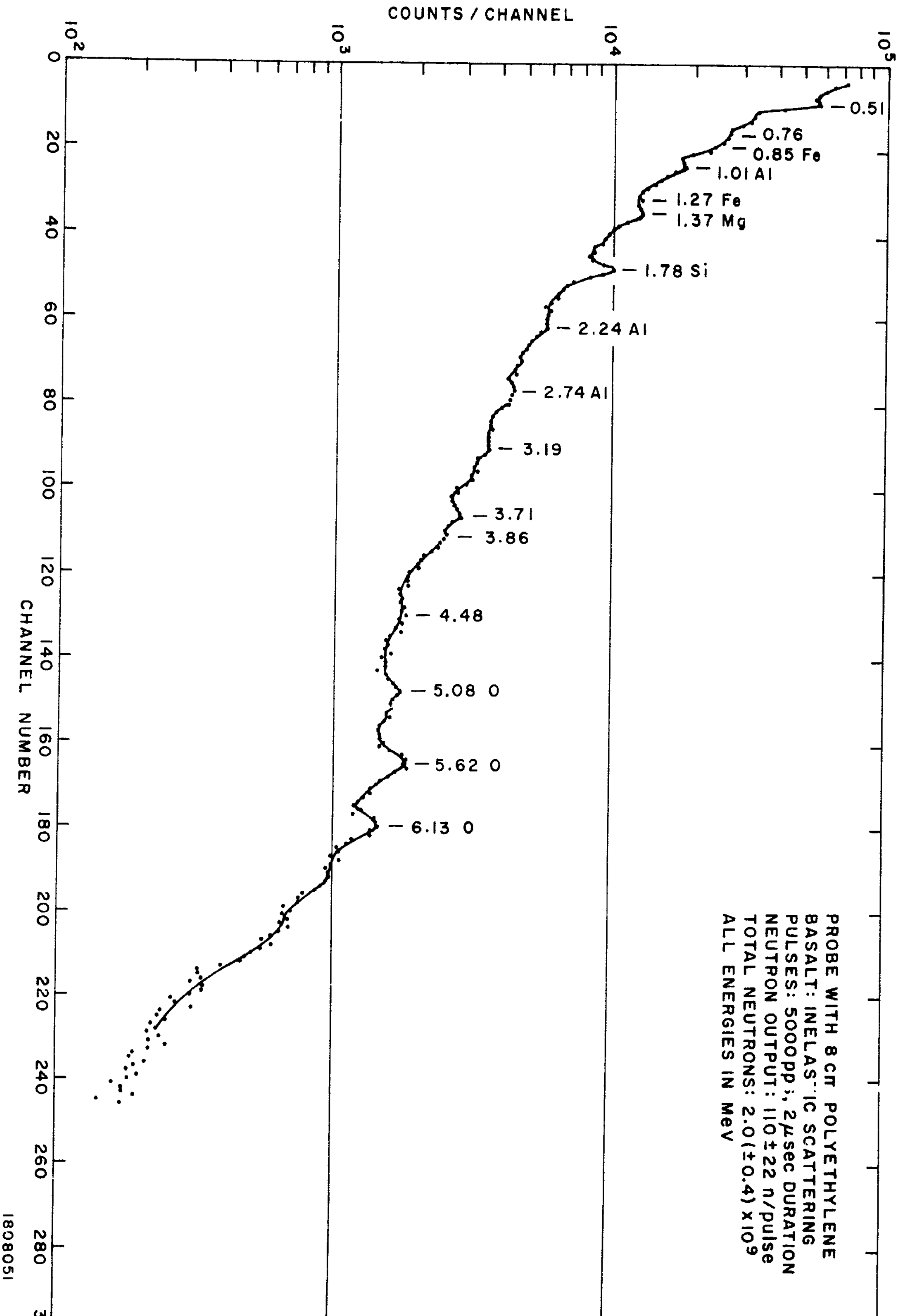

Figure 2 BASALT-INELASTIC SPECTRUM

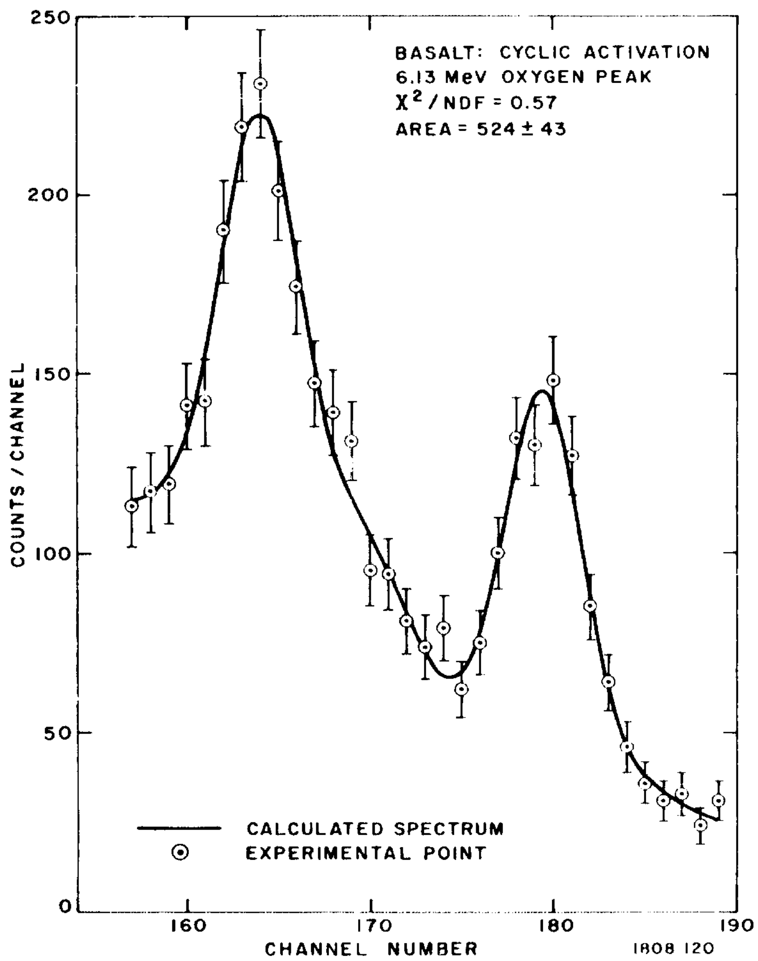

Figure 3 CALCULATED FIT TO 6.13 Mev OXYGEN PEAK

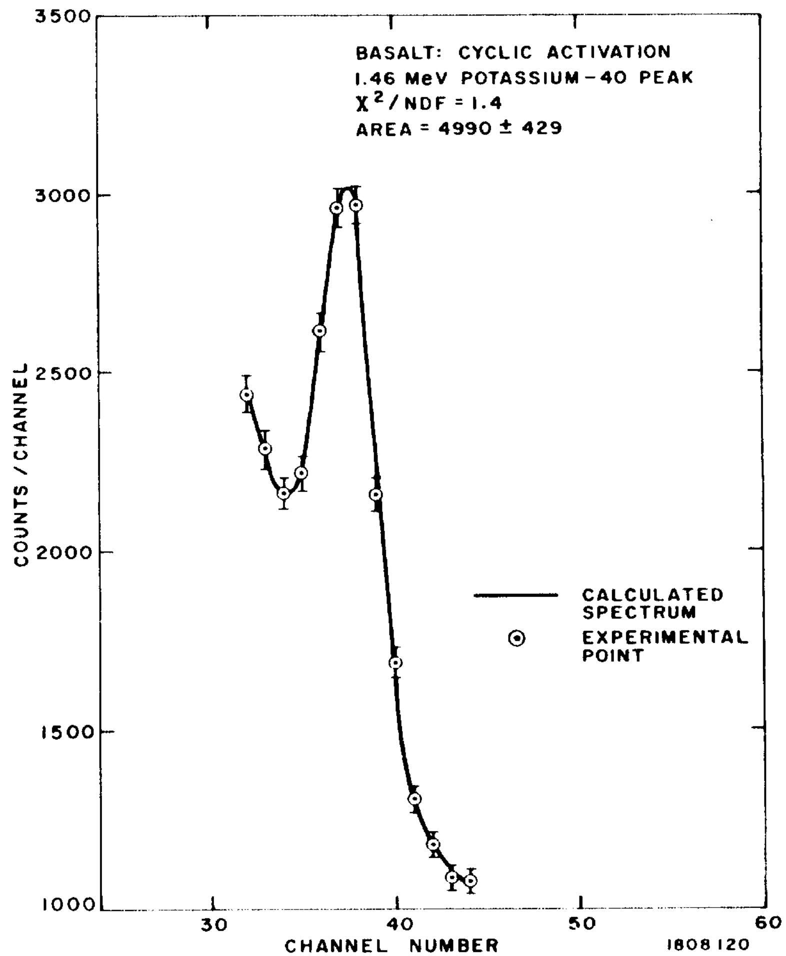

Figure 4 CALCULATED FIT TO 1.46 Mev POTASSIUM-40 PEAK

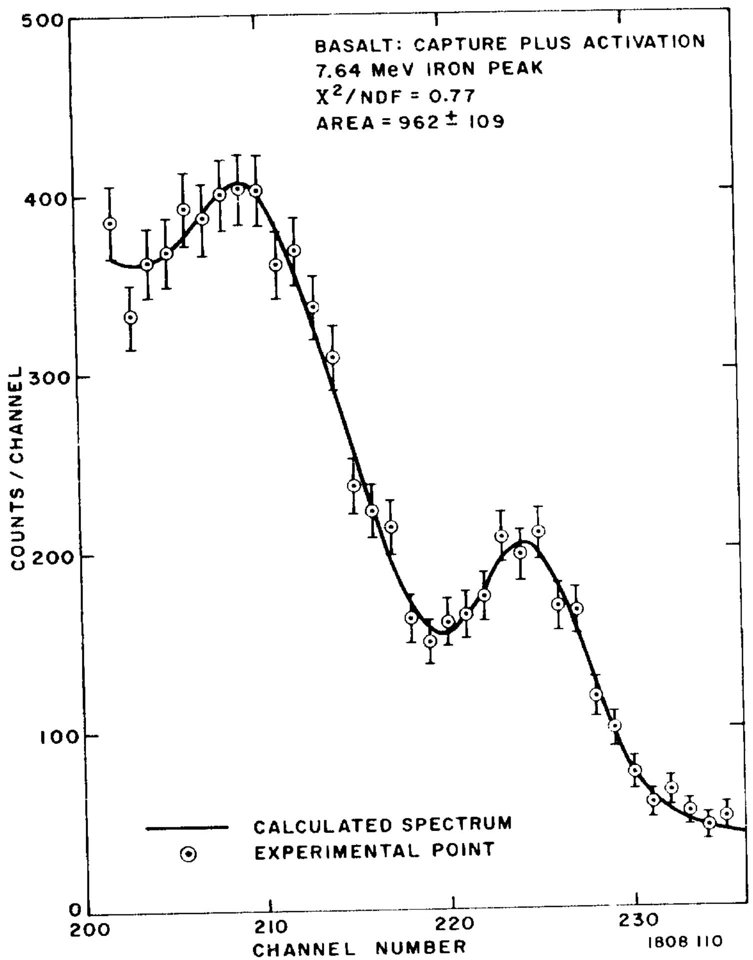

Figure 5 CALCULATED FIT TO 7.64 Mev IRON PEAK

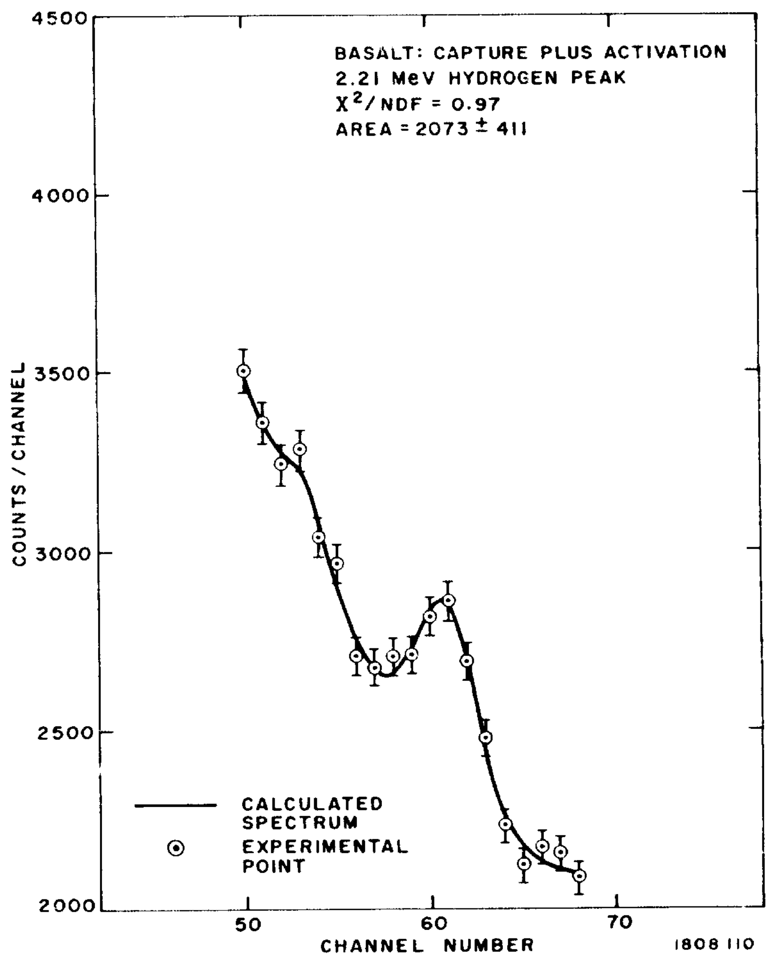

Figure 6 CALCULATED FIT TO 2.21 Mev HYDROGEN PEAK

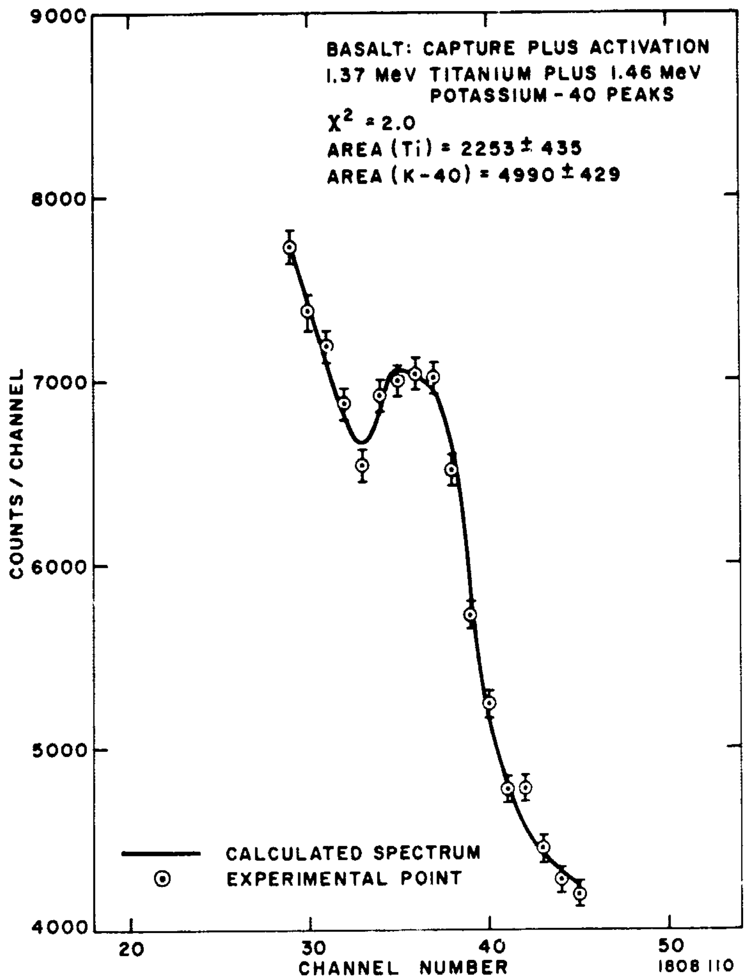

Figure 7 CALCULATED FIT TO 1.37 Mev TITANIUM PLUS 1.46 Mev POTASSIUM-40 DOUBLET

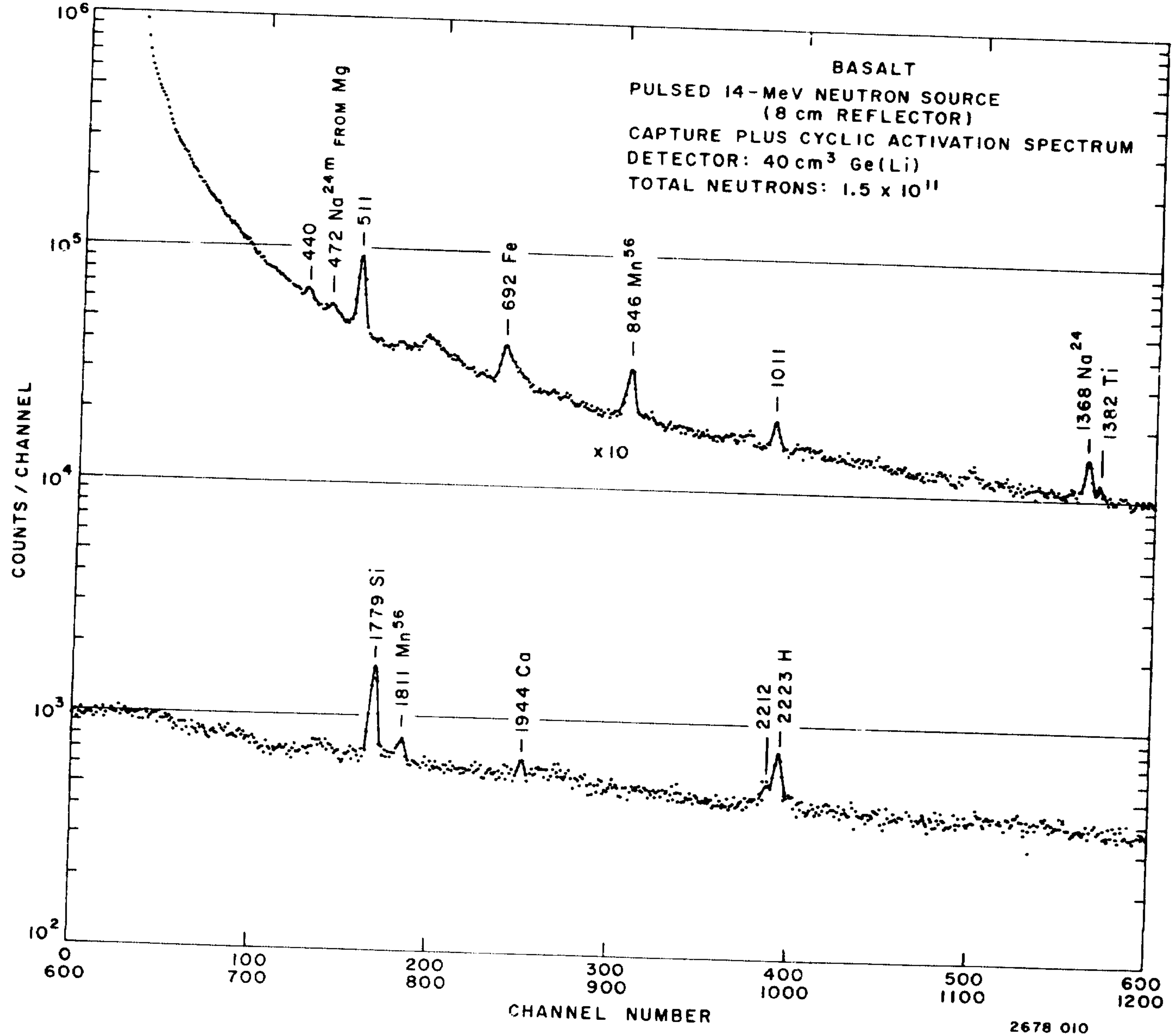

Figure 8 BASALT-CAPTURE AND CYCLIC ACTIVATION SPECTRA (40-cm3 Ge(Li) Detector)

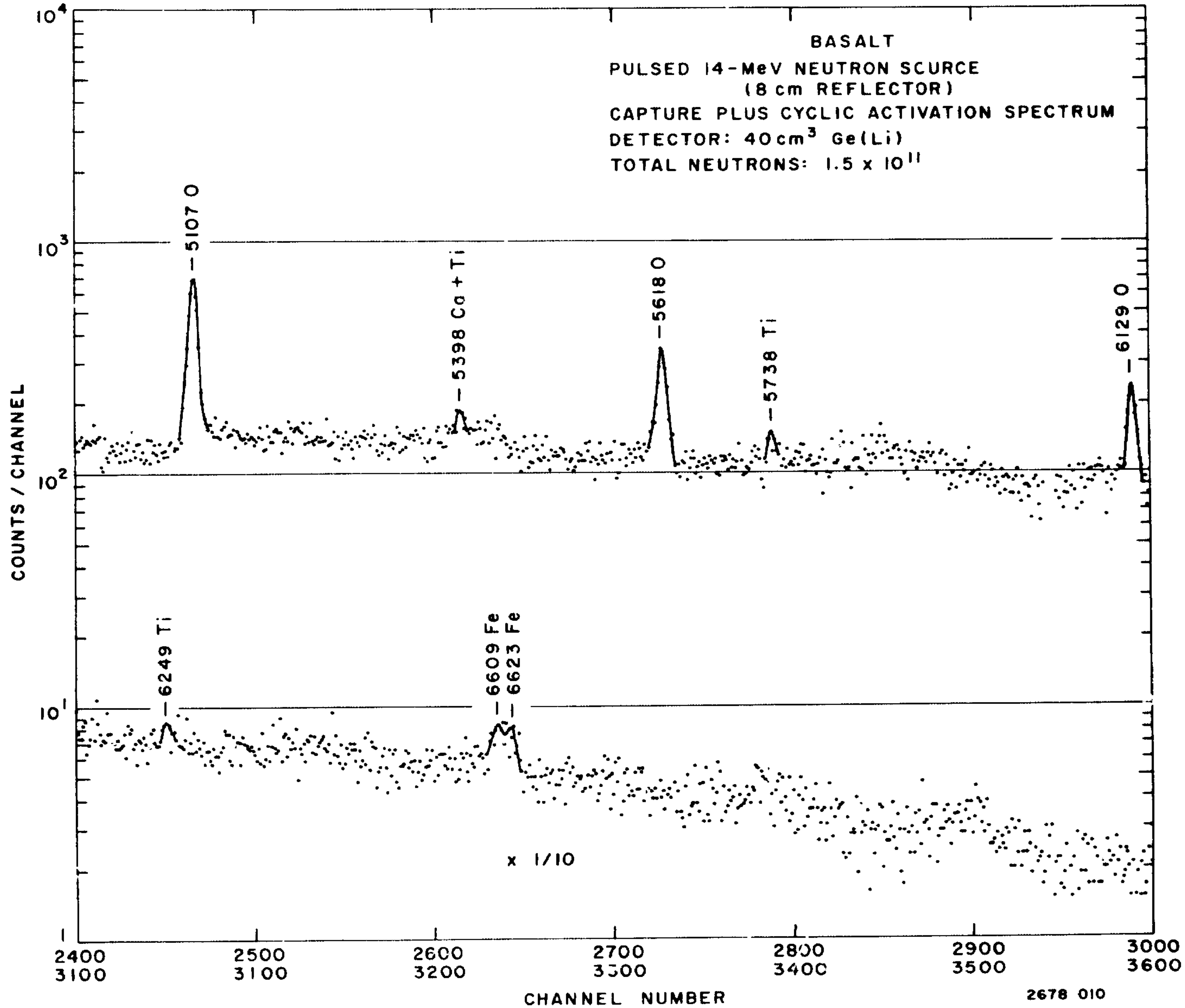

Figure 9 BASALT-CAPTURE AND CYCLIC ACTIVATION SPECTRA (40-cm^3 Ge(Li) Detector)