# A NEUTRON ACTIVATION ANALYSIS INVESTIGATION OF TRACEABLE ELEMENTS FROM AUTOMOBILE EXHAUST IN ROADSIDE SOIL AND VEGETATION

by

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This work is dedicated to my mother and

father, Mr. & Mrs. W. J. Oakes,

Jr. for their love and support

throughout my life.

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# I. INTRODUCTION

The purpose of this work was to demonstrate the effectiveness of neutron activation analysis in studying a complex environmental problem. Hence, the primary emphasis of this thesis will be on the principle of neutron activation analysis, on the experimental technique employed, the methods of data analysis and on the results. A brief introductory section on Automobile Pollution has been added to provide the reader with some insight into the factors affecting the results, and, through the references cited, additional information where desired. The author does not intend to analyze the environmental findings in any but the most general way.

The area chosen for study was the exhaust emitted by automobiles and its dispersion into the soil and selected plants near the highway. Since the dispersion would be airborne and could be either biologically active or inactive, it was decided to accumulate samples of a variety of types, viz. soil, surface accumulation on plants, and the plants themselves. Finally, several elements formed in the source of the contributing material, i.e., automobile exhaust, were studied to determine the most appropriate element to be used in studies of this type.

The findings indicated that, of the elements found in gasoline and in automobile exhaust, bromine most clearly indicated where some of the atmospheric components were going and therefore would be the most suitable element for neutron activation studies of atmos-

pheric and turbulence modeling and possibly for following biological effects of automobile traffic.

## II. AUTOMOBILE POLLUTION

### Introduction

The major man-made air pollution source of automobiles account for more than 60% of the total annual air pollutant emissions in North America (275).

Gasoline is highly volatile and the gas tank and carburetor lose hydrocarbons through evaporation (2). During an automobile engine operation, the fuel vapors from the carburetor and fuel tank are burned in the combustion chamber. The gasoline engine is imperfect and large amounts of unburned and partly burned gasoline are discharged from the exhaust; smaller amounts blow by the engine pistons to the crank case which is vented directly to the atmosphere (2). Figure 1 is an illustration showing the four main escape routes of pollution associated with gasoline from automobiles. The routes shown in the figure are numbered in the order of their importance to the total emission (241).

Some of the main pollutants from automobiles are unburned hydrocarbons, carbon monoxide, oxides of nitrogen, sulfur dioxide and particulates. In the past twenty years, the gaseous components in the exhaust stream have been widely investigated. Carbon monoxide (2, 35, 46-50, 54-56, 60, 117, 123), hydrocarbons (7-12, 15, 18, 27, 49, 101, 156), nitrogen oxides (55, 62, 71-73, 83, 222-226) and sulfur oxides (58, 59, 77, 78, 81, 82) have been studied with great interest because these components are emitted from the exhaust of gasoline engine in much larger quantities than are particulates as shown in Fig. 2.

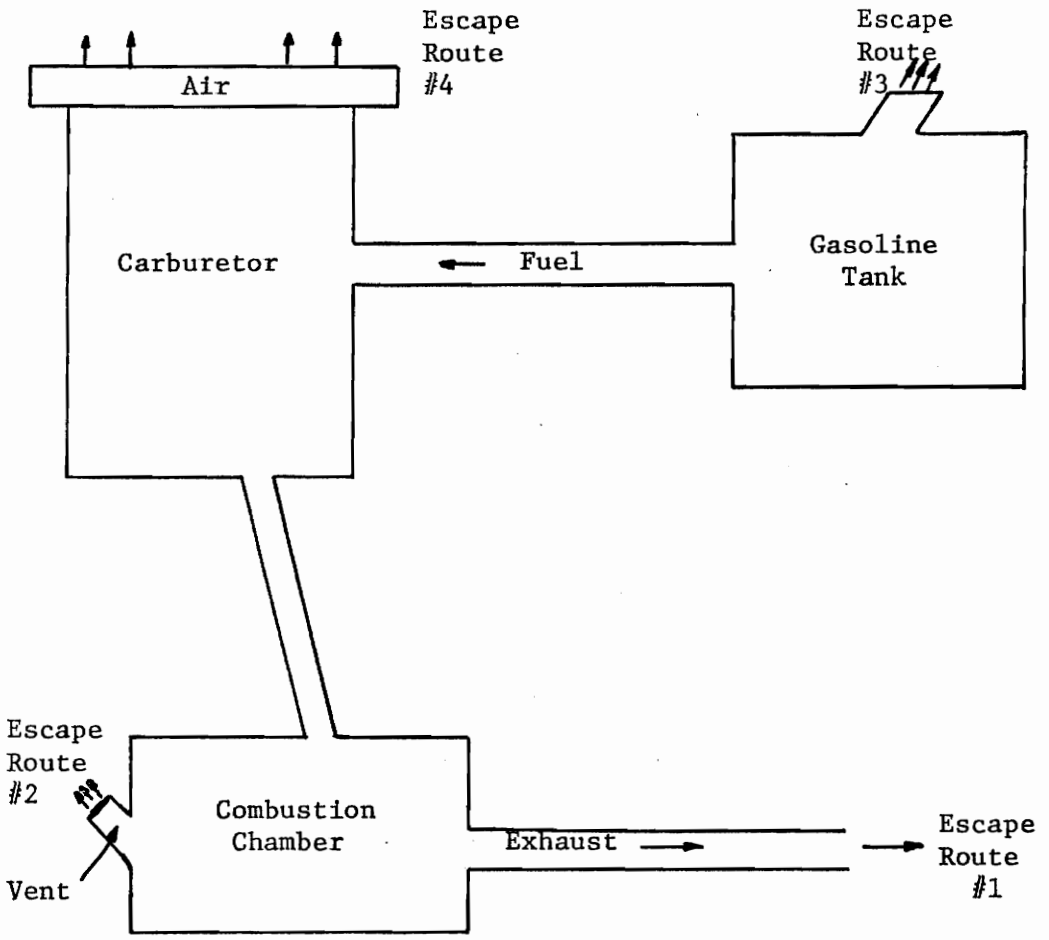



Figure 1[a]. Escape Routes for Gasoline in an Automobile

[a](From Samuel Williamson, Fundamentals Of Air Pollution, Addison-Wesley Publishing Co., Massachusetts, 1973, p. 314).

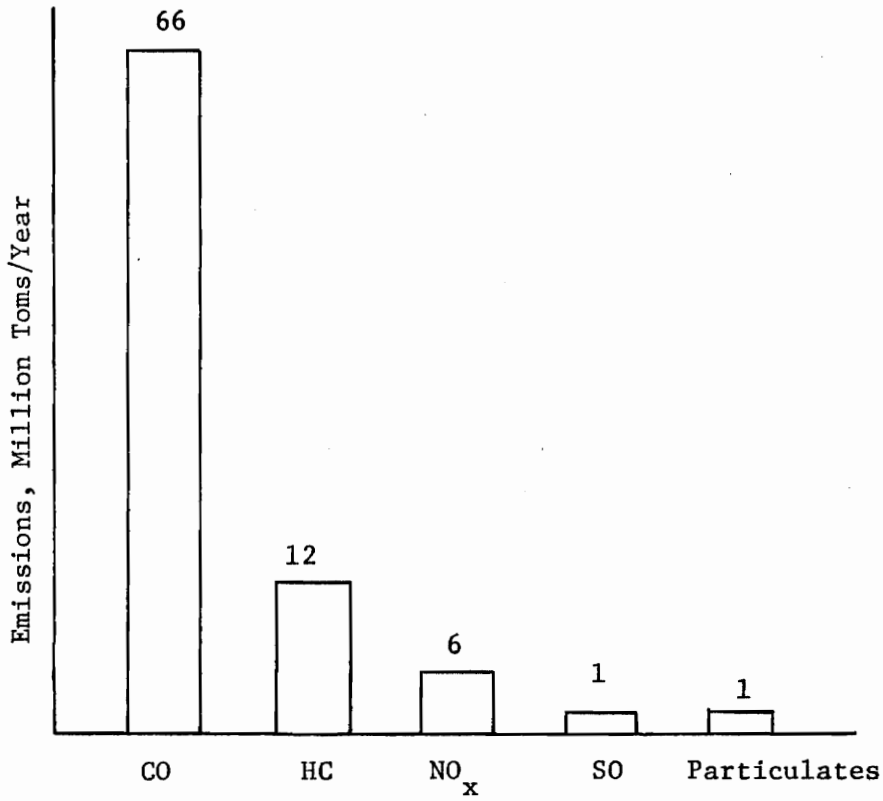



Figure 2[a]. Air Pollution in the United States from Automotive Sources

[a](From George S. Springer (Ed.), Engine Emissions Pollutant Formation and Measurement, Plenum Press, New York, 1973, p. 184).

Nevertheless, automobile engines produce about one million tons of particulate matter annually (72).

Driving cycles vary locally, therefore it is difficult to apply a general model to a region of interest when the model was not established in that region. The weight emitted, size distribution, shape and the chemical composition of the particulates are the major physical and chemical properties of particulates. Fuel composition, make of engine, wear and maintenance of engine, oil, geometry and design of the exhaust system, air to fuel ratio, surface area of the exhaust system, driving speed and load and the exhaust pressure and temperature are the major parameters contributing to these properties. These parameters vary from one automobile to another.

The temperature of the exhaust gas plays a significant role in the formation of particulates in the automobile system. Little information is available on the effect of temperature on exhaust particulate (219). One experiment (241) indicated that the total emission rate appeared to be extremely sensitive to the temperature of the exhaust gas. This effect is very noticeable above 600°F and below 200°F as shown in Table 1. Particulate emission is also affected by the type of engine and its operating condition (241).

## Exhaust Lead Compounds

Two of the most important factors influencing the efficiency of the internal combustion engine in automobiles are the combustion ratio and the octane rating (184, 187, 190, 231, 241). Tetraethyl lead

Table 1[a]

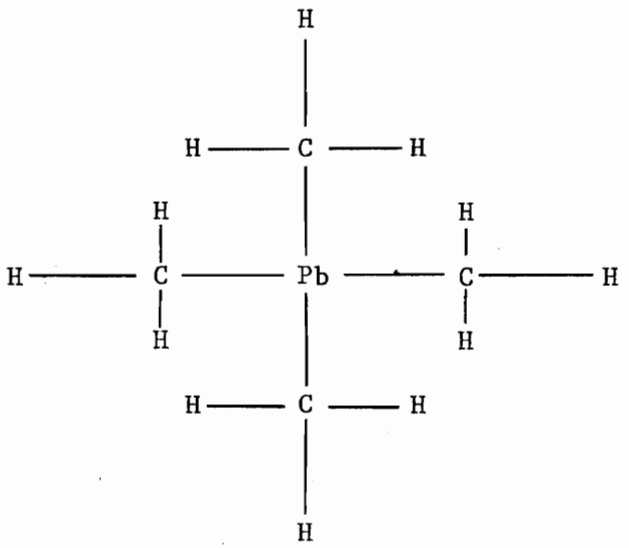
Temperature Versus Particle Concentration

of Automobile Exhaust Particulate

| Temperature (°F) | Particle Concentration ($mg/ft^3$) | Particle Emission (gm/mile) |
|---|---|---|
| 100 | 0.90 | 0.058 |
| 480 | 0.70 | 0.045 |
| 520 | 0.70 | 0.045 |
| 600 | 0.70 | 0.045 |
| 650 | 0.70 | 0.045 |
| 700 | 0.54 | 0.035 |
| 710 | 0.40 | 0.026 |
| 750 | 0.30 | 0.020 |
| 790 | 0.22 | 0.015 |
| 820 | 0.22 | 0.015 |

[a](From George S. Springer (Ed.), Engine Emissions, Plenum Press, New York, 1973, p. 195).

($[CH_3CH_2]Pb$) and tetramethyl lead ($[CH_3]_4Pb$) are added to the fuel to help produce molecular structures with better burning characteristics (142). The chemical structure (261) of tetramethyl lead is shown below. Adding these lead compounds to the fuel increases the octane rating but produces deposits of lead oxides and metallic lead which



Tetramethyl Lead

cause fouling of the values. Ethylene dibromide ($C_2H_4Br_2$) and ethylene dichloride ($C_2H_4Cl_2$) are added to gasoline as scavenging agents. These compounds react with the lead in the engine combustion chamber to form lead bromide (PbBr) compounds or lead chloride (PbCl) compounds which are emitted through the exhaust system (102, 142, 281).

The two main sources of atmospheric lead are industrial and automotive but in most areas the primary source is the automobile (279). Almost two-thirds of the lead consumed in gasoline is ex-

hausted to the atmosphere (11). Each year approximately 2.25(+8) kg. of particulate lead are dispersed into the atmosphere by automobile exhaust (232). In some areas of the northern hemisphere, the lead concentration is now about 1,000 times its natural background levels (167).

Particle diameters are an important factor in studying particle transport. It has been reported (66) in the area between 30 to 1750 ft of the roadside that 65% of the lead in the air consisted of particles with diameters under 2μ and 85% was under 4μ. The size distribution of lead particles in the air of widely different environments across the U.S. have been found to be very similar (55). The median diameter of the urban samples were 0.25μ and in 50% of the samples fell between 0.16μ and 0.43μ. One possible explanation of this uniformity in particle size is that the lead compounds form rapidly as they cool after being emitted in hot combustion stream (55).

Exhaust particles with diameters greater than 200μ were found to be composited of approximately 60 to 65% lead salts, 30 to 35% $Fe_2O_3$ and 2 to 3% soot and carbonaceous material. The compound PbBrCl is ~40 to 42% of these lead compounds with ~15 to 17% 2PbO · PbBrCl double salt and ~5 to 6% lead sulfate and lead phosphate (102). The major lead emission product in automobile exhaust with equivalent diameters of 2-10μ is lead bromochloride, PbClBr. In the smaller particle class (1μ), the alpha and beta forms of ammonium chloride and lead bromochloride, $NH_4Cl$ · 2PbClBr, $2NH_4Cl$ · PbClBr, are the major products with minor quantities of lead sulfate, $PbSO_4$, and a

mixed oxide-halide compound, $PbO \cdot PbClBr \cdot H_2O$ (140, 265). The physical and chemical characteristics of these compounds are mostly unknown except for the fact that they are unstable. The main formation of $2PbBrCl \cdot NH_4Cl$ takes place during cooling and mixing of exhaust with air (102). In some cases phosphorus compounds are added to fuel, producing up to 20% of the lead in the exhaust in the form of a phosphate-halide compound, $3Pb_3(PO_4)_2 \cdot PbBrCl$ (140).

A particulate concentration of 40-50μ g/l of exhaust was observed in an analysis of diluted automobile exhaust (171, 265). About 62-80% of the particulate mass had aerodynamic diameters below 2μ. About 40% of this particulate mass was lead compounds. Analysis of undiluted automobile exhaust have shown 90% by weight of the lead in the exhaust to have diameters below 0.5μ (42, 265). Automobile exhaust accounts for 98% of the total lead in the atmosphere that can be traced to its source (140). About 50% of the lead emitted in exhaust is removed from the atmosphere by gravity within a few hundred ft from the release point. The remaining lead stays airborne until removal by precipitation (140).

Nickel, manganese, magnesium, sodium, calcium, phosphorus and boron are also used as antiknock additives (8). Many of these additives escape out of the exhaust system and become air pollutant. Other additives to gasoline are metal deactivators, anti-icing compounds, lubricants, detergents, anti-oxidants compounds and anti-rust compounds (188). Copper, aluminum and iron oxides from the engine are released through the exhaust system (55).

Studies of automobile exhaust using X-ray diffraction (103, 113, 114) have shown the most abundant lead containing compounds to be lead bromochloride, PbBrCl. Small amounts of the alpha and beta forms of the double salt ammonium chloride • lead bromochloride, $NH_4Cl \cdot 2PbBrCl$ were found (187). Several other studies (102, 104, 115, 224) have also shown that PbBrCl and ammonium chloride compounds are the main lead sources.

The average chemical composition of particulate matter emitted from three types of automobiles using leaded gasoline is shown in Table 2. The average composition of exhausted particulate lead compounds detected in a X-ray diffraction analysis of two automobile exhaust streams are shown in Table 3.

These lead compounds are transported from their release point through the atmosphere and are deposited on plant surfaces or soil surfaces. The lead compounds may enter the plants through the leaf surfaces (17, 137, 216) or through the root system in the soil (38, 136, 137). The results of a study (169) indicated that the highest lead concentrations were found in the uppermost portion of plants. These lead compounds may have been surface absorbed material or some of it may have passed into the plant from the soil (169). In a study of corn tassels near a highway, it was found that high lead contamination was not removed by washing. The particle size of airborne lead is such that it could pass through open stomata. Lead was also found in plants grown in the soil near highways. This lead was absorbed directly from the soil (169). The amount of lead increased with

Table 2[a]

Average Chemical Composition of Particulate Matter Emitted From Three Types of Automobiles Using Leaded Gasoline

| Element | Range of Composition (%) | |
|---|---|---|
| | Fine Particles | Coarse Particles |
| Lead | 58-74 | 34-60 |
| Chlorine | 5.6-16.8 | 4.5-11.2 |
| Bromine | 8.2-21.3 | 9.2-23.6 |
| Iron | 0-1.3 | 1.2-11.2 |
| Sulfur | 0-1.9 | 0.2-2.3 |
| Carbon | 3.5-10.5 | 4.6-12.1 |

[a](From George S. Springer (Ed.), Engine Emissions, Plenum Press, New York, p. 207, 1973).

Table 3[a]

Weight % of Lead Compounds[b] in Automobile Exhaust

| | $PbCl \cdot Br$ | $\alpha$-$NH_4Cl \cdot 2PbCl \cdot Br$ | $\beta$-$NH_4Cl \cdot 2PbCl \cdot Br$ | $2NH_4Cl \cdot PbCl \cdot Br$ | $3Pb_3(PO_4)_2 \cdot PbCl \cdot Br$ |
|---|---|---|---|---|---|
| City Driving, Fuel + TEL Only | 68 | 24 | 6 | 2 | --- |
| City Driving, Sulfur added[c] | 70 | 30 | --- | --- | --- |
| City Driving, Phosphorus added[d] | 35 | 18 | 17 | 10 | 20 |
| Constant Speed 60 m.p.h. | 60 | 20 | 20 | --- | --- |
| Full-throttle accelerations | 85 | 10 | 5 | --- | --- |

[a](From George S. Springer (Ed.), Engine Emissions, Plenum Press, New York, 1973, p. 203).

[b]$PbSO_4$ and $PbO \cdot PbCl \cdot Br \cdot H_2O$ occured occasionally in concentrations of 5% or less.

[c]Sulfur content increased from 0.025 to 0.105 wt. % by added disulfide oil.

[d]0.4% theory phosphorus added in phosphorus additive.

traffic volume and decreased with distance from the highway. The greatest decrease was found to be between 30-100 ft from the highway. The distribution of lead found in the soil and plants with variations in traffic volumes and distance from the highway is very similar to the distribution of lead in air (169). Several studies (68, 175, 197, 198, 224, 226) have reported automotive lead compounds to be a significant contaminant of roadside soil. Almost all the lead compounds which accumulates in the soil remains within a few cm of the surface (181). High concentrations of PbBrCl have also been found in the bark of trees in the vicinity of a highway (249).

One study (232) reported about 50% of the airborne lead falls to the earth's surface within 30 m of the roadside. Another study (66), reported a 50% decrease in the airborne lead at 10-150 ft from the highway. Lead concentrations varying from 128 to 700 ppm were found in soil adjacent to the roadside of twelve different highways (137). In grass near a highway in Denver, Colorado, lead concentrations of as much as 3000 ppm were detected (13). An average of 115 ppm lead with a range of 10 to 700 ppm were found in some 16 types of vegetable samples within 50 ft of a road in Canadaros, New York (13).

Seasonal variations in airborne lead concentrations were observed in an investigation near U.S. Highway No. 1. The highest monthly averages were detected during the months of July and September (66). In other studies lead concentrations were shown much higher on the downwind side of the highway. Lead concentrations in the soil near U.S. Highway No. 1 on the downwind (east) side of the highway were much

higher than that of the west side (51). The lead concentrations detected in soil samples near the downwind side of a highway in Denver, Colorado indicated an average concentration of 515 ppm and ranged from 100 to 1000 ppm. These concentrations were found to be ~30% higher than on the upwind side at the roadside, ~70% higher 50 ft from the highway and ~30% higher 750 ft from the roadside. The lead concentrations versus distance decreased with distance except at 750 ft where a slight increase was found (277). Concentrations of lead found in grasses which grew adjacent to the road were greater than those away from the roadside (51).

Variations in the bromine-to-lead concentration ratio in atmospheric particulates, indicates a loss of halogens during atmospheric transport (80). When exposed to ultraviolet light, chemically pure PbBrCl decompass releasing free bromine and chlorine (187). In the absence of sunlight 70% of the exhausted lead particulates lose halogen, particularly bromine, within the first 20 min. after release (31, 211). The results of studies in Hawaii; Fairbanks, Alaska; and Cambridge, Massachusetts indicate that Br, but not Cl was depleted in lead aerosols. The extent of this depletion was found to be about the same in Fairbanks and Cambridge. The mechanism suggested for this phenomenon is the oxidation of Br, but not the more stable Cl, followed by volatilization of Br (55). The rate of production of Br and Cl gas by photochemical decomposition of lead bromochloride in carbon tetrachloride was determined in a laboratory study. These rates were used to calculate the rates at which Br and Cl might be

released into the atmosphere from lead bromochloride near a heavily traveled highway. The results indicated a release of 0.2 ppb by volume Br/hr and 0.1 ppb Cl/hr. In order to determine absolute values, the bromine and chlorine must be measured directly (55).

In the absence of sunlight, large decreases in the bromine-to-lead ratio of exhaust particulates were observed within the first hour after release (31, 211). Unidentified bromine and chlorine rich forms of PbBrCl have been detected in exhaust stream with no change in particulate composition as a function of time (165, 166). Assuming the major source of Br and Pb in automobile exhaust is the compound PbBrCl, little loss of Br has been detected in atmospheric particulates (185, 29) and in lake sediments (229).

Various concentrations of gaseous bromine have also been detected in the atmosphere. In most cases, the gaseous bromine concentrations are approximately equal to the particulate bromine concentrations (170). Oxidation of particulate bromine by ozone and other chemical oxidants or by photochemical processes has been suggested as a possible production of gaseous bromine (283). It was found in a study (187) where lead bromochloride particles were suspended in carbon tetrachloride that bromine was released by photochemical oxidation of bromine. Preliminary results of a study conducted in Cambridge, Massachusetts, indicated that a significant portion of the bromine produced by the combustion of leaded gasoline can be released to the gaseous phase with the gaseous bromine concentration being between 20 and 70% of the total bromine concentration (170). It should be noted

that this analysis was performed on a small number of samples which had limited changes of meteorological condition.

Bromine is chemically similar to chloride but in a study in the Boston area, size distribution in particles containing Br and Cl were quite different (98). Bromine was predominantly associated with small particles and, in most urban areas, originates from automobile exhaust (75, 98, 170) and the bromine-to-lead ratio in the particulate from automobile exhaust varies with time and atmosphere conditions (165). In Berkeley, California, a bromine-to-lead ratio of 0.312 was found in the atmosphere which is close to the ratio found in leaded gasoline (29). The ethyl fluid mixture of tetraethyl lead and ethylene dibromide and dichloride has the weight ratios lb:Br:Cl = 1.00:0.39:0.34 (283). A study of ten bark samples of white pine and elm trees near a highway showed large variations in lead but the lead/chloride/bromine ratio was found to fairly constant. The average ratio was 1.0/0.20/0.40 which in the case of bromine is close to that found in gasoline (107).

## Mechanisms Influencing Dispersion of Automobile Pollution

A detailed study of the factors influencing the dispersion of automobile pollution must include both macrometeorological and micrometeorological events. Macrometeorological events encompass the movement of large masses of air brought about by differences in temperature and pressure and the rotation of the earth. Micrometeorological events

encompass the local circulation and temperature variations (85).

A factor that restricts the movement of air will of course prevent the movement and dispersion of pollutants entering the atmosphere (71). The concentration of the pollutants on the earth surface or in the atmosphere is dependent on many factors. Some of these factors are: topography, wind speed, wind direction, temperature profiles and the amount of precipitation.

Atmospheric conditions near the source determine the specific path that air leaving the source will follow. These conditions also determine the extent to which the pollutant becomes chemically altered or diluted before reaching its target (243).

The importance of wind direction and speed on the dispersal of pollutants is obvious, but the variation of these two parameters with time of day and season of the year is an even greater factor (85). Meteorologic and/or topographic conditions in some areas favor the accumulation of pollutants (180).

Investigations into the topographic effects indicate that when the ground is smooth over a large area, the air flow will tend to be similarly smooth and when the ground is rough, the air passing over it will rise and fall in response to the surface undulations (139). A more detailed discussion of these mechanisms is beyond the scope of this thesis.

# III. NEUTRON ACTIVATION ANALYSIS (NAA) THEORY

## Introduction

Activation analysis is an analytical tool for qualitative and quantitative determination of the elements present in an unknown sample. Neutron irradiation of many elements creates radioactive isotopes. In neutron activation there are two phenomena taking place. First, a radioactive element is formed from the nucleus followed by radioactive decay in which an atom of one element changes spontaneously into an atom of another element. Gamma radiation associated with the radioactive decay often results from the de-excitation of the product nuclei. In this process, the energy of the nuclear transition is emitted as discrete quanta which are unique to that decay mode. Thus, for a given transition, one or more gamma rays are emitted with the same energies. This property makes gamma radiation useful for identifying specific radionuclides in the presence of many other radionuclides. The identification of several radionuclides simultaneously by their characteristic gamma ray energies has become an important method in activation analysis (132). The principles in activation analysis involve radioactive isotopic characteristics, interactions of radiation with matter and nuclear transformations (132).

## Neutron Interactions

Since the neutron is an uncharged particle, it can approach a target nucleus unhampered by the couloumb forces of electrostatic

interactions. The four most common neutron reactions are listed below: (94)

1) Neutron capture - This reaction involves the absorption of a neutron with the prompt emission of a gamma ray.
2) Transmutation - This reaction involves the absorption of a neutron with the subsequent release of a charged particle.
3) Fission - This reaction involves the absorption of a neutron and results in the splitting of the nucleus into two large fragments.
4) Scattering - This reaction is when the neutron transfers only part of its kinetic energy and escapes with less energy, generally with no significant change in the target nucleus.

The most common activation reaction is the neutron capture process. The nucleus produced in these reactions are often left in an excited state and decay from this unstable condition to a more stable one. During this decay process the following possibilities exist (94).

1) Electron emission
2) Positron emission
3) Electron capture
4) Alpha emission
5) Gamma emission.

In neutron activation analysis, detection of the gamma rays in the fifth process is the most common analytical mechanism.

## Interactions of Gamma Rays

Gamma rays are electromagnetic radiation which can be described as a quantum of energy called photons. The energy of a photon can be determined using Equation 1 (6).

$$E_\gamma = h\nu. \tag{1}$$

Where

$h$ = Planck's constant

$\nu$ = frequency of the photon.

The three main processes in which gamma rays interact with matter are: photoelectric effect, Compton effect and pair production. These interactions are of importance in the detection process and in processing the data. A detailed discussion of these interactions is given in this section and their role in the detection process will be discussed in the section entitled Gamma Interactions in the Detection Process.

At low energies (< 1 Mev), the most important gamma absorption process is the photoelectric effect. In the photoelectric effect, the photon transfers all of its energy to an orbital electron of an atom of the substance and ejects it from the atom. The interacting electron is ejected from the atom with kinetic energy $E_p$ which can be determined using Equation 2 (6).

$$E_p = h\nu - E_b. \tag{2}$$

Where

$h\nu$ = energy of the incident photon

$E_b$ = binding energy of the interacting electron.

A schematic diagram showing the photoelectric effect can be found in Fig. 3a. The cross section for this process is proportional to $Z^5$ (132) where Z is the number of protons in the nucleus.

In the photoelectric effect an electron from an inner orbital can be removed, leaving a vacancy in that orbital. This vacancy is filled by one of the outer electrons or a free electron giving up its excess energy by emitting a photon. These photons are called fluorescent radiation or X-rays. In some cases these X-rays strike electrons in higher orbital shells of the atom ejecting these electrons, which are called Auger electrons. A schematic diagram showing fluorescent radiation and Auger electrons can be found in Fig. 3b.

The Compton effect becomes predominant when the gamma energy is greater than 1 Mev and the photon energy is much greater than the binding energy of the interacting electron (132). In the Compton process, the incident photon gives up part of its energy to the interacting electron and is scattered at an angle Θ with the initial direction of the photon. In general the electron involved is a free or loosely bound electron. A schematic diagram showing the Compton effect can be found in Fig. 3c.

The energy of the scattered photon can be described using Equation 3 (6, 94, 132).

$$E_\gamma' = \frac{E_\gamma}{1 + E_\gamma/mc^2\ (1-\cos\Theta)}. \qquad (3)$$

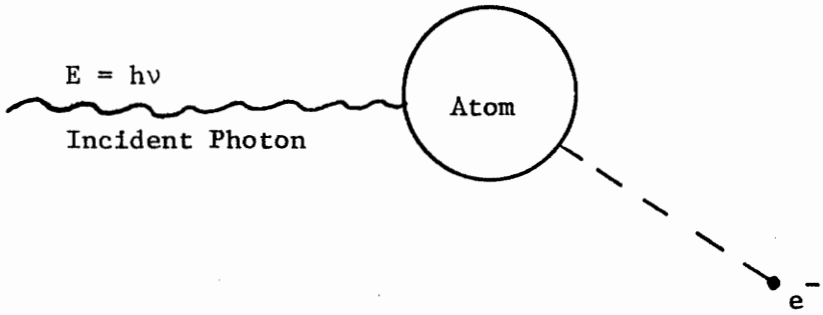
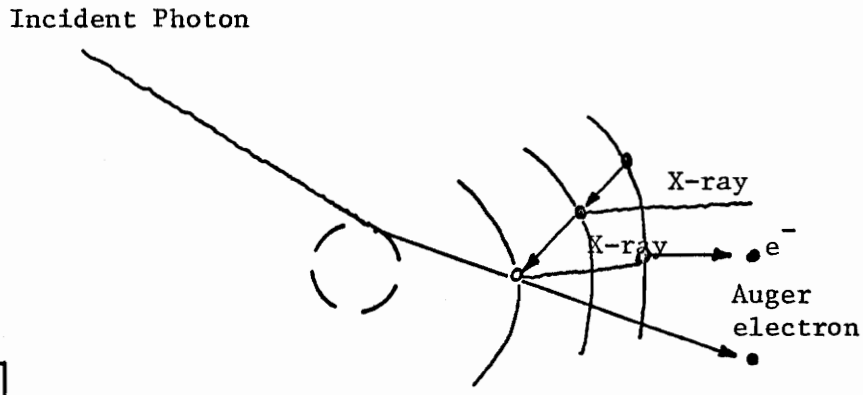



Figure 3a. Schematic of Photo-electric Effect

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• Electron

o Vacancy

Figure 3b. Schematic of Fluorescent Radiation and Auger Electron

Where

$E_\gamma$ = energy of the incident photon

m = rest mass of electron

c = velocity of light

$\Theta$ = angle of scattered photon.

The scattered electron energy ($E_e$) can be described using Equation 4.

$$E_e = E_\gamma - E_\gamma'. \tag{4}$$

At higher gamma energies (≥ 1.02 Mev), the pair production process becomes important (132). In this process the photon interacts with the electric field of the nucleus. The photon is absorbed to create a positive (positron) and negative (electron) pair. The minimum energy needed for pair production is given by Equation 5.

$$E = 2\ m_o\ c^2. \tag{5}$$

Where

$m_o$ = rest mass of a positron or electron

c = velocity of light.

The rest energy of an electron is 0.511 Mev, therefore, by solving Equation 5 it can be shown that the photon must have an energy ≧ 1.02 Mev for pair production to occur. The photon energy greater than 1.02 Mev is transferred to the electron-positron pair as kinetic energy. The electron and positron lose kinetic energy through ionization in

the substance and the positron, after coming to rest, interacts with an electron in a process called annihilation. In the annihilation process the mass of the particles are converted into two photons of 0.511 Mev each. After the annihilation process, the two photons are available to interact by the photoelectric or Compton effects. The cross section for the pair production process is proportional to $Z^2$ (132). A schematic diagram showing the pair production process is shown in Fig. 3d. The energy of the electron or positron can be determined using Equation 6.

$$E_{e^-} \text{ or } {}_{e^+} = 1.02 \text{ Mev} - E_\gamma/2. \tag{6}$$

Where

$E_\gamma$ = the energy (Mev) of incident gamma.

As noted above, 1.02 Mev is the energy needed to produce the pair. The remaining energy is divided equally between the two particles as kinetic energy.

## Decay Schemes

Radionuclides are characterized by their half-lives and decay schemes which are unique for each radionuclide. A decay scheme (disintegration scheme) is a representation of the decay modes of de-excitation and the energy levels of radionuclides. An illustration of a decay scheme is shown in Fig. 4a. Three β decay modes are shown in

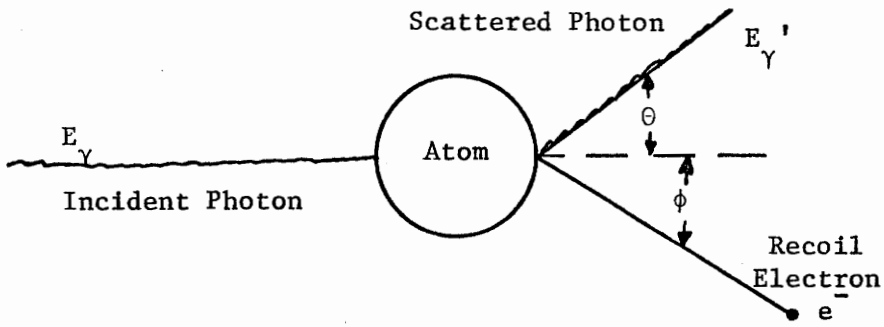



Figure 3c. Schematic of Compton Effect

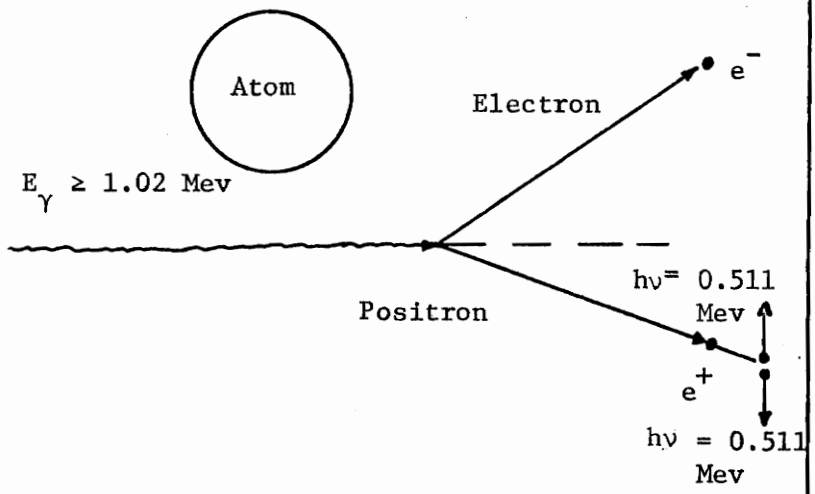



Figure 3d. Schematic of Pair Production Effect

the decay scheme. In two of the decay modes, after the β decay takes place, the isotope is left in an excited state and decays by characteric gamma emissions to the ground state. Although all possible gammas are shown, it would be possible for only $\gamma_2$ and $\gamma_3$ to occur or $\gamma_1$ and $\gamma_2$.

Figure 4b is an illustration showing a simple spectrum of the characteric gamma rays from the decay scheme shown in Fig. 4a. This illustration shows the relationship between the gammas emitted and the peaks indicated in a spectrum.

## Cross Sections and Reaction Rates

The cross section for a reaction is the probability of interaction and individual probabilities or cross sections can be summed to give the total probability. The total cross section is the sum of the absorption and scattering cross sections. For fissionable materials, the absorption cross section is the sum of the fission and radiative capture cross sections. The microscopic cross section, σ, may be considered as the cross sectional area of a hypothetical sphere surrounding the nucleus such that a neutron entering the sphere will react with the nucleus (186). The unit used for microscopic cross sections is the barn defined as $10^{-24}$ $cm^2$. In many cases the microscopic cross section of a nucleus is many times larger than the actual cross sectional area of the nucleus. Consider the following example, for $^{116}In$ (94).

The radius of a nucleus can be determined using Equation 7.

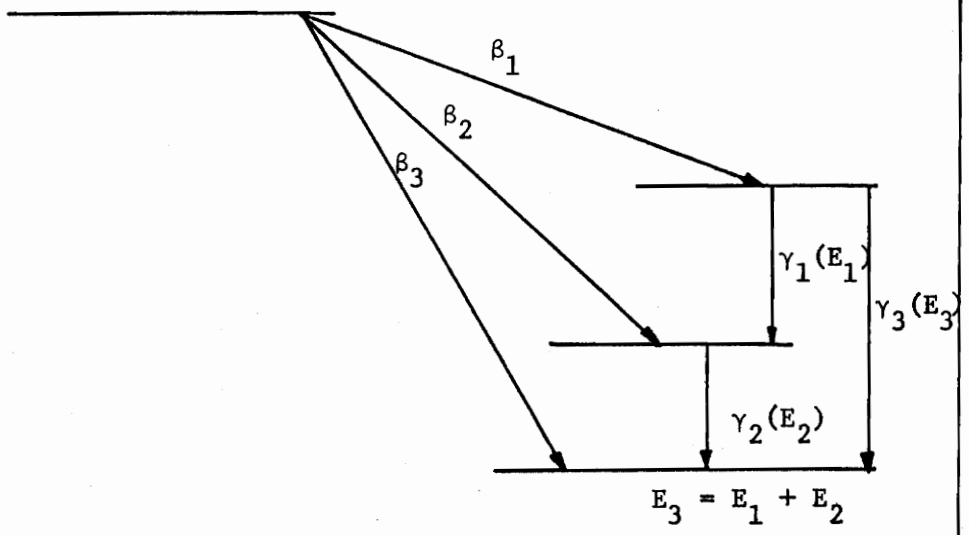



Figure 4a. Schematic of a Decay Scheme

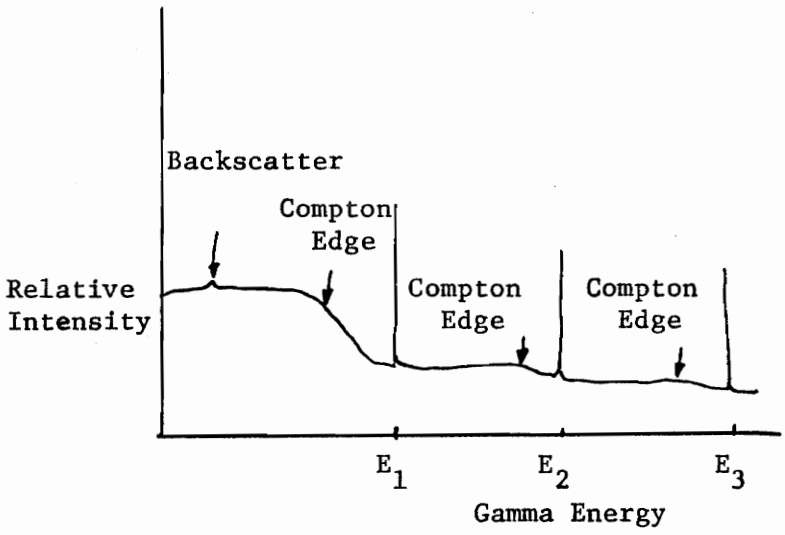



Figure 4b. Schematic of a Simple Spectrum

$$R = 1.4 \times 10^{-13} A\ 1/3. \tag{7}$$

Where

A = mass number

Constant = $1.4 \times 10^{-13} = r_o$.

The area of a nucleus can be determined using Equation 8.

$$\text{Area} = \pi R^2 \cong 6.16 \times 10^{-26} A\ 2/3. \tag{8}$$

Solving Equation 8 for $^{116}$In gives an area of $1.46 \times 10^{-24}$ cm$^2$ or 1.46 barns. However, the experimental thermal capture cross section is 205 barns. It is not possible to compute cross sections theoretically, therefore, they must be determined experimentally (94).

The target material contains N nuclei per cm$^3$ and the quantity, $N\Sigma$ is equivalent to the total cross section of the nuclei per cm$^3$ (89, 99, 186). This quantity is called the macroscopic cross section, $\Sigma$, of the material and is defined as (89, 99, 179, 186),

$$\Sigma = N\left(\frac{\text{nuclei}}{\text{cm}^3}\right) \sigma\ (\text{cm}^2) = N\ \sigma\ \frac{1}{\text{cm}}\ . \tag{9}$$

The number of nuclei per cubic centimeter, N, can be determined using Equation 10 (89, 179, 186).

$$N = \frac{\rho\ Na}{A}\ \frac{\text{atoms}}{\text{cm}^3}\ . \tag{10}$$

Where

$\rho$ = density of material = g/cm$^3$

Na = Avogadro's number = $6.023 \times 10^{23}$ atoms/gram-atom

A = Atomic weight = g/gram-atom.

The rate at which nuclear reactions occur can be determined using Equation 11 (89, 99, 186).

$$R = \Sigma \phi \text{ neutrons/cm}^3\text{-sec.} \tag{11}$$

Where

$\Sigma$ = Macroscopic cross section (1/cm)

$\phi$ = Neutron flux (neutrons/$cm^2$-sec).

The neutron flux, $\phi$, is defined as the product of the number of neutrons per cubic centimeter, n, and the velocity of these neutrons, v, as shown in Equation 12.

$$\phi = n \text{ (neutrons/cm}^3\text{) } v\text{(cm/sec)} = nv \text{ neutrons/cm}^2\text{-sec.} \tag{12}$$

The flux used in this study for activation was $1.2 \times 10^{12}$ n/$cm^2$-sec for short activations and $1.3 \times 10^{12}$ n/$cm^2$-sec for long activations.

## Abundance Determination

The abundance of an isotope can be determined by the absolute calibration of the counting system or by a comparator technique (53). The abundance of an isotope can be determined by the first method solving Equation 13.

$$\text{Abundance (ppm)} = \frac{N*A*\lambda*10^6}{60*F*\epsilon*b*\sigma*\phi*W*0.602}\left[\frac{1}{\left(1-e^{-\lambda t_a}\right)\left(1-e^{-\lambda t_c}\right)\left(e^{-\lambda t_w}\right)}\right] \tag{13}$$

Where

$N$ = Number of counts in the gamma peak.

$A$ = Atomic weight of the isotope $\left(\frac{1}{\text{mole}}\right)$.

$\lambda = \frac{0.693}{\text{Half-life}}$ = Decay constant of the isotope under investigation $\left(\frac{1}{\text{units of time}}\right)$.

$\epsilon$ = Detector efficiency at the gamma energy of the isotope.

$b$ = Branching ratio of the gamma.

$\sigma$* = Activation cross section of the isotope under investigation ($cm^2$).

$\phi$ = Neutron flux used for sample irradiation $\left(\frac{n}{cm^2 - sec}\right)$.

$W$ = Mass of sample (grams).

$t_a$ = Activation time (units of time).

$t_w$ = Wait time (units of time).

$t_c$ = Counting time (units of time).

*The cross section for an interaction is a measure of the probability for that interaction. The units of cross section are the barn. (1 barn = $10^{-24}$ $cm^2$).

The activation time is the time the sample was irradiated at flux $\phi$. The wait time is the time after irradiation until the beginning of counting. The counting time is the length of time the samples were counted.

The results obtained using the first technique can be no more reliable than are the nuclear constants used; such as cross sections (53). To avoid this problem the NAA program used for this investigation uses the comparator technique. A comparison is made of the unknown spectrum to previously run standards. This is discussed in the section entitled Neutron Activation Computer Program (VPI & SU).

## Gamma Interactions in the Detection Process

As discussed in a previous section, the three primary gamma-ray interaction processes in which incident photons give up all or part of their energy in a single event are: photoelectric effect, Compton scattering, and pair production.

In a photoelectric interaction, the total photon energy is absorbed by a bound atomic electron and is detected as the kinetic energy of that electron as it is ejected or as an X-ray or Auger electron emitted by the residual ion. The low energy X-ray have a high probability of being absorbed in a second photoelectric event before it can escape from the crystal. In the photoelectric effect, the total photon energy appears as electron kinetic energy; therefore, a monoenergetic gamma-ray would result in a monoenergetic peak with energy corresponding to the incident photon energy (132).

In the Compton scattering process, the photon is scattered by an electron with a partial energy loss. The electron kinetic energy lies between zero and an upper energy limit which is dependent on the incident photon energy. This scattering process gives rise to a con-

tinuous electron energy distribution between these limits. The Compton process is not as highly energy dependent as the photoelectric effect and is proportional to the Z of the scattering material (132).

Figure 5a is an illustration showing a spectrum representation of the Compton and photoelectric effect. This is the cumulative result of a large number of detected events. The degree to which the total absorption peak is broadened is a function of the energy resolution of the detector. The worse the energy resolution the more difficult it is to display separately gamma rays having energies close together. Shown in Fig. 5a are the photopeak of Ar-41 (1.29 Mev), Compton edge and the backscatter peak with the data taken by a scintillation spectrometer.

The pair production process has an energetic threshold equal to the combined positron-electron rest mass (1.02 Mev). The cross section increases rapidly above this threshold and is proportional to $Z^2$ of the scattering material. The total photon energy is absorbed and appears as the total kinetic energy of the positron-electron pair. The positron is unstable and will annihilate with an atomic electron.

During the positron annihilation process, two photons of energy 0.511 Mev are produced and emitted at 180° to each other. In most cases, both annihilation photons will escape. In such a case, a double escape peak will appear in the spectrum at an energy equal to the total absorption peak minus 1.02 Mev. There is a lower probability that only one annihilation photon will escape from the crystal creating a single escape peak at an energy equal to that of the total absorption

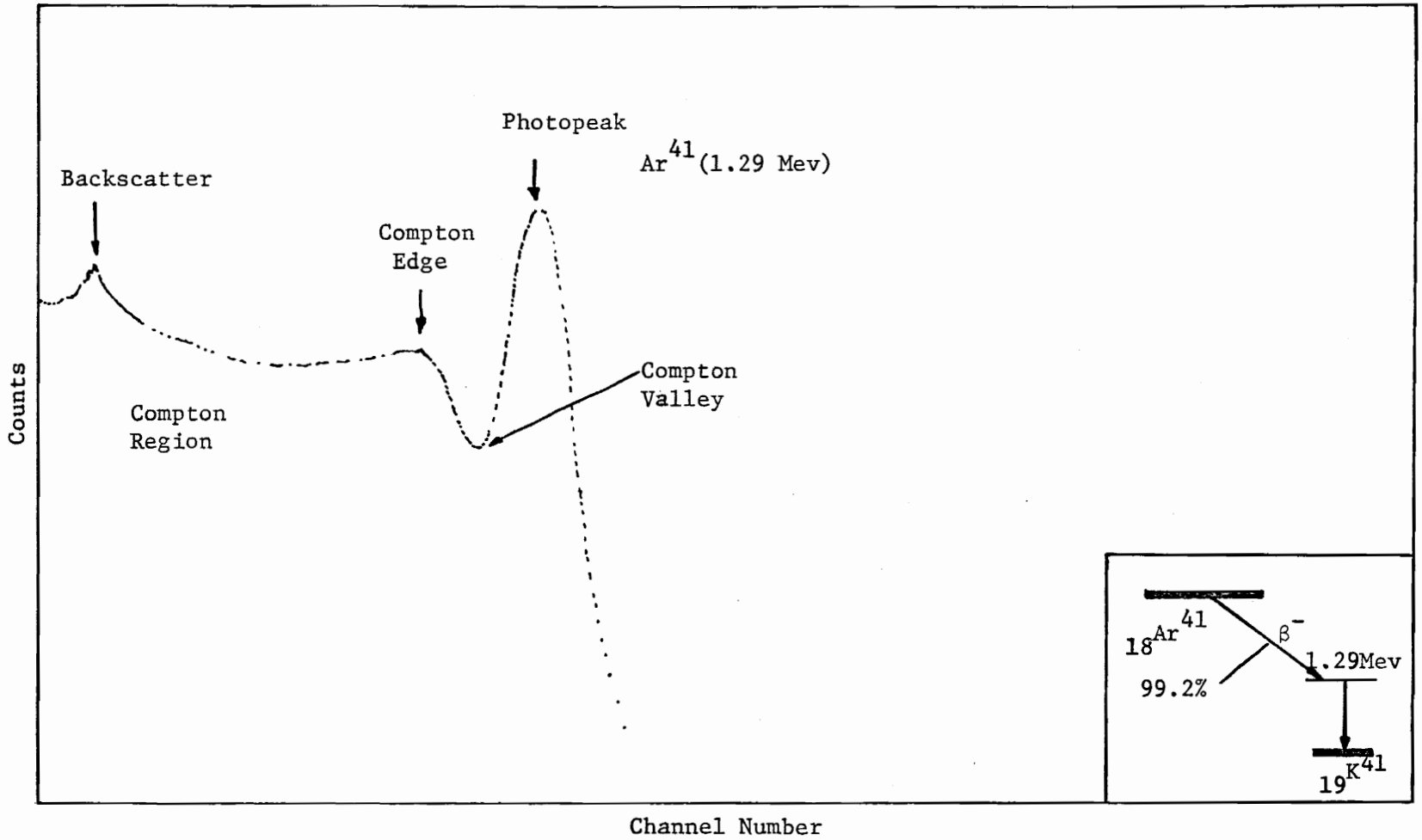



Figure 5a[a]. Compton Interaction Representation

[a](Adapted from Dr. A. K. Furr, Neutron Activation Analysis, p. 44, 1970).

peak minus 0.511 Mev. A low probability also exist for both photons being absorbed creating a full energy peak. Shown in Fig. 5b are the photopeak of Al-28 (1.78 Mev), the single (1.29 Mev) and the double (0.79 Mev) escape peaks, the annihilation peak and the backscatter peak. Again, the data taken with a scintillation spectrometer.

Frequently when an isotope emits two or more gamma rays in cascade, the photon production and interaction time are so short that the detector will produce a pulse that corresponds to the sum of the energies of the two gamma rays.

Figure 6a is an illustration showing the decay scheme for sodium-24 and Fig. 7a shows the decay scheme for cobalt-60. Figure 6b and Fig. 7b are computer plots of the data spectrum of a standard for sodium and cobalt, respectively. Cobalt-60 emits two major gamma rays of 1.17 and 1.33 Mev and sodium-24 emits two major gamma rays of 1.36 and 2.75 Mev. The sum peak of cobalt-60 (2.50 Mev) and the two escape peaks of sodium-24 (2.25 Mev and 1.74 Mev) are also illustrated in these figures. The data in these cases were taken with a Ge(Li) detector.

## Lithium Ion-Drifted P-I-N Semiconductor Theory

A semiconductor can be defined as a material whose resistance to electricity is between that of conductors and insulators (6, 132, 270). Quantum mechanical consideration of the band theory of solids can be used to explain the properties of semiconductors (284). When a group of atoms is brought together to form a solid, the neighboring atoms cause the energy levels associated with each atom to shift. After the

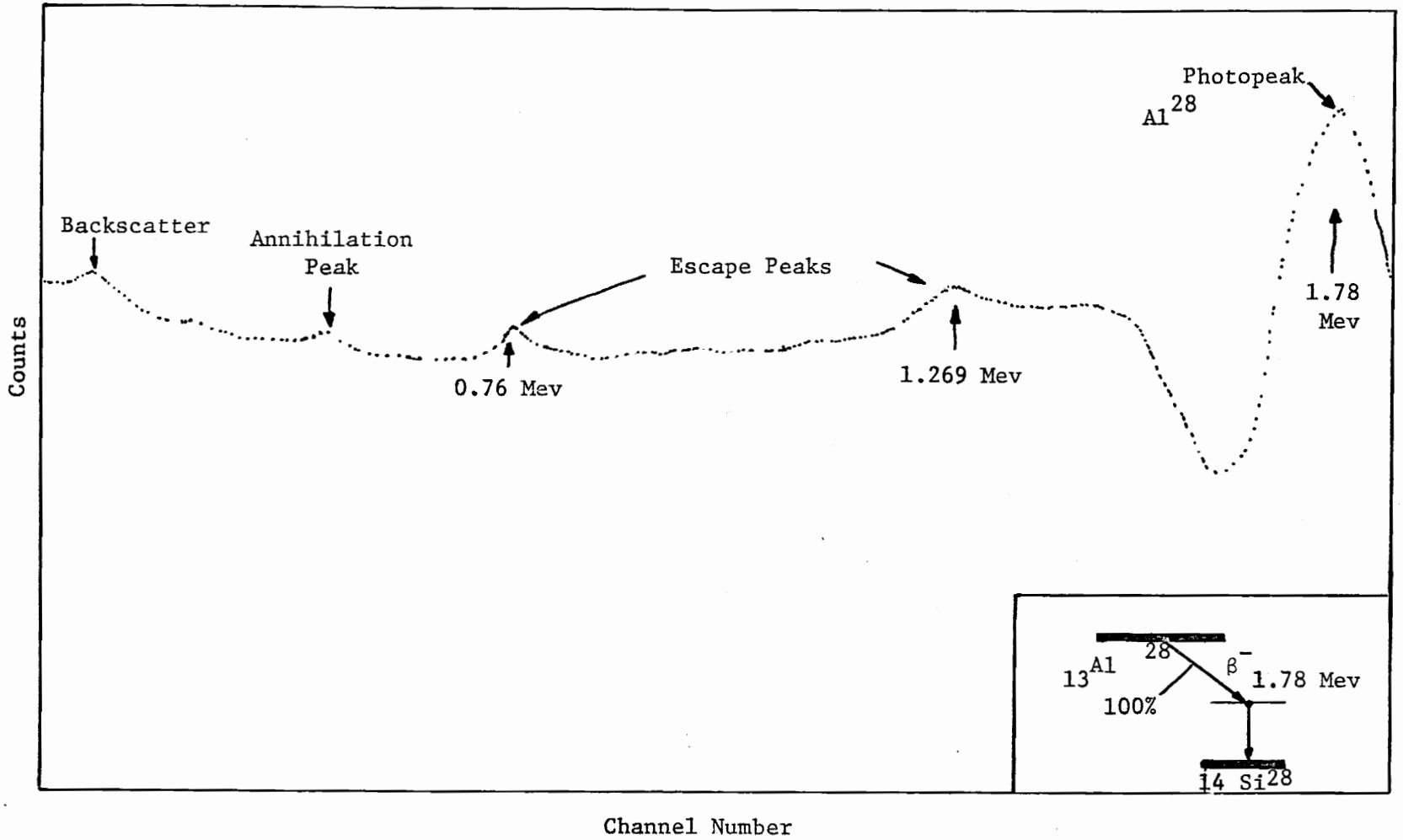



Figure 5b[a]. Annihilation and Escape Peak Representation

[a](Adapted from Dr. A. K. Furr, Neutron Activation Analysis, p. 45, 1970).

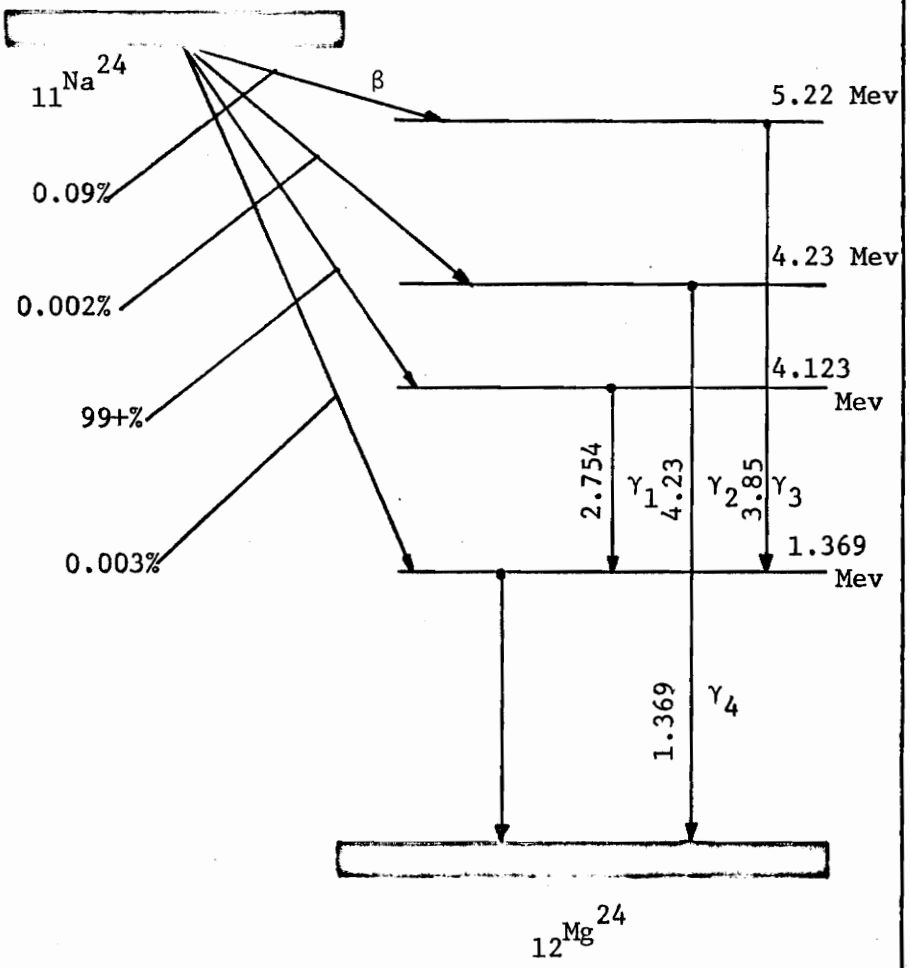



Figure 6a[a]. Decay Scheme - Na-24

[a](From C. Michael Lederer, Table of Isotopes (sixth Edition), p. 164, 1966).

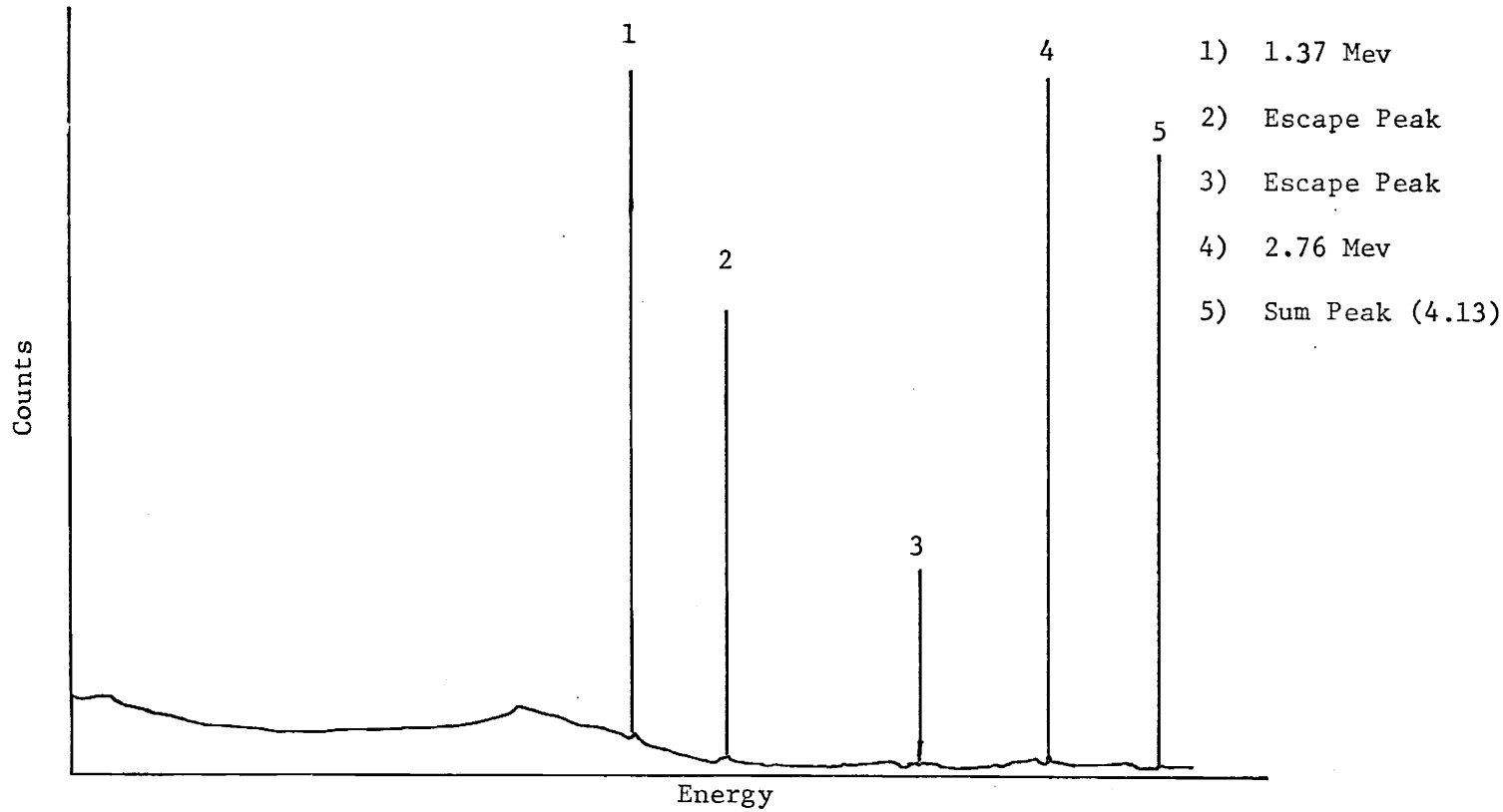



Figure 6b. Plot of Na-24 Standard

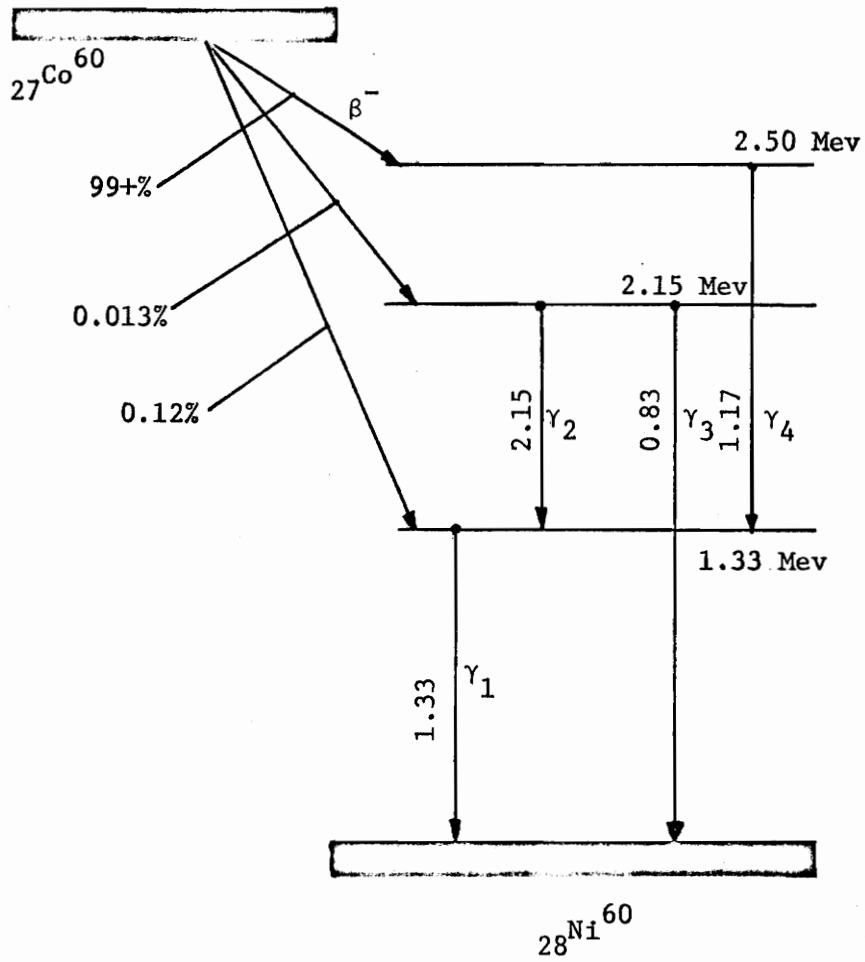



Figure 7a[a]. Decay Scheme Co- 60

[a](From C. Michael Lederer, Table of Isotopes, (Sixth Edition), p. 194 1966).

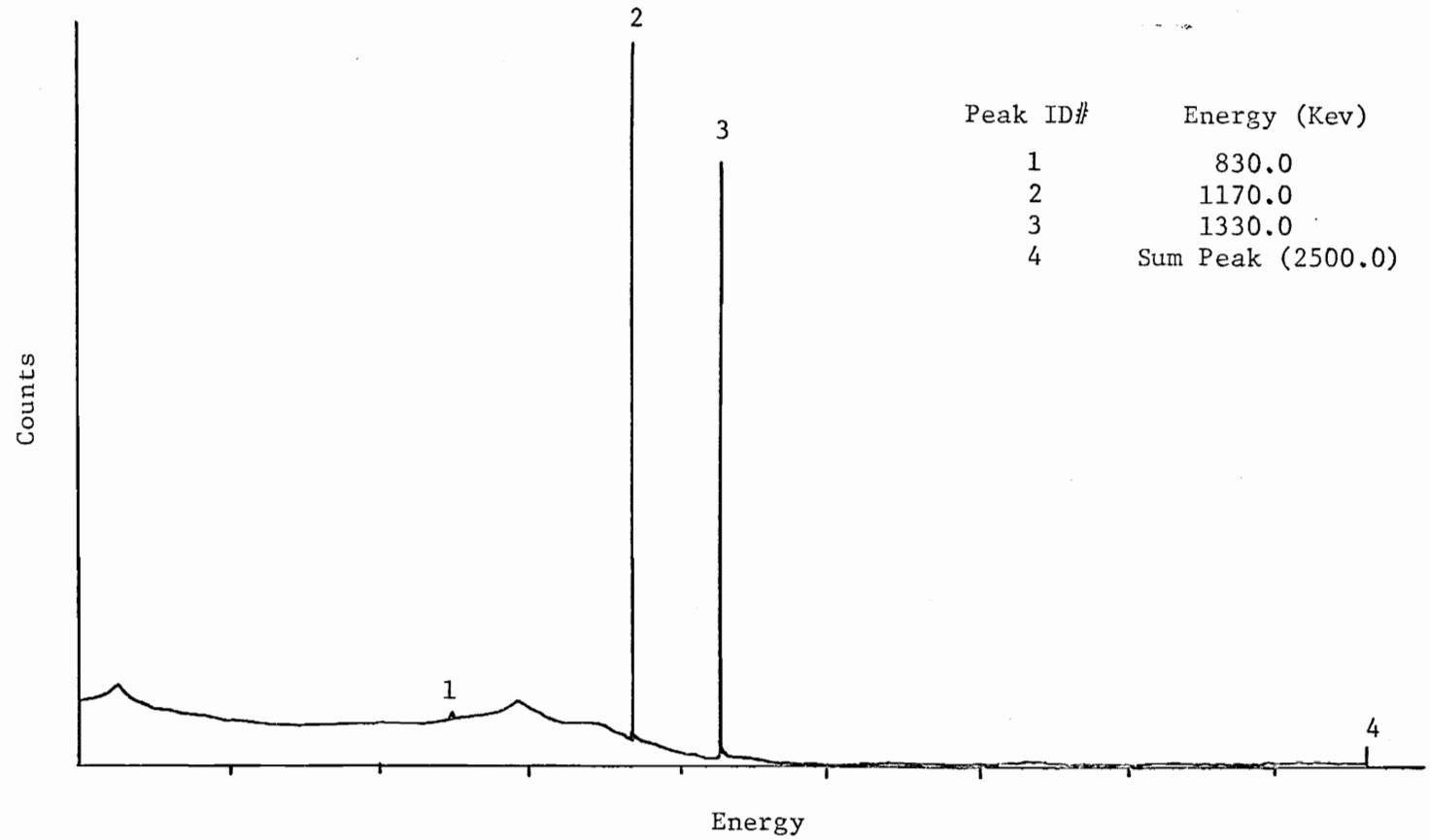



Figure 7b. Computer Plot of Co-60 Standard

shifting of these energy levels, the potential energy of each electron in the atom is changed. There is a significant shift in the potential energies of the outer electrons (270, 284). The inner and outer electronic energy levels of the atoms are considered in the band theory where, as groups of atoms form a solid, the sharp energy levels of the individual atoms become broadened into energy bands (94).

The two most important semiconductors are germanium and silicon. These elements are located in the fourth column of the periodic table and have four valence electrons. The discussion in this section will be restricted to germanium because it is the type of semiconductor used in the detector system used for this study. Germanium forms a tetrahedral crystal structure with each atom sharing one valence electron with each of the four nearest neighboring atoms. The valence electrons are tightly bound to individual atoms. The energy required to break a covalent bond is 0.66 ev for germanium (6, 53, 94, 132, 270, 284).

In semiconductors the conduction band is nearly empty of electrons and the valence band is almost filled with electrons (6, 132, 270). It is relatively easy to thermally excite electrons from the valence to the conduction band. The electrical conductivity of semiconductors increases with increasing temperature. As the temperature is increased, thermal agitation supplies some of the electrons with enough energy to jump into a higher band (132). The excited electrons act as conduction electrons (270). The valences or holes left in the lower level band by these electrons act as positive charge carriers (94).

Increasing temperature causes more electrons to transfer to the conduction band making the semiconductor a better conductor. The difference in conductivity of semiconductors is determined by the number density of electron transitions from the valence band to the conduction band (132, 270).

As stated above, when a covalent bond is broken, a vacancy or hole is created. In semiconductors the number of holes in the valence band are equal to the number of electrons in the conduction band (132, 270). At a given temperature the concentration of electrons and holes can be

$$n = p = N(E)\ e^{-E_g/2kT}. \qquad (14)$$

Where

$E_g$ = energy gap in ev

k = Boltzmann constant

T = absolute temperature.

N(E) = the number of allowed energy states per unit energy interval at 300°k

n = concentration of electrons

p = concentration of holes

kT = 0.026 ev (300°k).

N(E) is a property of the band structure of each semiconductor

$$N(E) \simeq 10^{19}.$$

If Equation 14 is solved for germanium at 300°k, the concentrations of holes and electrons is equal to $2.35 \times 10^{13}$ $cm^{-3}$ (132).

Impurities in the crystal lattice of semiconductors introduce sources of charge carriers and thus enhances the conductivity of the semiconductors (6, 132). As stated earlier, germanium is a member of group IV of the periodic table. The impurities in these crystal lattices are often atoms of chemical group V. Atoms of this group can have four of its valence electrons in the valence band of the crystal, leaving one electron loosely bound to its parent atom (132). These excess electrons are easily excited from the atom into the conduction band (6, 132, 270, 284). Impurities of this type donate an excess of negative carriers and are often called donors. The crystals formed with these impurities are called n-type semiconductors. A schematic diagram of this type semiconductor is shown in Fig. 8a.

Impurities in chemical group III create holes in the valence band (6, 132, 270). These elements lack valence electrons to complete the lattice bonds. Electrons with excitation energy above the valence band level often fill these holes. The transfer of these electrons leaves holes in the valence band without having mobile electrons in the conduction band (6, 132, 270). Impurities of this type accept electrons and leave an excess of positive hole carriers. The crystal formed with these impurities are called p-type semiconductors. A schematic diagram of this type of semiconductor is shown in Fig. 8b.

Lithium ion-drifted P-I-N junction semiconductors are widely used in gamma ray spectroscopy. Lithium, with three electrons serves to bind or fix excess electrons from group V impurities and greatly decreases the conductivity of the crystal. The same result can be

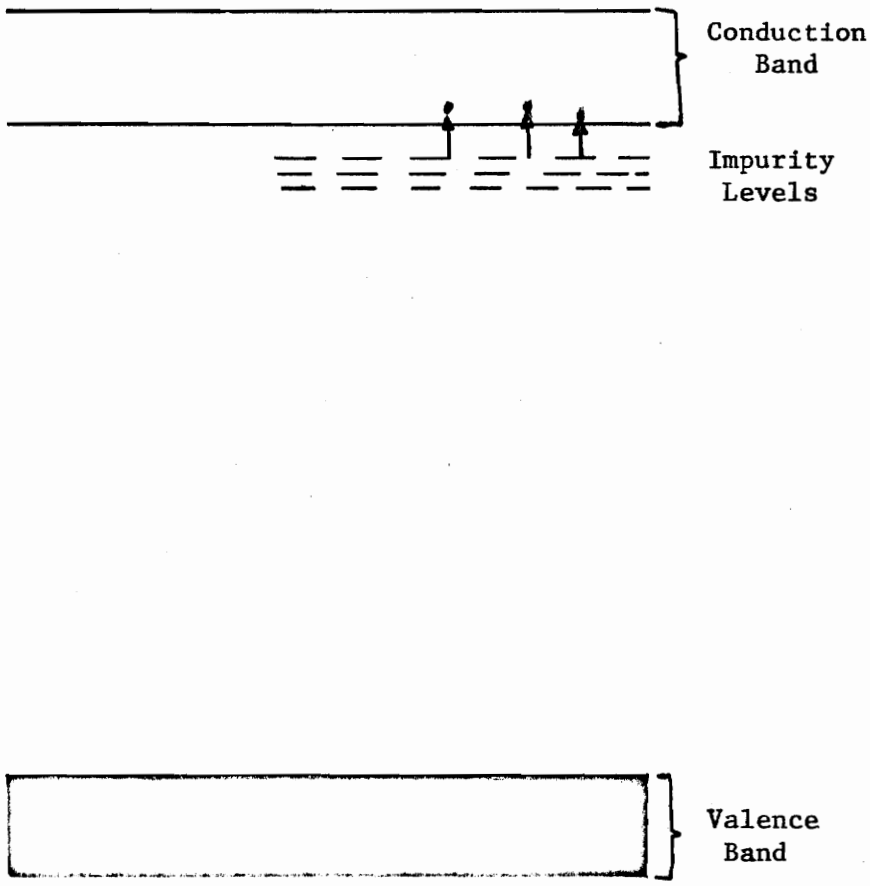



Figure 8a[a]. N-type Semiconductor

[a](From Marcelo, Alonso and Edward J. Finn, Fundamental University Physics Vol. 3, p. 266, 1968).

LEGEND

• electron

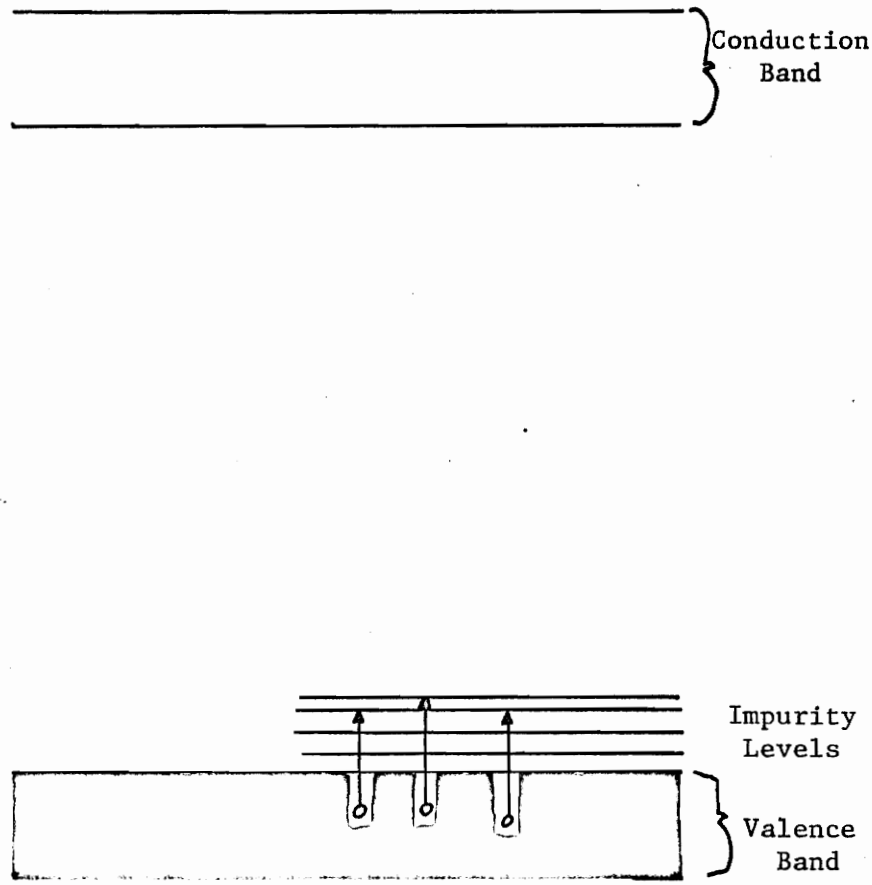



Figure 8b[a]. P-type Semiconductor

[a](From Marcelo Alonso and Edward J. Finn, Fundamental University Physics Vol. 3, p. 266, 1968).

LEGEND

o Valancy

achieved by improved purification of the crystal but at much greater cost. A significant increase in the efficiency for the absorption of gamma rays can be achieved by increasing the thickness of the depletion layers through the use of lithium drifting. The depletion region is the sensitive layer formed between the "n" and "p" type region when a bias voltage is applied. In this region the free electrons and holes are swept out by the applied voltage.

Germanium has a relatively high efficiency for gamma photoelectric effect absorption. The photoelectric absorption coefficient increases as $Z^5$. Germanium is about 40 times more effective than silicon (132). Higher atomic number semiconductors are being tried but so far have encountered problems. The variation of the absorption coefficient, for the photoelectric, Compton and pair production processes in germanium, as a function of energy is shown in Fig. 9. Direct ionization by the incident photon is the detection process used by semiconductor detector. Electron hole pairs are created during the ionization process and negative ions which are created in the depletion swept toward the positive (n-type) end (53, 132). Figures 10a and 10b are schematic diagrams showing the energy bands of a semiconductor material in general and germanium energy bands, respectively. In germanium, the energy expanded per ion pair is about 3 ev thus, an interacting 1 Mev photon would produce approximately 330,000 ion pairs. The number of ions created is directly related to the energy of the ionizing event. The current pulse representing the collected ions can be amplified and the amplitude of the resulting pulse is also

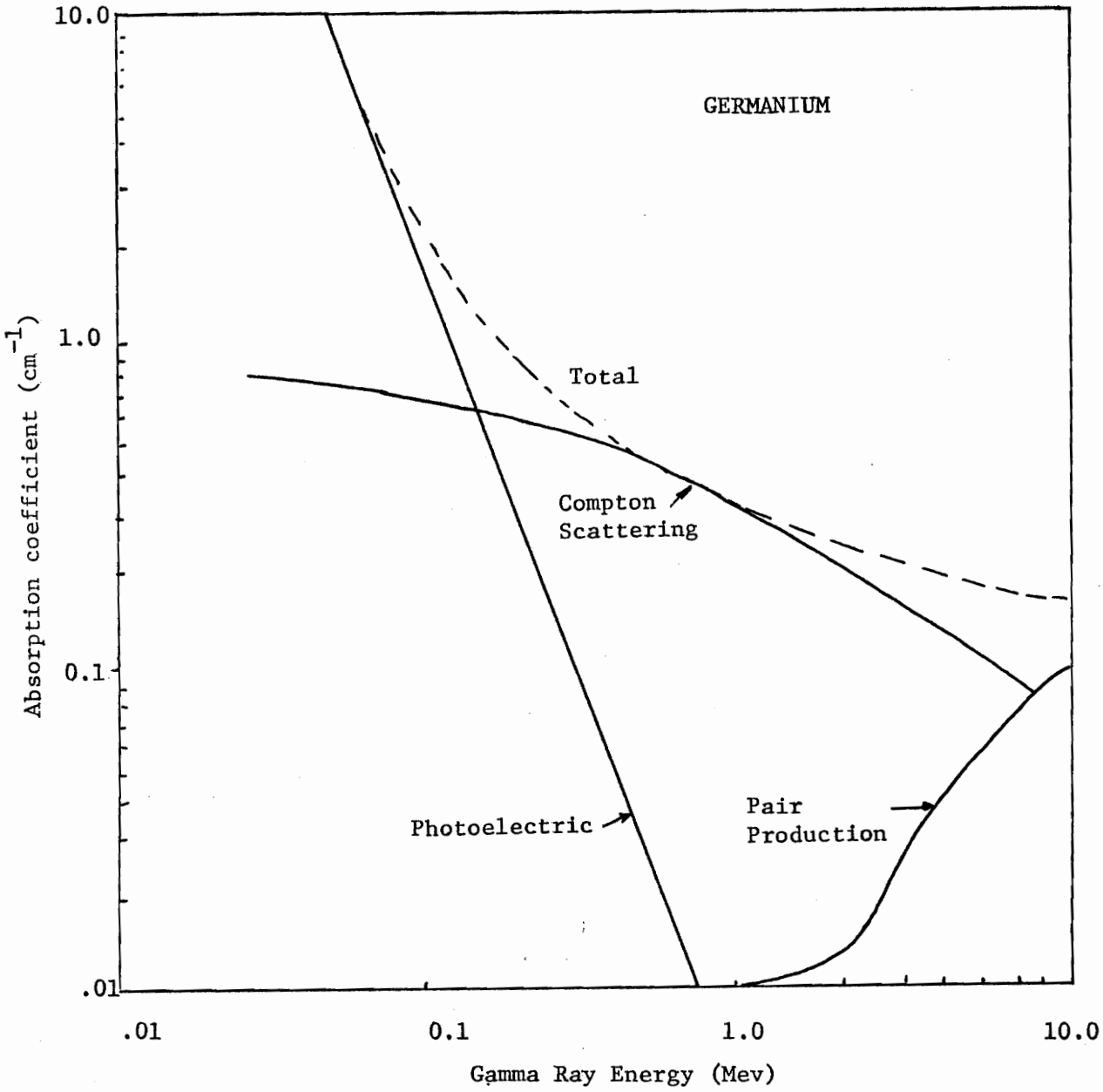



Figure 9[a]. Absorption Coefficient Versus Energy Germanium

[a](From Paul Kruger, Principles of Activation Analysis, Wiley-Interscience, p. 222, 1971).

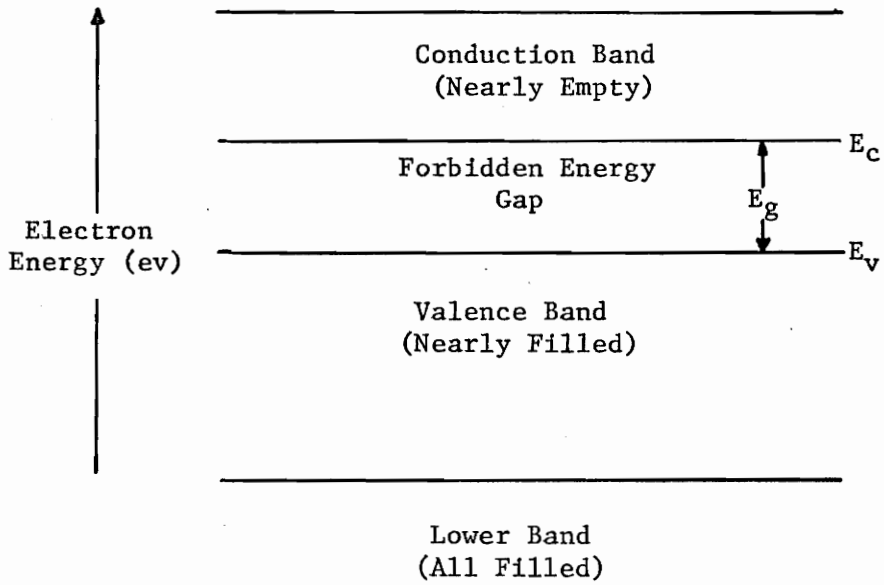



Figure 10[a]. Energy Band Diagram Of Semiconductor Material

[a](From Paul Kruger, Principles of Activation Analysis, Wiley-Interscience, p. 138, 1971).

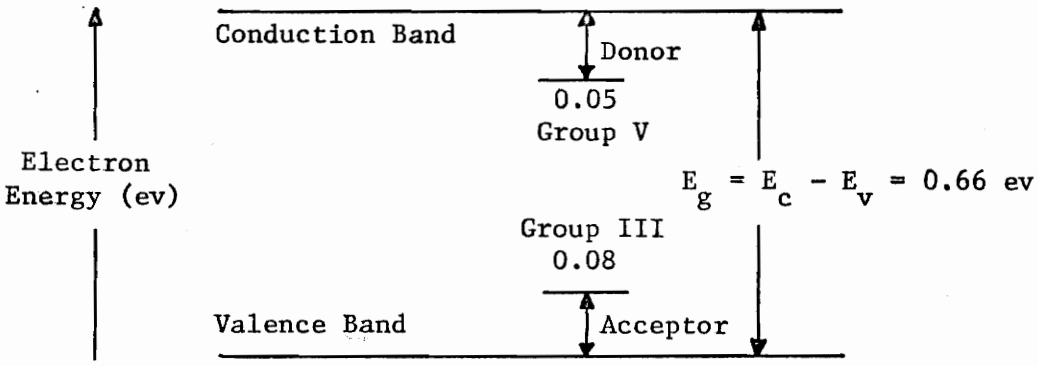



Figure 10b. Impurity Energy Levels In Germanium

[a](From Paul Kruger, Principles of Activation Analysis, Wiley-Interscience, p. 138, 1971).

related to the energy. Figure 11 is a simple illustration showing how these principles are applied to a detector. The large number of ion pairs that are produced is a statistical advantage of these type detectors (53). The output of the detector must be transformed into useful data. Some of the electrical equipment needed for this process is discussed in the following paragraphs.

The output of the detector is given as a series of electrical pulses which are separated by time. Each pulse represents the interaction of a unit of radiation with the detector. The amplitude of each electrical pulse is proportional to the gamma ray energy deposited in the detector. A preamplifier is essential when a solid state detector is used. The function of the preamplifier is to integrate the detector current and to provide a driver to the main amplifier. The preamplifier should be placed close to the detector in order to eliminate the capacitance of the cables since the pulse size is inversely proportional to the capacitance. The main amplifier is used to increase the size of the signal and to shape the pulses for further processing.

The signal is transferred from the amplifier to the multichannel analyzer (MCA) which is used to determine the energies and intensities of the gamma rays. As mentioned previously, each gamma ray emitting radionuclide produces a characteristic gamma ray spectrum in a detector system. The MCA is essentially a small computer whose functions are controlled by switches.

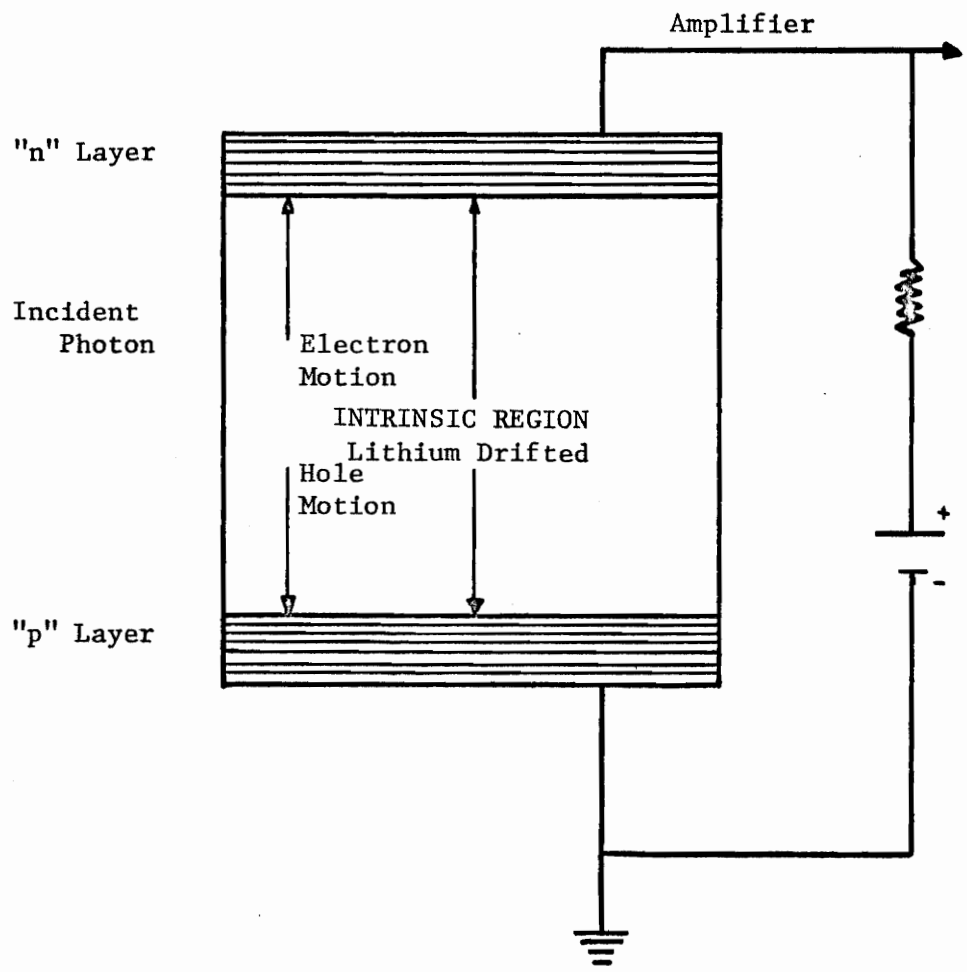



Figure 11[a]. Ge (Li) Detector

[a](Adopted from Gary M. Citrenbaum, "A Modified Generalized Stripping Technique For The Analysis Of Complex Gamma Spectra Generated In Neutron Activation Analysis", Unpublished Ph.D. dissertation, Virginia Polytechnic Institute and State University, 1972, p. 8).

The multichannel analyzer is operated in conjunction with an Analog-to-Digital Converter (ADC). In the ADC, the incoming pulse charges a capacitor and, at pulse maximum, the charging process is gated off and the capacitor is discharged by a constant current source until is is back to its initial level. During this discharging process, an oscillator runs at an accurately determined rate. The number of oscillations during the discharge sequence are recorded using a scalar with the number recorded representing an address or channel in the computer memory. At the end of the process, "one" is added to the previous content of the memory and the system is ready to process another pulse.

The analyzer used in this study had 4096 memory locations with each having a storage capacity of $2^{24} - 1$. At the completion of the counting process this information was transferred onto a 9-track computer compatible magnetic tape.

# IV. EXPERIMENTAL PROCEDURE

## Sample Collection and Preparation

### 1) Soil Samples

Starting at the roadside, soil samples were collected as described below (see Fig. 12a):

a) Five foot intervals for a distance of 300 ft.

b) Ten foot intervals for the next 50 ft.

c) Twenty-five foot intervals for the next 250 ft.

There were 76 sample locations and at each location, 10 soil samples were collected and mixed to form 1 sample. This mixing technique was used in an effort to eliminate possible inconsistencies with sampling of only one point at each location. The samples from each location were collected at points 5 ft apart parallel to the road. All samples were collected at a depth of about 1½ cm below the surface. Each sample was placed in a plastic bag, labeled and stored until sample preparation. During sample preparation, the soil samples were placed in premarked small virgin polythylene vials for storage until irradiation. These vials will be referred to henceforth as "sample" capsules. The "sample" capsules (right side of Fig. 14b were cylindrically shaped with approximate dimensions of 2.54 cm in height, and 1.27 cm in diameter. The weight of the soil sample, capsule identification number and sample identification assigned during sample collection were recorded. The weight of the soil samples

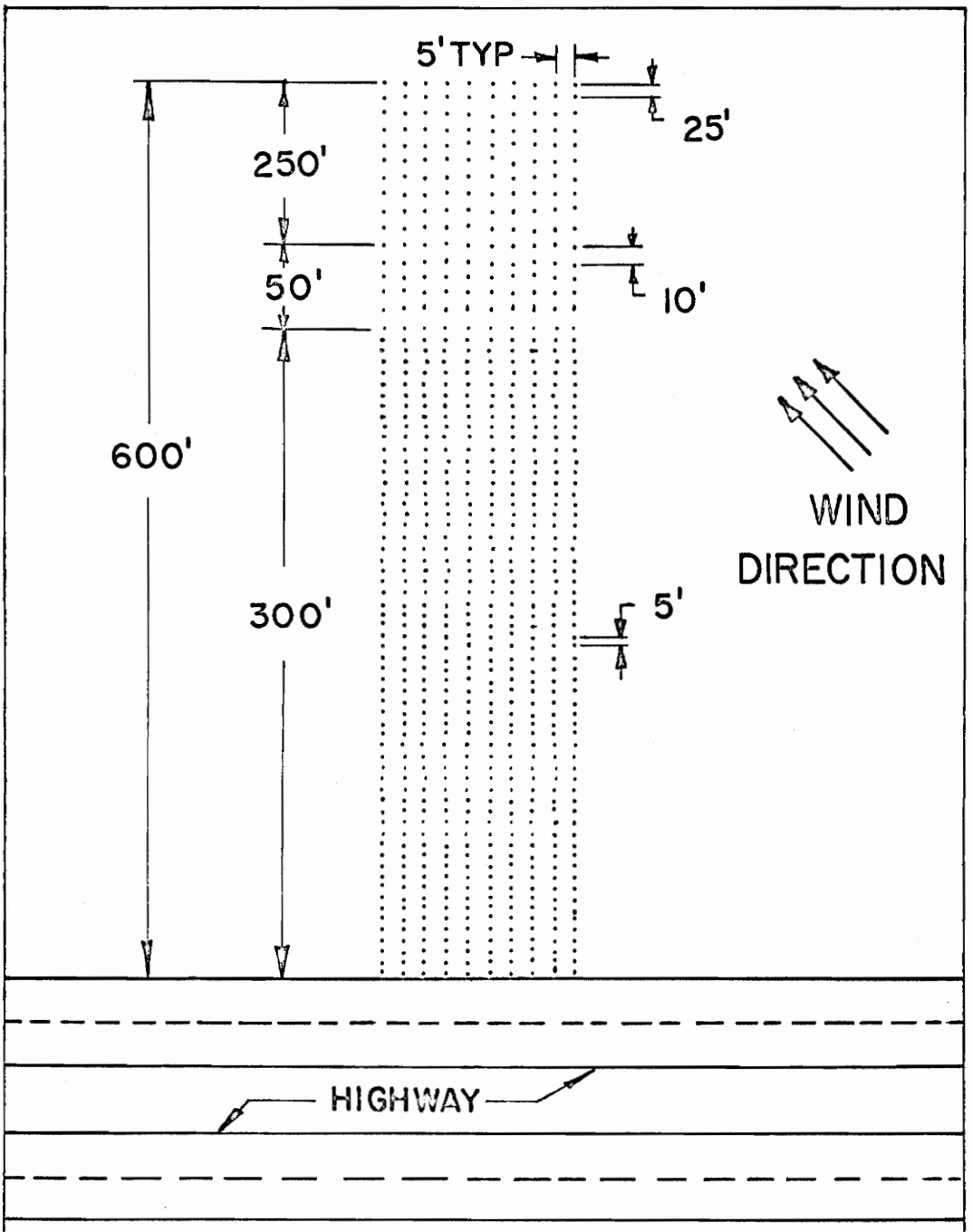



FIGURE 12a
COLLECTION LOCATIONS
OF SOIL AND GRASS SAMPLES

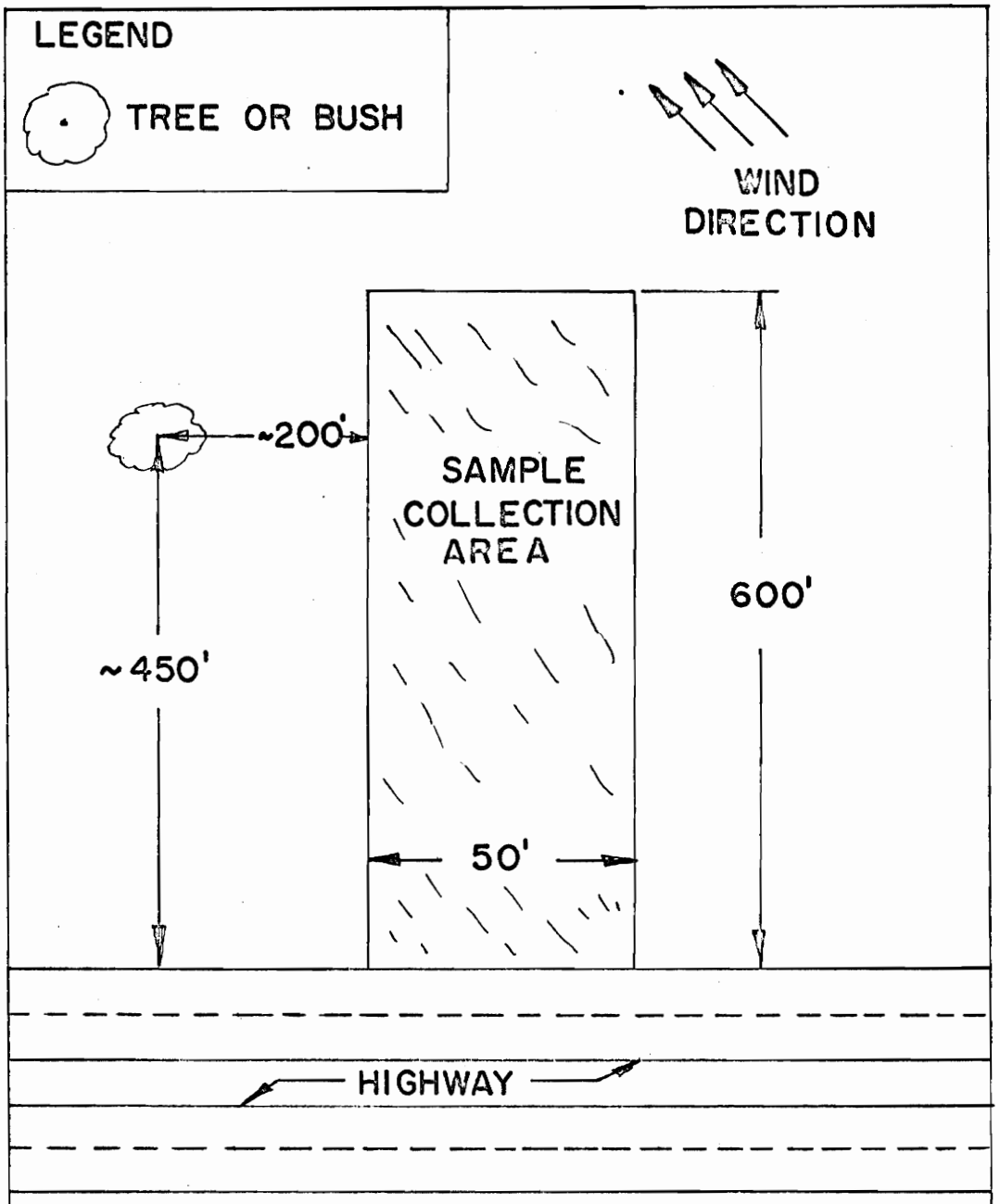



FIGURE 12b

LOCATION OF TREES AND BUSHES
HIGHWAY 1 - OAKRIDGE, TENN.

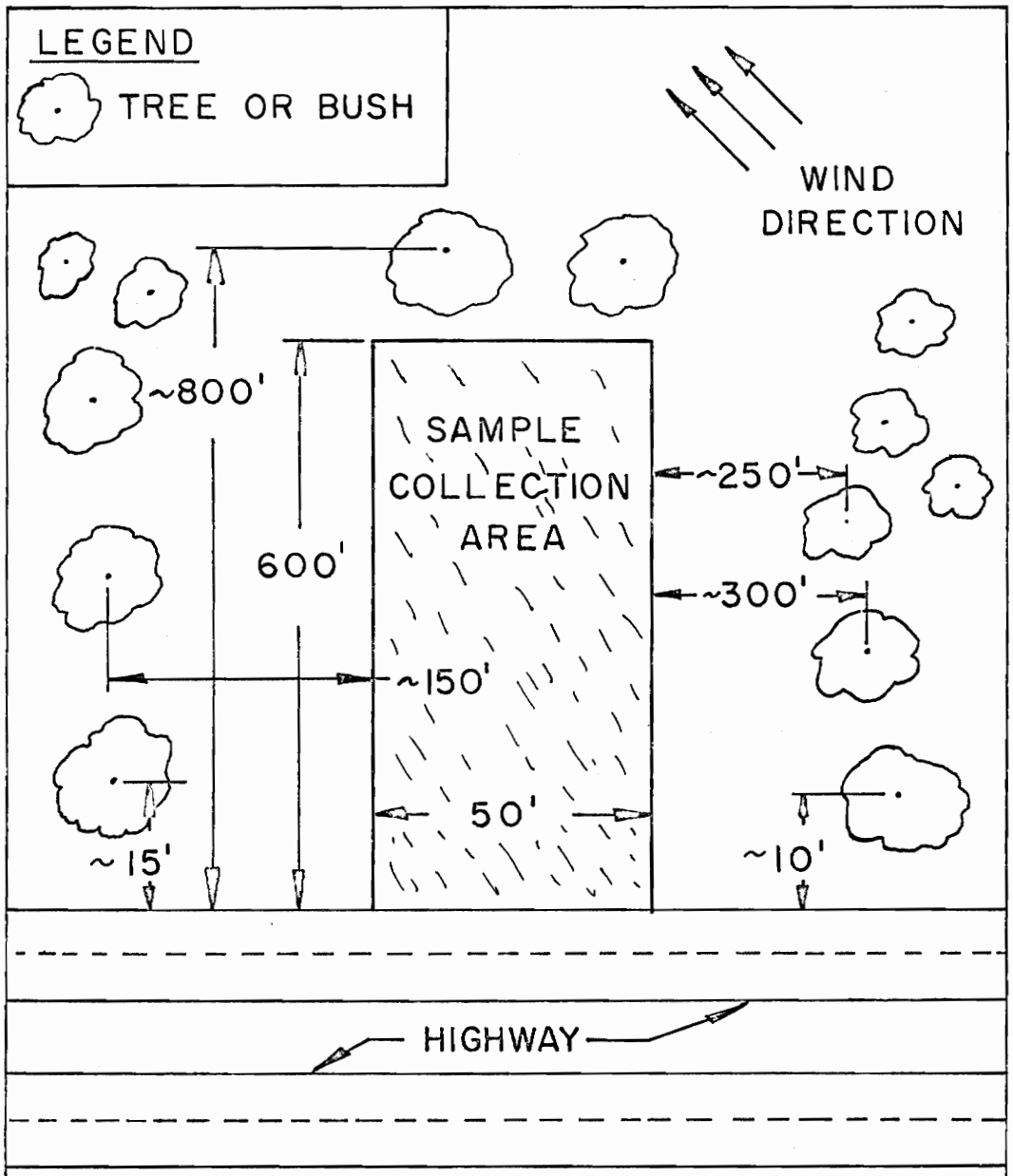



FIGURE 12c

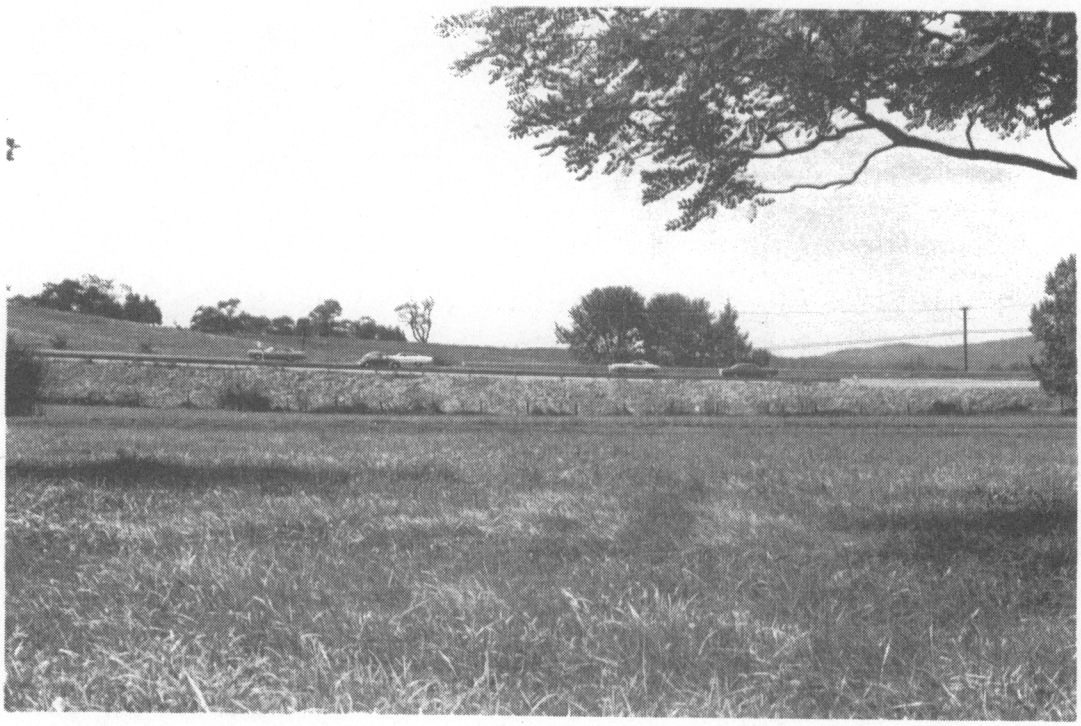
LOCATION OF TREES AND BUSHES
HIGHWAY 2 - BLACKSBURG, VA.

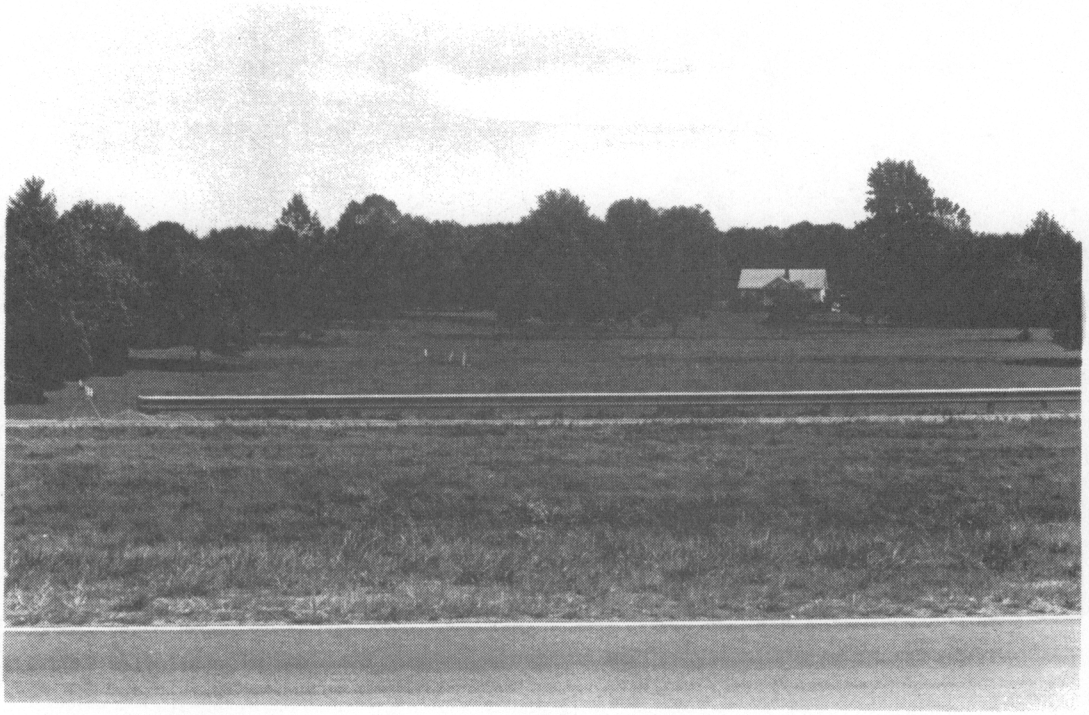
Figure 13a. View Looking Across Field at Sample Collection Location Near Oak Ridge, Tennessee

Figure 13b. View Looking From Site to Roadside at Sample Collection Location Near Oak Ridge, Tennessee

Figure 13c. View Looking From Site to Roadside at Sample Collection Location Near Blacksburg, Virginia

Figure 13d. View Looking From Roadside to Site at Sample Collection Location Near Blacksburg, Virginia





ranged from 0.6732 to 1.8564 g. Samples were not dried but lost moisture due to evaporation.

2) Grass Samples

Ten groups of grass samples were collected at each location described in the soil sample section. Each group consisted of 5 or 6 blades of grass ranging in length from 4 to 4½ cm. The species of grass collected has been identified as Poatrivialis (126). In order to investigate possible differences in concentration of elements in the distal and proximal portion of the blades, each blade was cut approximately in half. The blades were then placed in plastic bags, labeled and stored until sample preparation. During sample preparation, each group of grass samples, both distal and proximal portions, were washed 4 min. with 3.5 ml of triply deionized distilled water. The wash was then placed in "sample" capsules and stored until irradiation. The weight of the wash samples ranged from 0.3566 to 0.6284 g. After washing, the distal and proximal portion of the grass blades in each group of samples were blended together to form one sample. The distal and proximal portion of the grass samples were then placed in "sample" capsules and stored until irradiation. The weight of the grass samples ranged from 0.1228 to 0.2723 g.

3) Gasoline Samples

Gasoline samples were collected from gas pumps at four service stations in the Blacksburg area. The brands of gasoline collected were Texaco Regular and Premium, Exxon Regular and Plus, Phillips

Regular and 66-100 Plus Octane, and Shell Super. The gasoline samples were stored in glass jars until sample preparation. The preparation of gasoline samples was quite different from the other samples. Two major items had to be considered. First, safety from explosion of the gasoline in the reactor caused by heat and secondly, losses of gasoline components from evaporation. Various methods were tested. The best procedure found and the one used in this study is described in the following paragraph.

The "sample" capsules were sealed first and weighed. Distilled water was injected through the top of the capsule using a hypodermic needle and the weight of the water was determined. Gasoline was then injected through the top of the capsules using a hypodermic needle. The gasoline was added until there was a fifty-fifty mixture by volume of gasoline and distilled water. The small holes in the top of the capsules were sealed using a soldering gun. Next the weight of the gasoline was determined and samples were stored in a freezer until sample irradiation. This procedure was found to be acceptable. Several tests were run and it was found that there was approximately a 10% volume loss for short irradiation periods and a 25% volume loss for long irradiation periods. The weight of the gasoline in the samples ranged from 0.1745 to 0.3045 g.

4) Motor Oil Samples

Samples of motor oil were collected out of the cans in which they were purchased. The brands of motor oil collected were

Kendall 30w, Gulf Pride 20/20w, Havoline Texaco 20w, Quaker State 30w and Pennzoil 20w. During sample preparation, the motor oil samples were placed in "sample" capsules with a hypodermic needle. The weight of the oil samples ranged from 0.2357 to 0.5430 g.

5) Exhaust Samples

Pieces of filter paper (Whatman No. 1) were cut a little larger than the bottom of a small paper cup. The bottoms of the paper cups were removed and the pre-cut filter paper was placed inside. The paper cups were taped over the opening of the exhaust pipes of four automobiles. The cars were driven at 50 mph for approximately five minutes. The filter papers were then removed and stored in plastic bags until sample preparation. The efficiency of the filter paper was not known. Absolute concentrations were not needed. These filter samples were collected in order to assist in the identification and relative concentration of elements of particulates which fall out of exhaust gases. During sample preparation, the filter papers were removed from the plastic bags where they were stored since sample collection and placed in "sample" capsules. The weight of the material collected on the filter paper samples ranged from 0.1071 to 0.1228 g. Even though there have been many studies (2, 21, 29, 241) on the identification of elements in automobile exhaust particles, these samples were collected in order to determine which elements could be readily identified at the Virginia Polytechnic Institute Neutron Acti-

vation Laboratory.

All samples were handled with plastic gloves during sample collection and preparation for activation. Extreme caution was taken to prevent contamination of samples during handling.

Plant and soil samples were obtained on July 30, 1973 along Lafayette Drive, Oak Ridge, Tenn. (Highway No. 1) and plant and soil samples were obtained on July 15, 1973 along U.S. 460 (Highway No. 2) between Christiansburg and Blacksburg, Va.

## Sample Irradiation

All samples were irradiated in a 100 Kw, thermal, Argonaut-type, light water cooled and moderated, graphite reflected, heterogenous reactor. A cross sectional view of the reactor assembly is shown in Fig. 16a.

All samples were activated twice; first, for short periods of time, ranging from 10 sec. to 2 min. on which spectrum analyses of short lived isotopes were performed and secondly, for long periods of time, ranging from 6-8 hr. on which spectrum analyses of long lived isotopes were performed.

For short activations the samples were transferred into and out of the reactor by means of the pneumatic "rabbit" system shown in Fig. 16b. The pneumatic "rabbit" transfer system is a pressurized system using nitrogen gas at 40 lbs./in.$^2$ to force the transfer capsules into and out of the reactor core.

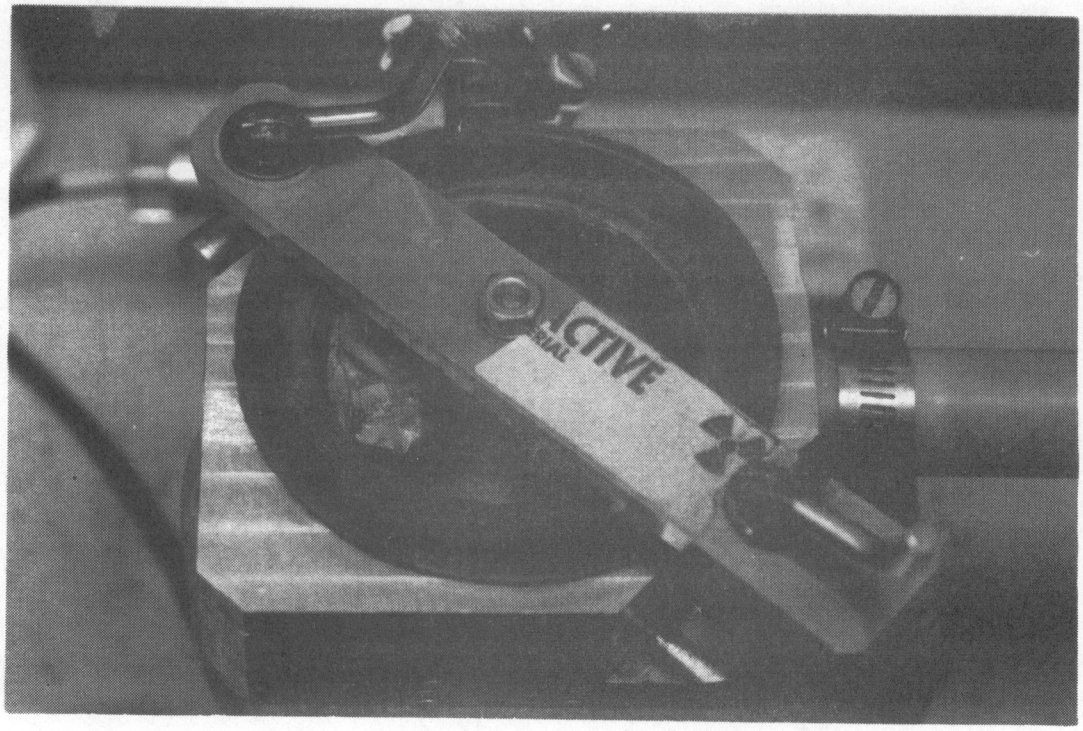
The "sample" capsules (right side of Fig. 14b) were placed in larger transfer capsules (left side of Fig. 14b. These transfer capsules are cylindrical shaped with approximate dimensions of 4.63 cm in height and 2.10 cm in diameter. The transfer capsules were then placed in a small transfer chamber (Fig. 14a center). The top of the transfer chamber was clamped down and sealed.

The rabbit system transferred the sample from the Neutron Activation Laboratory into the southeastern stringer (Fig. 16b) in the center reflector of the reactor core where the neutron flux is 1.2 x $10^{12}$ n/cm$^2$-sec. The transfer time was less than 1 sec. each way. Once the sample had been activated for the preset time the nitrogen gas was turned on automatically returning the sample to the rabbit box (Fig. 17a and into the transfer chamber (Fig. 13a). At this point, the sample was surveyed for radiation levels and those with low radiation levels (< 10 mr/hr) were prepared for counting. The samples with higher radiation levels were left in the rabbit box and allowed to decay until levels permitted preparation for counting. Figures 15a and 15b show the rabbit box, rabbit control panel and rabbit entrance into the reactor.

For long activations, the "sample" capsules were placed in a container which was manually dropped into the central stringer on top of the reactor core (Fig. 15b) where the neutron flux is 1.3 x $10^{12}$ n/cm$^2$-sec. Once the samples had been activated the desired length of time, the reactor was shut down allowing samples to decay overnight. The samples were then removed from the stringer and placed in a lead

Figure 14a. Rabbit Transfer Chamber

Figure 14b. Rabbit Transfer Capsule
and Sample Capsule


ACTIVE
SEAL

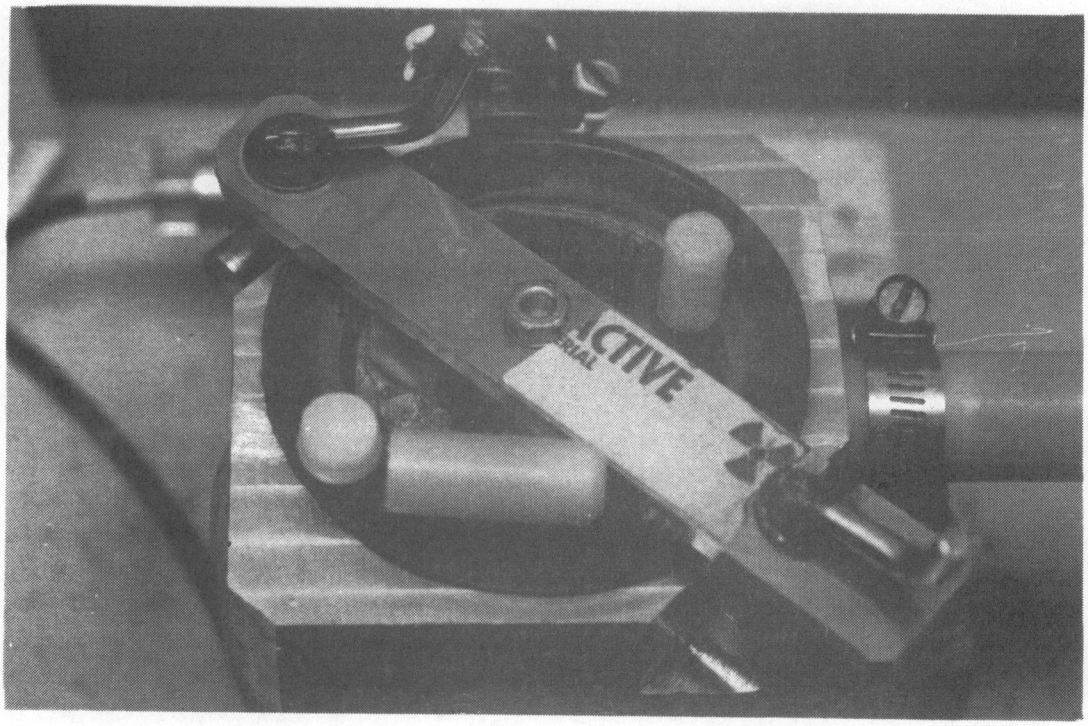
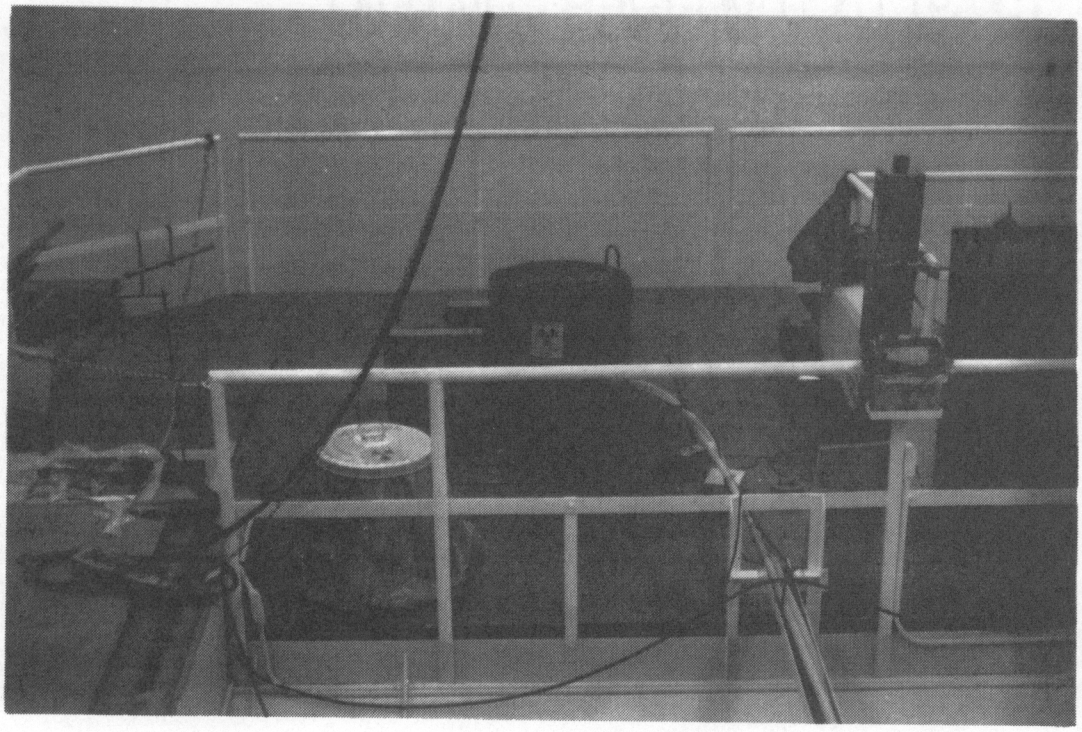

ACTIVE
SEAL

Figure 15a. Top View of Reactor

Figure 15b. Rabbit Box and Rabbit Control Panel



POTENTIAL
CONTAMINATED
AREA

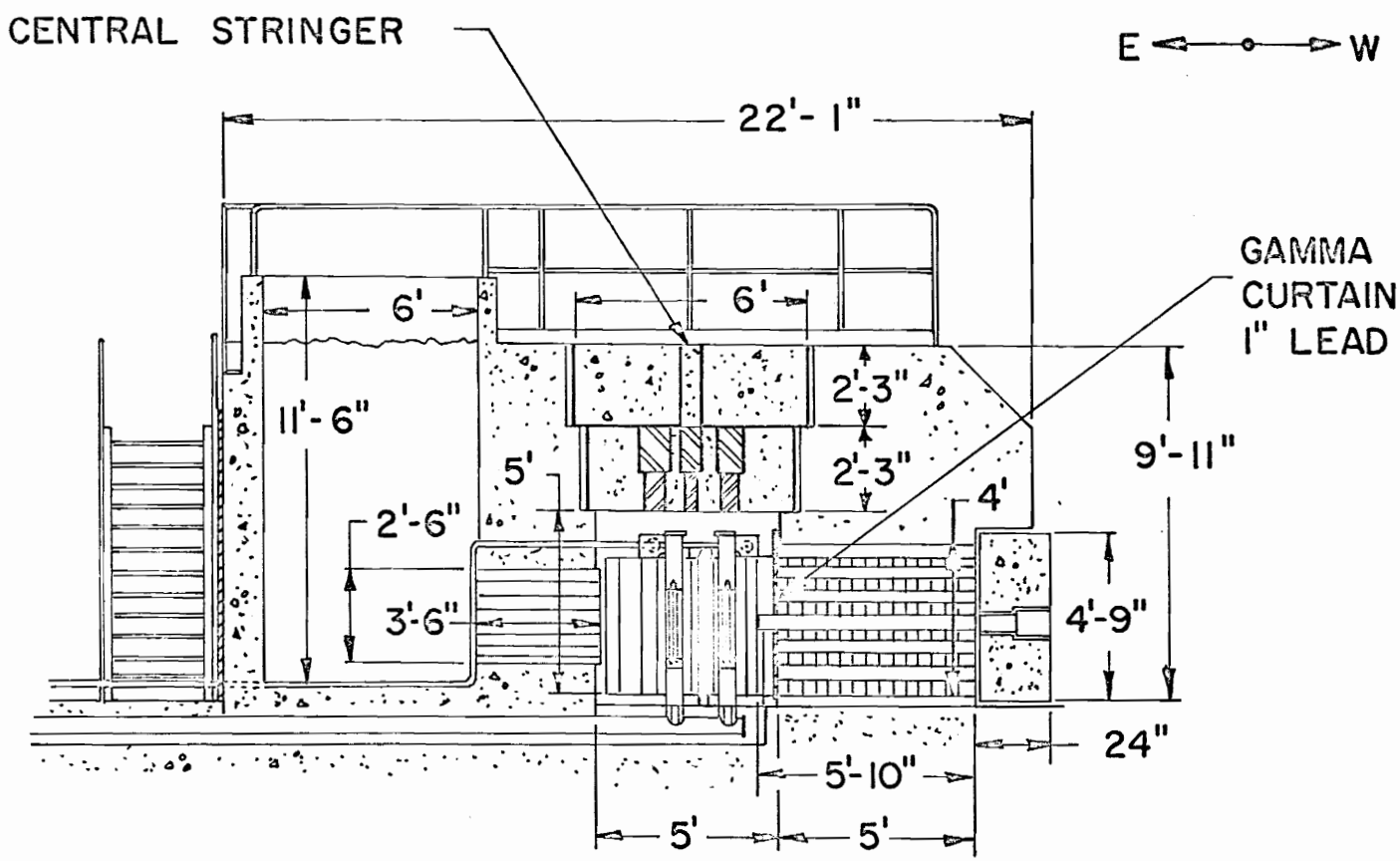



FIGURE 16a
V.P.I. REACTOR
EAST TO WEST CUTTING PLANE, LOOKING SOUTH

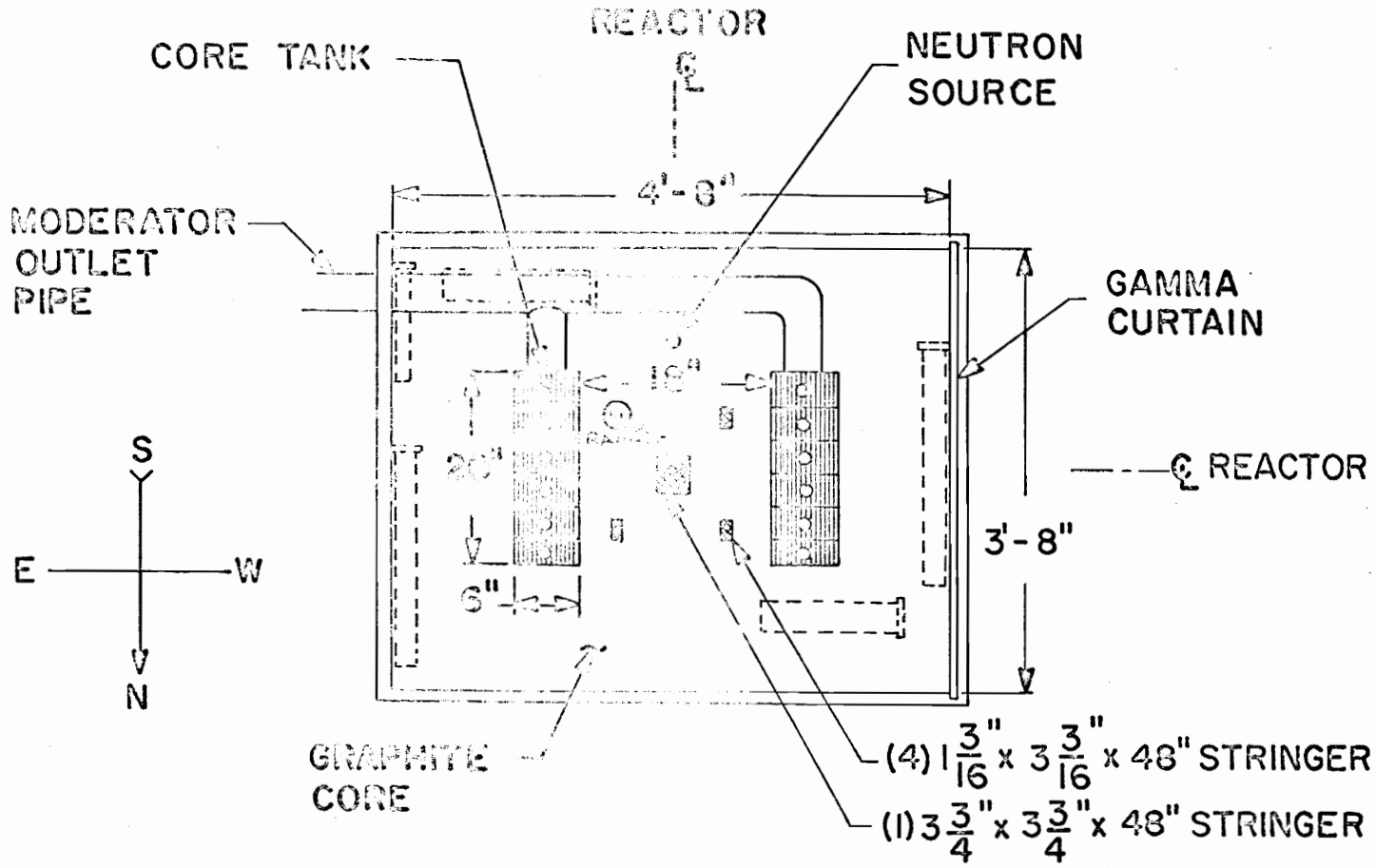



FIGURE - 16b
V.P.I. REACTOR CORE - TOP VIEW

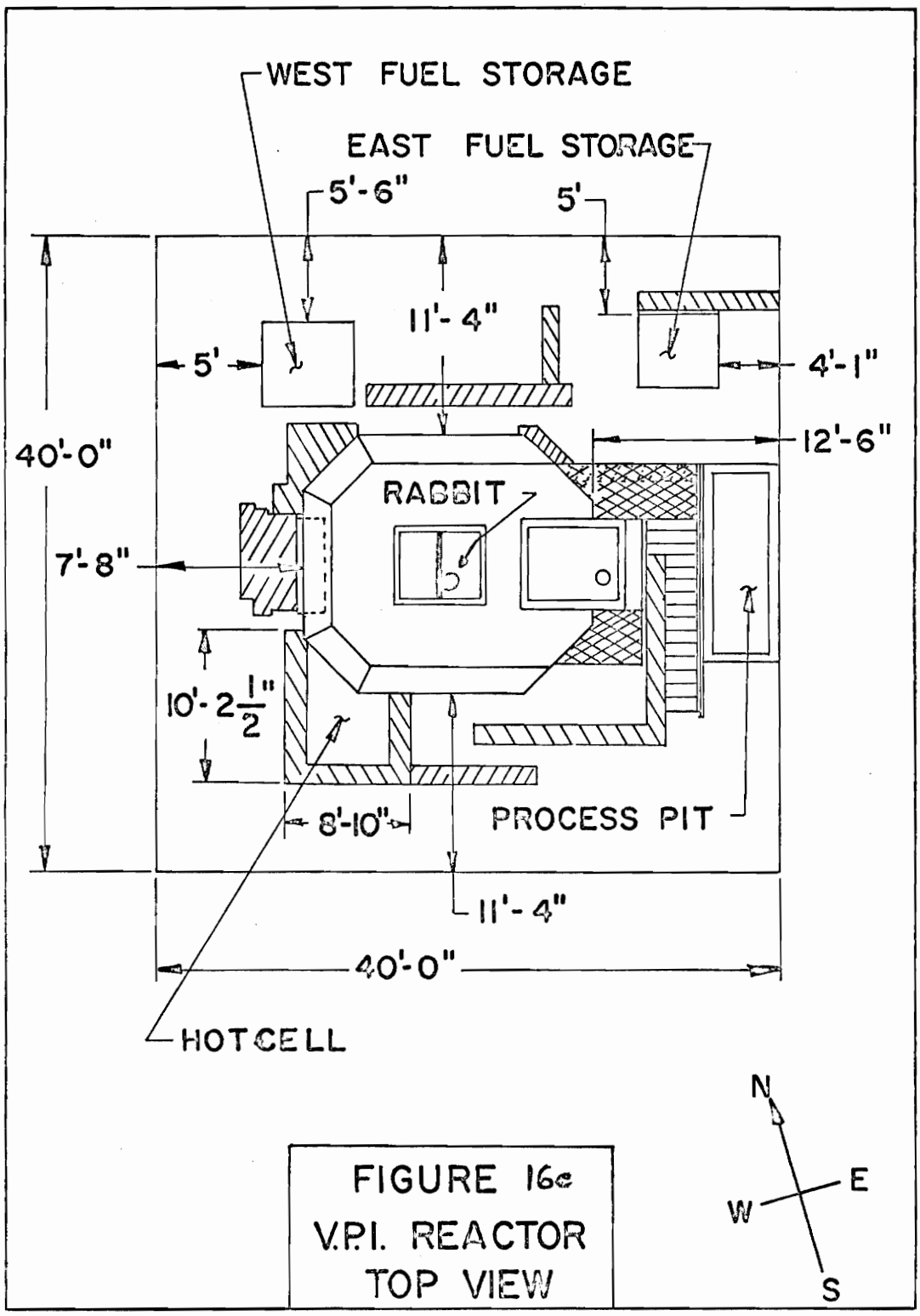



FIGURE 16c
V.P.I. REACTOR
TOP VIEW

container where they were stored until radiation levels were low enough to allow preparation for counting. Activation times, decay times and counting times were recorded for later use in the computer program described in Appendix A.

## Sample Counting and Data Storage System

The Neutron Activation Analysis Laboratory at Virginia Polytechnic Institute and State University has a Nuclear Data 4420 system (Fig. 17b) consisting of the following:

1) A high resolution lithium-ion drifted germanium detector (Ge(Li)).
2) An internal 24,000 word computer memory.
3) The analyzer contains 4096 memory locations or channels with a storage capacity of $2^{24}$ -1 per channel.
4) The readout options of the system are:
   (a) teletype unit
   (b) chart recorder
   (c) visual scope display
   (d) paper computer tape
   (e) magnetic tape unit.

A block diagram of the system can be found in Fig. 17a. Short activated samples were counted for 8 min. and long activated samples were counted for 1 hr. The spectrum data was transferred to, and stored on magnetic tape until data interpretation was performed using the Virginia Polytechnic Institute and State University IBM 370 Computer.

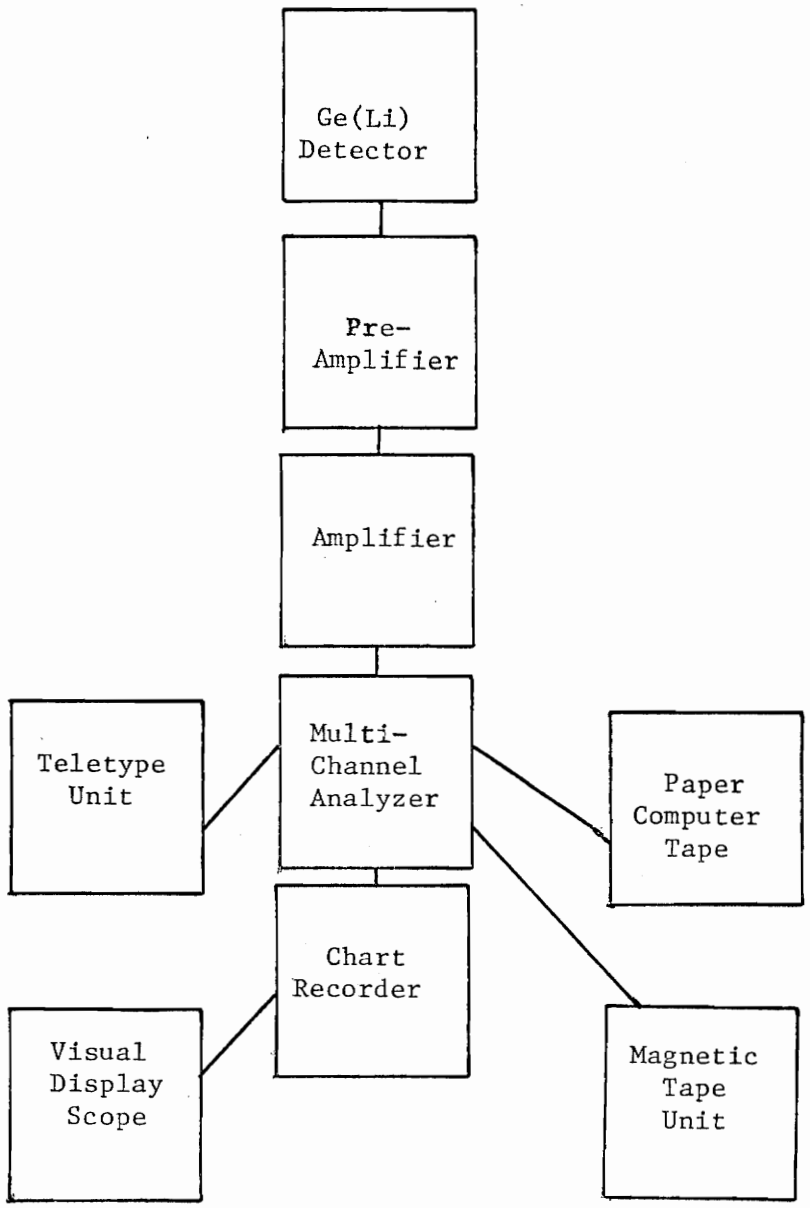
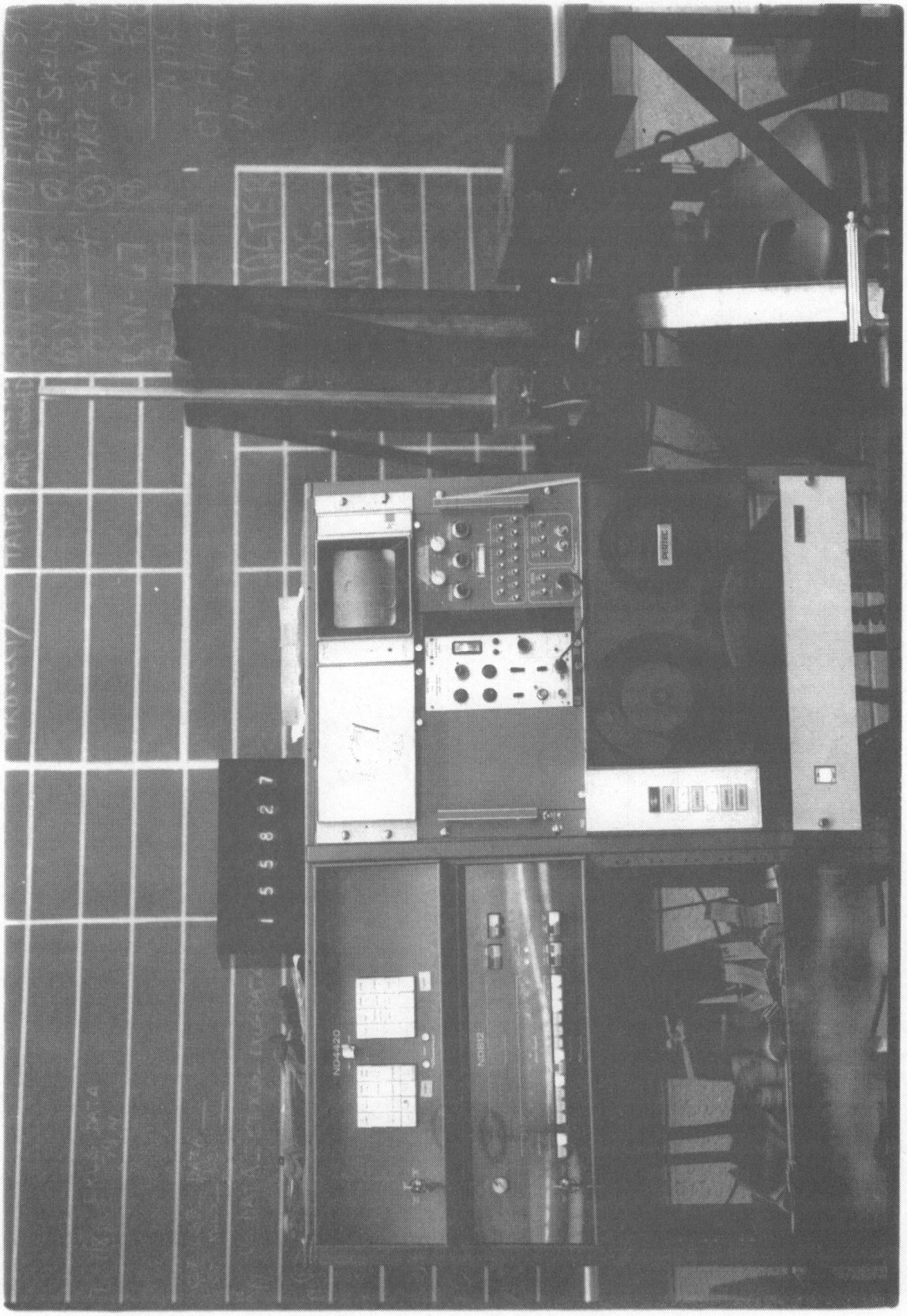



Figure 17a. Block Diagram of Counting System of V.P.I. & S.U. NAA Laboratory

Figure 17b. Counting System of the
V.P.I. & S.U. NAA Laboratory


1 5 5 8 2 7
NO.5620
NO.602

## Background Levels

Several empty "sample" capsules, several unused pieces of filter paper (Whatman No. 1), and several samples of the distilled water used for washing the grass samples were activated and a spectrum analysis was performed on the data. The "sample" capsules were chosen for their relative freedom from activatable contaminants. Copper-64 found in the "sample" capsule was the only isotope of importance to this study that was identified in the above samples. There was a wide variation of the copper concentration in the capsules and therefore no copper was reported in the Results section of this work. The natural background of the laboratory was checked several times and no isotopes of importance to this work were identified.

## General Soil Test

A mixture of the soil samples for each sample location was sent to the VPI&SU Soil Testing Laboratory for testing and the results are shown in Table 4.

## Climatological Data

In an air dispersion study, information on temperatures, precipitation levels, wind speed and wind direction is important. This type of data was not collected at the sample locations during this study. Appendix D contains data received from the National Oceanic and Atmospheric Administration of the U.S. Department of Commerce for the Roanoke and Knoxville areas and data was collected approximately

Table 4

Soil Testing Results

| Sample Location | pH | Calcium CaO | Magnesium MgO | Phosphate $P_2O_5$ | Potash $K_2O$ |
|---|---|---|---|---|---|
| Blacksburg | 6.8 | very high | very high | very high | very high |
| Oak Ridge | 6.9 | very high | very high | medium | high |

30 miles from the sample locations. In future studies of this type, it is recommended that weather stations be set up on site.

## Elevation

Highway planning maps were used to determine the elevation of the two highways. These maps were obtained from the Virginia Highway Department for the Blacksburg highway and the City Department of Oak Ridge for the Oak Ridge highway.

In the sample areas, greater detail of small changes in elevation than was available from the planning maps was needed. A tripod and surveying equipment was used to obtain these elevation changes every 5 ft starting at the roadside and extending outward 600 ft.

These changes are plotted in the bottom portion of the concentration versus distance graphs shown in the Results section of this work. These changes appear drastic due to the scale chosen. However, the variations were realistically quite moderate but it was felt of value to show small changes in elevation. Further discussion on the elevation effects is contained in the Results section of this work.

## Data Identification Procedure

Capsule identification numbers and sample identification numbers were recorded during sample preparation.

During irradiation the information needed for input to the NAA Computer Program listed in Appendix A was recorded on data forms and this information was placed on computer data cards which

were submitted with the Job Control Cards necessary to execute the NAA Computer Program.

Figure 18a is an example of the data format used and Fig. 18b is an example of the data card used. The first four columns contain information concerning activation time and counting time.

Column one is the time the sample entered the reactor given as the day of the year, 078, the hour, 09, the minute, 42, and the sec., 00. Column two is the time out of the reactor. Subtracting the number in column one from the number in column two, the irradiation time will be obtained, which in this case is 5 hr. Column three is the time counting started and column four is the time the counting stopped. Subtracting the number in column three from the number in column four will yield the count time which in this case is 1 hr. Subtracting the number in column two from the number in column three, the wait time will be obtained, which in this case is 6004 min. Column five contains the weight of the sample in grams. Column six contains the flux divided by $10^{10}$. Column seven is the sample identification which corresponds to the identification on the sample capsule. Column eight contains the tape identification. Column nine is the tagword which is the identification on the tape that identifies the spectrum data.

## Standard Gamma Library (V. P. I. & S. U.)

In 1971, the staff of the Neutron Activation Laboratory at Virginia Polytechnic Institute and State University under the direction of Dr. A. K. Furr began compiling a standard library rather

| Act. Time In | Act. Time Out | Count Str. Time | Count Stp. Time | Weight | Flux | Sample I.D. | Tagword & Tape | |
|---|---|---|---|---|---|---|---|---|
| 078094200 | 078144200 | 082184600 | 082194600 | 0.4033 | 130 | OA 10 | 8N | 000188 |

Figure 18a. Sample Data Form

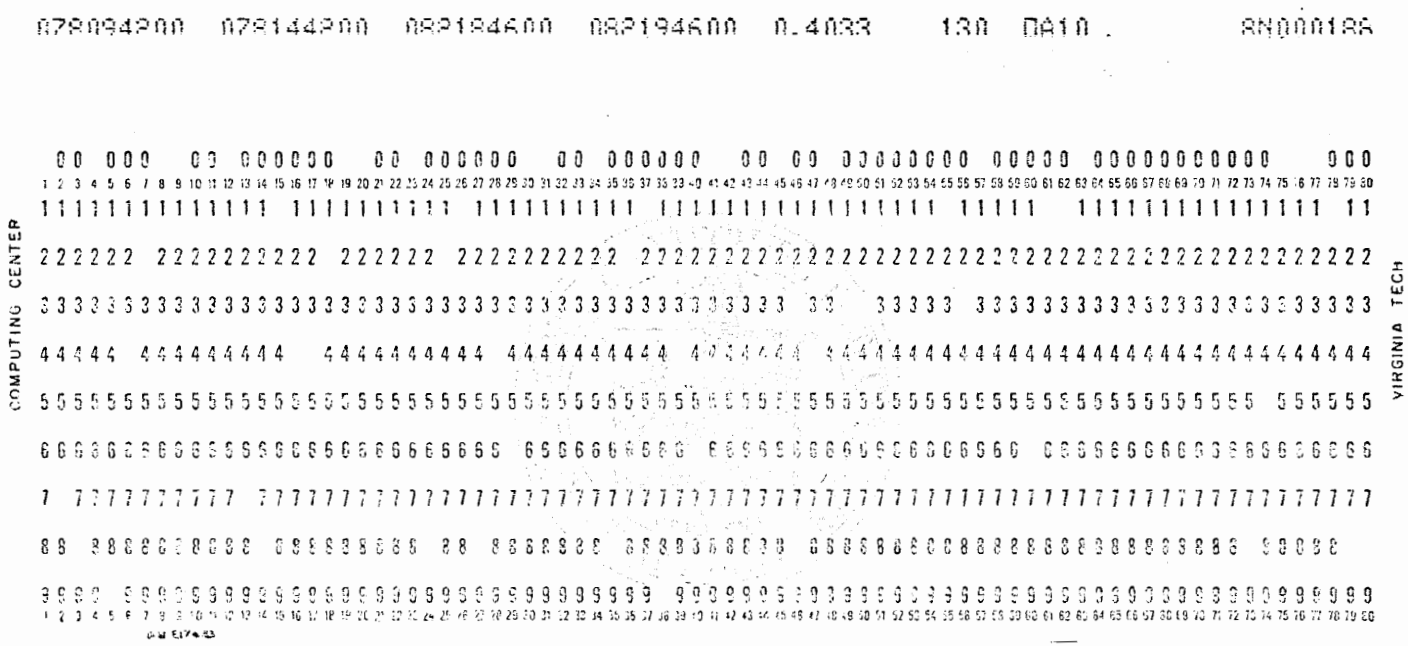



Figure 18b. Sample Data Card

than using data from the literature which had been previously employed. The present standard library consists of some 65 elements. The value of this library is that the spectrum of pure elemental standards were generated on the same counting system as the unknown spectrum to which it will be applied. This minimizes systematic errors. Appendix C contains some of the information from the standard library for these elements. Since bromine is one of the important elements in this study, Fig. 19a shows a decay scheme for Bromine-82 and Fig. 19b is a computer plot of the data spectrum of a standard for bromine.

## Neutron Activation Computer Program (V. P. I. & S. U.)

A description of the computer program used to analyze the spectrum data stored on magnetic tape is given in this section. During this discussion the reader should refer to the program listing given in Appendix A.

### Main Program

| Card I.D. | Brief Description |
|---|---|
| Main 335 | Read Statement |

| Variable Name | Description |
|---|---|
| TID | Time sample entered the reactor in days |
| TIH | Time sample entered the reactor in hours |
| TIM | Time sample entered the reactor in minutes |
| TIS | Time sample entered the reactor in seconds |
| TOD | Time sample was removed from the reactor in days |

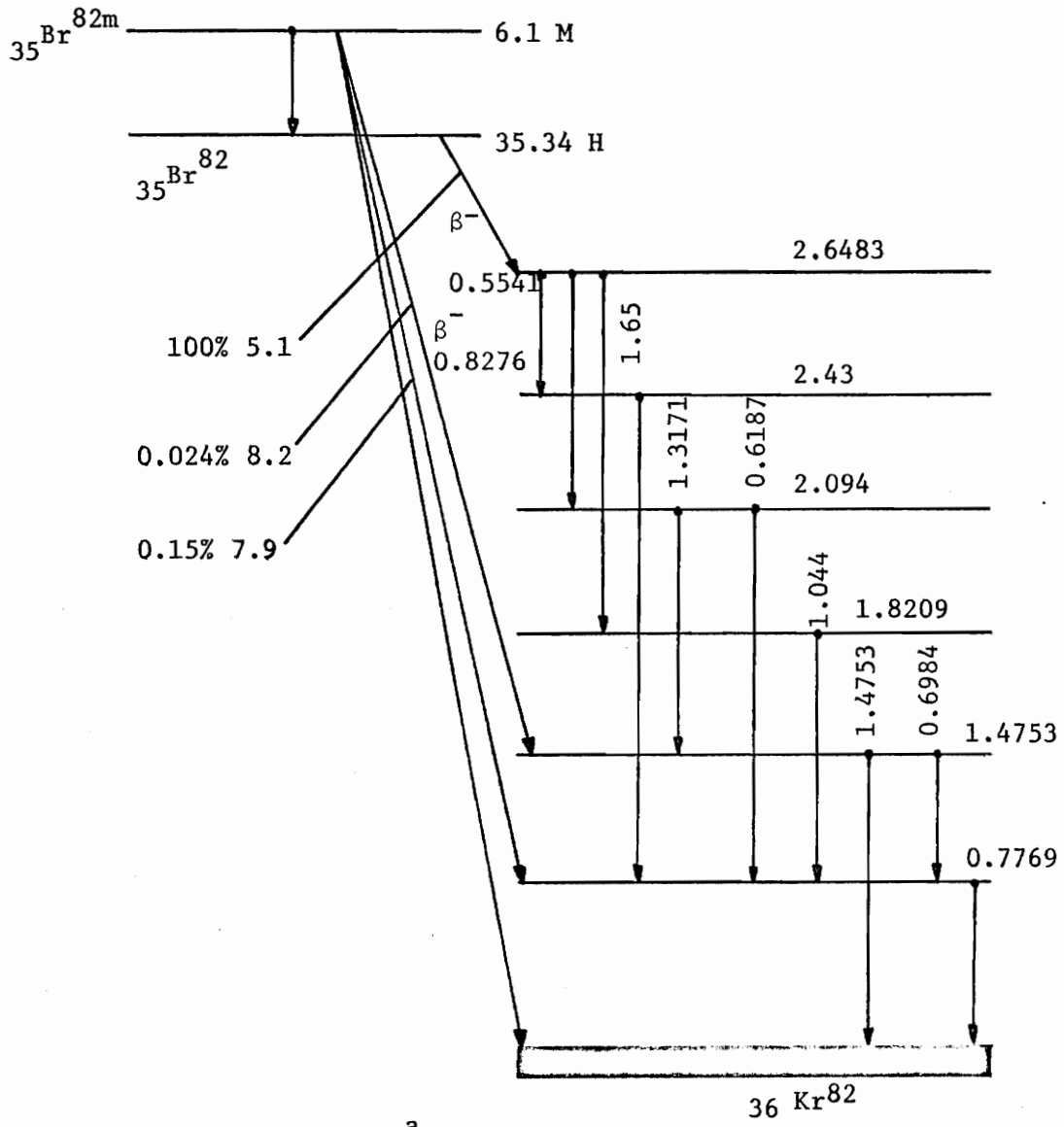
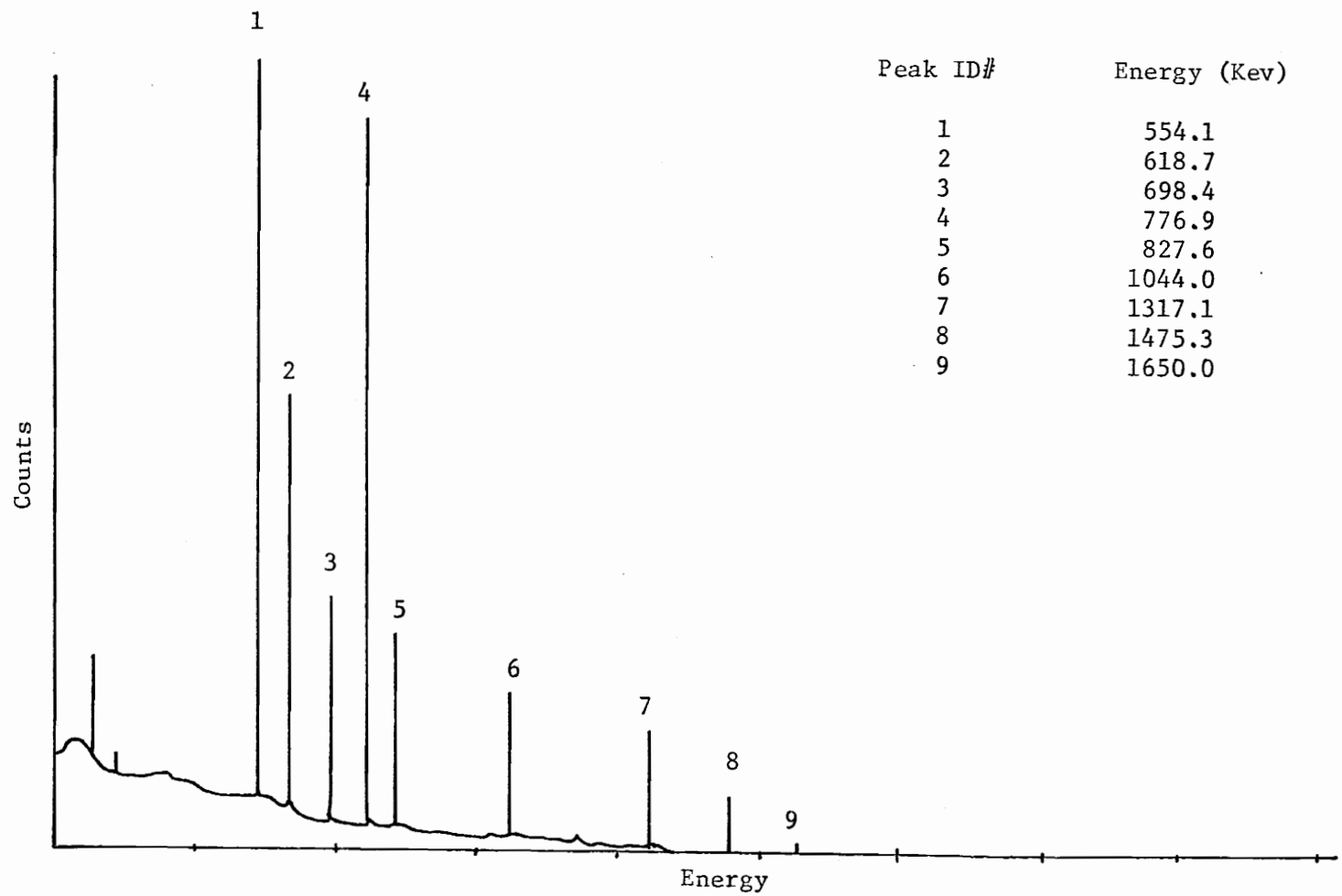



Figure 19a[a]. Decay Scheme Br - 82

[a](From C. M. Lederer, Table of Isotopes, John Wiley & Sons, New York, Sixth Edition, p. 217, 1966).




| Peak ID# | Energy (Kev) |
|---|---|
| 1 | 554.1 |
| 2 | 618.7 |
| 3 | 698.4 |
| 4 | 776.9 |
| 5 | 827.6 |
| 6 | 1044.0 |
| 7 | 1317.1 |
| 8 | 1475.3 |
| 9 | 1650.0 |

Figure 19b. Computer Plot of Br-82 Standard

| | |
|---|---|
| TOH | Time sample was removed from the reactor in hours |
| TOM | Time sample was removed from the reactor in minutes |
| TOS | Time sample was removed from the reactor in seconds |
| TCD | Time sample started counting in days |
| TCH | Time sample started counting in hours |
| TCM | Time sample started counting in minutes |
| TCS | Time sample started counting in seconds |
| WT | Weight of sample (grams) |
| IFLUX | Thermal neutron flux $\frac{\text{neutrons}}{\text{cm}^2\text{-sec}}$ *10 |
| W1,W2,W3 | Sample identification number |
| NTAG | Tape tagword |

| Card I.D. | Brief Description |
|---|---|
| Main 380-395 | Converts times read in on card (main 335) to seconds |
| Main 400 | Calculation of activation time |
| Main 405 | Calculation of wait time |
| Main 410 | Calculation of counting time |
| Main 470 | Read and store library information |

| Variable | Brief Description |
|---|---|
| ELE | Element name |

| | |
|---|---|
| ISOT | Isotope mass number |
| HF | Half Life |
| Energy | Gamma energy |
| SA | Specific Activity |
| KFLAG | Half-life code for counting sequence |
| IPFLAG | Forced double-peak code |
| Main 535-675 | This group of cards reads and writes the spectrum from the tape and converts it to decimal numbers. |
| Main | Calls the subroutine FIT to analyze the spectrum. |

## Subroutine FIX

This subroutine controls the analysis of the spectrum. In this subroutine the subroutine FIXUP is called first. FIXUP corrects for any energy shift. Fix converts from energy to channel number. If the peak the program is examining is small, a fit over a small number of data points is performed. If the peak the program is examining is large, a fit over a large number of data points is performed.

Subroutine NAAFIT is called to fit the data to a function if the number of data points is greater than the number of fitting parameters.

Once the curve fit had been completed subroutine CONPPM was called to determine ppm from peak area and sample times.

In the case where there are multiple peaks for the same isotope an average is calculated.

## Subroutine FIXUP

This routine corrects for shifts in energy and determines which peak to normalize. The three peaks examined are the sodium 2754 KeV peak, potassium 1461 KeV peak and aluminum 1779 KeV peak.

## Subroutine CONPPM

This subroutine determines the concentration in ppm using the following equation.

$$ppm = \frac{AREA*ALAM*10^6}{FLUX*SA*WT*EXPA*EXPC*EXPW} \quad . \tag{15}$$

Where

AREA = area of peak

ALAM = .693/HF = .693/Half Life

EXPA = 1-EXP (-ALTA)

= $1-e^{-}$ ALAM * Tact

EXPC = 1-EXP (ALTC)

= $1-e^{-}$ ALAM * Tcount

EXPW = EXP (-ALTW)

= $e^{-}$ ALAM * Twait

WT = Weight of Sample

SA = Specific Activity

FLUX = Neutron Flux

## Subroutine NAAFIT

Subroutine NAAFIT initializes and checks parameters for curve fit. This routine finds errors in data values and converts from channel number to energy.

## Subroutine SMOOTH

This routine uses a five point smooth of the data and is normally bypassed since close peaks may be lost.

## Subroutine STRIP

This subroutine strips out interference peaks.

## Subroutine CURFIT

This subroutine makes a least-squares fit to a function using the algorithm of Marquardt. The function can have parameters that are non-linear. The Marquardt algorithm combines an analytical solution and a gradient search. The solution is developed from linearizing the fitting function (291).

## Subroutine FDERIV

This subroutine evaluates the derivatives of the Gaussian plus quadratic polynomial function of Equation 16,

$$y(x) = a_1 \exp\left[-\tfrac{1}{2}\left(\frac{x-a_2}{a_1}\right)^2\right] + a_4 + a_5 x + a_6 x^2 . \qquad (16)$$

The derivatives are evaluated analytically,

$$\text{DERIV}(J) = \frac{\partial_y(X_I)}{\partial_{a_J}} \tag{17}$$

with six different expressions for the six possible derivatives (23). These derivatives are calculated for the subroutine CURFIT.

Subroutine MATINV

This subroutine inverts a square symmetric matrix and calculates its determinant. The inverted matrix is substituted into the same array as the original matrix (23).

Function FUNCTN

This function evaluates terms of a function for non-linear least-squares search with form of a Gaussian peak plus quadratic polynomial. FUNCTN is very good for fitting a Gaussian peak with a slowly changing background (23).

Function FCHISØ

This function evaluates $\chi^2$ for a set of data points and a fitted function. FCHISØ can be used to evaluate $\chi^2$ for functions with linear or non-linear coefficients (23).

Function SUM

This function subtracts out the quadratic background for the curve and sums up the area.

# V. RESULTS

## Introduction

Most of the discussion contained in this section will be concerned with the elements of bromine and chlorine for the following reasons:

1) A large percentage of automobile exhaust particulate matter is lead compounds containing bromine and chlorine.
2) The detection sensitivity of the V.P.I. & S.U. Neutron Activation System is very good for both elements, viz. ~ 3 ppb for bromine and ~ 38 ppb for chlorine.
3) The concentrations of bromine and chlorine found in the gasoline and on the filter paper samples in this study were among the highest.

The elements detected by neutron activation both on the filter paper samples and in the gasoline or oil samples are listed in Table 5. Column two of the table contains the range of concentrations (ppm) of these elements that were detected on the filter paper samples. The efficiency of the filter is not known, therefore, the concentrations given in Table 5 are not absolute.

The results contained in this section are felt to be sound for the following reasons:

1) A large number of samples were collected from each highway.
2) Two highways were studied.
3) A blending method was used during sample preparation.

Table 5

Concentrations of Elements Detected on Filter Paper Exposed to Automobile Exhaust

| Element | Range of Concentrations (parts per million) |
|---|---|
| Aluminum | 81.5 to 129.8 |
| Antimony | 0.8 to 1.3 |
| Arsenic | 3.5 to 5.7 |
| Barium | 42.8 to 107.5 |
| Bromine | 136.1 to 328.5 |
| Cadmium | 1.3 to 3.8 |
| Calcium | 171.5 to 257.8 |
| Chlorine | 86.7 to 237.0 |
| Chromium | 6.8 to 7.3 |
| Magnesium | 65.9 to 129.7 |
| Manganese | 1.37 to 1.75 |
| Samarium | 0.2 to 0.4 |
| Sodium | 238.4 to 288.0 |
| Titanium | 10.1 to 25.1 |

4) The computer program used for the analysis of the neutron activation results has been found through extended use to yield very consistent results.

5) The statistical error limits shown in the plots contained in this chapter represent two standard deviations which gives a 95% confidence limit.

## Bromine (Br)

Plots of the bromine concentrations versus distance from the highway that were detected in the soil samples, distal and proximal portion of the grass blades and the wash off the distal and proximal portion of the grass blades from Highway No. 1 are given in Figs. 20, 21 and 22 respectively. Figs. 23, 24 and 25 are plots of the bromine concentrations versus distance from Highway No. 2 detected in the soil samples, distal and proximal portion of the grass blades and the wash off the distal and proximal portion of the grass blades, respectively. The bromine concentrations detected in the proximal portion of the grass blades and in the wash from the proximal portion of the grass blades from Highway No. 1 were at such low levels that the plots were barely noticeable in Figs. 21 and 22.

There seems to be a direct relationship between the build-up of the bromine concentration producing the major peaks shown in Fig. 20 and the increases in the elevation at the sample locations. The relationship between these peaks and the elevation during the build-up phase of the major peaks can be seen in Table 6. The distances from

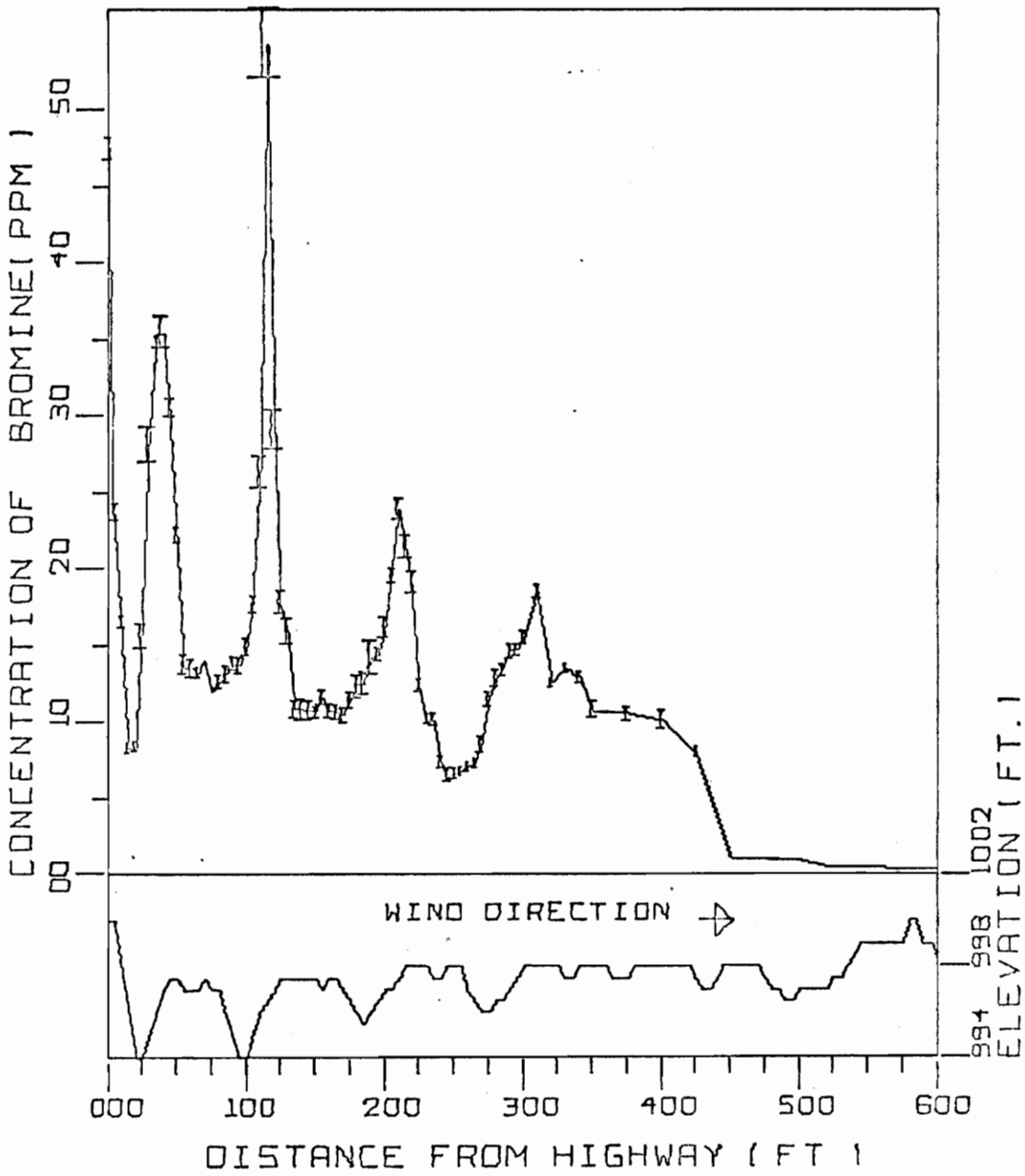



Figure 20. Concentration (ppm) of Bromine Detected in Soil Samples Versus Distance (ft) from Highway No. 1

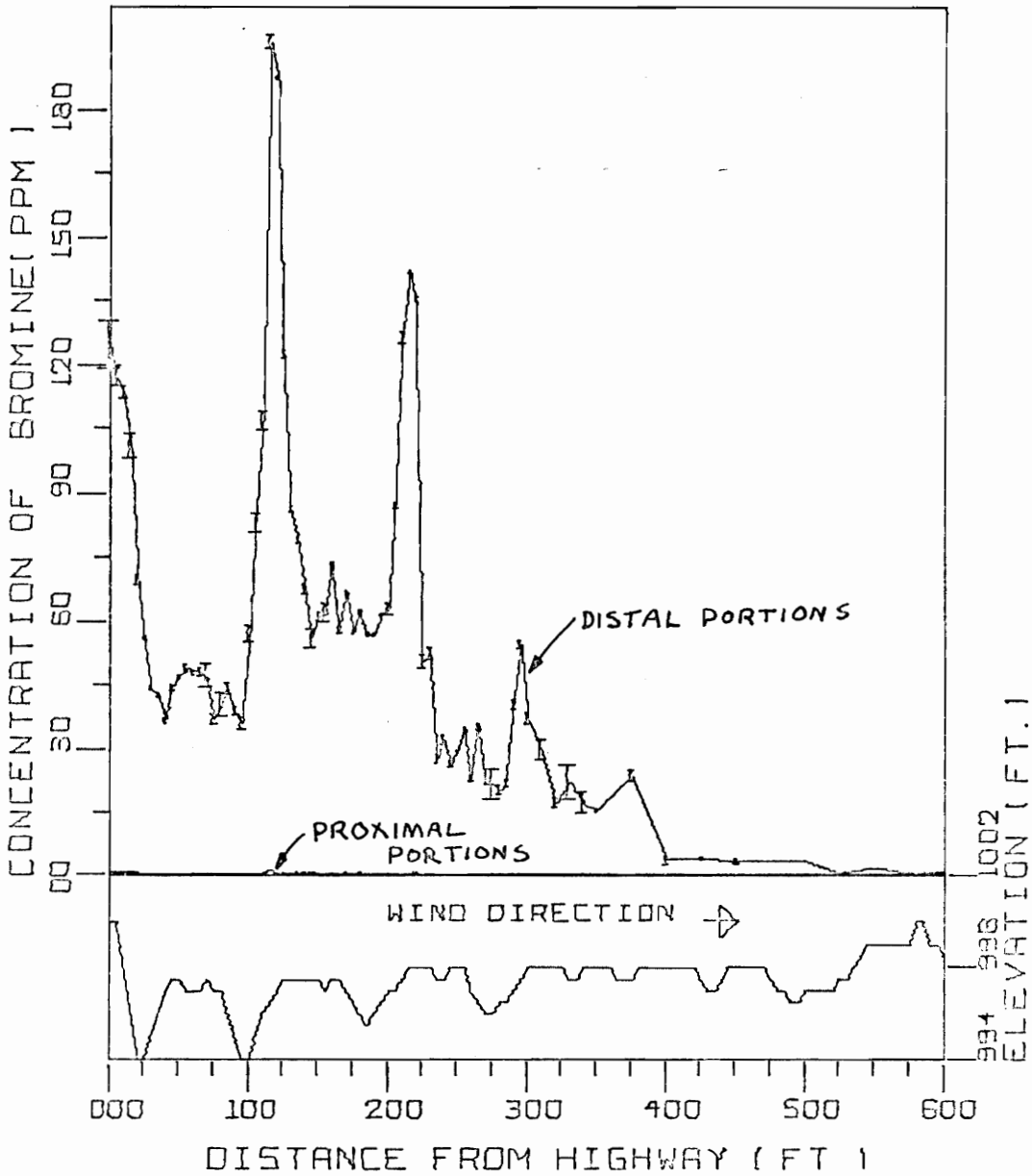



Figure 21. Concentration (ppm) of Bromine Detected in the Distal and Proximal Portion of Grass Blades Versus Distance (ft) from Highway No. 1

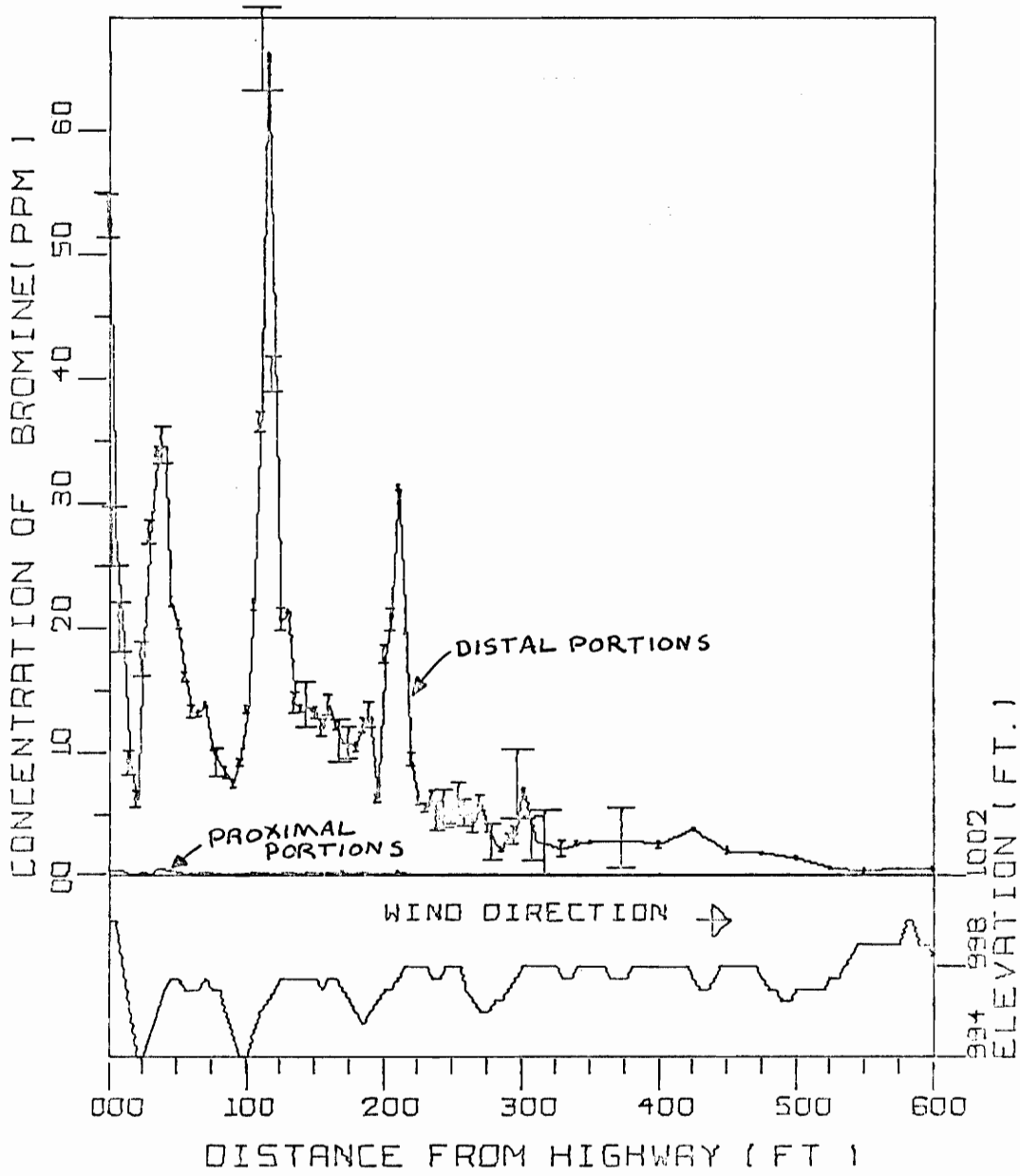



Figure 22. Concentration (ppm) of Bromine Detected in Wash Off the Distal and Proximal Portion of Grass Blades Versus Distance (ft) from Highway No. 1

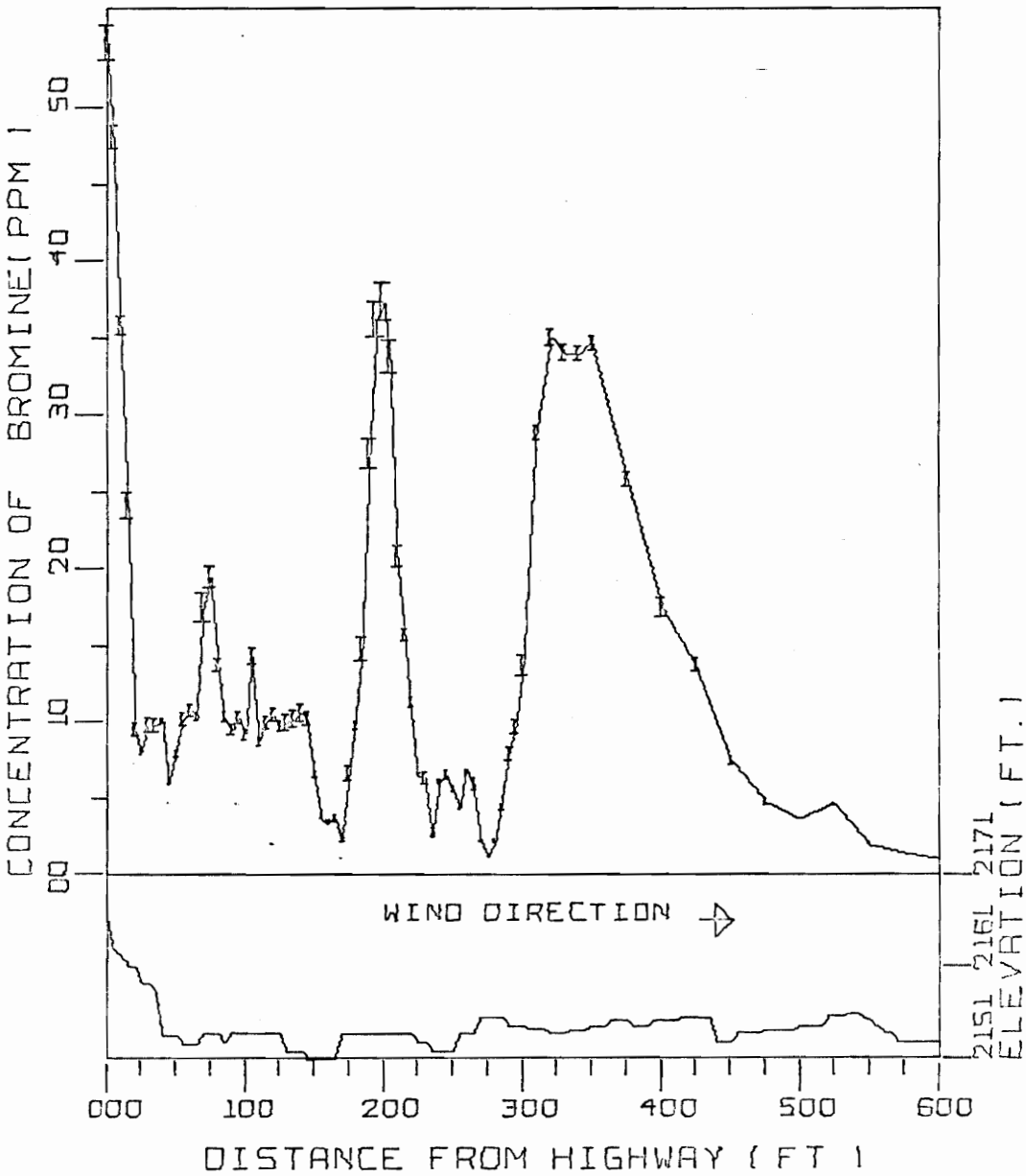



Figure 23. Concentration (ppm) of Bromine Detected in Soil Samples Versus Distance (ft) from Highway No. 2

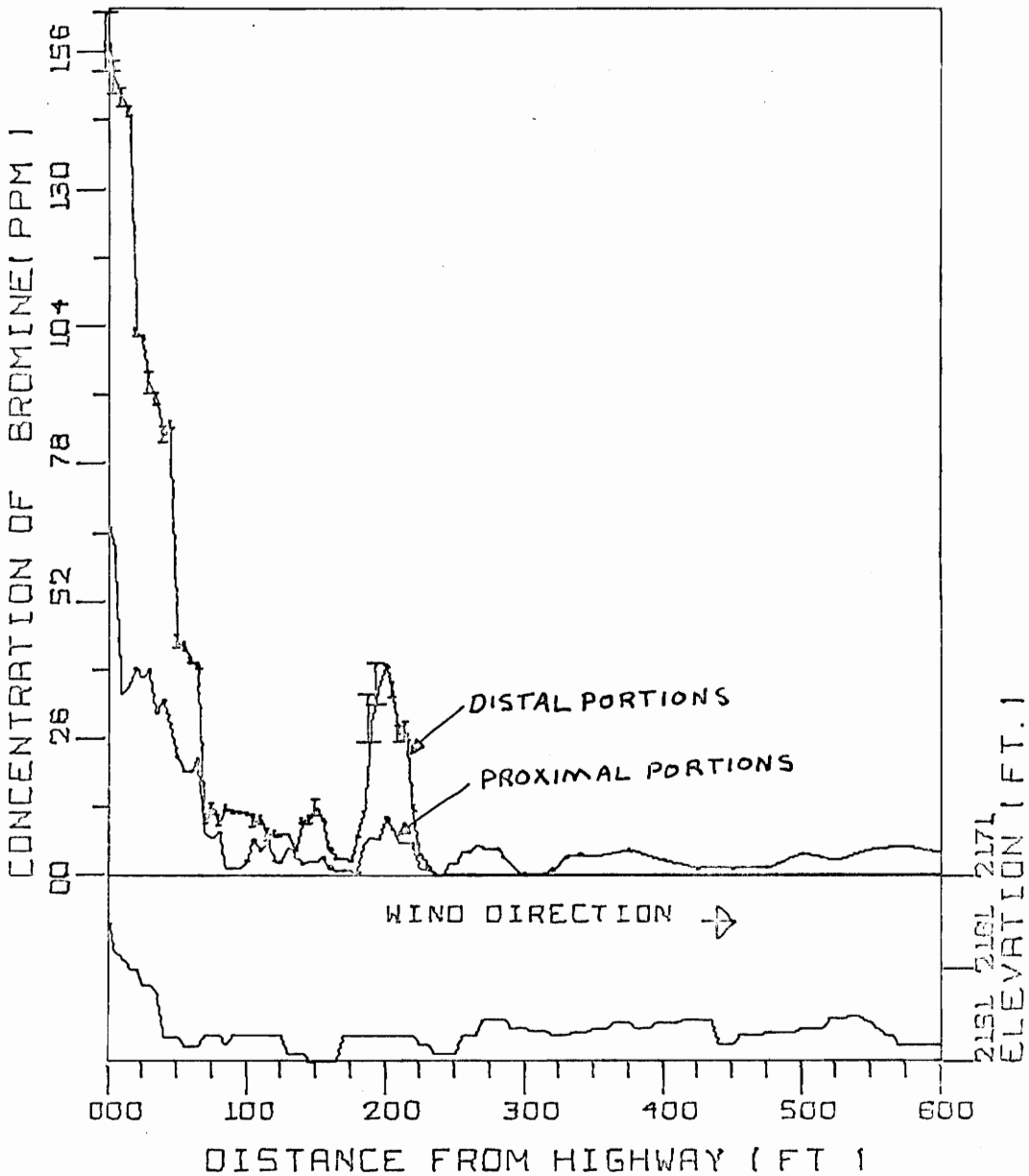



Figure 24. Concentration (ppm) of Bromine Detected in the Distal and Proximal Portion of Grass Blades Versus Distance (ft) from Highway No. 2

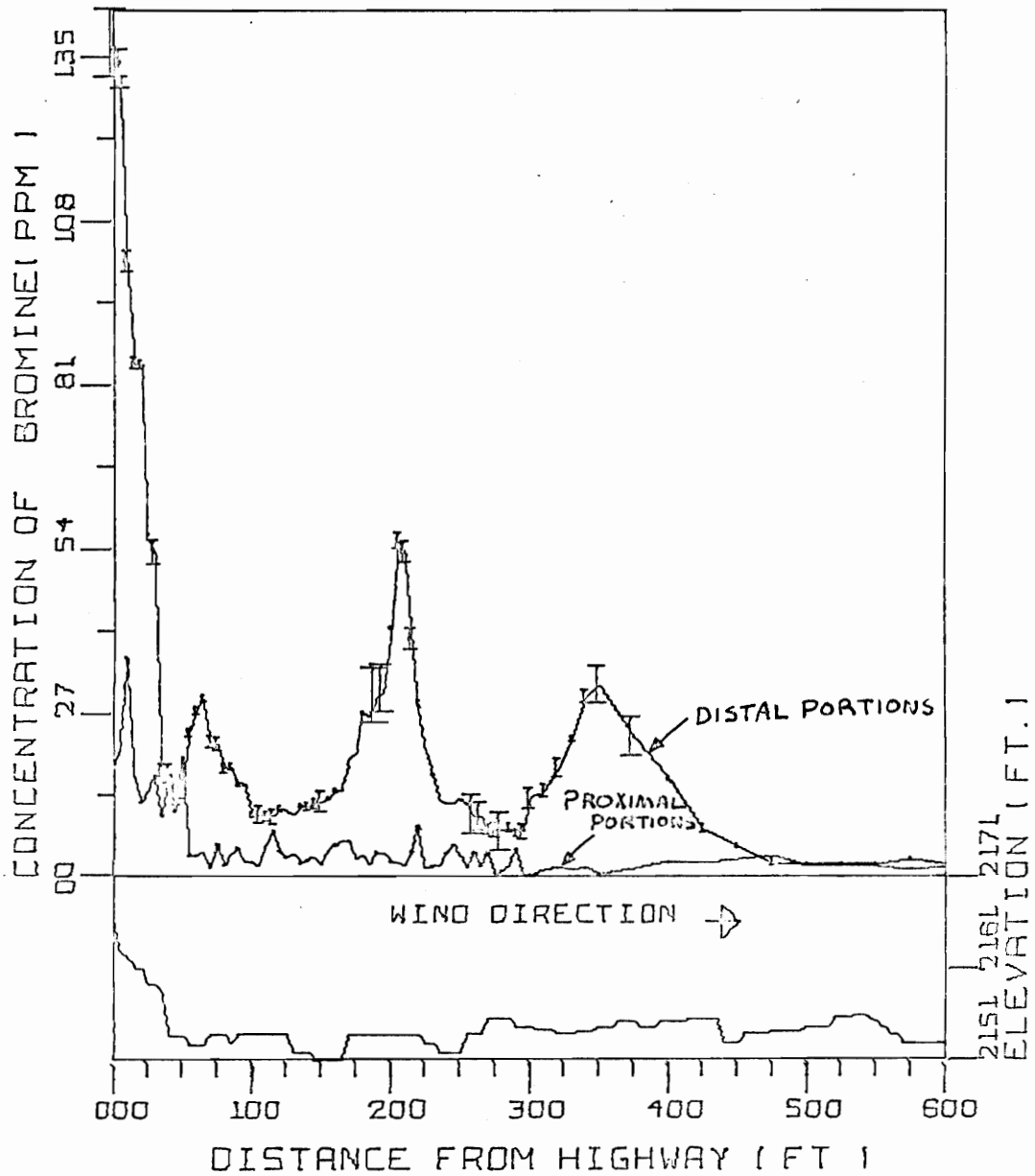



Figure 25. Concentration (ppm) of Bromine Detected in Wash Off the Distal and Proximal Portion of Grass Blades Versus Distance (ft) from Highway No. 2

the highway at which these peaks reached a maximum are very close to the distances at which the elevation stopped increasing. On the other hand, the starting point of these increases in concentration and elevation differ a great deal more. The base lines of peaks 2, 3 and 4 identified in Table 6 range over small valleys resulting from decreases in elevation from 2-4 ft. At 450 ft from Highway No. 1, the bromine concentration detected in the soil was much lower than that found in samples closer to the highway and remained at a low concentration out to 600 ft from the highway.

The plot of the bromine concentrations detected in the distal portion of the grass blades shown in Fig. 21 has several similarities to that of the plot of the concentrations detected in the soil samples shown in Fig. 20. The location of the maximum point of the larger peaks appearing at 0, 115, 215 and 300 ft in Fig. 21 corresponds closely to the location of the maximum point of four of the five major peaks shown in Fig. 20. The third largest peak shown in Fig. 20 located at 40 ft from the roadside was not detected in the grass, but a small peak was found at 60 ft as shown in Fig. 21. The base line of the peaks in Fig. 21 are smaller than the corresponding peaks in Fig. 20. The bromine concentrations shown in Fig. 21 appear almost entirely in the distal portion of the grass blades. At 400 ft from Highway No. 1, the bromine concentrations detected in the distal portion of the grass blades decreased and remained at a low level out to 600 ft from the highway.

Table 6

Location of Increases in Elevation

and Bromine Concentrations in Soil Samples from Highway No. 1

| Distances at Which the Increase in Elevation Started and Stopped (ft) | Peak No. | Distance at Which the Increase in Bromine Concentration Started and Stopped (ft) |
|---|---|---|
| 25 to 45 | 1 | 20 to 40 |
| 100 to 125 | 2 | 75 to 115 |
| 185 to 215 | 3 | 170 to 210 |
| 280 to 305 | 4 | 250 to 310 |

The plot of the bromine concentrations detected in the wash off the distal portion of the grass blades shown in Fig. 22 is also similar to the plot of the concentrations detected in the soil samples shown in Fig. 20. The location of the maximum point of the larger peaks appearing in Fig. 22 correspond closely to the location of the maximum point of the larger peaks shown in Fig. 20. Peaks with maximums appearing at 0, 40 and 115 ft in both figures were very similar but those peaks in Fig. 22 have a broader base line and are sharper than those appearing in Fig. 20. The maximum concentration points of peaks shown in Fig. 22 are very close to those shown in Fig. 20. The bromine concentrations in the wash appeared almost entirely in the distal portion of the grass blades as shown in Fig. 22. The bromine concentrations detected in the wash off the distal portion of the grass blades decreased to a low level at 500 ft from Highway No. 1 and remained at a low level out to 600 ft from the roadside.

Examination of Fig. 23 shows no obvious direct relationship between the build-up of the bromine concentrations in the soil samples and the increases in the elevation of the sample locations at Highway No. 2. As shown in Fig. 23, three of the four major bromine concentration peaks with maximum points at 60, 105 and 200 ft from the roadside have base lines that range over flat sample areas and the peak with a maximum point at 320 ft is very broad with its base line covering an area with a varying elevation. The bromine concentrations decreased continuously between 375 and 500 ft from the roadside. A small concentration peak was found with its maximum point located 525

ft from the roadside at which point the concentration continued to decrease out to 600 ft.

Examination of Fig. 24 also shows no clear relationship between the build-up of the bromine concentration peaks in the distal portion of the grass blades and the increases in the elevation of the sample locations at Highway No. 2, Also, there was very little similarity in the locations of the maximum point of the major bromine concentration peaks detected in the distal portion of the grass blades and the locations of the maximum point of the concentration peaks found in the soil samples from Highway No. 2. The bromine concentration in the grass samples from Highway No. 2 reached a low much faster than did the concentration in the samples from Highway No. 1 and the soil samples from Highway No. 2. The concentration dropped off to a low at 235 ft from Highway No. 2 and remained at a fairly low level out to 600 ft from the roadside.

The bromine concentrations in the proximal portion of the grass blades from Highway No. 2 shown in Fig. 24 were found to be much higher in comparison to the distal portions than were those from Highway No. 1 as shown in Fig. 24. In many of the sample locations at Highway No. 2, the concentrations in the distal and proximal portion of the grass blades were very close and in some cases were found to be equal.

The bromine concentration in the wash off the distal portion of the grass blades from Highway No. 2 shown in Fig. 25 have several similarities to that of the plot of the concentrations in the soil

samples shown in Fig. 23. The locations of the maximum point of the larger peaks appearing at 0, 65, 205 and 350 ft in Fig. 25 correspond closely to the location of the maximum point of the four major peaks found in the soil samples shown in Fig. 23. The length of the base lines of the peaks shown in Fig. 25 are also very close to those shown in Fig. 23. The bromine concentrations in the wash off the grass blades reached a low level around 475 ft from Highway No. 2 and remained at a low level out to 600 ft from the roadside. The concentrations in the wash off the proximal portion of the grass blades, as in the plant samples themselves, were much higher compared to the distal portion than were those from Highway No. 1 as shown in Fig. 22.

## Chlorine (Cl)

Plots of the chlorine concentrations versus distance from the highway detected in the soil samples, distal and proximal portion of the grass blades and the wash off the distal and proximal portion of the grass blades from Highway No. 1 are given in Figs. 26, 27 and 28, respectively. Figures 29, 30, and 31 are plots of the chlorine concentrations versus distance from Highway No. 2 detected in the soil samples, distal and proximal portion of the grass blades and the wash off the distal and proximal portion of the grass blades, respectively. The chlorine concentrations detected in the wash from the proximal portion of the grass blades from Highway No. 1 were at such low levels that the plot was barely noticeable in Fig. 28.

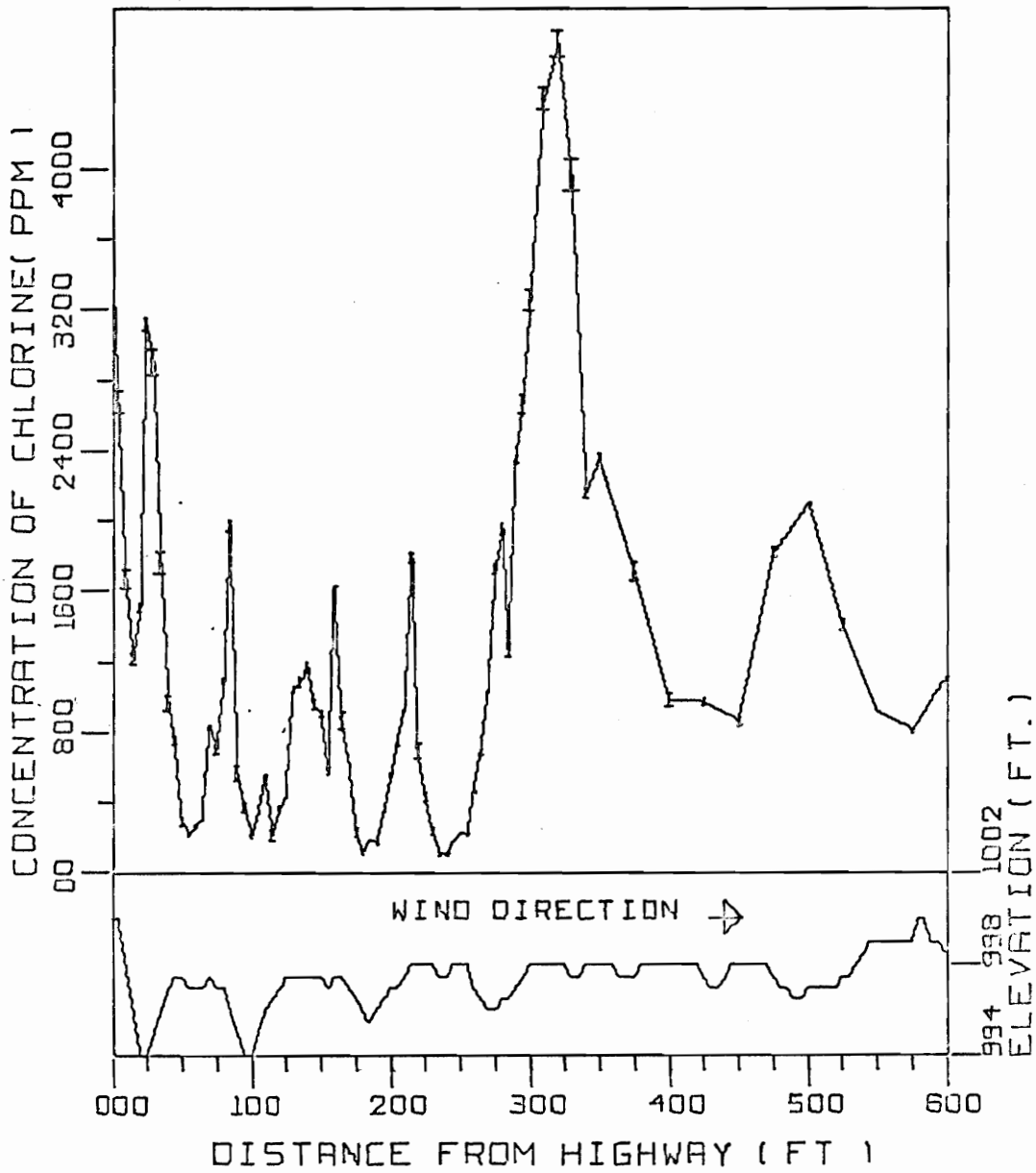



Figure 26. Concentration (ppm) of Chlorine Detected in Soil Samples Versus Distance (ft) from Highway No. 1

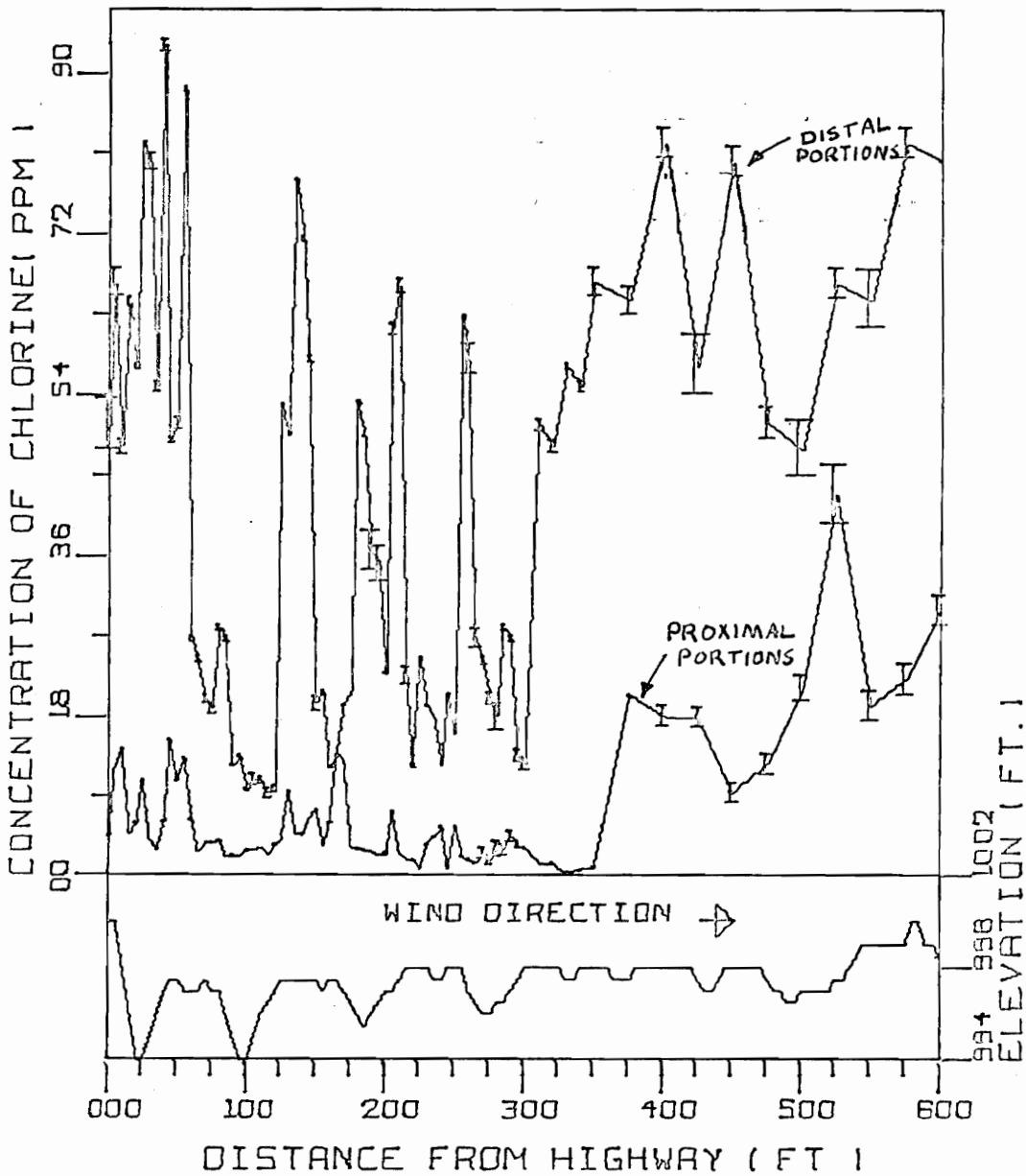



Figure 27. Concentration (ppm) of Chlorine Detected in the Distal and Proximal Portion of Grass Blades Versus Distance (ft) from Highway No. 1

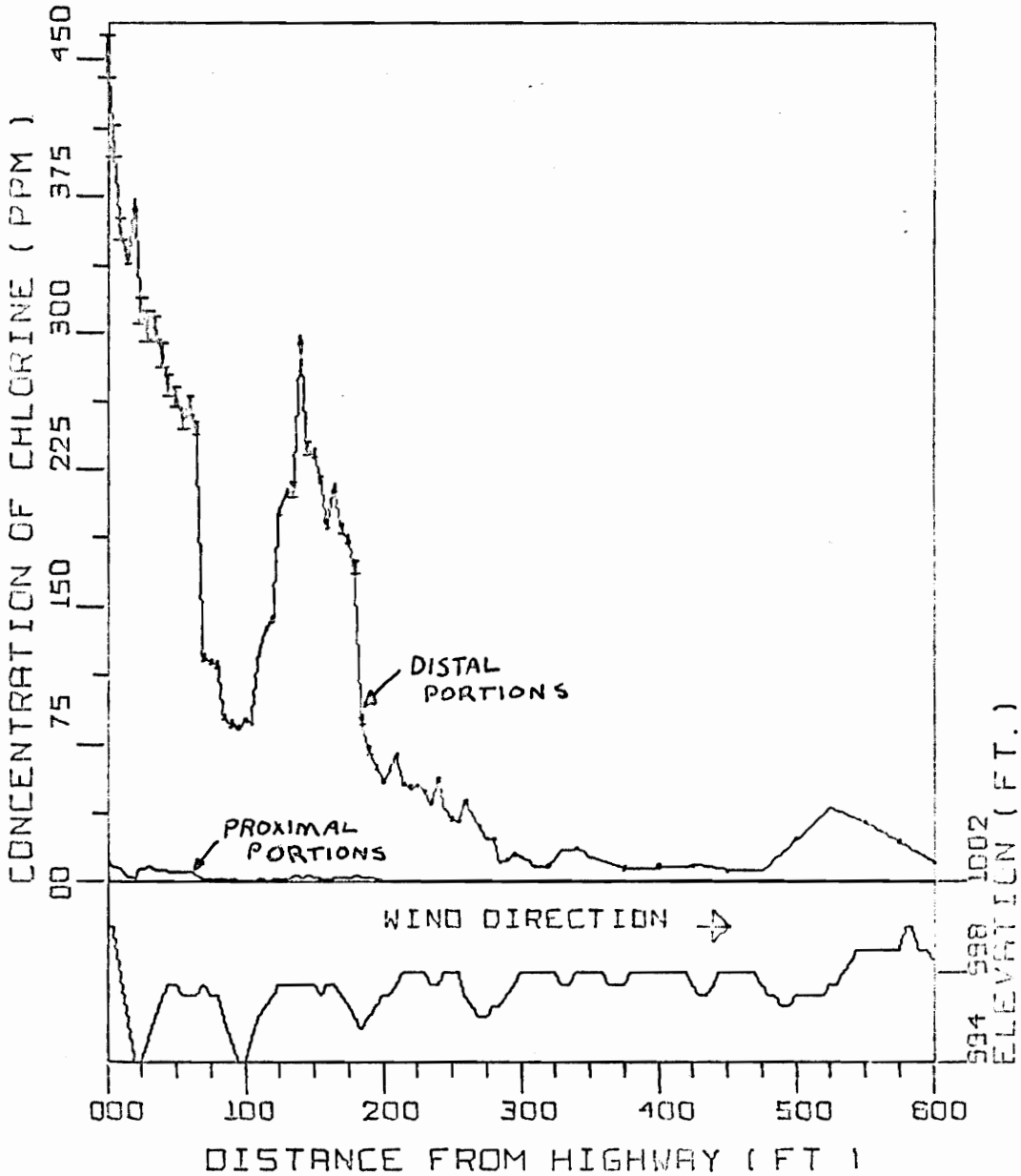



Figure 28. Concentration (ppm) of Chlorine Detected in Wash Off the Distal and Proximal Portion of Grass Blades Versus Distance (ft) from Highway No. 1

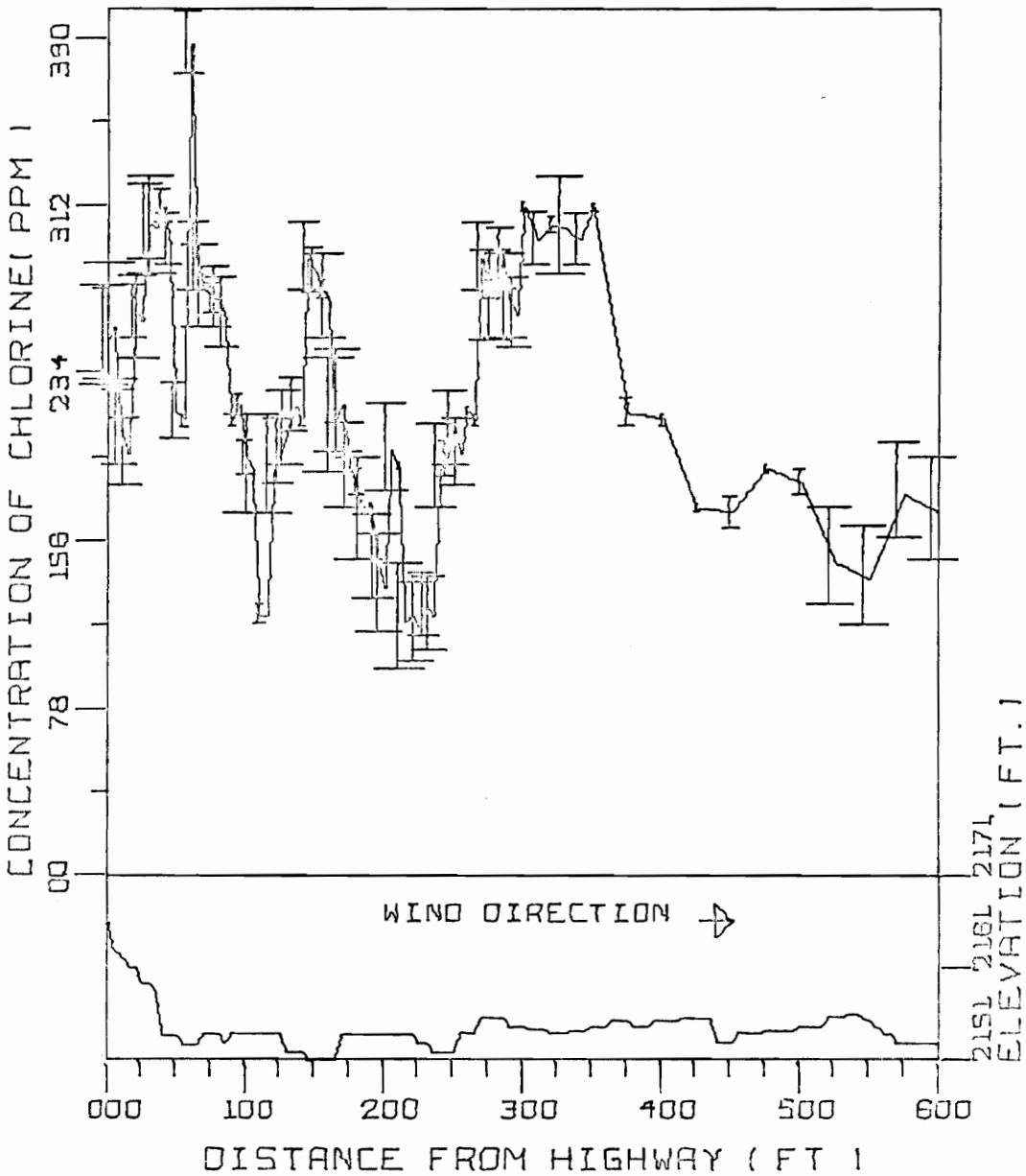



Figure 29. Concentration (ppm) of Chlorine Detected in Soil Samples Versus Distance (ft) from Highway No. 2

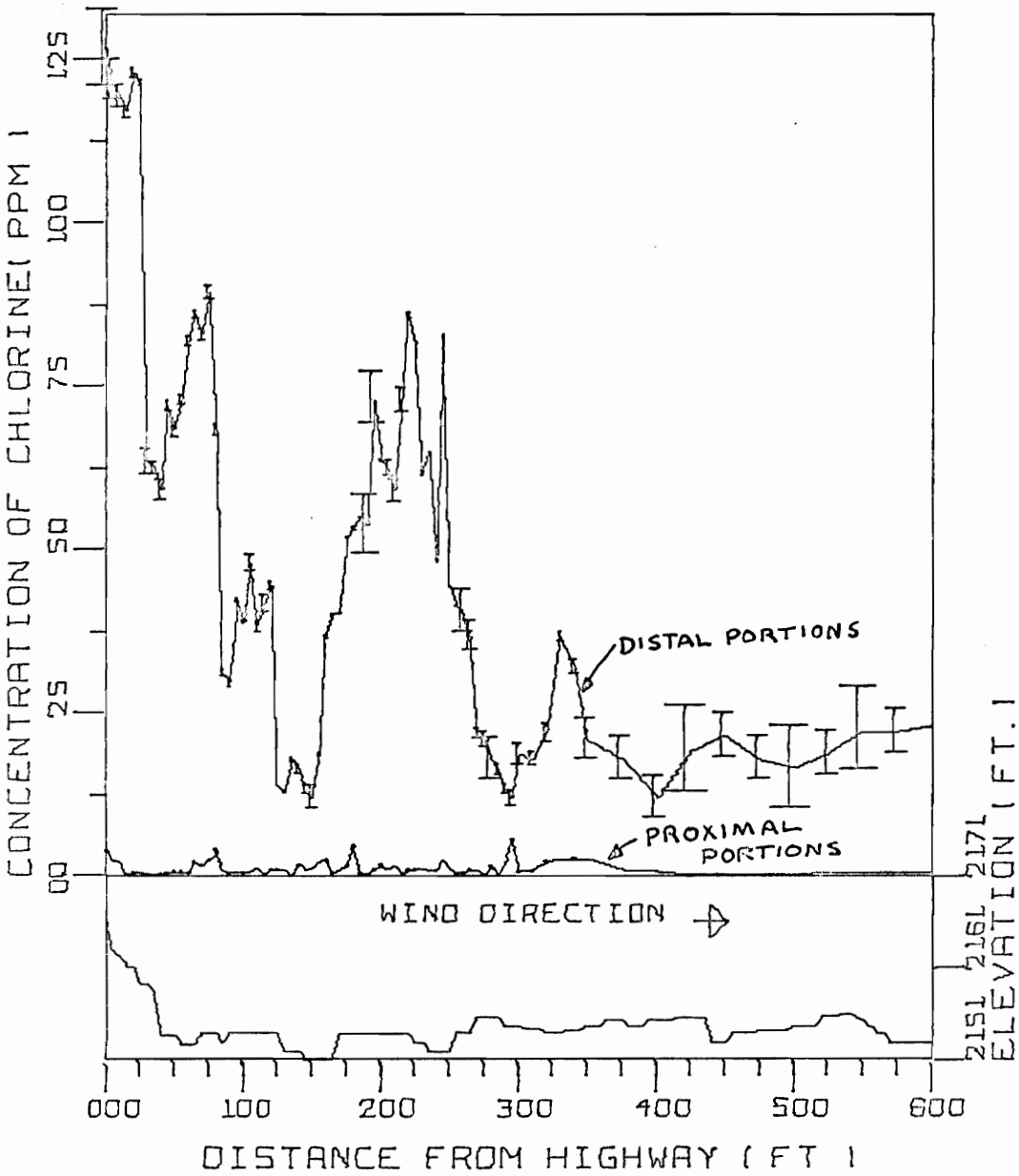



Figure 30. Concentration (ppm) of Chlorine Detected in the Distal and Proximal Portion of Grass Blades Versus Distance (ft) from Highway No. 2

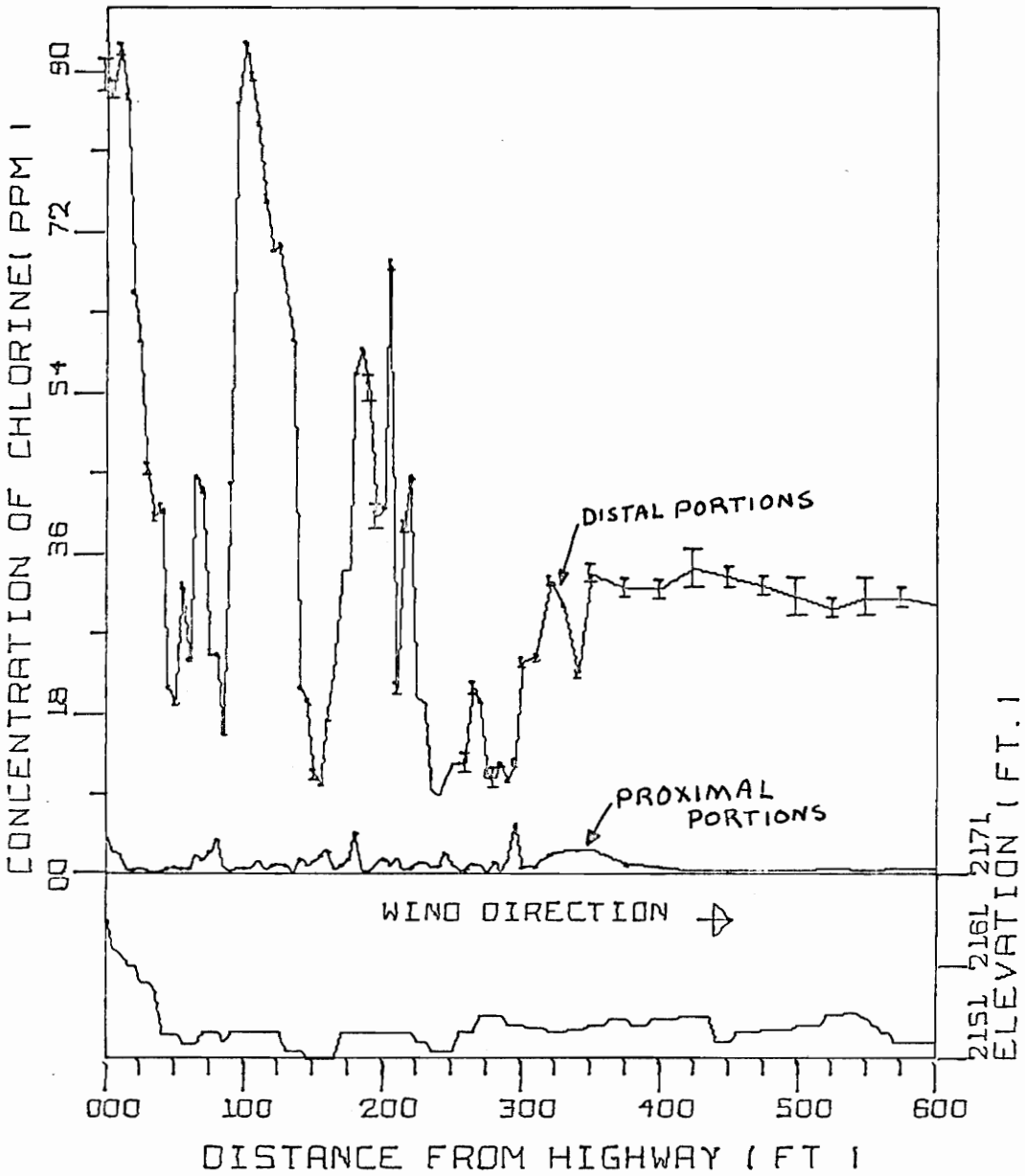



Figure 31. Concentration (ppm) of Chlorine Detected in Wash Off the Distal and Proximal Portion of Grass Blades Versus Distance (ft) from Highway No. 2

No significant relationship was found between the build-up of the chlorine concentration in the soil samples and the increases in the elevation of the sample locations at Highway No. 1. Beyond 60 ft from the highway, all the maximum points of the concentration peaks except for the one at 110 ft appeared at sample locations with smooth elevations. The chlorine concentrations did not show a decreasing trend as a function of distance from the roadside. Concentrations detected in the soil samples from Highway No. 1, were much higher than detected in the samples from Highway No. 2.

No similarities were found in the plots of the chlorine concentrations detected in the soil samples shown in Fig. 26 and the grass samples shown in Fig. 27. As shown in Fig. 27, the concentrations detected in the grass samples changed rapidly as a function of distance and no distinct patterns were noticed. Chlorine concentrations in the distal portion of the grass blades were found to be much higher than detected in the proximal portions but these concentrations are much lower than those found in the soil.

In comparison of Figs. 26 (soil), 27 (grass), 28 (wash), no similarities were noticed. As shown in Fig. 28, the concentrations show a general decreasing trend as a function of distance from the highway. At 290 ft from Highway No. 1, the chlorine concentrations reached a low level and remained low out to 600 ft from the highway. The concentrations detected in the wash off the distal portion of the grass blades were much higher than was found in the plants themselves. As shown in Fig. 28, the chlorine concentrations appear almost entirely

in the wash off the distal portions.

The plot of the chlorine concentrations detected in the soil samples versus distance from Highway No. 2 shown in Fig. 29 is a fairly smooth curve. At about 300 ft from the roadside, the concentration begins a decreasing pattern and shows only a slight increase around 550 ft. As mentioned earlier, the chlorine concentrations detected in the soil from Highway No. 2 were much less than detected in samples from Highway No. 1.

The general shape of the plot shown in Fig. 30 is quite different from the one shown in Fig. 29. There is an overall decreasing pattern in the chlorine concentrations detected in the distal portion of the grass blades as a function of distance from the roadside out to about 350 ft. No relationship was found between the build-up of the peaks and the increases in the elevation of the sample locations. After about 85 ft the base lines of the major peaks are over sample areas with flat elevations. As shown in Fig. 30, the concentrations appear almost entirely in the distal portions of the grass blades which was not the case for the grass samples from Highway No. 1. Between 350 ft and 600 ft from the highway the chlorine concentrations detected in the distal portions were fairly constant.

The plot of the chlorine concentrations detected in the wash off the grass samples from Highway No. 2 shown in Fig. 31 has several similarities to that of the plot shown in Fig. 30. The location of the concentration peaks shown in Fig. 31 are fairly close to the peaks shown in Fig. 30. As shown in Fig. 31, the concentration appear al-

most entirely in the wash off the distal portion of the grass blades. Between 350 ft and 600 ft from the highway the chlorine concentration detected in the wash off the distal portion of the grass blades were fairly constant.

In the soil samples from Highway No. 1, there were four Br (Fig. 20) and Cl (Fig. 26) concentration peaks with maximum points appearing at similar locations. These locations are 0, 115, 210 and 310 ft from the roadside for the bromine plot and 0, 110, 220 and 315 ft for the chlorine plot. In the soil samples from Highway No. 2, there were five Br (Fig. 23) and Cl (Fig. 29) concentration peaks with maximum points appearing at similar locations. These locations are 0, 40, 75, 140 and 200 ft from the roadside for the bromine plot and 0, 40, 75, 145 and 205 ft for the chlorine plot. Even with these similarities the overall shape of the plots discussed above were found to be quite different.

In the grass samples from Highway No. 1, there were six Br (Fig. 21) and Cl (Fig. 27) concentration peaks with maximum points appearing at similar locations. These locations were at 0, 60, 170, 215, 265 and 385 ft for the bromine plot and at 0, 65, 180, 210, 260 and 395 ft for the chlorine plot. In the grass samples from Highway No. 2, there were three Br (Fig. 24) and Cl (Fig. 30) concentration peaks with maximum points appearing at similar locations. These locations were at 0, 85 and 200 ft from the roadside for the bromine plot and at 0, 75 and 195 ft for the chlorine plot. The concentrations detected in the proximal portion of the grass blades shown in Fig. 27

(chlorine) were much higher in comparison to the distal portions than were those shown in Fig. 23 (bromine). In the samples from Highway No. 2, the concentrations detected in the proximal portion of the grass blades in Fig. 24 (bromine) were much higher in comparison to the distal portions than were those shown in Fig. 30 (chlorine). The overall shape of the curves shown in Figs. 21 and 27 is quite different but, in Figs. 24 and 30 the overall shape of the curve is very similar.

In the wash samples from Highway No. 1, there were five Br (Fig. 22) and Cl (Fig. 28) concentration peaks with maximum points appearing at similar locations. These locations were at 0, 130, 145, 210 and 255 ft from the roadside for the bromine plot and at 0, 135, 155, 220 and 260 ft for the chlorine plot. In the wash samples from Highway No. 2, there were six Br (Fig. 25) and Cl (Fig. 31) concentration peaks with maximum points appearing at similar locations. These locations were at 0, 65, 85, 205, 260 and 350 ft from the roadside for the bromine plot and at 0, 60, 95, 200, 255 and 345 ft for the chlorine plot. The concentrations detected in the wash off the proximal portion of the grass blades shown in Figs. 22 and 29 were similar in comparison to the wash off the distal portions. In the samples from Highway No. 2, the concentrations in the wash off the proximal portion of the grass blades shown in Fig. 25 (bromine) were much higher in comparison to the distal portions than were those shown in Fig. 31 (chlorine). About 400 ft from the highway, all four figures discussed above exhibited a leveling out of the concentrations detected in the wash.

## Other Elements

This section contains some of the results of the other elements. Most of the plots shown in this section are given for general interest. No noticeable patterns were found in the soil, grass or wash for these elements.

### Aluminum (Al)

The concentration of aluminum versus distance from the highway detected in the soil samples, distal and proximal portion of the grass blades and the wash off the distal and proximal portion of the grass blades from Highway No. 1 are plotted in Figs. 32, 33 and 34, respectively. As shown in Figs. 33 and 34, the concentrations detected in the distal and proximal portion of the grass blades were the same but those found in the wash were quite different. In the wash samples, much higher Al concentrations were detected in the distal portion of the grass blades than in the proximal portion.

### Sodium (Na)

The concentration of sodium versus distance from the highway detected in the soil samples, distal and proximal portion of the grass blades and the wash off the distal and proximal portion of the grass blades from Highway No. 1 are plotted in Figs. 35, 36, and 37, respectively. As shown in Figs. 36 and 37 the sodium concentrations detected in the distal and proximal portion of the grass blades were the same but small differences were found in the wash samples.

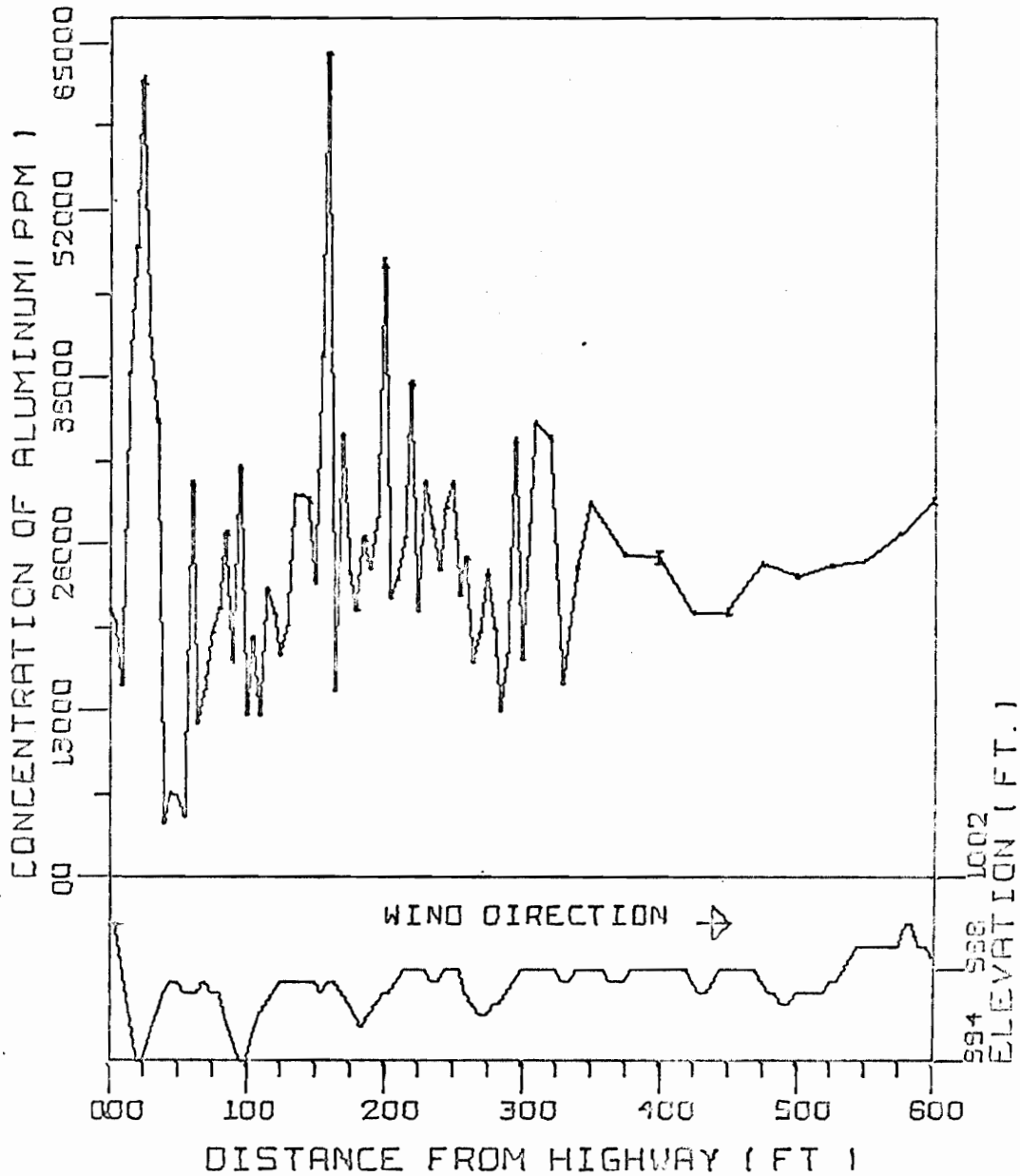



Figure 32. Concentration (ppm) of Aluminum Detected in Soil Samples Versus Distance (ft) from Highway No. 1

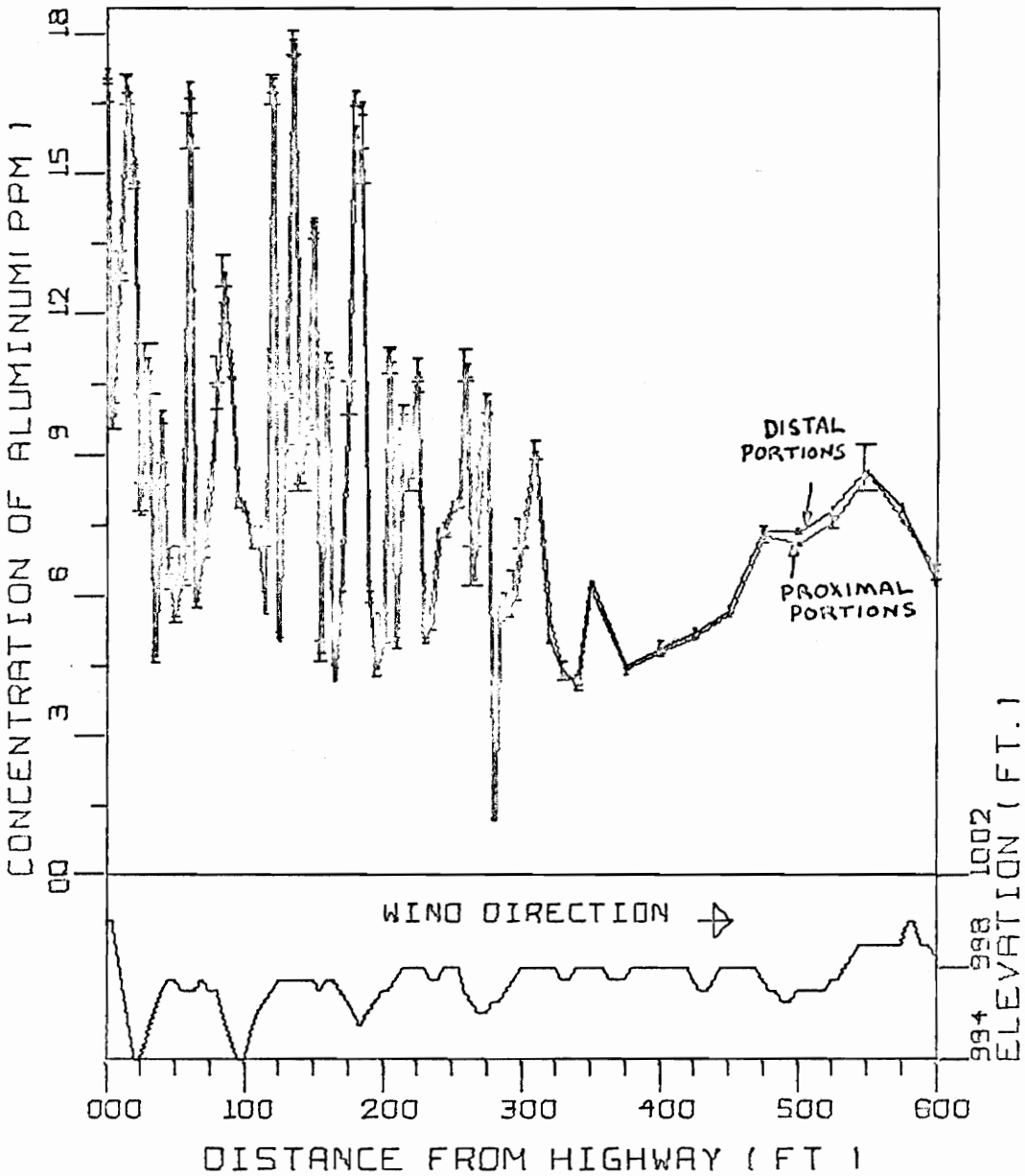



Figure 33. Concentration (ppm) of Aluminum Detected in the Distal and Proximal Portion of Grass Blades Versus Distance (ft) from Highway No. 1

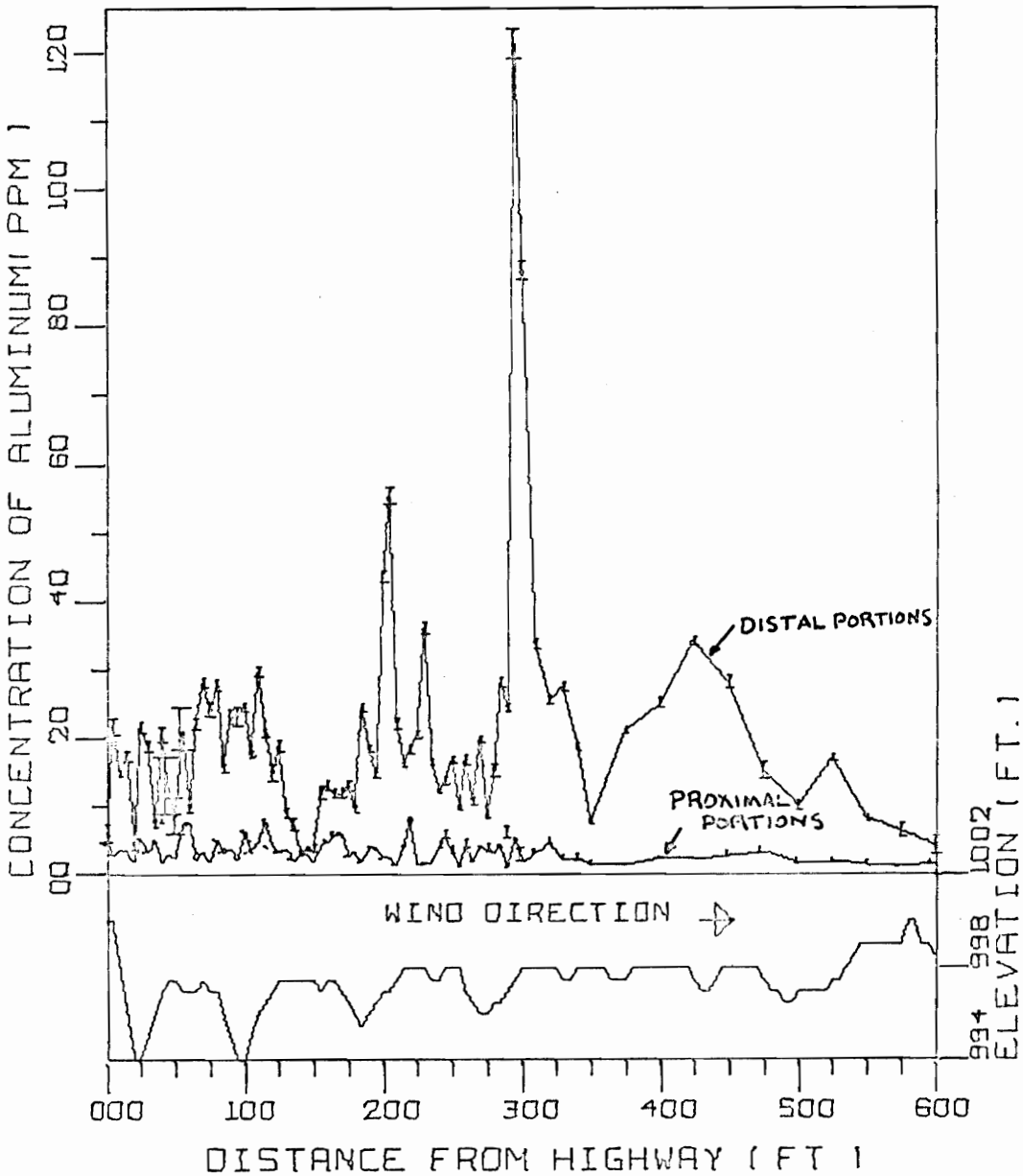



Figure 34. Concentration (ppm) of Aluminum Detected in Wash Off the Distal and Proximal Portion of Grass Blades Versus Distance (ft) from Highway No. 1

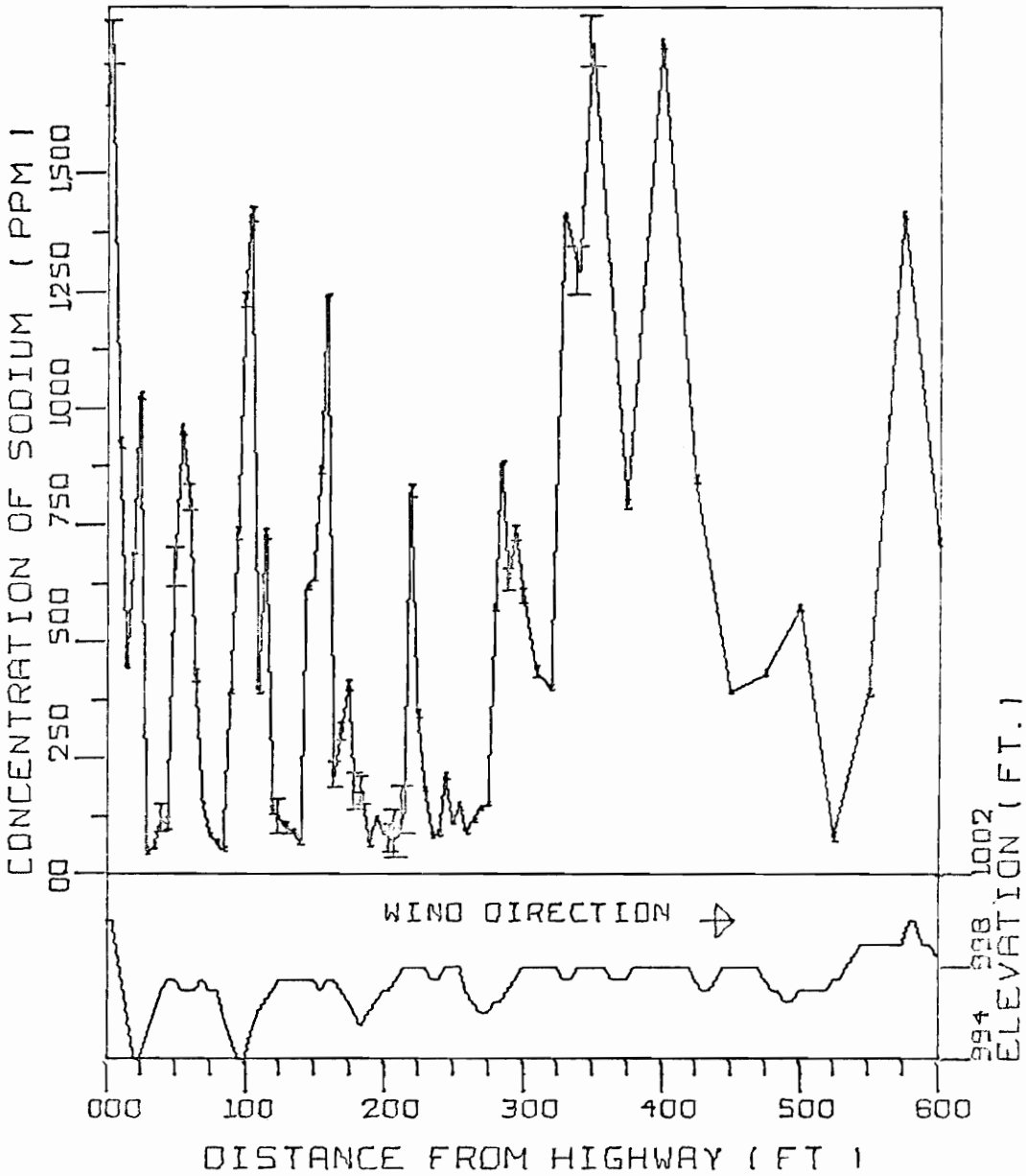



Figure 35. Concentration (ppm) of Sodium Detected in Soil Samples Versus Distance (ft) from Highway No. 1

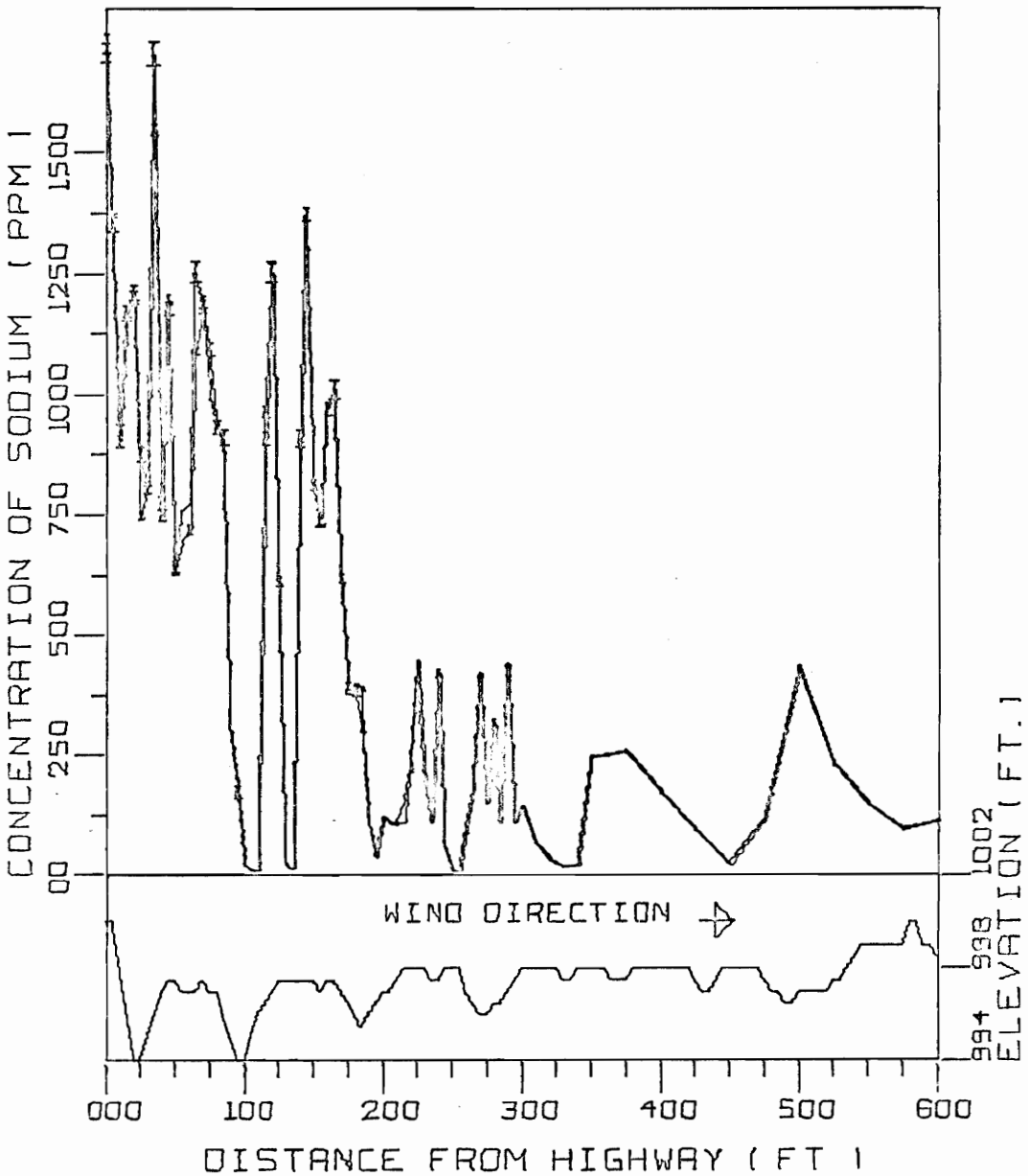



Figure 36. Concentration (ppm) of Sodium Detected in the Distal and Proximal Portion of Grass Blades Versus Distance (ft) from Highway No. 1

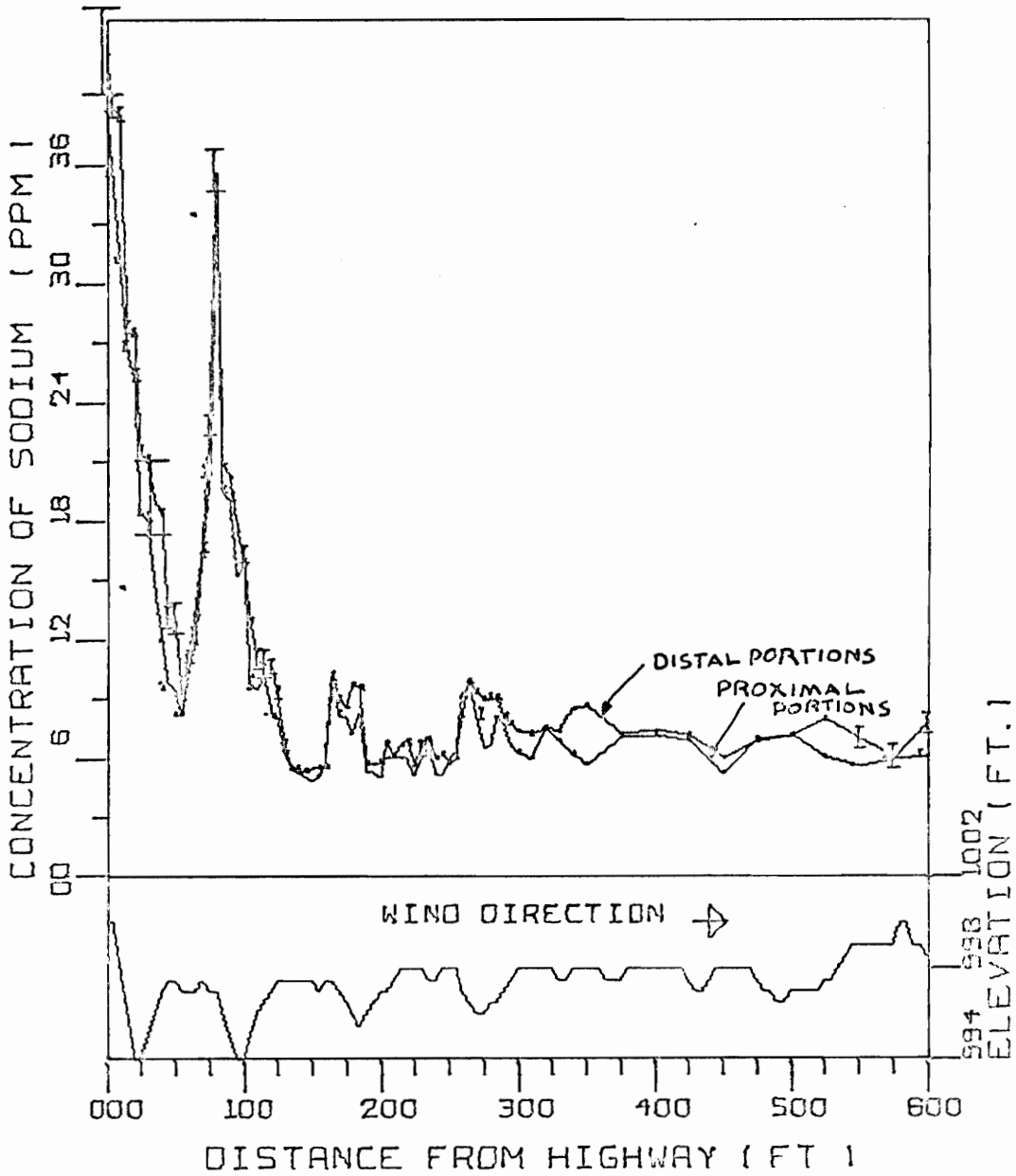



Figure 37. Concentration (ppm) of Sodium Detected in Wash Off the Distal and Proximal Portion of Grass Blades Versus Distance (ft) from Highway No. 1

## Calcium (Ca)

The concentration of calcium versus distance from the highway detected in the soil samples near Highway No. 1 are plotted in Fig. 38.

## Manganese (Mn)

The concentration of manganese versus distance from the highway detected in the soil samples near Highway No. 1 are plotted in Fig. 39.

## Arsenic (As)

The concentration of arsenic versus distance from the highway detected in the soil samples near Highway No. 1 are plotted in Fig. 40.

## Chromium (Cr)

The concentration of chromium versus distance from the highway detected in the soil samples near Highway No. 1 are plotted in Fig. 41.

## Titanium (Ti)

The concentration of titanium versus distance from the highway detected in the soil samples near Highway No. 1 are plotted in Fig. 42.

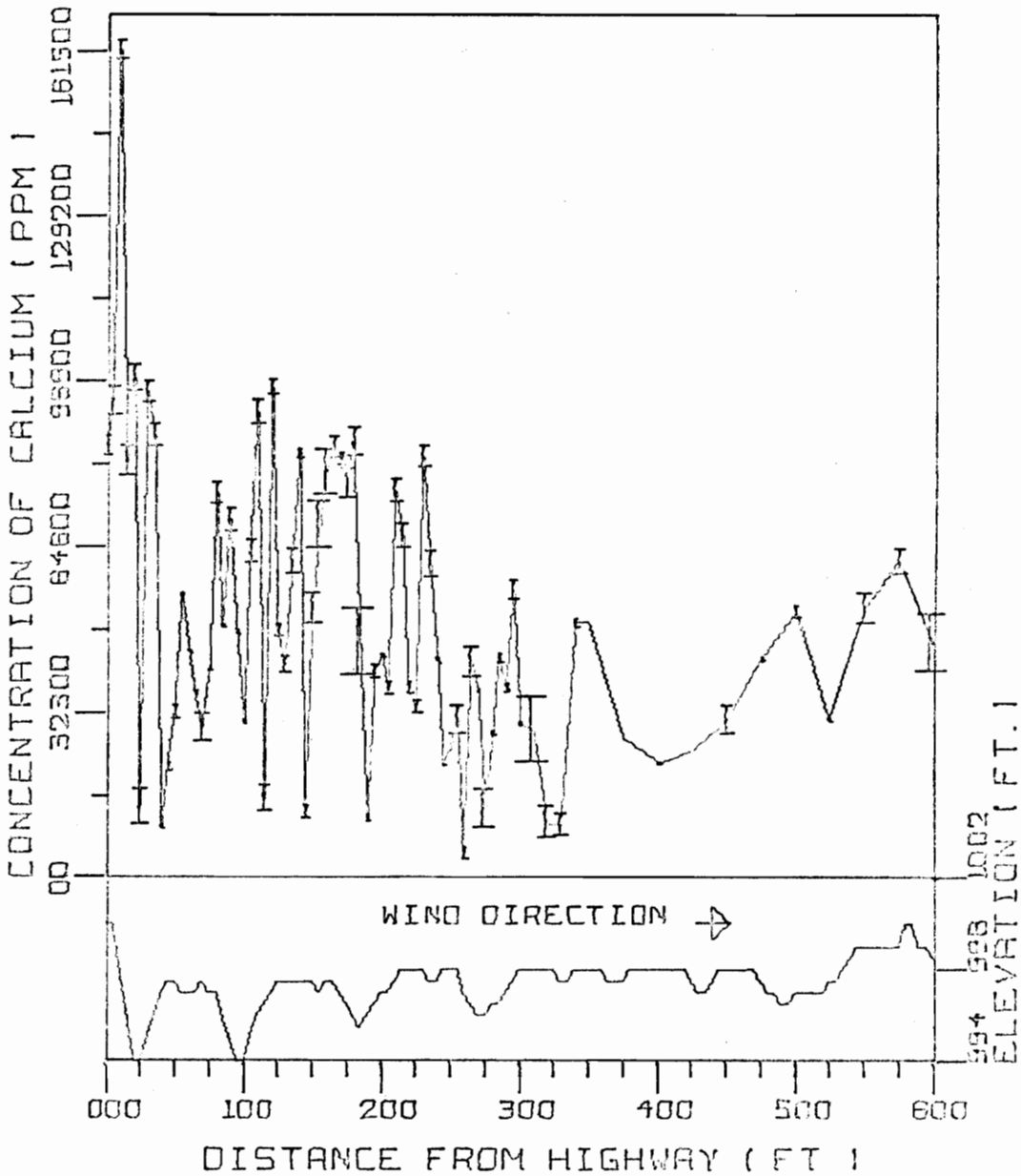



Figure 38. Concentration (ppm) of Calcium Detected in Soil Samples Versus Distance (ft) from Highway No. 1

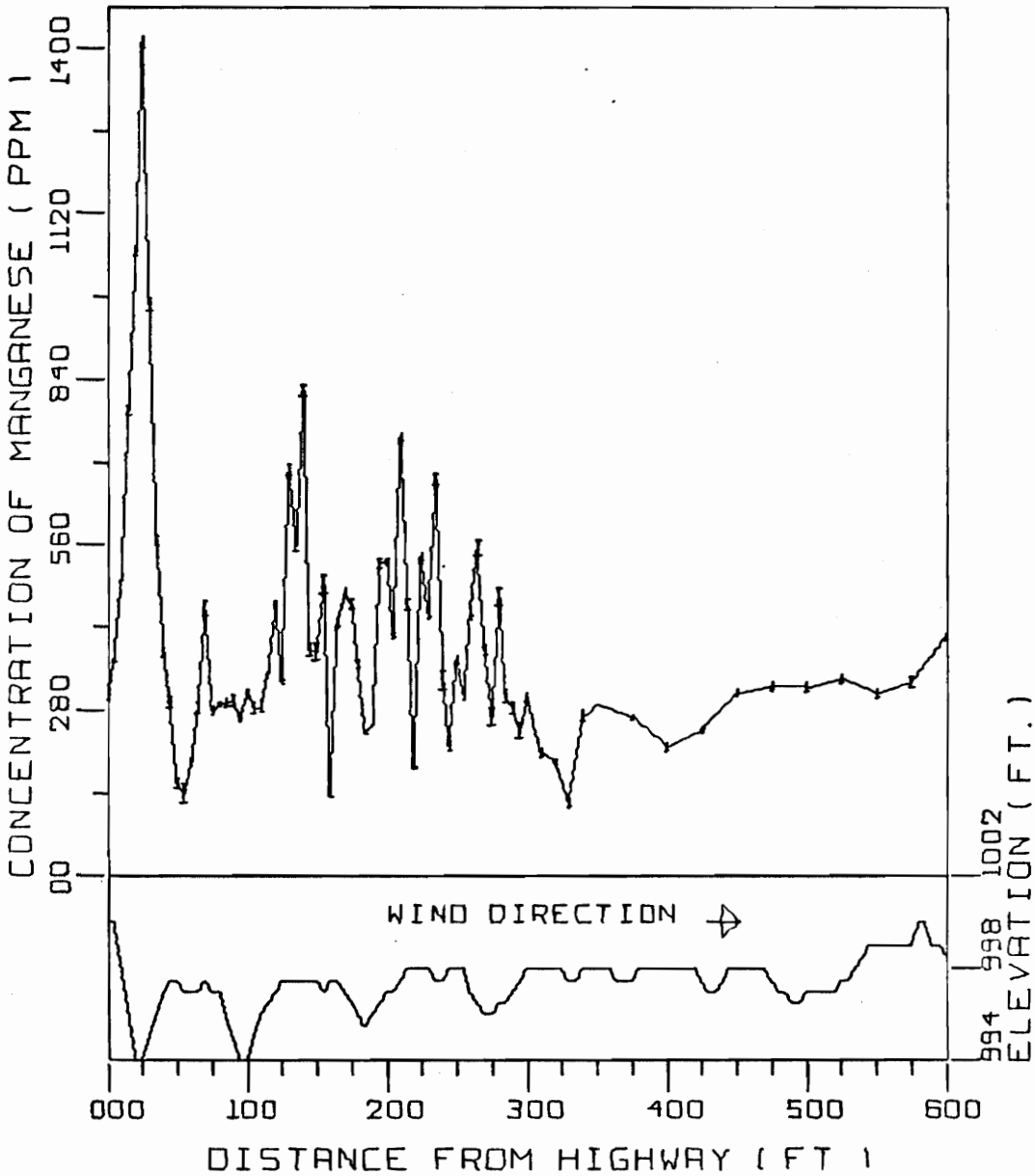



Figure 39. Concentration (ppm) of Manganese Detected in Soil Samples Versus Distance (ft) from Highway No. 1

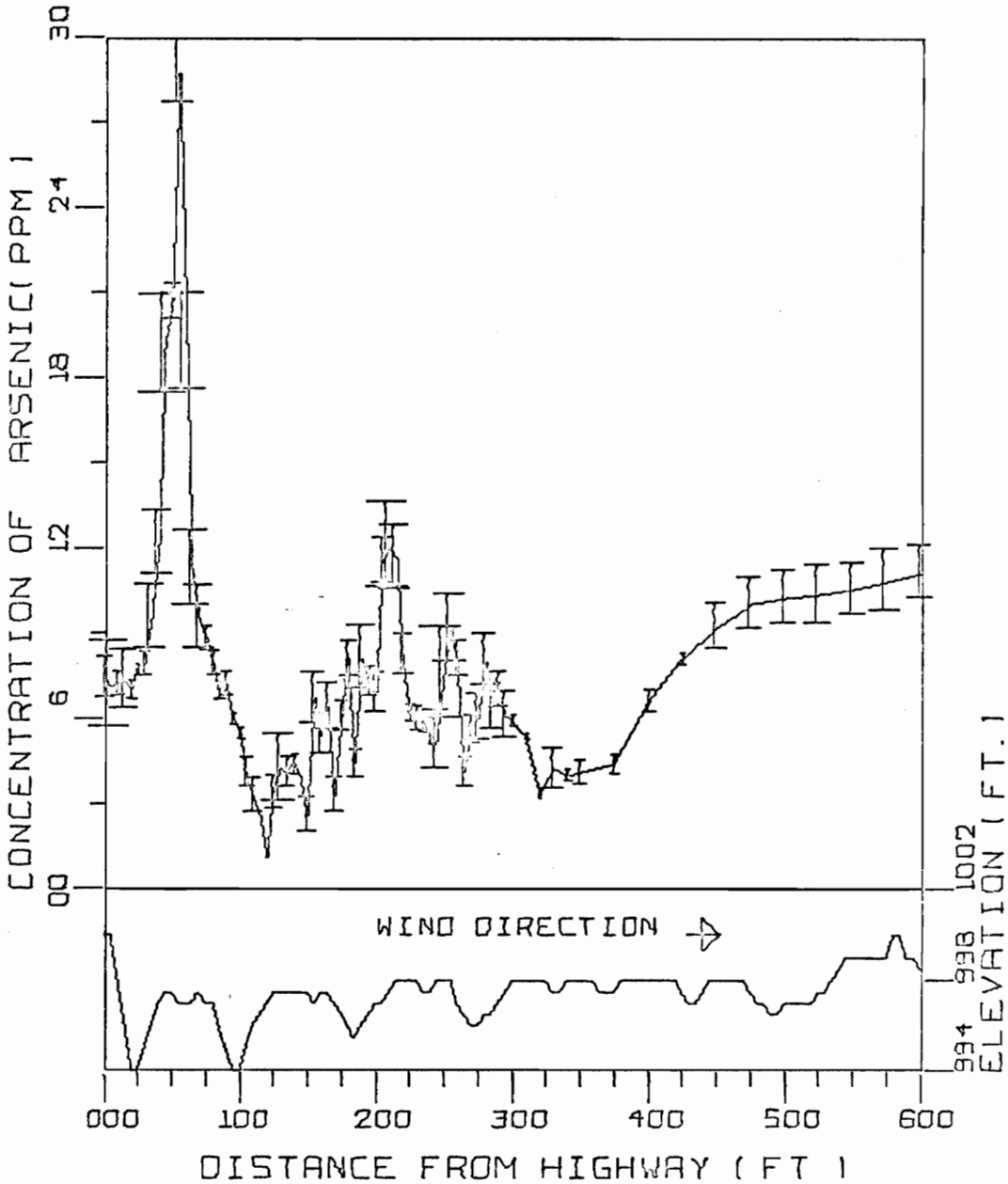



Figure 40. Concentration (ppm) of Arsenic Detected in Soil Samples Versus Distance (ft) from Highway No. 1

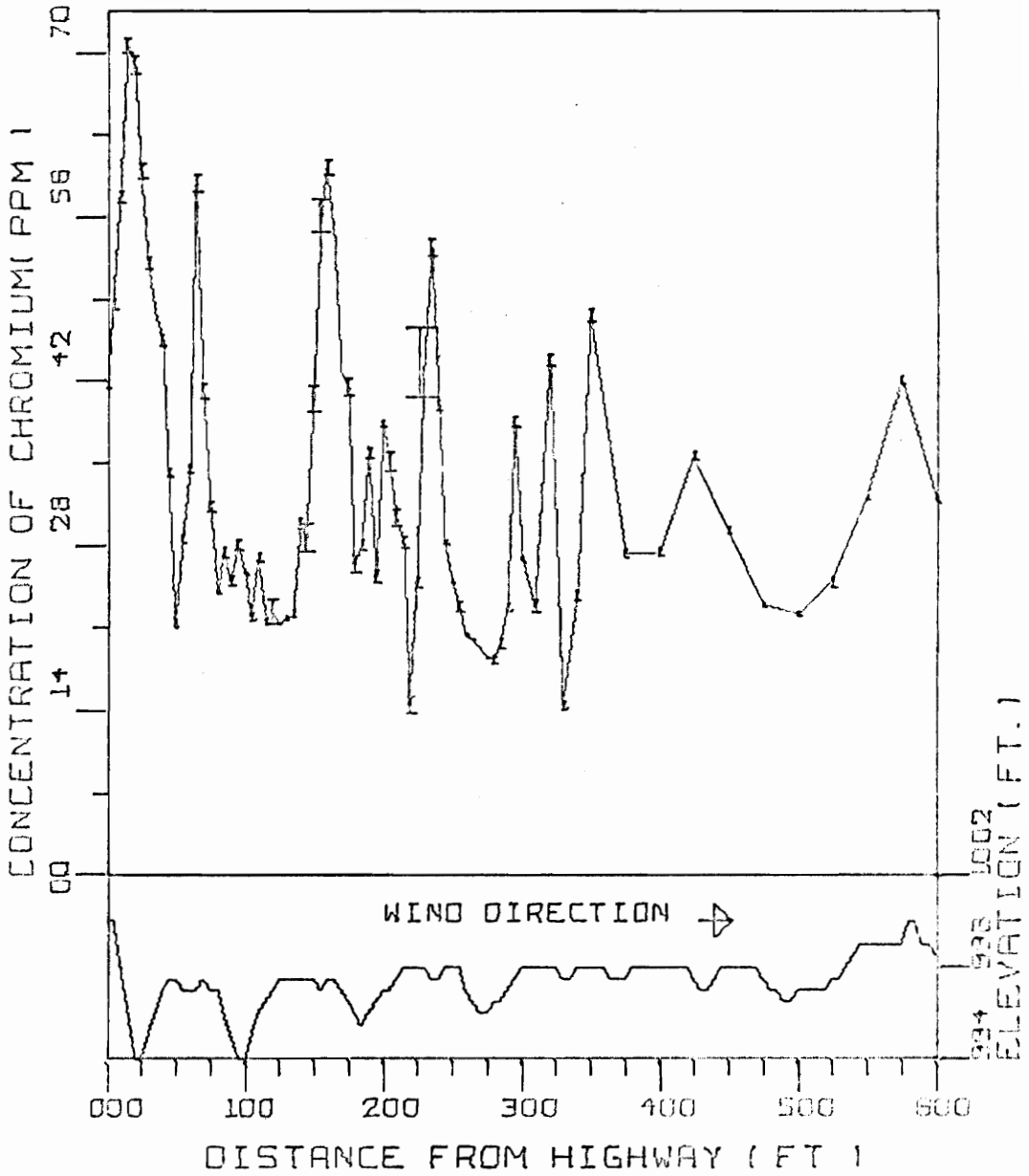



Figure 41. Concentration (ppm) Chromium Detected in Soil Samples Versus Distance (ft) from Highway No. 1

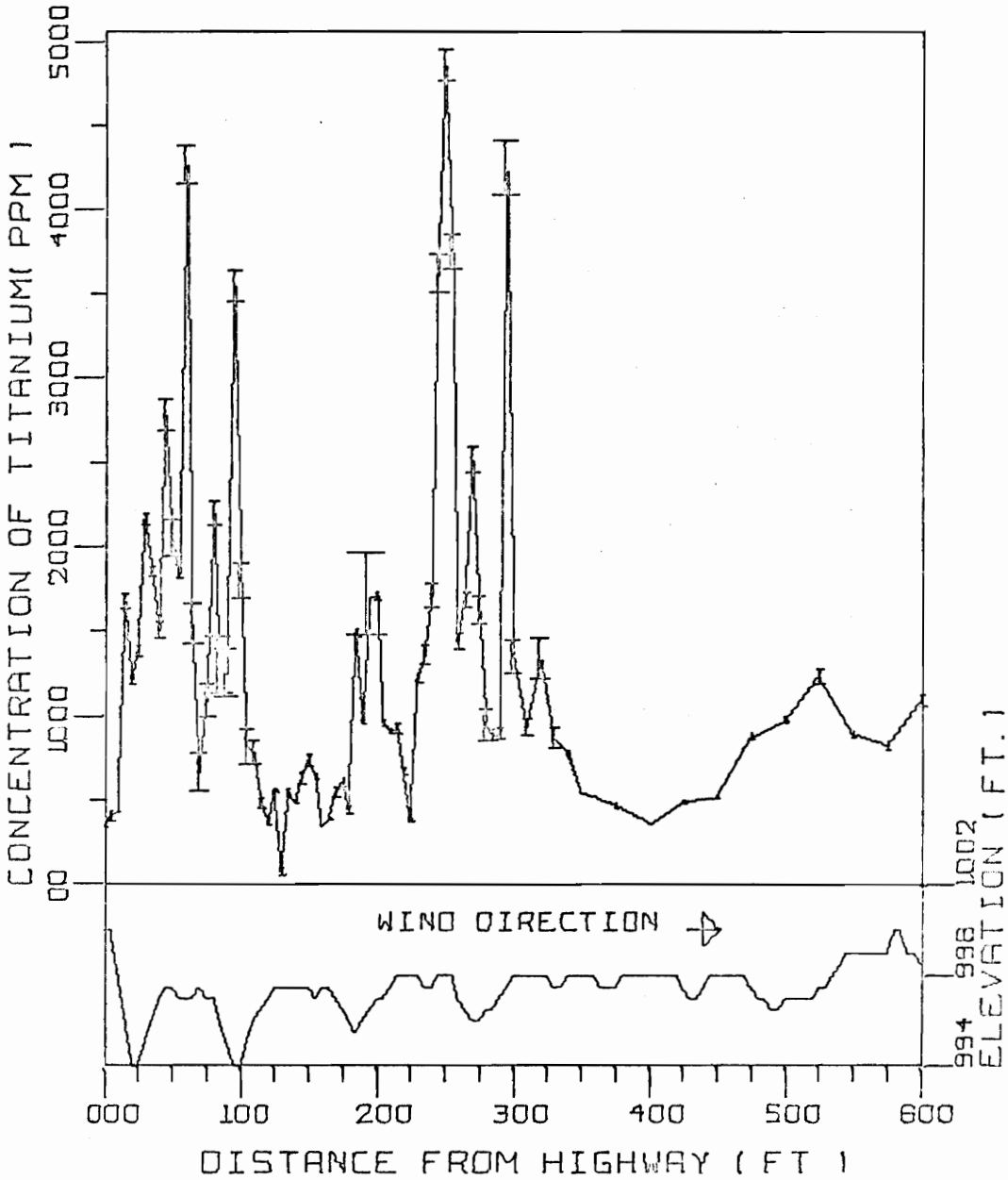



Figure 42. Concentration (ppm) of Titanium Detected in Soil Samples Versus Distances (ft) from Highway No. 1

# VI. SUMMARY

The purpose of this work was to demonstrate the effectiveness of Neutron Activation Analysis in studying a complex environmental problem. The area chosen for study was the exhaust emitted by automobiles and its dispersion into the soil and selected plants near highways.

The major elements detected both in a typical gasoline or oil sample and on filter paper exposed to automobile exhaust were: aluminum, antimony, arsenic, barium, bromine, cadmium, calcium, chlorine, chromium, magnesium, manganese, samarium, sodium and titanium. The discussion of results in this work was limited to the elements of bromine and chlorine for the reasons given in the introduction of section V.

The bromine results indicate:

1) Bromine had a tendency to concentrate in the distal portion of the grass blades. Since the distribution patterns of the bromine concentrations detected in the grass and wash samples are found to be very similar, the mechanism involved may be surface adhesion or absorption, biological concentration from the soil or bromine vapor movement.
2) Bromine concentrations tended to drop off generally at distances further out from the highway. The results indicated much higher bromine concentrations in the soil, grass and wash samples closer to the highway. The concentrations

became fairly constant around 400 ft from Highway No. 1 and 475 ft from Highway No. 2.

3) At distances close to the highway there was indication that a relationship between the build-up of bromine concentrations peaks and changes in the elevation of the sample locations existed. The results from Highway No. 1 supported this relationship, however, the data from Highway No. 2 did not. The presence of numerous trees at the site of Highway No. 2 very likely affected air flow patterns which possible influenced bromine distribution patterns.

4) Concentrations were found to be the highest in the grass samples, second highest in the wash off the grass samples and lowest in the soil samples. This was true in the samples from both highways, possibly an indication of biological concentration.

The chlorine results indicate:

1) Chlorine had a tendency to concentrate in the distal portion of the grass blades as did bromine. The highest chlorine concentrations were detected in the distal portion of the grass blades and in the wash off the distal portion of the grass blades samples from both highways.

2) Chlorine concentrations tended to drop off at distances further out from the highway in the grass samples from Highway No. 2 and the wash off the grass samples from both

highways. No indication was found in other samples.

3) The chlorine concentrations were found to be the highest in the soil samples from both highways. In the samples from Highway No. 1, the second highest concentrations were found in the wash and the lowest were found in the grass. This was reversed in the samples from Highway No. 2. However, the natural levels of chlorine in the soil were proportionally much higher than were found for bromine. This could have masked to some extent highway effects. Also, the particles involved could be different and have substantially different diffusion patterns.

Of these two elements, bromine probably most clearly indicates where some of the atmospheric components were going and therefore would be the most suitable element for neutron activation studies of atmospheric and turbulence modeling and possibly for following biological effects studies of automobile traffic. If bromine could be used to infer indirectly lead distribution, then biological effects due to lead might be important where the bromine peaks were found.

More work must be done to develop the procedures used in this study in order to make a more reliable technique for the indication of automobile pollution. It is felt that neutron activation analysis, the computer program and analytical techniques described in this work employed in conjunction with an air monitoring program and possibly wind tunnel experiments would provide an effective tool for establishing computer models to predict the environmental impact of automobiles

on the regions near highways.

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# APPENDIX A
## LISTING OF NAA COMPUTER PROGRAM

```
C     MAIN PROGRAM                                                      MAIN   5
C     ALL IMPORTANT DECISIONS ARE MADE ON THE BASIS OF INSUFFICIENT DATAMAIN  10
C                                                                       MAIN  15
C     NAA SPECTRUM ANALYSIS PROGRAM DEVELOPED DURING 1974 FOR HD4420.   MAIN  20
C     COMMENTED BY ALAN HAWTHORNE  8/74.                                MAIN  25
C                                                                       MAIN  30
C     VARIABLES DEFINED AT BEGINNING OF EACH SUBPROGRAM FOR EASY        MAIN  35
C     REFERENCE.  VARIABLES OCCURRING IN MORE THAN ONE SUBROUTINE       MAIN  40
C     WILL BE LISTED ONLY ONCE.  INDEXING COUNTERS NOT LISTED.          MAIN  45
C                                                                       MAIN  50
C     MAIN PROGRAM VARIABLE LISTING.                                    MAIN  55
C                                                                       MAIN  60
C     EL=ARRAY OF LIBRARY ELEMENT NAMES.                                MAIN  65
C     ELE=ELEMENT NAME READ FROM LIBRARY.                               MAIN  70
C     GA=ARRAY OF LIBRARY GAMMA ENERGES.                                MAIN  75
C     ENERGY=GAMMA ENERGY READ FROM LIBRARY.                            MAIN  80
C     H=ARRAY OF LIBRARY HALF-LIVES.                                    MAIN  85
C     HF=HALF-LIFE READ FROM LIBRARY.                                   MAIN  90
C     ID=ARRAY OF SPECTRUM DATA POINTS                                  MAIN  95
C     IDATA=VALUE OF DATA POINT IN HEXADECIMAL                          MAIN 100
C     IDP=ARRAY OF LIBRARY FORCED DOUBLE-PEAK CODES                     MAIN 105
C     IDT=ARRAY OF SAMPLE INFORMATION INPUT FROM TAPE                   MAIN 110
C     IET=ELAPSED TIME READ FROM TAPE                                   MAIN 115
C     IFILE=FILE NUMBER COUNTER                                         MAIN 120
C     IFLAG=ARRAY OF LIBRARY HALF-LIFE CODES FOR COUNTING SEQUENCE      MAIN 125
C                                                                       MAIN 130
C     ILIB=NUMBER OF LIBRARY CARDS INPUT                                MAIN 135
C     IPFLAG=FORCED DOUBLE-PEAK CODE READ FROM LIBRARY                  MAIN 140
C     ISO=ARRAY OF LIBRARY ISOTOPE MASS NUMBERS                         MAIN 145
C     ISOT=ISOTOPE MASS NUMBERS READ FROM LIBRARY                       MAIN 150
C     ITAG=TAGWORD READ FROM TAPE                                       MAIN 155
C     KFLAG=HALF-LIFE CODE FOR COUNTING SEQUENCE READ FROM LIBRARY      MAIN 160
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C     LASTAG=LAST TAGWORD OF INPUT SEQUENCE                             MAIN 165
C     MTAG=ARRAY OF TAGWORDS FROM CARD READER                           MAIN 170
C     NPTS=NUMBER OF SPECTRUM POINTS                                    MAIN 175
C     NTAG=TAGWORD INPUT FROM CARD READER                               MAIN 180
C                                                                       MAIN 185
C     SA=SPECIFIC ACTIVITY READ FROM LIBRARY                            MAIN 190
C     SP=ARRAY OF LIBRARY SPECIFIC ACTIVITIES                           MAIN 195
C                                                                       MAIN 200
C     TA=SAMPLE ACTIVATION TIME                                         MAIN 205
C     TC=SAMPLE COUNT TIME                                              MAIN 210
C     TW=SAMPLE WAIT TIME                                               MAIN 215
C     WT=SAMPLE WEIGHT                                                  MAIN 220
C     XLUX=FLUX CODE FOR SAMPLE ACTIVATION                              MAIN 225
C                                                                       MAIN 230
C                                                                       MAIN 235
C     DIMENSION SPACE FOR STORAGE OF LIBRARY AND DATA.                  MAIN 240
      COMMON ID(4010)                                                   MAIN 245
      DIMENSION MTAG(100)                                               MAIN 250
      DIMENSION EL(200), ISO(200), H(200), EN(200), SP(200), IFLAG(200),MAIN 255
     1 IDP(200)                                                         MAIN 260
      DIMENSION AFLUX(100), ATA(100), ATW(100), ATC(100), AWT(100), A1(1MAIN 265
     100), A2(100), A3(100), IDATA(4010), Y(60)                         MAIN 270
      INTEGER TID,TIH,TIM,TIS,TCD,TCH,TCM,TCS,TSD,TSH,TSMAIN 280
     1M,TSS                                                             MAIN 285
      DOUBLE PRECISION SI,SO,SC,SS                                      MAIN 275
C     CALL FOR SPECIFIC FORTRAN ERROR LISTINGS.                         MAIN 290
      CALL ERRSET (207,256,10)                                          MAIN 295
      CALL ERRSET (208,256,-1)                                          MAIN 300
      CALL ERRSET (209,256,10)                                          MAIN 305
C     INITIALIZE COUNTERS.                                              MAIN 310
      I=0                                                               MAIN 315
      ID=0                                                              MAIN 320
```

```
      IFILE=0                                                           MAIN 325
C     INPUT AND STORE TAGWORDS OF SPECTRUMS TO BE PROCESSED.            MAIN 330
10    READ (5,55) TID,TIH,TIM,TIS,TOD,TOH,TOM,TOS,TCD,TCH,TCM,TCS,TSD,TSMAIN 335
     1H,TSM,TSS,WT,IFLUX,W1,W2,W3,NTAG                                  MAIN 340
      IF (NTAG.EQ.000000) GO TO 15                                      MAIN 345
      IC=IC+1                                                           MAIN 350
      WRITE (6,60) TID,TIH,TIM,TIS,TOD,TOH,TOM,TOS,TCD,TCH,TCM,TCS,TSD,TMAIN 355
     1SH,TSM,TSS,WT,IFLUX,W1,W2,W3,NTAG                                 MAIN 360
      FLUX=IFLUX                                                        MAIN 365
      IF (FLUX.EQ.0.0) FLUX=130.0                                       MAIN 370
      AFLUX(IC)=FLUX                                                    MAIN 375
      SI=TID*86400+TIH*3600+TIM*60+TIS                                  MAIN 380
      SO=TOD*86400+TOH*3600+TOM*60+TOS                                  MAIN 385
      SC=TCD*86400+TCH*3600+TCM*60+TCS                                  MAIN 390
      SS=TSD*86400+TSH*3600+TSM*60+TSS                                  MAIN 395
      DTA=SO-SI                                                         MAIN 400
      DTW=SC-SO                                                         MAIN 405
      AWT(IC)=WT                                                        MAIN 410
      DTC=SS-SC                                                         MAIN 415
      ATA(IC)=DTA/60.                                                   MAIN 420
      ATW(IC)=DTW/60.                                                   MAIN 425
      ATC(IC)=DTC/60.                                                   MAIN 430
      A1(IC)=W1                                                         MAIN 435
      A2(IC)=W2                                                         MAIN 440
      A3(IC)=W3                                                         MAIN 445
      MTAG(IC)=NTAG                                                     MAIN 450
      LASTAG=NTAG                                                       MAIN 455
      GO TO 10                                                          MAIN 460
C     READ AND STORE LIBRARY INFORMATION.                               MAIN 465
15    READ (5,70) ELE,ISOT,HF,ENERGY,SA,KFLAG,IPFLAG                    MAIN 470
      IF (ISOT.EQ.0) GO TO 20                                           MAIN 475
      I=I+1                                                             MAIN 480
```

```
      EL(I)=ELE                                                         MAIN 485
      ISO(I)=ISOT                                                       MAIN 490
      H(I)=HF                                                           MAIN 495
      EN(I)=ENERGY                                                      MAIN 500
      SP(I)=SA                                                          MAIN 505
      IFLAG(I)=KFLAG                                                    MAIN 510
      IDP(I)=IPFLAG                                                     MAIN 515
      ILIB=I                                                            MAIN 520
      IF (I.EQ.200) GO TO 20                                            MAIN 525
      GO TO 15                                                          MAIN 530
C     READ SPECTRUM AND CONVERT TO DECIMAL #'S IF TAGWORD MATCHES THAT  MAIN 535
C     REQUESTED                                                         MAIN 540
20    READ (10,65,END=45) ITAG,(IDATA(II),II=1,4010)                    MAIN 545
      IFILE=IFILE+1                                                     MAIN 550
      ITAG=ICHANG(ITAG)                                                 MAIN 555
      ITAG=IC(ITAG)                                                     MAIN 560
      DO 25 IT=1,IC                                                     MAIN 565
      TAG=MTAG(IT)                                                      MAIN 570
      JTAG=TAG/1000.                                                    MAIN 575
      ATAG=JTAG                                                         MAIN 580
      TAG=TAG-ATAG*1000.                                                MAIN 585
      JITAG=TAG                                                         MAIN 590
      IF (ITAG.NE.MTAG(IT).AND.ITAG.NE.JITAG) GO TO 25                  MAIN 595
      GO TO 30                                                          MAIN 600
25    CONTINUE                                                          MAIN 605
      GO TO 20                                                          MAIN 610
30    DO 35 I=1,4010                                                    MAIN 615
      IDATA(I)=ICHANG(IDATA(I))                                         MAIN 620
      ID(I)=IC(IDATA(I))+1                                              MAIN 625
35    CONTINUE                                                          MAIN 630
      NPTS=4000                                                         MAIN 635
C     WRITE DATA OF SPECTRUM TO BE PROCESSED.                           MAIN 640
```

```
      WRITE (6,75) ITAG,(IZZ,IZZ=1,20)                                  MAIN 645
      DO 40 III=1,200                                                   MAIN 650
      IZ=(III-1)*20                                                     MAIN 655
      IZTWN=IZ+20                                                       MAIN 660
      IZP1=IZ+1                                                         MAIN 665
      WRITE (6,80) IZ,(ID(JJ),JJ=IZP1,IZTWN)                            MAIN 670
40    CONTINUE                                                          MAIN 675
      WRITE (6,85) IFILE                                                MAIN 680
C     CALL SUBROUTINE TO OBTAIN SAMPLE INPUT INFORMATION.               MAIN 685
      TA=ATA(IT)                                                        MAIN 690
      TW=ATW(IT)                                                        MAIN 695
      TC=ATC(IT)                                                        MAIN 700
      WT=AWT(IT)                                                        MAIN 705
      W1=A1(IT)                                                         MAIN 710
      W2=A2(IT)                                                         MAIN 715
      W3=A3(IT)                                                         MAIN 720
      XLUX=AFLUX(IT)                                                    MAIN 725
      I=ILIB                                                            MAIN 730
C     CALL SUBROUTINE TO ANALIZE SPECTRUM.                              MAIN 735
      CALL FIT (TA,TW,TC,XLUX,WT,ITAG,EL,ISO,H,EN,SP,I,IFLAG,IDP,W1,W2,WMAIN 740
     13)                                                                MAIN 745
C     IF THIS IS NOT LAST TAGWORD, READ ANOTHER SPECTRUM FROM TAPE.     MAIN 750
      IF (ITAG.EQ.LASTAG) GO TO 50                                      MAIN 755
45    GO TO 20                                                          MAIN 760
50    CONTINUE                                                          MAIN 765
      STOP                                                              MAIN 770
C                                                                       MAIN 775
C                                                                       MAIN 780
55    FORMAT (4(I3,I2,I2,I2,2X),F8.5,2X,I3,2X,2A4,A2,5X,I6)             MAIN 785
60    FORMAT (1X,4(I3,I2,I2,I2,2X),F8.5,2X,I3,2X,2A4,A2,5X,I6)          MAIN 790
65    FORMAT (100A3,100A3,56A3,/,3X,100A3,100A3,55A3,/,3X,100A3,100A3,55MAIN 795
     1A3,/,3X,100A3,100A3,55A3,/,3X,100A3,100A3,55A3,/,3X,100A3,100A3,55MAIN 800
```

```
      2A3,/,3X,100A3,100A3,55A3,/,3X,100A3,100A3,55A3,/,3X,100A3,100A3,55MAIN 805
      3A3,/,3X,100A3,100A3,55A3,/,3X,100A3,100A3,55A3,/,3X,100A3,100A3,55MAIN 810
      4A3,/,3X,100A3,100A3,55A3,/,3X,100A3,100A3,55A3,/,3X,100A3,100A3,55MAIN 815
      5A3,/,3X,100A3,100A3,55A3)                                          MAIN 820
70     FORMAT (A2,4X,I3,4X,F10.2,4X,F5.0,4X,E9.3,4X,I2,20X,I1)            MAIN 825
75     FORMAT (1H1,10X,11H TAG WORD= ,I8,/,10X,20I6)                      MAIN 830
80     FORMAT (1X,I4,5X,20I6)                                             MAIN 835
85     FORMAT (13H FILE NUMBER=,I8)                                       MAIN 840
       END                                                                MAIN 845
```

```
      SUBROUTINE FIT (TA,TW,TC,XLUX,WT,ITAG,EL,ISC,H,EN,SP,NC,IFLAG,IDP,FITX    5
     1W1,W2,W3)                                                         FITX   10
C     THIS ROUTINE CONTROLS ANALYSIS OF SPECTRUM.                       FITX   15
C                                                                       FITX   20
C     FIT VARIABLE LISTING                                              FITX   25
C     A=ARRAY OF FITTING PARAMETERS                                     FITX   30
C     AC=ARRAY OF INITIAL GUESS PARAMETERS                              FITX   35
C     AREA=AREA UNDER THE PEAK                                          FITX   40
C     BKG=STRAIGHT LINE ESTIMATE OF BACKGROUND                          FITX   45
C     CHISQR=CHI-SQUARED VALUE OF FIT                                   FITX   50
C     ERROR=% ERROR                                                     FITX   55
C     IISC=TEMPORARY STORAGE OF MASS NUMBER USED FOR AVERAGING          FITX   60
C     IL=LEFT LIMIT OF FITTING (MIN. PT.)                               FITX   65
C     IR=RIGHT LIMIT OF FITTING (MAX. PT.)                              FITX   70
C     IWIDE=WITH OF EXCLUDED REGION AROUND CENTROID                     FITX   75
C     K=HALF-LIFE CODE                                                  FITX   80
C     KDP=DOUBLE PEAK FIT CODE                                          FITX   85
C     KEXIT=FLAG TO SIGNAL EXIT TO NEXT PEAK                            FITX   90
C     NC=NUMBER OF LIBRARY CARDS                                        FITX   95
C     NOPK=CHANNEL NUMBER OF PEAK ( INTEGER )                           FITX  100
C     NPTS=NUMBER OF POINTS FIT                                         FITX  105
C     NTERMS=NUMBER OF FITTING PARAMETERS                               FITX  110
C     PPM=PARTS PER MILLION CONCENTRATION                               FITX  115
C     PPT=TEMPORARY STORAGE OF PPM FOR AVERAGING                        FITX  120
C     REPK=CHANNEL NUMBER OF PEAK ( REAL )                              FITX  125
C     SHIFT=MULTIPLICATIVE ENERGY CORRECTION                            FITX  130
C     SUM1=ESTIMATE OF BACKGROUND EXCLUDING CENTER POINTS               FITX  135
      COMMON ID(4010)                                                   FITX  140
      DOUBLE PRECISION ARRAY                                            FITX  145
C     DIMENSION SPACE FOR VARIABLES.                                    FITX  150
      DIMENSION X(60), Y(60), SIGMAY(60), A(9), YFIT(60), AC(3), CHI(10)FITX  155
     1, BETA(9), DERIV(9), IK(9), JK(9), ALPHA(9,9), APRAY(9,9), B(9)   FITX  160
```

```
      DIMENSION KF(200), IST(200), I2(200), EL(200), ISO(200), H(200), EFITX 165
     1N(200), SP(200), IFLAG(200), IDP(200)                            FITX 170
C     INITIALIZE VALUES                                                FITX 175
      CHISQR=0.                                                        FITX 180
C     SUM2=ESTIMATE OF TOTAL AREA                                      FITX 185
C     TS=ELAPSED LIVE TIME                                             FITX 190
C     TRIP=CODE TO SELECT PROPER LIBRARY CARDS                         FITX 195
C     X=ARRAY OF PEAK DATA POINTS ( CHAN. NUMBERS )                    FITX 200
C     Y=ARRAY OF RAW PEAK VALUES ( DATA )                              FITX 205
C     YFIT= ARRAY OF FITTED PEAK VALUES                                FITX 210
C                                                                      FITX 215
      AC(1)=5.0                                                        FITX 220
      NTERMS=8                                                         FITX 225
      IISO=0                                                           FITX 230
      I5=1                                                             FITX 235
      PP=0                                                             FITX 240
      NPTS=40                                                          FITX 245
C     CALL SUBROUTINE TO CORRECT FOR ANY ENERGY SHIFT.                 FITX 250
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```
      CALL FIXUP (X,Y,SIGMAY,NPTS,NTERMS,A,YFIT,AC,FLAMDA,ALPHA,BETA,DERFITX 255
     1IV,CHI,ARRAY,B,IK,JK,CHISQR,SHIFT,TW,DW)                          FITX 260
C     WRITE SAMPLE INFORMATION.                                         FITX 265
      WRITE (6,85) TA,TW,TC,WT,ITAG,W1,W2,W3                            FITX 270
      WRITE (6,90) XLUX                                                 FITX 275
      WRITE (6,105)                                                     FITX 280
      DO 80 II=1,NC                                                     FITX 285
      KEXIT=0                                                           FITX 290
      TRIP=0.0                                                          FITX 295
      K=IFLAG(II)                                                       FITX 300
C     DETERMINE IF LIBRARY CARD SHOULD BE USED FOR GIVEN WAIT TIME.     FITX 305
      IF (K.EQ.1.AND.TW.LE.1.) TRIP=1.0                                 FITX 310
      IF (K.EQ.3.AND.TW.LE.30.) TRIP=1.0                                FITX 315
      IF (K.EQ.5.AND.TW.LE.120.) TRIP=1.0                               FITX 320
      IF (K.EQ.7.AND.TW.LE.5000.) TRIP=1.0                              FITX 325
      IF (K.EQ.9.AND.TW.LE.14400.) TRIP=1.0                             FITX 330
      IF (K.EQ.6.AND.TW.GT.120..AND.TW.LE.7200.) TRIP=1.0               FITX 335
      IF (K.EQ.12.AND.TW.GT.120.) TRIP=1.0                              FITX 340
      IF (K.EQ.15.AND.TW.GT.120..AND.TW.LE.14400.) TRIP=1.0             FITX 345
      IF (K.EQ.8.AND.TW.GT.10000.) TRIP=1.0                             FITX 350
      IF (TRIP.NE.1.0) GO TO 80                                         FITX 355
      ELE=EL(II)                                                        FITX 360
      ISOT=ISO(II)                                                      FITX 365
      HF=H(II)                                                          FITX 370
      ENERGY=EN(II)                                                     FITX 375
      SA=SP(II)                                                         FITX 380
      KDP=IDP(II)                                                       FITX 385
C     DETERMINE CHANNEL # FOR GIVEN GAMMA ENERGY.                       FITX 390
C     DETERMINE CHANNEL NUMBER FOR GIVEN GAMMA ENERGY.                  FITX 395
      REPK=(-1.36+1.262*ENERGY)/SHIFT                                   FITX 400
C     END OF CHANNEL CALCULATION FUNCTION CONTINUE SPECTRUM ANALYSIS    FITX 405
C     CONTROL ROUTINE.                                                  FITX 410
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```
      REPK=REPK+0.5                                                     FITX 415
      NCPK=REPK                                                         FITX 420
      AC(1)=3.5                                                         FITX 425
C     DETERMINE RANGE OF ENERGY DEVIATION ALLOWED.                      FITX 430
      IF (ENERGY.GE.2500.) AC(1)=5.0                                    FITX 435
      IF (ENERGY.EQ.844..OR.ENERGY.EQ.847.) AC(1)=1.5                   FITX 440
      AC(2)=ENERGY/SHIFT                                                FITX 445
      SUM1=0.                                                           FITX 450
      SUM2=0.                                                           FITX 455
      YMIN=999999                                                       FITX 460
      KLEFT=NCPK-12                                                     FITX 465
      IK1=KLEFT+7                                                       FITX 470
C     ESTIMATE SIZE OF PEAK.                                            FITX 475
      DO 5 J=KLEFT,IK1                                                  FITX 480
5     SUM1=SUM1+ID(J)                                                   FITX 485
      KRIT=NCPK+11                                                      FITX 490
      IK2=KRIT-7                                                        FITX 495
      DO 10 J=IK2,KRIT                                                  FITX 500
10    SUM1=SUM1+ID(J)                                                   FITX 505
      SUM1=SUM1/2.                                                      FITX 510
      IK1=IK1+1                                                         FITX 515
      IK2=IK2-1                                                         FITX 520
      DO 15 J=IK1,IK2                                                   FITX 525
15    SUM2=SUM2+ID(J)                                                   FITX 530
      IF (SUM1.LT..8*SUM2) GO TO 20                                     FITX 535
C     IF PEAK IS SMALL FIT OVER SMALL #OF DATA POINTS.                  FITX 540
      NPTS=12                                                           FITX 545
      IWIDE=2                                                           FITX 550
      GO TO 25                                                          FITX 555
C     IF PEAK IS LARGE FIT OVER LARGE # OF DATA POINTS.                 FITX 560
20    NPTS=40                                                           FITX 565
      IF (AC(2).LT.150.0) NPTS=30                                       FITX 570
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```
      IWIDE=6                                                           FITX 575
25    CONTINUE                                                          FITX 580
C     FIND MIN. DATA PT. TO LEFT AND RIGHT OF CENTROID.                 FITX 585
      IP1=NOPK-(NPTS/2)                                                 FITX 590
      IP2=NOPK+(NPTS/2)-1                                               FITX 595
      ILEFT=NOPK-(IWIDE/2)-1                                            FITX 600
      IRITE=NOPK+(IWIDE/2)                                              FITX 605
      DO 30 I=IP1,ILEFT                                                 FITX 610
      K=0                                                               FITX 615
      IF (ID(I).LE.YMIN) K=1                                            FITX 620
      IF (K.EQ.1) YMIN=ID(I)                                            FITX 625
30    IF (K.EQ.1) IL=I                                                  FITX 630
      YMIN=999999                                                       FITX 635
      DO 35 I=IRITE,IP2                                                 FITX 640
      K=0                                                               FITX 645
      IF (ID(I).LT.YMIN) K=1                                            FITX 650
      IF (K.EQ.1) YMIN=ID(I)                                            FITX 655
35    IF (K.EQ.1) IR=I                                                  FITX 660
      NPTS=IR-IL+1                                                      FITX 665
      DO 40 I=IL,IR                                                     FITX 670
      J=I-IL+1                                                          FITX 675
      Y(J)=ID(I)                                                        FITX 680
      X(J)=I                                                            FITX 685
40    CONTINUE                                                          FITX 690
      NTERMS=8                                                          FITX 695
C     IF # OF DATA PTS. IS LESS THAN # OF FITTING PARAMETERS USE        FITX 700
C     STRAIGHT LINE BKGD. APPROXIMATION.                                FITX 705
C     IF# OF DATA PTS. IS GREATER THAN # OF FITTING PARAMETERS CALL     FITX 710
C     ROUTINE TO FIT DATA TO FUNCTION.                                  FITX 715
      IF (NPTS.GT.NTERMS) GO TO 50                                      FITX 720
      BKG=(ID(IL)+ID(IR))*NPTS/2                                        FITX 725
      AREA=0.                                                           FITX 730
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```
      DO 45 I=IL,IR                                                     FITX 735
45    AREA=ID(I)+AREA                                                   FITX 740
      AREA=AREA-BKG                                                     FITX 745
      IF (AREA.LE.0.) GO TO 75                                          FITX 750
      A(1)=0.                                                           FITX 755
      A(3)=AC(2)                                                        FITX 760
      ERROR=SQRT(AREA+BKG)/AREA*100.                                    FITX 765
      GO TO 55                                                          FITX 770
50    CALL NAAFIT (X,Y,SIGMAY,NPTS,NTERMS,A,YFIT,AC,FLAMDA,ALPHA,BETA,DEFITX 775
     1RIV,CHI,ARRAY,B,IK,JK,CHISQR,KDP,DW)                              FITX 780
C     IF THE AMPLITUDE OR WIDTH PARAMETERS OF FIT ARE NEGATIVE          FITX 785
C     GO TO NEXT LIBRARY ENTRY.                                         FITX 790
      IF (A(1).LT.0.) KEXIT=10                                          FITX 795
      IF (A(2).LT.0.) KEXIT=10                                          FITX 800
      IF (KEXIT.EQ.10) GO TO 75                                         FITX 805
C     CALL FUNCTION TO FIND AREA OF THE FITTED PEAK.                    FITX 810
      AREA=SUM(YFIT,NPTS,X,A)                                           FITX 815
C     DETERMINE % ERROR.                                                FITX 820
      ERROR=AC(3)/A(1)*100.                                             FITX 825
C     IF ERROR GREATER THAN 100% OR AREA/AMP. GREATER THAN6 , THEN      FITX 830
C     GO TO NEXT LIBRARY ENTRY.                                         FITX 835
      IF (ERROR.GT.100.) GO TO 75                                       FITX 840
      IF (AREA/A(1).GT.6.) GO TO 75                                     FITX 845
55    PPM=0.                                                            FITX 850
C     CALL SUBROUTINE TO DETERMINE PPM FROM PEAK AREA AND SAMPLE TIMES. FITX 855
      CALL CONPPM (SA,HF,TA,TW,TC,XLUX,WT,AREA,PPM)                     FITX 860
C     CORRECT FOR ENERGY SHIFT.                                         FITX 865
      A(3)=A(3)*SHIFT                                                   FITX 870
      NCPK=REPK                                                         FITX 875
C     IF MULTIPLE PEAKS OF SAME ISOTOPE, THEN AVERAGE THE RESULTS.      FITX 880
      IF (IISO.NE.ISOT) GO TO 60                                        FITX 885
      PP=PP+PPM                                                         FITX 890
```

```
      I5=I5+1                                                           FITX 895
      GO TO 70                                                          FITX 900
60    IF (I5.LE.1) GO TO 65                                             FITX 905
      PPT=PP/I5                                                         FITX 910
      WRITE (6,95) EELE,IISO,PPT,I5                                     FITX 915
      I5=1                                                              FITX 920
65    PP=PPM                                                            FITX 925
70    WRITE (6,100) ELE,ISOT,A(1),AREA,ERROR,NOPK,NPTS,PPM,SA,ENERGY,A(3FITX 930
     1)                                                                 FITX 935
      IISO=ISOT                                                         FITX 940
      EELE=ELE                                                          FITX 945
75    CONTINUE                                                          FITX 950
80    CONTINUE                                                          FITX 955
      RETURN                                                            FITX 960
C                                                                       FITX 965
C                                                                       FITX 970
85    FORMAT (18H  ACTIVATION TIME=,F7.3,13H   WAIT TIME=,F10.3,14H   COFITX 975
     1UNT TIME=,F7.3,10H   WEIGHT=,F7.5,7H   TAG=,I6,3X,3HID=,5X,2A4,A2/FITX 980
     2/)                                                                FITX 985
90    FORMAT (8H   FLUX=,F4.0//)                                        FITX 990
95    FORMAT (4X,23HMEAN CONCENTRATION OF  ,A3,1H-,I3,6H  IS  ,1PE10.4,1FITX 995
     10H   USING  ,I2,7H  PEAKS)                                        FITX1000
100   FORMAT (2X,A3,1H-,I3,1PE12.4,2X,E12.4,6X,0PF4.1,1H%,6X,I4,5X,I2,6XFITX1005
     1,1PE12.4,4X,E9.3,5X,0PF7.2,6X,F7.2)                               FITX1010
105   FORMAT (124H ELEMENT-     PEAK          PEAK          PCT.      PEAFITX1015
     1K   NO. OF    CONCENTRATION     SP. ACT.     THEORETICAL   CALCULAFITX1020
     2TED ,/,124H ISOTOPE    AMPLITUDE      AREA          ERROR      NO.FITX1025
     3  PTS. USED      (PPM)      (CTS/MIN-GM)       ENERGY       ENERGYFITX1030
     4   ,/,102X,22H(KEV)        (KEV)     ,/,130(1H-))                 FITX1035
      END                                                               FITX1040
```

```
      SUBROUTINE FIXUP (X,Y,SIGMAY,NPTS,NTERMS,A,YFIT,AC,FLAMDA,ALPHA,BEFIXP   5
     1TA,DERIV,CHI,ARRAY,B,IK,JK,CHISQR,SHIFT,TW,DW)                    FIXP  10
C        THIS ROUTINE ALLOWS FOR CORRECTION DUE TO SHIFT IN ENERGY      FIXP  15
      COMMON ID(4010)                                                   FIXP  20
      DIMENSION X(NPTS), Y(NPTS), SIGMAY(NPTS), A(NTERMS), YFIT(NPTS), AFIXP  25
     1C(3), ALPHA(NTERMS,NTERMS), BETA(NTERMS), DERIV(NTERMS), CHI(10), FIXP  30
     2ARRAY(NTERMS,NTERMS), B(NTERMS), IK(NTERMS), JK(NTERMS), CHISQR(10FIXP  35
     3)                                                                 FIXP  40
      DOUBLE PRECISION ARRAY                                            FIXP  45
C        INITALIZE VALUES                                               FIXP  50
      SHIFT=1.                                                          FIXP  55
      KDP=2                                                             FIXP  60
C        DETERMINES WHICH PEAK TO NORMALIZE                             FIXP  65
      IF (TW.LE.10.) GO TO 25                                           FIXP  70
      IF (TW.GE.15000.) GO TO 15                                        FIXP  75
      NAPK=3474                                                         FIXP  80
C        SODIUM 2754 KEV PEAK                                           FIXP  85
      AC(2)=2754.                                                       FIXP  90
      IP1=NAPK-NPTS/2                                                   FIXP  95
      IP2=NAPK+NPTS/2-1                                                 FIXP 100
      DO 5 I=IP1,IP2                                                    FIXP 105
      J=I-IP1+1                                                         FIXP 110
      Y(J)=(ID(I))                                                      FIXP 115
      X(J)=I                                                            FIXP 120
5     CONTINUE                                                          FIXP 125
      CALL NAAFIT (X,Y,SIGMAY,NPTS,NTERMS,A,YFIT,AC,FLAMDA,ALPHA,BETA,DEFIXP 130
     1RIV,CHI,ARRAY,B,IK,JK,CHISQR,KDP,DW)                              FIXP 135
      IF (A(3).LT.2748.0) GO TO 10                                      FIXP 140
      CHECK=A(1)/AC(3)                                                  FIXP 145
      IF (CHECK.LT.2.0) GO TO 10                                        FIXP 150
      SHIFT=AC(2)/A(3)                                                  FIXP 155
      WRITE (6,45) A(3)                                                 FIXP 160
```

```
      GO TO 40                                                          FIXP 165
10    IF (TW.GE.10000.) GO TO 15                                        FIXP 170
      GO TO 35                                                          FIXP 175
C        POTASSIUM 1461 KEV PEAK                                        FIXP 180
15    AC(2)=1461.0                                                      FIXP 185
      KPK=1043                                                          FIXP 190
      IP1=KPK-NPTS/2                                                    FIXP 195
      IP2=KPK+NPTS/2-1                                                  FIXP 200
      DO 20 I=IP1,IP2                                                   FIXP 205
      J=I-IP1+1                                                         FIXP 210
      Y(J)=ID(I)                                                        FIXP 215
      X(J)=I                                                            FIXP 220
20    CONTINUE                                                          FIXP 225
      CALL NAAFIT (X,Y,SIGMAY,NPTS,NTERMS,A,YFIT,AC,FLAMDA,ALPHA,BETA,DEFIXP 230
     1RIV,CHI,ARRAY,B,IK,JK,CHISQR,KDP,DW)                              FIXP 235
      IF (A(3).LT.1450.0) GO TO 35                                      FIXP 240
      CHECK=A(1)/AC(3)                                                  FIXP 245
      IF (CHECK.LT.2.0) GO TO 35                                        FIXP 250
      SHIFT=AC(2)/A(3)                                                  FIXP 255
      WRITE (6,55) A(3)                                                 FIXP 260
      GO TO 40                                                          FIXP 265
C        ALUMINUM 1779 KEV PEAK                                         FIXP 270
25    AC(2)=1779.                                                       FIXP 275
      LPK=2244                                                          FIXP 280
      IP1=LPK-NPTS/2                                                    FIXP 285
      IP2=LPK+NPTS/2-1                                                  FIXP 290
      DO 30 I=IP1,IP2                                                   FIXP 295
      J=I-IP1+1                                                         FIXP 300
      Y(J)=ID(I)                                                        FIXP 305
30    X(J)=I                                                            FIXP 310
      CALL NAAFIT (X,Y,SIGMAY,NPTS,NTERMS,A,YFIT,AC,FLAMDA,ALPHA,BETA,DEFIXP 315
     1RIV,CHI,ARRAY,B,IK,JK,CHISQR,KDP,DW)                              FIXP 320
```

```
      IF (A(3).LT.1772.) GO TO 35                                       FIXP 325
      CHECK=A(1)/AC(3)                                                  FIXP 330
      IF (CHECK.LT.2.0) GO TO 35                                        FIXP 335
      SHIFT=AC(2)/A(3)                                                  FIXP 340
      WRITE (6,60) A(3)                                                 FIXP 345
      GO TO 40                                                          FIXP 350
35    WRITE (6,50)                                                      FIXP 355
40    CONTINUE                                                          FIXP 360
      RETURN                                                            FIXP 365
C                                                                       FIXP 370
C                                                                       FIXP 375
45    FORMAT (10X,39H.....A SODIUM PEAK HAS BEEN DETECTED AT,F8.2,16H KEFIXP 380
     1V RATHER THAN,/,14X,58H AT ITS TRUE ENERGY OF 2754.0 KEV. CONSEQUEFIXP 385
     2NTLY ,AN ENERGY,/,14X,56H CORRECTION HAS BEEN APPLIED BY MEANS OF FIXP 390
     3A GAIN SHIFT.../// )                                              FIXP 395
50    FORMAT (1X,/,10X,65H....NO SODIUM PEAK HAS BEEN DETECTED. CONSEQUEFIXP 400
     1NTLY, NO CORRECTION,/,14X,61H FOR DETECTOR GAIN SHIFT VARIATIONS HFIXP 405
     2AS  BEEN APPLIED TO THIS,/,14X,14H SPECTRUM.....,/)               FIXP 410
55    FORMAT (10X,40H...A POTASSIUM PEAK HAS BEEN DETECTED AT,F8.2,15H KFIXP 415
     1EV RTHER THAN,/,14X,58H AT ITS TRUE ENERGY OF 1461.0 KEV. CONSEQUEFIXP 420
     2NTLY, AN ENERGY,/,14X,58H CORRECTION HAS BEEN APPLIED BY MEANS OF FIXP 425
     3A GAIN SHIFT.....,///)                                            FIXP 430
60    FORMAT (10X,40H...AN ALUMINUM PEAK HAS BEEN DETECTED AT,F8.2,15H KFIXP 435
     1EV RTHER THAN,/,14X,58H AT ITS TRUE ENERGY OF 1779.0 KEV. CONSEQUEFIXP 440
     2NTLY, AN ENERGY,/,14X,56H CORRECTION HAS BEEN APPLIED BY MEANS OF FIXP 445
     3A GAIN SHIFT.../// )                                              FIXP 450
      END                                                               FIXP 455
```

```
      SUBROUTINE CONPPM (SA,HF,TA,TW,TC,XLUX,WT,AREA,PPM)
      ALAM=.693/HF
      ALTA=ALAM*TA
      ALTC=ALAM*TC
      ALTW=ALAM*TW
      IF (ALTA.GE..003) GO TO 5
      EXPA=ALTA
      GO TO 10
5     EXPA=1.-EXP(-ALTA)
10    IF (ALTC.GE..003) GO TO 15
      EXPC=ALTC
      GO TO 20
15    EXPC=1.-EXP(-ALTC)
20    IF (ALTW.GE..003) GO TO 25
      EXPW=1.-ALTW
      GO TO 30
25    EXPW=EXP(-ALTW)
30    PPM=(AREA*ALAM*10.**6)/(SA*WT*EXPA*EXPC*EXPW)
      A=XLUX/120.
      PPM=PPM/A
      RETURN
      END
```

```
      SUBROUTINE NAAFIT (X,Y,SIGMAY,NPTS,NTERMS,A,YFIT,AC,FLAMDA,ALPHA,BNAFT    5
     1ETA,DERIV,CHI,ARRAY,B,IK,JK,CHISQR,KDP,CW)                          NAFT   10
C                                                                         NAFT   15
C     THIS ROUTINE INITALIZES AND CHECKS PARAMETERS FOR THE CURVE FIT.    NAFT   20
C     INITIALIZE VALUES.                                                  NAFT   25
      DOUBLE PRECISION ARRAY                                              NAFT   30
      DIMENSION X(NPTS), Y(NPTS), SIGMAY(NPTS), A(NTERMS), YFIT(NPTS), ANAFT   35
     1C(3), CHI(10), ALPHA(NTERMS,NTERMS), BETA(NTERMS), DERIV(NTERMS), NAFT   40
     2ARRAY(NTERMS,NTERMS), B(NTERMS), IK(NTERMS), JK(NTERMS), ABSDER(9)NAFT   45
      DIMENSION CKY(60)                                                   NAFT   50
      IF (NPTS.LE.NTERMS) GO TO 50                                        NAFT   55
      ICHI=0                                                              NAFT   60
5     FLAMDA=.001                                                         NAFT   65
      ICHI=ICHI+1                                                         NAFT   70
      YMAX=0.0                                                            NAFT   75
      XMAX=0.0                                                            NAFT   80
      KJ=0                                                                NAFT   85
      DO 10 I=1,NPTS                                                      NAFT   90
C     FIND ERROR IN DATA VALUES AND CONVERT FROM CHANNEL # TO ENERGY.     NAFT   95
      SIGMAY(I)=SQRT(Y(I))                                                NAFT  100
      IF (ICHI.GT.1) GO TO 10                                             NAFT  105
      X(I)=1.08+.792214*X(I)                                              NAFT  110
10    CONTINUE                                                            NAFT  115
      DO 15 I=1,NPTS                                                      NAFT  120
      K=0                                                                 NAFT  125
C     DETERMINE MAXIMUM VALUE OF INTERVAL.                                NAFT  130
      IF (Y(I).GT.YMAX) K=1                                               NAFT  135
      IF (K.EQ.1) YMAX=Y(I)                                               NAFT  140
      IF (K.EQ.1) XMAX=X(I)                                               NAFT  145
15    IF (K.EQ.1) KJ=I                                                    NAFT  150
C     INITIAL ESTIMATE FOR FITTING PARAMETERS.                            NAFT  155
      A(1)=YMAX                                                           NAFT  160
```

```
      A(2)=1.46+.0005*AC(2)                                             NAFT 165
      A(2)=.426*A(2)                                                    NAFT 170
      A(3)=XMAX                                                         NAFT 175
      A(4)=Y(1)                                                         NAFT 180
      A(5)=.05                                                          NAFT 185
      A(6)=.0005                                                        NAFT 190
      I=KJ-1                                                            NAFT 195
      A(8)=AC(2)-XMAX                                                   NAFT 200
      IF (ABS(A(8)).GT.AC(1)) GO TO 20                                  NAFT 205
      NTERMS=6                                                          NAFT 210
C     CHECK FOR DOUBLE PEAK CRITERIA.                                   NAFT 215
      IF (KDP.EQ.1) GO TO 20                                            NAFT 220
      GO TO 25                                                          NAFT 225
20    DD=A(8)/(XMAX-X(I))                                               NAFT 230
C     INITIAL ESTIMATE FOR DOUBLE PEAK PARAMETERS                       NAFT 235
      IKJ=DD                                                            NAFT 240
      IKJ=IKJ+KJ                                                        NAFT 245
      IF (IKJ.GT.NPTS) IKJ=NPTS                                         NAFT 250
      IF (IKJ.LT.1) IKJ=1                                               NAFT 255
      A(7)=Y(IKJ)                                                       NAFT 260
25    CONTINUE                                                          NAFT 265
      L=0                                                               NAFT 270
30    L=L+1                                                             NAFT 275
      D=XMAX                                                            NAFT 280
      DW=YMAX                                                           NAFT 285
C     CALL ROUTINE TO FIT DATA POINTS.                                  NAFT 290
      CALL CURFIT (X,Y,SIGMAY,NPTS,NTERMS,A,FLAMDA,YFIT,CHISQR,AC,ALPHA,NAFT 295
     1BETA,DERIV,ARRAY,B,IK,JK,D,KDP,DW)                                NAFT 300
      DO 35 J=1,NTERMS                                                  NAFT 305
C     CHECK FOR GOODNESS OF FIT.                                        NAFT 310
      IF (DERIV(J).EQ.0.) GO TO 35                                      NAFT 315
      ABSDER(J)=ABS(DERIV(J))                                           NAFT 320
```

```
      IF (ABSDER(J).GT.1.0E+37) GO TO 50                                NAFT 325
      IF (ABSDER(J).LT.1.0E-35) GO TO 50                                NAFT 330
35    CONTINUE                                                          NAFT 335
      CHI(L)=CHISQR                                                     NAFT 340
      IF (CHISQR.EQ.0.0) GO TO 50                                       NAFT 345
      IF (L.EQ.1) GO TO 30                                              NAFT 350
      DELCHI=(CHI(L-1)-CHI(L))/CHI(L-1)                                 NAFT 355
C     CHECK # OF ITTERATIONS.                                           NAFT 360
      IF (L.EQ.8) GO TO 40                                              NAFT 365
      IF (DELCHI.GT.0.05) GO TO 30                                      NAFT 370
40    IF (AC(2).EQ.2754.) GO TO 45                                      NAFT 375
      IF (AC(2).EQ.1461.) GO TO 45                                      NAFT 380
      IF (AC(2).EQ.1779.) GO TO 45                                      NAFT 385
      DIFEN=A(3)-AC(2)                                                  NAFT 390
      DIFEN=ABS(DIFEN)                                                  NAFT 395
C     CHECK FOR NEED TO USE DOUBLE PEAK.                                NAFT 400
      IF (DIFEN.LE.AC(1)) GO TO 45                                      NAFT 405
      IF (ICHI.EQ.3) GO TO 50                                           NAFT 410
C     STRIP PEAK OUT, SMOOTH, AND REFIT.                                NAFT 415
      CALL STRIP (X,Y,A,YFIT,NPTS,NTERMS)                               NAFT 420
      P=2.0                                                             NAFT 425
      CALL SMOOTH (NPTS,P,Y)                                            NAFT 430
      GO TO 5                                                           NAFT 435
45    CONTINUE                                                          NAFT 440
      RETURN                                                            NAFT 445
50    CONTINUE                                                          NAFT 450
      AC(3)=2.0*ABS(A(1))                                               NAFT 455
      RETURN                                                            NAFT 460
      END                                                               NAFT 465
```

```
      SUBROUTINE SMOOTH (NPTS,P,Y)                                      SMTH   5
C        THIS ROUTINE USES A 5 POINT SMOOTH OF THE DATA                 SMTH  10
C        P=THE JUMP CODE                                                SMTH  15
C        Y=THE ARRAY OF DATA                                            SMTH  20
      COMMON ID(4010)                                                   SMTH  25
      DIMENSION Y(60)                                                   SMTH  30
      N=NPTS-2                                                          SMTH  35
      DO 10 J=3,N                                                       SMTH  40
      J1=J-2                                                            SMTH  45
      J2=J-1                                                            SMTH  50
      J3=J+1                                                            SMTH  55
      J4=J+2                                                            SMTH  60
      IF (P.EQ.2.0) GO TO 5                                             SMTH  65
      Y1=3.*ID(J1)-12.*ID(J2)-17.*ID(J)-12.*ID(J3)+3.*ID(J4)            SMTH  70
      Y2=-1.0*Y1/35.                                                    SMTH  75
      JY=Y2                                                             SMTH  80
      ID(J)=JY                                                          SMTH  85
      IF (ID(J).LE.0) ID(J)=1                                           SMTH  90
      GO TO 10                                                          SMTH  95
5     Y1=3.*Y(J1)-12.*Y(J2)-17.*Y(J)-12.*Y(J3)+3.*Y(J4)                 SMTH 100
      Y2=-1.0*Y1/35.                                                    SMTH 105
      JY=Y2                                                             SMTH 110
      Y(J)=JY                                                           SMTH 115
      IF (Y(J).LE.0.0) Y(J)=1.0                                         SMTH 120
10    CONTINUE                                                          SMTH 125
      RETURN                                                            SMTH 130
      END                                                               SMTH 135
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```
      SUBROUTINE STRIP (X,Y,A,YFIT,NPTS,NTERMS)                         STRP   5
C        THIS ROUTINE STRIPS OUT INTERFERENCE PEAKS                     STRP  10
      DIMENSION X(NPTS), Y(NPTS), YFIT(NPTS), A(NTERMS)                 STRP  15
      DO 5 I=1,NPTS                                                     STRP  20
      D=1.0                                                             STRP  25
      YFIT(I)=FUNCTN(X,I,A,NPTS,NTERMS,D)                               STRP  30
      Y(I)=Y(I)-YFIT(I)                                                 STRP  35
      IF (Y(I).LT.1.0) Y(I)=1.0                                         STRP  40
5     CONTINUE                                                          STRP  45
      NTERMS=8                                                          STRP  50
      D=0.0                                                             STRP  55
      WRITE (6,10) A(3)                                                 STRP  60
      RETURN                                                            STRP  65
C                                                                       STRP  70
C                                                                       STRP  75
10    FORMAT (1X,19H STRIP DATA AROUND ,E12.4)                          STRP  80
      END                                                               STRP  85
```

```
      SUBROUTINE CURFIT (X,Y,SIGMAY,NPTS,NTERMS,A,FLAMDA,YFIT,CHISQR,AC,CRFT   5
     1ALPHA,BETA,DERIV,ARRAY,B,IK,JK,D,KDP,DW)                          CRFT  10
C        THIS ROUTINE MAKES A LEAST-SQUARES FIT TO A NON-LINEAR FUNCTIONCRFT  15
C        FOR FURTHER REFERENCE SEE 'DATA REDUCTION AND ERROR ANALYSIS ' CRFT  20
C        BY BEVINGTON                                                   CRFT  25
      DOUBLE PRECISION ARRAY,DSQRT                                      CRFT  30
      DIMENSION X(NPTS), Y(NPTS), SIGMAY(NPTS), A(NTERMS), YFIT(NPTS), ACRFT  35
     1C(3), ALPHA(NTERMS,NTERMS), BETA(NTERMS), DERIV(NTERMS), ARRAY(NTECRFT  40
     2RMS,NTERMS), B(NTERMS), IK(NTERMS), JK(NTERMS)                    CRFT  45
      DIMENSION WEIGHT(60), ABSDER(9)                                   CRFT  50
      XMAX=0                                                            CRFT  55
      NFREE=NPTS-NTERMS                                                 CRFT  60
      IF (NFREE) 5,5,10                                                 CRFT  65
5     CHISQR=0.0                                                        CRFT  70
      GO TO 100                                                         CRFT  75
C       EVALUATE WEIGHTS                                                CRFT  80
10    DO 20 I=1,NPTS                                                    CRFT  85
      IF (I.EQ.1) GO TO 15                                              CRFT  90
      IF (SIGMAY(I)**2.EQ.0.0) SIGMAY(I)=SIGMAY(I-1)                    CRFT  95
15    CONTINUE                                                          CRFT 100
      WEIGHT(I)=1.0/SIGMAY(I)**2                                        CRFT 105
20    CONTINUE                                                          CRFT 110
      DO 25 J=1,NTERMS                                                  CRFT 115
      BETA(J)=0.0                                                       CRFT 120
      DO 25 K=1,J                                                       CRFT 125
25    ALPHA(J,K)=0.0                                                    CRFT 130
      DO 35 I=1,NPTS                                                    CRFT 135
      CALL FDERIV (X,I,A,NPTS,NTERMS,DERIV,D)                           CRFT 140
      DO 30 J=1,NTERMS                                                  CRFT 145
      BETA(J)=BETA(J)+WEIGHT(I)*(Y(I)-FUNCTN(X,I,A,NPTS,NTERMS,D))*DERIVCRFT 150
     1(J)                                                               CRFT 155
      DO 30 K=1,J                                                       CRFT 160
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30    ALPHA(J,K)=ALPHA(J,K)+WEIGHT(I)*DERIV(J)*DERIV(K)                CRFT 165
35    CONTINUE                                                         CRFT 170
      DO 40 J=1,NTERMS                                                 CRFT 175
      DO 40 K=1,J                                                      CRFT 180
40    ALPHA(K,J)=ALPHA(J,K)                                            CRFT 185
      DO 45 I=1,NPTS                                                   CRFT 190
45    YFIT(I)=FUNCTN(X,I,A,NPTS,NTERMS,D)                              CRFT 195
      CHISQ1=FCHISQ(Y,SIGMAY,NPTS,NFREE,MODE,YFIT)                     CRFT 200
50    DO 60 J=1,NTERMS                                                 CRFT 205
      DO 55 K=1,NTERMS                                                 CRFT 210
      IF (ALPHA(J,J)*ALPHA(K,K).EQ.0.) A(1)=-1.0                       CRFT 215
      IF (A(1).LT.0.) CHISQR=0.0                                       CRFT 220
      IF (A(1).LT.0.) GO TO 100                                        CRFT 225
55    ARRAY(J,K)=ALPHA(J,K)/SQRT(ALPHA(J,J)*ALPHA(K,K))                CRFT 230
60    ARRAY(J,J)=1.0+FLAMDA                                            CRFT 235
      CALL MATINV (ARRAY,NTERMS,DET,IK,JK)                             CRFT 240
      IF (DET) 65,105,65                                               CRFT 245
65    DO 70 J=1,NTERMS                                                 CRFT 250
      B(J)=A(J)                                                        CRFT 255
      DO 70 K=1,NTERMS                                                 CRFT 260
70    B(J)=B(J)+BETA(K)*ARRAY(J,K)/SQRT(ALPHA(J,J)*ALPHA(K,K))         CRFT 265
      WM=(.0003*AC(2)+.4)                                              CRFT 270
      WMIN=WM-WM*.5                                                    CRFT 275
      WMAX=WM+WM*.75                                                   CRFT 280
      IF (B(2).LT.WMIN) B(2)=WMIN                                      CRFT 285
      IF (B(2).GT.WMAX) B(2)=WMAX                                      CRFT 290
      IF (B(2).GT.DW*1.5) B(1)=DW                                      CRFT 295
      IF (B(3).GT.(XMAX+AC(1))) B(3)=XMAX+AC(1)                        CRFT 300
      IF (B(3).LT.(XMAX-AC(1))) B(3)=XMAX-AC(1)                        CRFT 305
      IF (NTERMS.EQ.6) GO TO 75                                        CRFT 310
      DEL=(NPTS*0.4)-1.0                                               CRFT 315
      IF (B(8).GT.DEL) B(8)=DEL                                        CRFT 320
```

```
      IF (B(8).LT.-DEL) B(8)=-DEL                                       CRFT 325
75    DO 80 I=1,NPTS                                                    CRFT 330
80    YFIT(I)=FUNCTN(X,I,B,NPTS,NTERMS,D)                               CRFT 335
      CHISQR=FCHISQ(Y,SIGMAY,NPTS,NFREE,MODE,YFIT)                      CRFT 340
      IF (CHISQ1-CHISQR) 85,90,90                                       CRFT 345
85    FLAMDA=10.0*FLAMDA                                                CRFT 350
      GO TO 60                                                          CRFT 355
90    DO 95 J=1,NTERMS                                                  CRFT 360
      A(J)=B(J)                                                         CRFT 365
95    CONTINUE                                                          CRFT 370
      IF (ARRAY(1,1)/ALPHA(1,1).LT.0.) AC(3)=2.0*A(1)                   CRFT 375
      IF (ARRAY(1,1)/ALPHA(1,1).LT.0.) GO TO 100                        CRFT 380
      AC(3)=DSQRT(ARRAY(1,1)/ALPHA(1,1))                                CRFT 385
      FLAMDA=FLAMDA/10.0                                                CRFT 390
100   RETURN                                                            CRFT 395
105   AC(3)=2.0*A(1)                                                    CRFT 400
      RETURN                                                            CRFT 405
      END                                                               CRFT 410
```

```
      SUBROUTINE FDERIV (X,I,A,NPTS,NTERMS,DERIV,D)                     DRIV   5
C        THIS ROUTINE CONTAINS THE DERIVATIVES OF THE ROUTINE 'FUNCTN'  DRIV  10
C        FOR FURTHER REFERENCE SEE 'DATA REDUCTION AND ERROR ANALYSIS ' DRIV  15
C        BY BEVINGTON                                                   DRIV  20
      DIMENSION A(NTERMS), DERIV(NTERMS), X(NPTS), DER(7)               DRIV  25
      K=0                                                               DRIV  30
      XI=X(I)                                                           DRIV  35
5     K=K+1                                                             DRIV  40
      Z=(XI-A(3))/A(2)                                                  DRIV  45
      Z2=Z**2                                                           DRIV  50
      IF (Z2.LT.50.) GO TO 15                                           DRIV  55
      DO 10 J=1,NTERMS                                                  DRIV  60
10    DERIV(J)=0.0                                                      DRIV  65
      GO TO 20                                                          DRIV  70
15    DERIV(1)=EXP(-Z2/2)                                               DRIV  75
      DERIV(3)=A(1)*DERIV(1)*Z/A(2)                                     DRIV  80
      DERIV(2)=DERIV(3)*Z                                               DRIV  85
20    DERIV(4)=1.0                                                      DRIV  90
      DERIV(5)=XI                                                       DRIV  95
      DERIV(6)=XI**2                                                    DRIV 100
      IF (NTERMS.EQ.6) GO TO 35                                         DRIV 105
      IF (K.EQ.2) GO TO 25                                              DRIV 110
      IF (K.EQ.3) GO TO 30                                              DRIV 115
      XI=X(I)-A(8)                                                      DRIV 120
      DER(1)=DERIV(1)                                                   DRIV 125
      DER(2)=DERIV(2)                                                   DRIV 130
      DER(3)=DERIV(3)                                                   DRIV 135
      DER(4)=DERIV(4)                                                   DRIV 140
      DER(5)=DERIV(5)                                                   DRIV 145
      DER(6)=DERIV(6)                                                   DRIV 150
      GO TO 5                                                           DRIV 155
25    CONTINUE                                                          DRIV 160
```

```
      DER(2)=DER(2)+DERIV(2)                                            DRIV 165
      DER(3)=DER(3)+DERIV(3)                                            DRIV 170
      DERIV(7)=DERIV(1)                                                 DRIV 175
      XI=X(I)-A(3)                                                      DRIV 180
      TEMP=A(3)                                                         DRIV 185
      A(3)=A(8)                                                         DRIV 190
      GO TO 5                                                           DRIV 195
30    CONTINUE                                                          DRIV 200
      DERIV(1)=DER(1)                                                   DRIV 205
      DERIV(2)=DER(2)                                                   DRIV 210
      DERIV(4)=DER(4)                                                   DRIV 215
      DERIV(5)=DER(5)                                                   DRIV 220
      DERIV(6)=DER(6)                                                   DRIV 225
      DERIV(8)=DERIV(3)                                                 DRIV 230
      DERIV(3)=DER(3)                                                   DRIV 235
      A(3)=TEMP                                                         DRIV 240
35    RETURN                                                            DRIV 245
      END                                                               DRIV 250
```

```
      SUBROUTINE MATINV (ARRAY,NORDER,DET,IK,JK)                        MTNV   5
C        THIS ROUTINE INVERTS AN N-ORDERED MATRIX                       MTNV  10
C        FOR FURTHER REFERENCE SEE 'DATA REDUCTION AND ERROR ANALYSIS ' MTNV  15
C        BY BEVINGTON                                                   MTNV  20
      DOUBLE PRECISION ARRAY,AMAX,SAVE,DABS,ABSARR                      MTNV  25
      DIMENSION ARRAY(NORDER,NORDER), IK(NORDER), JK(NORDER)            MTNV  30
5     DET=1.0                                                           MTNV  35
      DO 100 K=1,NORDER                                                 MTNV  40
      AMAX=0.                                                           MTNV  45
10    DO 20 I=K,NORDER                                                  MTNV  50
      DO 20 J=K,NORDER                                                  MTNV  55
      IF (DABS(AMAX)-DABS(ARRAY(I,J))) 15,15,20                         MTNV  60
15    AMAX=ARRAY(I,J)                                                   MTNV  65
      IK(K)=I                                                           MTNV  70
      JK(K)=J                                                           MTNV  75
20    CONTINUE                                                          MTNV  80
      IF (AMAX) 30,25,30                                                MTNV  85
25    DET=0.0                                                           MTNV  90
      GO TO 135                                                         MTNV  95
30    I=IK(K)                                                           MTNV 100
      IF (I-K) 10,45,35                                                 MTNV 105
35    DO 40 J=1,NORDER                                                  MTNV 110
      SAVE=ARRAY(K,J)                                                   MTNV 115
      ARRAY(K,J)=ARRAY(I,J)                                             MTNV 120
40    ARRAY(I,J)=-SAVE                                                  MTNV 125
45    J=JK(K)                                                           MTNV 130
      IF (J-K) 10,60,50                                                 MTNV 135
50    DO 55 I=1,NORDER                                                  MTNV 140
      SAVE=ARRAY(I,K)                                                   MTNV 145
      ARRAY(I,K)=ARRAY(I,J)                                             MTNV 150
55    ARRAY(I,J)=-SAVE                                                  MTNV 155
60    DO 70 I=1,NORDER                                                  MTNV 160
```

```
      IF (I-K) 65,70,65                                                 MTNV 165
65    ARRAY(I,K)=-ARRAY(I,K)/AMAX                                       MTNV 170
70    CONTINUE                                                          MTNV 175
      DO 85 I=1,NORDER                                                  MTNV 180
      DO 85 J=1,NORDER                                                  MTNV 185
      IF (I-K) 75,85,75                                                 MTNV 190
75    IF (J-K) 80,85,80                                                 MTNV 195
80    ABSARR=ARRAY(I,K)*ARRAY(K,J)*1.0D+10                              MTNV 200
      ABSARR=DABS(ABSARR)                                               MTNV 205
      IF (ABSARR.LT.1.0D-64) DET=0.0                                    MTNV 210
      IF (DET.EQ.0.0) GO TO 135                                         MTNV 215
      ARRAY(I,J)=ARRAY(I,J)+ARRAY(I,K)*ARRAY(K,J)                       MTNV 220
85    CONTINUE                                                          MTNV 225
      DO 95 J=1,NORDER                                                  MTNV 230
      IF (J-K) 90,95,90                                                 MTNV 235
90    ARRAY(K,J)=ARRAY(K,J)/AMAX                                        MTNV 240
95    CONTINUE                                                          MTNV 245
      ARRAY(K,K)=1.0/AMAX                                               MTNV 250
100   DET=DET*1.0                                                       MTNV 255
      DO 130 L=1,NORDER                                                 MTNV 260
      K=NORDER-L+1                                                      MTNV 265
      J=IK(K)                                                           MTNV 270
      IF (J-K) 115,115,105                                              MTNV 275
105   DO 110 I=1,NORDER                                                 MTNV 280
      SAVE=ARRAY(I,K)                                                   MTNV 285
      ARRAY(I,K)=-ARRAY(I,J)                                            MTNV 290
110   ARRAY(I,J)=SAVE                                                   MTNV 295
115   I=JK(K)                                                           MTNV 300
      IF (I-K) 130,130,120                                              MTNV 305
120   DO 125 J=1,NORDER                                                 MTNV 310
      SAVE=ARRAY(K,J)                                                   MTNV 315
      ARRAY(K,J)=-ARRAY(I,J)                                            MTNV 320
```

```
125   ARRAY(I,J)=SAVE                                    MTNV 325
130   CONTINUE                                           MTNV 330
135   RETURN                                             MTNV 335
      END                                                MTNV 340
```

```
FUNCTION IC (N)                                                         ICNN   5
IHTH=N/16**5                                                            ICNN  10
ITTH=(N-IHTH*16**5)/16**4                                               ICNN  15
ITH=(N-IHTH*16**5-ITTH*16**4)/16**3                                     ICNN  20
IH=(N-IHTH*16**5-ITTH*16**4-ITH*16**3)/16**2                            ICNN  25
IT=(N-IHTH*16**5-ITTH*16**4-ITH*16**3-IH*16**2)/16                      ICNN  30
IU=N-IHTH*16**5-ITTH*16**4-ITH*16**3-IH*16**2-IT*16                     ICNN  35
IC=IHTH*10**5+ITTH*10**4+ITH*10**3+IH*10**2+IT*10+IU                    ICNN  40
RETURN                                                                  ICNN  45
END                                                                     ICNN  50
```

```
      FUNCTION FUNCTN (X,I,A,NPTS,NTERMS,D)                              FNCT   5
C        THIS FUNCTION CONTAINS THE GAUSSIAN CURVE PLUS A QUADRATIC      FNCT  10
C        BACKGROUND                                                      FNCT  15
C        FOR FURTHER REFERENCE SEE 'DATA REDUCTION AND ERROR ANALYSIS '  FNCT  20
C        BY BEVINGTON                                                    FNCT  25
      DIMENSION X(NPTS), A(NTERMS)                                       FNCT  30
5     XI=X(I)                                                            FNCT  35
      FUNCTN=0.0                                                         FNCT  40
      IF (D.EQ.1.0) NTERMS=6                                             FNCT  45
      IF (D.EQ.1.0) GO TO 10                                             FNCT  50
      FUNCTN=A(4)+A(5)*XI+A(6)*XI**2                                     FNCT  55
10    CONTINUE                                                           FNCT  60
      Q=XI-A(3)                                                          FNCT  65
      Z=Q/A(2)                                                           FNCT  70
      Z2=Z**2                                                            FNCT  75
      IF (Z2.GT.50.) GO TO 15                                            FNCT  80
      FUNCTN=FUNCTN+A(1)*EXP(-Z2/2)                                      FNCT  85
      IF (NTERMS.EQ.6) GO TO 15                                          FNCT  90
      Q=Q-A(8)                                                           FNCT  95
      Z=Q/A(2)                                                           FNCT 100
      Z2=Z**2                                                            FNCT 105
      IF (Z2.GT.50.) GO TO 15                                            FNCT 110
      FUNCTN=FUNCTN+A(7)*EXP(-Z2/2)                                      FNCT 115
15    RETURN                                                             FNCT 120
      END                                                                FNCT 125
```

```
      FUNCTION FCHISQ (Y,SIGMAY,NPTS,NFREE,MODE,YFIT)                   CISQ   5
C        THIS FUNCTION DETERMINES THE VALUE OF CHI-SQUARED              CISQ  10
C        FOR FURTHER REFERENCE SEE 'DATA REDUCTION AND ERROR ANALYSIS ' CISQ  15
C        BY BEVINGTON                                                   CISQ  20
      DOUBLE PRECISION CHISQ,WEIGHT                                     CISQ  25
      DIMENSION Y(NPTS), SIGMAY(NPTS), YFIT(NPTS)                       CISQ  30
5     CHISQ=0.0                                                         CISQ  35
      IF (NFREE) 10,10,15                                               CISQ  40
10    FCHISQ=0.0                                                        CISQ  45
      GO TO 25                                                          CISQ  50
15    DO 20 I=1,NPTS                                                    CISQ  55
      WEIGHT=1.0/SIGMAY(I)**2                                           CISQ  60
20    CHISQ=CHISQ+WEIGHT*(Y(I)-YFIT(I))**2                              CISQ  65
      FREE=NFREE                                                        CISQ  70
      FCHISQ=CHISQ/FREE                                                 CISQ  75
25    RETURN                                                            CISQ  80
      END                                                               CISQ  85
```

```
      FUNCTION SUM (YFIT,NPTS,X,A)                                      SUMM   5
C        THIS FUNCTION SUBRACTS QUADRATIC BACKGROUND FROM THE CURVE AND SUMM  10
C        SUMS THE AREA                                                  SUMM  15
      DIMENSION YFIT(NPTS), X(NPTS), A(8)                               SUMM  20
      SUM=0.0                                                           SUMM  25
      DO 5 I=1,NPTS                                                     SUMM  30
5     SUM=SUM+YFIT(I)-(A(4)+A(5)*X(I)+A(6)*X(I)**2)                     SUMM  35
      RETURN                                                            SUMM  40
      END                                                               SUMM  45
```

APPENDIX B

ISOTOPE LIBRARY LISTING

| Elements and Isotopes | Halflife (min) | Energy (kev) | Channel Number |
|---|---|---|---|
| Sm-153 | 2808.00 | 70.0 | 86 |
| Hg-197 | 3888.00 | 78.0 | 97 |
| Ho-166 | 1608.00 | 80.0 | 99 |
| Lu-176 | 221.40 | 88.0 | 109 |
| Dy-165 | 141.00 | 94.0 | 117 |
| Gd-160 | 3.70 | 102.0 | 127 |
| Sm-153 | 2808.00 | 103.0 | 128 |
| Sm-155 | 22.30 | 104.0 | 129 |
| Yb-177 | 0.11 | 104.0 | 129 |
| U-238 | 3384.00 | 106.0 | 132 |
| Dy-165 | 1.26 | 108.0 | 134 |
| Er-171 | 450.00 | 111.0 | 138 |
| Yb-175 | 6034.00 | 113.0 | 141 |
| Lu-177 | 9662.00 | 113.0 | 141 |
| Nd-151 | 12.40 | 117.0 | 146 |
| Eu-152 | 558.00 | 122.0 | 152 |
| Er-171 | 450.00 | 124.0 | 155 |
| Hf-181 | 63792.00 | 133.0 | 166 |
| Yb-175 | 6034.00 | 138.0 | 172 |
| Se-75 | 172800.00 | 138.0 | 172 |

| Elements and Isotopes | Halflife (min) | Energy (kev) | Channel Number |
|---|---|---|---|
| Nd-151 | 12.40 | 139.0 | 174 |
| Sm-155 | 22.30 | 141.0 | 176 |
| Mo-99 | 3988.80 | 142.0 | 177 |
| Ce-141 | 46800.00 | 145.0 | 181 |
| Ta-182 | 16.20 | 147.0 | 184 |
| Yb-177 | 114.00 | 150.0 | 187 |
| Dy-165 | 1.26 | 154.0 | 192 |
| Se-77 | 0.29 | 162.0 | 203 |
| Ba-139 | 82.80 | 166.0 | 208 |
| Nd-151 | 12.40 | 171.0 | 214 |
| Nd-151 | 12.40 | 175.0 | 219 |
| Ta-182 | 16.20 | 185.0 | 232 |
| O-19 | 0.42 | 200.0 | 251 |
| Lu-177 | 9662.00 | 208.0 | 261 |
| Nd-148 | 103.80 | 211.0 | 264 |
| Ba-131 | 16776.00 | 216.0 | 271 |
| Yb-177 | 0.11 | 226.0 | 283 |
| Sm-155 | 22.30 | 246.0 | 309 |
| Nd-151 | 12.40 | 255.0 | 320 |
| Se-75 | 172800.00 | 265.0 | 333 |
| Nd-151 | 12.40 | 269.0 | 338 |
| U-238 | 3384.00 | 278.0 | 349 |
| Hg-203 | 67680.00 | 279.0 | 350 |

| Elements and Isotopes | Halflife (min) | Energy (kev) | Channel Number |
|---|---|---|---|
| Yb-175 | 6034.00 | 282.0 | 354 |
| Gd-160 | 3.70 | 284.0 | 357 |
| Ce-137 | 2040.00 | 293.0 | 368 |
| Er-171 | 450.00 | 296.0 | 372 |
| Th-232 | 39455.00 | 300.0 | 377 |
| Er-171 | 450.00 | 308.0 | 387 |
| Th-282 | 39455.00 | 312.0 | 392 |
| Gd-160 | 3.70 | 315.0 | 396 |
| Cr-51 | 40032.00 | 320.0 | 402 |
| Ti-51 | 5.80 | 320.0 | 402 |
| La-140 | 2414.00 | 329.0 | 413 |
| Sn-125 | 9.70 | 332.0 | 417 |
| Cd-115 | 3182.00 | 336.0 | 422 |
| Eu-153 | 558.00 | 344.0 | 432 |
| Dy-165 | 141.00 | 361.0 | 454 |
| Dy-165 | 1.26 | 361.0 | 454 |
| Gd-160 | 3.70 | 361.0 | 454 |
| Sr-87 | 169.00 | 388.0 | 488 |
| Yb-175 | 6034.00 | 397.0 | 499 |
| Au-198 | 3888.00 | 412.0 | 518 |
| In-116 | 54.00 | 417.0 | 524 |
| Er-171 | 450.00 | 420.0 | 528 |
| Nd-151 | 12.40 | 423.0 | 532 |

| Elements and Isotopes | Halflife (min) | Energy (kev) | Channel Number |
|---|---|---|---|
| Zn-69 | 828.00 | 439.0 | 552 |
| I-128 | 25.00 | 443.0 | 557 |
| Pt-199 | 30.00 | 475.0 | 598 |
| W-187 | 1434.00 | 479.0 | 603 |
| Hf-181 | 63792.00 | 482.0 | 606 |
| La-140 | 2414.00 | 487.0 | 613 |
| Ba-131 | 16776.00 | 496.0 | 624 |
| Cu-64 | 768.00 | 511.0 | 643 |
| Dy-165 | 1.26 | 515.0 | 648 |
| Dy-165 | 141.00 | 515.0 | 648 |
| Cd-115 | 3182.40 | 527.0 | 663 |
| Nd-148 | 103.80 | 540.0 | 680 |
| As-76 | 1584.00 | 559.0 | 704 |
| Sb-122 | 4032.00 | 564.0 | 710 |
| Cs-134 | 1077480.00 | 605.0 | 762 |
| Br-80 | 17.60 | 617.0 | 777 |
| Dy-165 | 141.00 | 633.0 | 797 |
| Sb-124 | 86832.00 | 646.0 | 813 |
| Nd-148 | 103.80 | 654.0 | 823 |
| As-76 | 1584.00 | 657.0 | 827 |
| Br-80 | 17.60 | 666.0 | 839 |
| Ru-105 | 266.40 | 676.0 | 851 |
| W-187 | 1434.00 | 685.0 | 863 |

| Elements and Isotopes | Halflife (min) | Energy (kev) | Channel Number |
|---|---|---|---|
| Br-82 | 2116.80 | 698.0 | 879 |
| Dy-165 | 141.00 | 715.0 | 900 |
| Ru-105 | 266.40 | 724.0 | 912 |
| Mo-99 | 3988.80 | 740.0 | 932 |
| Br-82 | 2116.80 | 776.0 | 977 |
| Pt-199 | 30.00 | 791.0 | 996 |
| Cs-134 | 1077480.00 | 796.0 | 1003 |
| Ia-140 | 2414.00 | 815.0 | 1027 |
| Eu-152 | 558.00 | 963.0 | 1213 |
| Eu-152 | 558.00 | 1003.0 | 1264 |
| Mg-27 | 9.50 | 1014.0 | 1278 |
| Cu-66 | 5.10 | 1039.0 | 1309 |
| Rb-86 | 26927.99 | 1077.0 | 1357 |
| In-116 | 54.00 | 1097.0 | 1383 |
| Fe-59 | 64800.00 | 1099.0 | 1385 |
| Zn-65 | 352800.00 | 1115.0 | 1405 |
| Sc-46 | 120960.00 | 1121.0 | 1413 |
| Co-60 | 2764656.00 | 1173.0 | 1478 |
| Ta-182 | 165744.00 | 1189.0 | 1499 |
| Ta-182 | 165744.00 | 1221.0 | 1539 |
| Fe-59 | 64800.00 | 1292.0 | 1629 |
| Ar-41 | 109.80 | 1293.0 | 1630 |
| Eu-152 | 558.00 | 1315.0 | 1658 |

| Elements and Isotopes | Halflife (min) | Energy (kev) | Channel Number |
|---|---|---|---|
| Co-60 | 2764656.00 | 1333.0 | 1680 |
| Cu-64 | 768.00 | 1347.0 | 1698 |
| Na-24 | 900.00 | 1369.0 | 1726 |
| Ho-166 | 1608.00 | 1380.0 | 1740 |
| V-52 | 3.75 | 1434.0 | 1808 |
| Ni-65 | 153.60 | 1482.0 | 1868 |
| K-42 | 744.00 | 1525.0 | 1923 |
| La-140 | 2414.00 | 1596.0 | 2012 |
| F-20 | 0.19 | 1634.0 | 2060 |
| Cl-38 | 37.10 | 1642.0 | 2070 |
| Sb-124 | 86832.00 | 1691.0 | 2132 |
| Al-28 | 2.30 | 1779.0 | 2243 |
| Mn-56 | 154.20 | 1811.0 | 2284 |
| Cl-38 | 37.10 | 2168.0 | 2734 |
| Na-24 | 900.00 | 2754.0 | 3474 |
| Ca-49 | 8.80 | 3084.0 | 3890 |
| S-37 | 5.07 | 3103.0 | 3914 |

# APPENDIX C
## PLOTTING PROGRAM LISTING

```
      DIMENSION YA(80),YB(80),XZX(80),XZY(80)
      DIMENSION   EBB(6),XC(12),NN(2,6)
      DIMENSION LCC(5),LCCC(5)
      DIMENSION X(121),Y(304),LAB(5),LABA(4),XX(121),YY(121),LBBB(4)
      DIMENSION LAA(6),LBB(6)
      DIMENSION EE(200),A(25),B(25),DD(25)
      READ(5,10)(XX(I),I=1,121)
      READ(5,11)(YY(I),I=1,121)
      READ(5,100)(X(I),I=1,76)
      READ(5,600)(Y(I),I=1,304)
      READ(5,1)(LCC(I),I=1,4)
      READ(5,101)(LAB(I),I=1,5)
      READ(5,708)(LABA(I),I=1,4)
      READ(5,708)(LBBB(I),I=1,4)
      READ(5,709)(LCCC(I),I=1,5)
      READ(5,166) ((NN(I,J),I=1,2),J=1,6)
166   FORMAT(6(A4,A2))
 708  FORMAT(4A4)
709   FORMAT(5A4)
1     FORMAT(4A4)
10    FORMAT(12F6.0/13F6.0/13F6.0/13F6.0/13F6.0/13F6.0/13F6.0/13F
     16.0/5F6.0)
 600  FORMAT(11F7.2/11F7.2/11F7.2/11F7.2/11F7.2/11F7.2/13F7.2/13F6.2/13F
     16.2/13F6.2/13F6.2/13F6.2/11F6.2/11F7.2/11F7.2/11F7.2/11F7.2/11F7.2
     2/11F7.2/13F7.2/13F6.2/13F6.2/13F6.2/13F6.2/13F6.2/11F6.2)
11    FORMAT(12F6.1/13F6.1/13F6.1/13F6.1/13F6.1/13F6.1/13F6.1/13F6.1/13F
     16.1/5F6.1)
100   FORMAT(12F6.2/12F6.2/12F6.2/12F6.2/12F6.2/12F6.2/4F6.2)
101   FORMAT(5A4)
102   FORMAT(2A4)
 200  FORMAT(4A4)
201   FORMAT(5A4)
```

```
      CALL SCALE(XX,121,4.5,XXMIN,DDX,1)
      XA=157.8
      XAA=XA/4.5
      XB=13.0
      XBB=XB/XAA
      DO 167 I=1,12
      RI=I
      XC(I)=XBB*RI
 167  CONTINUE
      CALL SCALE(YY,121,0.75,YYMIN,DDY,1)
      CALL PLOT(1.,3.,-3)
      CALL SLINE(XX,YY,121,1,0,12)
      CALL SCALE(X,76,4.5,XMIN,DX,1)
      CALL SCALE(Y,304,4.5,YMIN,DY,1)
      DO 50 I=1,76
      YA(I)=Y(I)
50    CONTINUE
      DO 51 I=1,76
      YB(I)=Y(I+76)
51    CONTINUE
      DO 52 I=1,152
      EE(I)=Y(I+152)
52    CONTINUE
      CALL PLOT(0.,0.,3)
      CALL PLOT(0.,1.,2)
      CALL PLOT(4.5,1.,2)
C  XAXIS LABEL AND MARKS
      CALL PLOT(0.,0.,3)
      CALL PLOT(4.5,0.,2)
      CALL PLOT(0.,0.,3)
      CALL SYMBOL(0.,0.,.2,'|',180.0,1)
      DD(1)=0.0
```

```
      DO 300 I=1,6
      A(I)=DD(1)+.7500
      DD(1)=A(I)
      CALL SYMBOL(A(I),0.,.2,'|',180.0,1)
300   CONTINUE
      DD(1)=0.
      DO 301 I=1,23
      B(I)=DD(1)+.1875
      DD(1)=B(I)
      CALL SYMBOL(B(I),0.,.1,'|',180.0,1)
301   CONTINUE
      CALL SYMBOL(-.1,-.32,.1,'000',0.,3)
      CALL SYMBOL(.6500,-.32,.1,'100',0.,3)
      CALL SYMBOL(1.40,-.32,.1,'200',0.,3)
      CALL SYMBOL(2.15,-.32,.1,'300',0.,3)
      CALL SYMBOL(2.90,-.32,.1,'400',0.,3)
      CALL SYMBOL(3.65,-.32,.1,'500',0.,3)
      CALL SYMBOL(4.40,-.32,.1,'600',0.,3)
      CALL SYMBOL(0.55,-.6,.12,'DISTANCE FROM HIGHWAY ( FT. )',0.,29)
      CALL SYMBOL(1.5,0.75,.1,'WIND DIRECTION',0.,14)
      CALL SYMBOL(3.3,.755,.4,6,270.,-1)
C  YAXIS LABEL AND MARK
      CALL PLOT(0.,1.,3)
      CALL PLOT(0.,5.5,2)
      CALL PLOT(0.,1.,3)
      CALL SYMBOL(2.3,5.26,.1,LCC,0.,13)
      CALL SYMBOL(2.3,5.11,.1,LAB,0.,15)
      CALL SYMBOL(2.3,4.87,.1,LABA,0.,16)
      CALL SYMBOL(2.3,4.71,.1,LBCB,0.,16)
      CALL SYMBOL(2.3,4.56,.1,LCCC,0.,19)
      CALL PLOT(0.,5.5,3)
      CALL PLOT(0.,5.7,2)
```

```
      CALL PLOT(4.5,5.7,2)
      CALL PLOT(4.5,1.,2)
      CALL PLOT(4.5,0.,3)
      CALL PLOT(4.5,1.,2)
      CALL SYMBOL(4.5,.5,.2,'|',270.,1)
      CALL SYMBOL(4.5,0.,.2,'|',270.,1)
      CALL SYMBOL(4.5,1.,.2,'|',270.,1)
      CALL SYMBOL(4.79,0.,.1,'2151',90.,4)
      CALL SYMBOL(4.79,.5,.1,'2161',90.,4)
      CALL SYMBOL(4.79,1.,.1,'2171',90.,4)
      CALL SYMBOL(4.95,0.,.12,'ELEVATION ( FT. )',90.,17)
      CALL PLOT(0.,1.,-3)
      CALL SYMBOL(0.,0.,.2,'|',90.,1)
      CALL SYMBOL(0.,XC(1),.1,'|',90.,1)
      CALL SYMBOL(0.,XC(2),.2,'|',90.,1)
      CALL SYMBOL(0.,XC(3),.1,'|',90.,1)
      CALL SYMBOL(0.,XC(4),.2,'|',90.,1)
      CALL SYMBOL(0.,XC(5),.1,'|',90.,1)
      CALL SYMBOL(0.,XC(6),.2,'|',90.,1)
      CALL SYMBOL(0.,XC(7),.1,'|',90.,1)
      CALL SYMBOL(0.,XC(8),.2,'|',90.,1)
      CALL SYMBOL(0.,XC(9),.1,'|',90.,1)
      CALL SYMBOL(0.,XC(10),.2,'|',90.,1)
      CALL SYMBOL(0.,XC(11),.1,'|',90.,1)
      CALL SYMBOL(0.,XC(12),.2,'|',90.,1)
      DO 104  I=1,6
      II=2*I
      BBB(I)=XC(II)-.4
104   CONTINUE
      CALL SYMBOL(-.22,-.1,.1,'00',90.,2)
      DO 106 I=1,6
      CALL SYMBOL(-.22,BBB(I),.1,NN(1,I),90.,6)
```

```
106   CONTINUE
      CALL SYMBOL(-.42000,0.00,.12,'CONCENTRATION OF  BROMINE( PPM )',90
     1.,32)
      DO 700 I=1,152
      EE(I)=EE(I)*6.
 700  CONTINUE
      CALL SLINE(X,YA,76,1,0,2)
      DO 801  I=1,76
      XZX(I)=X(I)-(.45*EE(I))
      YA(I)=YA(I)-(.45*EE(I))
801   CONTINUE
      DO 900 I=1,76
      CALL SYMBOL(XZX(I),YA(I),EE(I),'I',0.,1)
900   CONTINUE
      CALL SLINE(X,YB,76,1,0,2)
      DO 802 I=1,76
      J=I+76
      XZY(I)=X(I)-(.45*EE(J))
      YB(I)=YB(I)-(.45*EE(J))
802   CONTINUE
      DO 901   I=1,76
      J=I+76
      CALL SYMBOL(XZY(I),YB(I),EE(J),'I',0.,1)
901   CONTINUE
      CALL PLOT(0.0,0.0,-4)
      STOP
      END
```

APPENDIX D

CLIMATOLOGICAL DATA IN THE AREAS OF THE HIGHWAYS

Knoxville and Oak Ridge, Tennessee Area

a) Temperature °F

June 1974

| Date | Maximum | Minimum | Average | Average Dew Point |
|---|---|---|---|---|
| 1 | 82 | 67 | 75 | 63 |
| 2 | 74 | 62 | 68 | 60 |
| 3 | 81 | 59 | 70 | 56 |
| 4 | 84 | 64 | 74 | 59 |
| 5 | 82 | 58 | 70 | 57 |
| 6 | 78 | 65 | 72 | 63 |
| 7 | 85 | 65 | 75 | 64 |
| 8 | 83 | 65 | 74 | 65 |
| 9 | 85 | 66 | 76 | 67 |
| 10 | 82 | 68 | 75 | 64 |
| 11 | 80 | 58 | 69 | 56 |
| 12 | 79 | 63 | 71 | 56 |
| 13 | 80 | 58 | 69 | 55 |
| 14 | 83 | 59 | 71 | 58 |
| 15 | 82 | 64 | 73 | 61 |
| 16 | 78 | 58 | 68 | 55 |
| 17 | 73 | 53 | 63 | 49 |

June 1974 (Continued)

| Date | Maximum | Minimum | Average | Average Dew Point |
|---|---|---|---|---|
| 18 | 77 | 51 | 64 | 53 |
| 19 | 84 | 54 | 72 | 61 |
| 20 | 86 | 69 | 78 | 68 |
| 21 | 87 | 72 | 80 | 69 |
| 22 | 90 | 74 | 82 | 67 |
| 23 | 78 | 63 | 71 | 59 |
| 24 | 71 | 58 | 65 | 54 |
| 25 | 72 | 54 | 63 | 52 |
| 26 | 75 | 50 | 63 | 49 |
| 27 | 68 | 60 | 64 | 54 |
| 28 | 68 | 60 | 64 | 54 |
| 29 | 82 | 56 | 69 | 53 |
| 30 | 86 | 58 | 72 | 55 |
| Average for the Month | 79.8 | 61.1 | 70.5 | 58 |

July 1974

| | | | | |
|---|---|---|---|---|
| 1 | 86 | 67 | 77 | 62 |
| 2 | 90 | 65 | 78 | 61 |
| 3 | 88 | 68 | 78 | 64 |
| 4 | 85 | 69 | 77 | 64 |
| 5 | 84 | 70 | 77 | 65 |
| 6 | 85 | 69 | 77 | 66 |

July 1974 (Continued)

| Date | Maximum | Minimum | Average | Average Dew Point |
|---|---|---|---|---|
| 7 | 88 | 71 | 80 | 68 |
| 8 | 86 | 68 | 77 | 67 |
| 9 | 88 | 67 | 78 | 66 |
| 10 | 88 | 68 | 78 | 66 |
| 11 | 87 | 71 | 79 | 67 |
| 12 | 84 | 69 | 77 | 63 |
| 13 | 87 | 62 | 75 | 59 |
| 14 | 90 | 65 | 78 | 63 |
| 15 | 92 | 68 | 80 | 64 |
| 16 | 88 | 70 | 79 | 66 |
| 17 | 92 | 68 | 80 | 64 |
| 18 | 92 | 73 | 83 | 68 |
| 19 | 84 | 71 | 78 | 68 |
| 20 | 88 | 70 | 79 | 69 |
| 21 | 87 | 67 | 77 | 65 |
| 22 | 86 | 65 | 76 | 64 |
| 23 | 77 | 71 | 74 | 65 |
| 24 | 86 | 71 | 79 | 68 |
| 25 | 88 | 68 | 78 | 68 |
| 26 | 80 | 70 | 75 | 68 |
| 27 | 90 | 71 | 81 | 68 |
| 28 | 90 | 68 | 79 | 65 |
| 29 | 90 | 68 | 79 | 67 |

July 1974 (Continued)

| Date | Maximum | Minimum | Average | Average Dew Point |
|---|---|---|---|---|
| 30 | 86 | 65 | 76 | 55 |
| 31 | 87 | 62 | 75 | 56 |
| Average for the Month | 87.1 | 68.1 | 77.7 | 65 |

b) Precipitation[a]

| June | | July | |
|---|---|---|---|
| Date | Water Equivalent in. | Date | Water Equivalent in. |
| 1 | .16 | 1 | 0 |
| 2 | T | 2 | 0 |
| 3 | 0 | 3 | 0 |
| 4 | 0 | 4 | 0 |
| 5 | T | 5 | T |
| 6 | 1.34 | 6 | T |
| 7 | 0 | 7 | .25 |
| 8 | T | 8 | T |
| 9 | 0 | 9 | .19 |
| 10 | .25 | 10 | 0 |
| 11 | 0 | 11 | 1.26 |
| 12 | .05 | 12 | 0 |
| 13 | 0 | 13 | 0 |
| 14 | 0 | 14 | 0 |
| 15 | 0 | 15 | T |

June and July (Continued)

| Date | Water Equivalent in. | Date | Water Equivalent in. |
|---|---|---|---|
| 16 | .64 | 16 | 0 |
| 17 | 0 | 17 | 0 |
| 18 | 0 | 18 | 0 |
| 19 | 0 | 19 | 1.04 |
| 20 | T | 20 | .14 |
| 21 | .02 | 21 | 0 |
| 22 | 0 | 22 | T |
| 23 | .16 | 23 | T |
| 24 | 0 | 24 | .01 |
| 25 | .08 | 25 | 0 |
| 26 | 0 | 26 | .03 |
| 27 | 0 | 27 | T |
| 28 | T | 28 | 0 |
| 29 | 0 | 29 | 0 |
| 30 | 0 | 30 | 0 |
| | | 31 | 0 |

[a]T-Amount too small to measure

c) Wind

| June | | July | |
|---|---|---|---|
| Date | Average Speed M.P.H. | Date | Average Speed M.P.H. |
| 1 | 9.6 | 1 | 8.3 |
| 2 | 6.0 | 2 | 6.8 |

June and July (Continued)

| Date | Average Speed M.P.H. | Date | Average Speed M.P.H. |
|---|---|---|---|
| 3 | 8.2 | 3 | 6.2 |
| 4 | 5.2 | 4 | 6.9 |
| 5 | 5.5 | 5 | 6.3 |
| 6 | 5.3 | 6 | 3.5 |
| 7 | 5.9 | 7 | 5.9 |
| 8 | 5.9 | 8 | 6.8 |
| 9 | 7.5 | 9 | 5.8 |
| 10 | 10.8 | 10 | 4.5 |
| 11 | 5.8 | 11 | 6.8 |
| 12 | 7.3 | 12 | 7.8 |
| 13 | 4.0 | 13 | 4.5 |
| 14 | 3.6 | 14 | 3.6 |
| 15 | 8.6 | 15 | 4.9 |
| 16 | 9.6 | 16 | 8.9 |
| 17 | 4.6 | 17 | 6.2 |
| 18 | 6.9 | 18 | 6.8 |
| 19 | 7.6 | 19 | 8.3 |
| 20 | 6.0 | 20 | 6.0 |
| 21 | 9.6 | 21 | 6.8 |
| 22 | 10.9 | 22 | 5.9 |
| 23 | 11.4 | 23 | 8.1 |
| 24 | 10.2 | 24 | 4.2 |
| 25 | 6.3 | 25 | 5.6 |

June and July (Continued)

| Date | Average Speed M.P.H. | Date | Average Speed M.P.H. |
|---|---|---|---|
| 26 | 6.8 | 26 | 5.2 |
| 27 | 8.2 | 27 | 6.0 |
| 28 | 7.5 | 28 | 3.7 |
| 29 | 7.1 | 29 | 5.6 |
| 30 | 9.4 | 30 | 6.0 |
| | | 31 | 5.8 |

## Roanoke and Blacksburg, Virginia Area

a) Temperature °F

June 1974

| Date | Maximum | Minimum | Average | Average Dew Point |
|---|---|---|---|---|
| 1 | 75 | 63 | 69 | 63 |
| 2 | 72 | 60 | 66 | 61 |
| 3 | 79 | 60 | 70 | 58 |
| 4 | 79 | 55 | 67 | 57 |
| 5 | 80 | 51 | 66 | 56 |
| 6 | 79 | 60 | 70 | 62 |
| 7 | 75 | 62 | 69 | 60 |
| 8 | 76 | 61 | 69 | 62 |
| 9 | 88 | 59 | 74 | 64 |
| 10 | 91 | 65 | 78 | 66 |
| 11 | 81 | 60 | 71 | 52 |
| 12 | 78 | 55 | 67 | 52 |

June 1974 (Continued)

| Date | Maximum | Minimum | Average | Average Dew Point |
|---|---|---|---|---|
| 13 | 78 | 47 | 63 | 52 |
| 14 | 74 | 59 | 67 | 60 |
| 15 | 78 | 54 | 66 | 60 |
| 16 | 75 | 58 | 67 | 60 |
| 17 | 72 | 50 | 61 | 47 |
| 18 | 78 | 47 | 63 | 50 |
| 19 | 84 | 51 | 68 | 58 |
| 20 | 90 | 67 | 79 | 64 |
| 21 | 88 | 67 | 78 | 64 |
| 22 | 88 | 67 | 78 | 64 |
| 23 | 79 | 60 | 70 | 62 |
| 24 | 75 | 54 | 65 | 52 |
| 25 | 78 | 54 | 66 | 53 |
| 26 | 78 | 54 | 66 | 55 |
| 27 | 69 | 58 | 64 | 59 |
| 28 | 63 | 57 | 60 | 59 |
| 29 | 76 | 55 | 66 | 57 |
| 30 | 85 | 55 | 70 | 58 |
| Average for the Month | 78.7 | 57.7 | 68.1 | 58 |

July 1974

| | | | | |
|---|---|---|---|---|
| 1 | 87 | 68 | 78 | 61 |

July 1974 (Continued)

| Date | Maximum | Minimum | Average | Average Dew Point |
|---|---|---|---|---|
| 2 | 90 | 64 | 77 | 66 |
| 3 | 91 | 67 | 79 | 65 |
| 4 | 89 | 69 | 79 | 65 |
| 5 | 75 | 66 | 71 | 67 |
| 6 | 80 | 66 | 73 | 68 |
| 7 | 89 | 64 | 77 | 68 |
| 8 | 91 | 65 | 78 | 67 |
| 9 | 91 | 64 | 78 | 65 |
| 10 | 90 | 65 | 78 | 66 |
| 11 | 84 | 66 | 75 | 65 |
| 12 | 81 | 62 | 72 | 56 |
| 13 | 87 | 55 | 71 | 56 |
| 14 | 93 | 60 | 77 | 57 |
| 15 | 92 | 66 | 79 | 61 |
| 16 | 86 | 65 | 76 | 60 |
| 17 | 82 | 60 | 71 | 61 |
| 18 | 89 | 64 | 77 | 68 |
| 19 | 83 | 66 | 75 | 66 |
| 20 | 86 | 61 | 74 | 60 |
| 21 | 77 | 62 | 70 | 57 |
| 22 | 83 | 56 | 70 | 57 |
| 23 | 70 | 59 | 65 | 51 |
| 24 | 82 | 64 | 73 | 65 |

July 1974 (Continued)

| Date | Maximum | Minimum | Average | Average Dew Point |
|---|---|---|---|---|
| 25 | 81 | 67 | 74 | 67 |
| 26 | 82 | 67 | 75 | 69 |
| 27 | 86 | 66 | 76 | 67 |
| 28 | 88 | 67 | 78 | 67 |
| 29 | 88 | 65 | 77 | 67 |
| 30 | 83 | 62 | 73 | 59 |
| 31 | 84 | 60 | 72 | 59 |
| Average for the Month | 85.2 | 63.8 | 74.5 | 63 |

b) Precipitation[a]

| June | | July | |
|---|---|---|---|
| Date | Water Equivalent in. | Date | Water Equivalent in. |
| 1 | .18 | 1 | 0 |
| 2 | .13 | 2 | 0 |
| 3 | 0 | 3 | 0 |
| 4 | 0 | 4 | 0 |
| 5 | 0 | 5 | .18 |
| 6 | T | 6 | .01 |
| 7 | T | 7 | T |
| 8 | T | 8 | 0 |
| 9 | 0 | 9 | 0 |
| 10 | .14 | 10 | 0 |

June and July (Continued)

| Date | Water Equivalent in. | Date | Water Equivalent in. |
|---|---|---|---|
| 11 | 0 | 11 | .02 |
| 12 | 0 | 12 | 0 |
| 13 | .06 | 13 | 0 |
| 14 | .61 | 14 | 0 |
| 15 | 0 | 15 | .43 |
| 16 | .24 | 16 | 0 |
| 17 | 0 | 17 | 0 |
| 18 | 0 | 18 | .40 |
| 19 | 0 | 19 | T |
| 20 | 0 | 20 | 0 |
| 21 | 0 | 21 | 0 |
| 22 | 0 | 22 | 0 |
| 23 | .02 | 23 | .12 |
| 24 | 0 | 24 | .89 |
| 25 | .02 | 25 | .10 |
| 26 | 0 | 26 | 1.34 |
| 27 | .97 | 27 | T |
| 28 | .56 | 28 | 0 |
| 29 | 0 | 29 | .22 |
| 30 | 0 | 30 | 0 |
| | | 31 | 0 |

[a]T-amount too small to measure.

c) Wind

| June | | July | |
|---|---|---|---|
| Date | Average Speed M.P.H. | Date | Average Speed M.P.H. |
| 1 | 5.9 | 1 | 8.5 |
| 2 | 9.5 | 2 | 6.8 |
| 3 | 7.3 | 3 | 8.8 |
| 4 | 4.8 | 4 | 8.9 |
| 5 | 6.0 | 5 | 5.0 |
| 6 | 8.3 | 6 | 5.2 |
| 7 | 8.8 | 7 | 5.6 |
| 8 | 4.3 | 8 | 4.8 |
| 9 | 5.6 | 9 | 4.2 |
| 10 | 7.2 | 10 | 8.6 |
| 11 | 10.9 | 11 | 6.3 |
| 12 | 8.9 | 12 | 6.9 |
| 13 | 6.0 | 13 | 5.5 |
| 14 | 5.6 | 14 | 4.5 |
| 15 | 8.5 | 15 | 11.7 |
| 16 | 8.2 | 16 | 7.6 |
| 17 | 9.2 | 17 | 2.7 |
| 18 | 6.2 | 18 | 5.9 |
| 19 | 5.6 | 19 | 9.9 |
| 20 | 10.5 | 20 | 8.2 |
| 21 | 10.9 | 21 | 6.8 |
| 22 | 9.9 | 22 | 6.0 |

June and July (Continued)

| Date | Average Speed M.P.H. | Date | Average Speed M.P.H. |
|---|---|---|---|
| 23 | 7.3 | 23 | 4.9 |
| 24 | 9.2 | 24 | 5.3 |
| 25 | 6.8 | 25 | 4.9 |
| 26 | 6.9 | 26 | 7.8 |
| 27 | 7.8 | 27 | 5.8 |
| 28 | 5.8 | 28 | 5.6 |
| 29 | 7.5 | 29 | 6.6 |
| 30 | 10.1 | 30 | 6.8 |
| | | 31 | 6.0 |

# VITA

The author was born on June 14, 1950 in Danville, Virginia, where he attended primary and secondary schools. He received a B.S. degree in Nuclear Science with an option in Chemistry from Virginia Polytechnic Institute and State University in June, 1973. The author spent six months during the academic year of 1972-73 at Oak Ridge National Laboratory in the Health Physics Division on an Undergraduate AEC Health Physics Traineeship. He entered graduate school at Virginia Polytechnic Institute and State University in June, 1973 as a Nuclear Science and Engineering major. The author married the former Terry Lynne Jenkins in June, 1974.

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Thomas Wyatt Oakes

Thomas Wyatt Oakes

# A NEUTRON ACTIVATION ANALYSIS INVESTIGATION OF TRACEABLE ELEMENTS FROM AUTOMOBILE EXHAUST IN ROADSIDE SOIL AND VEGETATION

by

Thomas Wyatt Oakes

(ABSTRACT)

The purpose of this work was to demonstrate the effectiveness of neutron activation analysis in studying a complex environmental problem. The area chosen for study was the exhaust emitted by automobiles and its dispersion into soil and selected plants near highways. The elements chosen for this study were the major traceable components of gasoline and automobile exhaust. Variations in the concentrations of these trace elements in soil, grass and wash off the grass at various distances from two highways were investigated.

Of the elements found in gasoline and in automobile exhaust, bromine most clearly indicated where some of the atmospheric components were going and, therefore, would be the most suitable element for neutron activation studies of atmospheric and turbulence modeling and possibly for following biological effects of automobile traffic.