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X-ray excited optical luminescence of polynuclear aromatic hydrocarbons

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X-ray excited optical luminescence of

polynuclear aromatic hydrocarbons

by

Gregory Joseph Oestreich

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER 1: INTRODUCTION

The search for cancer-causing agents began in 1775 when physicians observed an abnormally high occurrence of cancer of the scrotum in chimney sweeps. Today, the carcinogenic and mutagenic properties of polynuclear aromatic hydrocarbons (PAHs), a major component of soot, are well known (1,2). All humans are exposed to many natural and man made sources of PAHs. These compounds are produced in hydrocarbon-fueled combustion processes, both natural (e.g. forest fires (3)) and controlled (e.g. internal combustion engines, (4) fuel-rich flames (5)). In addition to the many existing sources of PAHs, the dwindling supply of petroleum threatens to add another source of PAHs, as coal becomes an energy substitute. PAHs occur in coal tar pitch (6,7), in the environment surrounding coke production (8), in coal conversion processes (9), in coal liquification products (10-12), and even in coal (13).

Once formed, the PAHs can enter the atmosphere and the food chain. The modern coal-burning power plant is one example of a particularly dangerous source of atmospheric PAHs. The PAHs formed in the combustion process enter the atmosphere as gases and subsequently condense on the particulate matter formed in the boiler (14) and finally escape into the environment by being immobilized on the very fine particulate matter not removed by precipitators. In this form the PAHs are inhaled deeply into the lungs and become imbedded in tissue. The localized concentrations of PAHs in the lung tissues represents a serious health hazard. PAHs also enter the body during the consumption of nourishment and water. Fresh water supplies contain PAHs in the range from 1 part per trillion in ground water to 100 parts per trillion and higher in industrially-polluted surface water (15,16). Certain foods contain large quantities of PAHs. Smoked and charcoal broiled foods have been shown to be dietary sources of PAHs. In one study the content of PAHs ranged from 0 to 141 part per billion in smoked foods and from 0 to 164 part per billion in charcoal broiled foods (17). In a more general study PAHs were found at trace levels in meat, fish, poultry, root vegetables, beverages, dairy products, oils, fats and shortenings (18). The occurrence of PAHs in the diet is an important source of human exposure to carcinogenic substances.

The many different sources and the varied composition of PAH-contaminated materials presents the analytical chemist with a serious problem. Sensitive and selective analytical methods for the characterization of PAHs are required. For these reasons and because of the potentially hazardous exposure of humans to PAHs in industrial (19) and natural environments, there is increasing interest in new analytical concepts for the qualitative and quantitative determination of these compounds at trace and ultratrace levels (20).

PAHs occur in natural and man-made substances at trace and ultratrace levels in complex matrices (21-24,18). Therefore, sensitive and selective analytical techniques are required to characterize PAH mixtures. Because PAHs are highly luminescent materials (25,26), fluorimetric and phosphorimetric methods are favored for PAH characterization. Unfortunately, broad-band emission of most PAH systems prevents the simultaneous determination of several PAHs and limits the selectivity of luminescent methods.

To improve the selectivity of the luminescent methods for PAH systems, solid state techniques are often used. Two approaches for sharpening the luminescent emission are line-narrowing fluorescence spectroscopy (27,28) and mixed-crystal spectroscopy (29,30,31). Line-narrowing fluorescence spectroscopy employs a laser to excite only those PAH molecules in a particular environment within a low temperature matrix (e.g. glass, crystal or Shpol'skii). Molecules with vibrational levels in the first singlet electronic state which coincide with the laser frequency are excited. After vibrational deactivation these molecules are in equal energy excited states and fluoresce in a narrow frequency range. This technique has been demonstrated with an argon ion laser for anthracene and pyrene (32). Greatly improved selectivity should be possible with a tunable dye laser in place of the argon ion laser. The second approach requires choice of a solvent or matrix in which the PAHs can reside in a few particular orientations. If PAHs are dissolved in n-alkanes (pentane to nonane) and the resulting solutions are cooled to a temperature in the range of 4 K to 77 K, narrow-lined emission is observed under UV excitation. The impurity PAH molecules in the n-alkane host are held in substitutional sites and lattice broadening of their emission is not observed. These quasilinear spectra are a manifestation of the Shpol'skii effect (33-35). A review of the Shpol'skii effect (36) summarizes the systems which display this behavior. The variety of systems listed suggests the phenomena is quite common. The application of the Shpol'skii effect, excited by UV radiation, to the determination of 3,4-benzopyrene, a potent carcinogen, is well-documented (37-40).

The major drawbacks to luminescence analysis using the Shpol'skii effect are instrumental limitations (41). Scattered radiation from the excitation source is a particularly serious limitation since internal reflection occurs within the n-alkane snows formed upon freezing. The technique known as X-ray Excited Optical Luminescence (XEOL), which employs x-ray excitation, eliminates the problem of crosstalk between emission from the excitation source and luminescenct emission from the sample. The conventional sources (e.g. lasers, mercury lamps, xenon arcs etc.) (42) are replaced by an x-ray tube. XEOL is a sensitive analytical technique capable of detecting impurities at the fractional part per billion level in appropriate solid or gaseous environments (43,44). In an earlier publication (45) we reported the first observation of the Shpol'skii effect from PAHs in n-alkanes under x-ray excitation. The observation of quasilinear fluorescence and phosphorescence of PAHs under x-ray excitation suggested the combination of XEOL and the Shpol'skii effect might be a viable approach to the simultaneous multicomponent determination of complex PAH mixtures.

Another advantage gained by combining the Shpol'skii effect and XEOL is nonspecific excitation of the sample. The coincidence of the absorption band of the PAH molecule and the emission frequency of the excitation source is not a requirement because resonance processes are not responsible for direct excitation of the PAH molecules. Instead, highly selective energy transfer processes are responsible for the sensitized luminescence which is observed from trace PAHs contained in n-alkane microcrystals (45). The observation of sensitized luminescence indicates XEOL should be a sensitive method for the determination of PAHs in Shpol'skii matrices.

To visualize the processes which occur in the proposed excitation mechanism, an energy level diagram of the

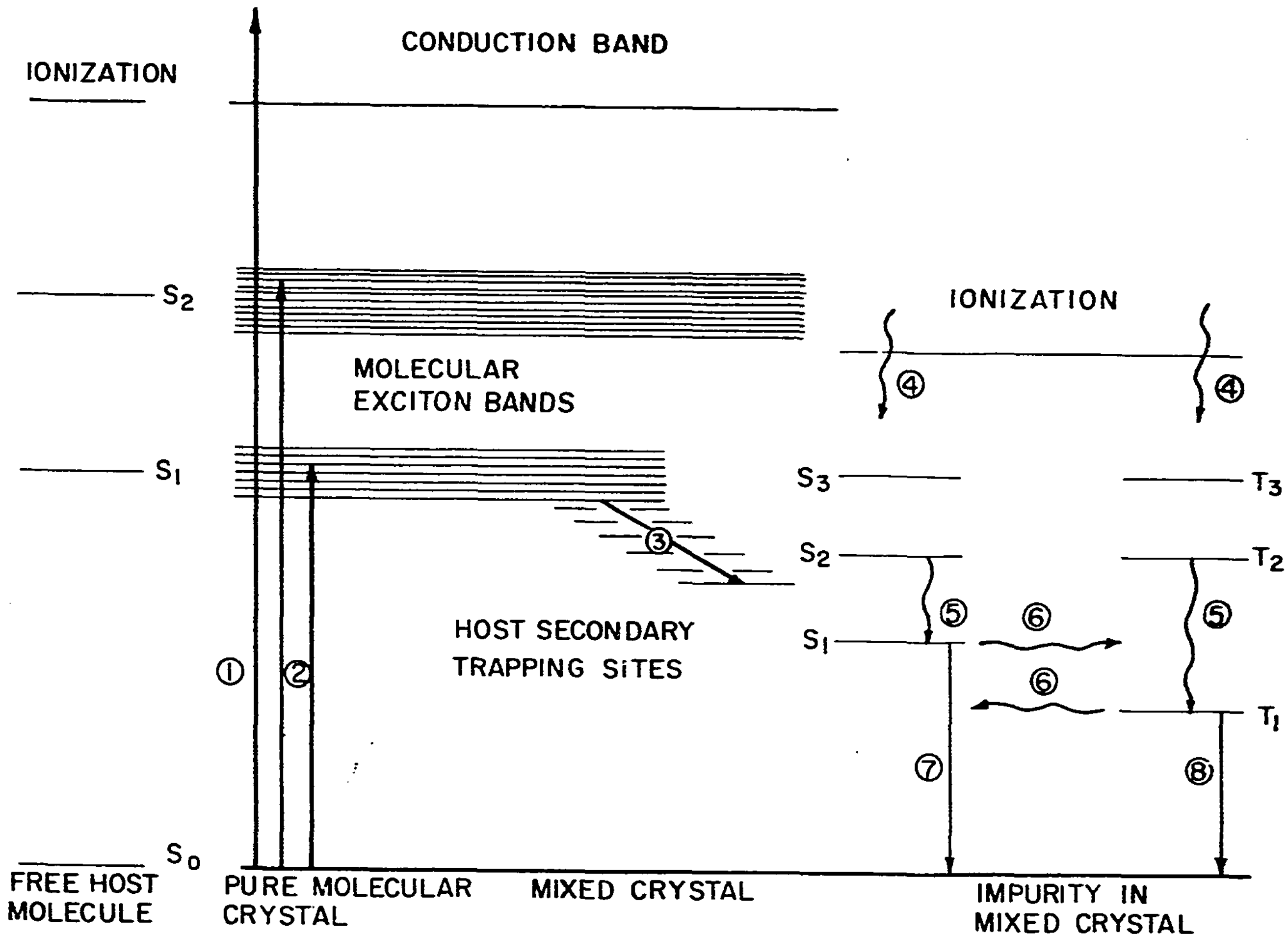

Figure 1. Energy level diagram for a n-alkane-PAH system at 10 K. The numbered transitions are; 1. Formation of the primary photoelectron, 2. Collisional population of molecular exciton bands, 3. Exciton trapped by perturbed host molecule, 4. Recombination, 5. Internal conversion followed by vibrational deactivation, 6. Intersystem crossing, 7. Fluorescence and 8. Phosphorescence.

n-alkane-PAH system at 10 K is presented in Figure 1. An explanation of the excitation mechanism begins with the energy levels of the free host molecule on the left side of Figure 1. The ground state, first two excited singlet electronic states, and the ionization limit are shown. To simplify the diagram, the vibrational levels were not drawn. In the solid state, the ground state and the ionization limit of the free host molecule are analogous to the valence and conduction bands of an ionic crystal. The singlet electronic states of the free host molecule broaden into molecular exciton bands which are characteristic of a molecular assembly of many host molecules. These molecular exciton bands are the transmission lines of the excitation energy. The perturbation exerted by an impurity molecule on neighboring host molecules results in the formation of host secondary trapping sites, shown in the mixed crystal region of the diagram. These perturbed host molecules are important in the selective capture of excitons by the impurity molecules. Finally, on the right side of Figure 1 the energy levels of a typical PAH are depicted as discrete states. The use of a Shpol'skii solvent traps the PAHs in identical environments in the crystal lattice and prevents broadening of the singlet and triplet excited electronic states. The observed optical signal is a composite of fluorescence and phosphorescence transitions of PAH molecules trapped in the lattice.

The first step in the excitation mechanism is the interaction of x-ray photons with the sample or the sample holder. X-ray photons interact with matter in three ways; 1. Photoelectric effect, 2. Compton effect and 3. Pair production (46,47). At the energies used in XEOL experiments (typically 60 kV.) only the photoelectric effect occurs. Atoms of the solvent or sample holder may absorb an x-ray photon and eject a primary photoelectron with energy in excess of several keV. (process No. 1 in Figure 1). The excited atoms relax by the emission of characteristic fluorescence x-rays or the ejection of Auger electrons. The primary photoelectron, fluorescent x-rays and the Auger electrons collisionally excite neighboring atoms in a cascade process.

The collisional excitation of electrons and atoms of host molecules populates the molecular exciton bands (process No. 2 in Figure 1). The exciton wave migrates through the molecular assembly and the excitation is delocalized (31). As the exciton propagates through the microcrystal it may enter a region in which an impurity molecule is trapped in the lattice. If the exciton migrates to a perturbed host molecule a phonon is produced and the exciton no longer possesses enough energy to migrate freely in the microcrystal. The exciton continues toward the impurity with the production of additional phonons (process No. 3 in Figure 1) until the impurity traps the exciton and is excited electronically or ionized. The inability of the exciton to return to the bulk of the crystal after the production of phonons near the impurity sites results in the funneling of excitation energy to the impurity. Recombination, internal conversion and intersystem crossing with vibrational deactivation (processes No. 4, 5 and 6 in Figure 1) occur in the impurity. Fluorescence (process No. 7 in Figure 1) and phosphorescence (process No. 8 in Figure 1) return the PAH molecule to the ground state. Thus, the highly selective energy transfer processes produce the optical signal.

The sharp line spectra resulting from the Shpol'skii effect make spectral resolution of several PAHs possible and endow the XEOL technique with some selectivity. However, no monochromator is capable of resolving all lines. Even with the Shpol'skii effect, overlap occurs in the fluorescent and phosphorescent emission of PAHs. Time resolved spectroscopy (TRS) coupled with XEOL would further improve the selectivity of the method. The technique of time resolved spectroscopy (48-50) allows separation of overlapping luminescence of PAHs on the basis of their luminescent decay constants. Since PAHs possess a large range of fluorescent and phosphorescent decay constants (26), it should be possible to time resolve fluorescent components and phosphorescent components. A pulsed excitation source is required to perform the time resolution experiment. Before coupling XEOL and TRS a pulsed x-ray source has to be constructed.

This dissertation describes the development of XEOL-TRS as a method for the analysis of PAHs. The modification of a medical x-ray unit for use as a pulsed x-ray source under computer control is discussed. The ability to time resolve phosphorescent mixtures but not fluorescent mixtures because of x-ray pulse characteristics is reported. Finally, analytical data is presented on the analysis of synthetic PAH mixtures and other systems that might be amenable to study by the XEOL-TRS technique are suggested.

CHAPTER 2: FACILITIES

Experimental Facilities

The experimental facilities, used as basic components in a simple XEOL system, are described in an early publication (51). The basic components plus the additional components of the pulsed XEOL system used in the present study are summarized in Table 1.

In Figures 2 and 3 the essential hardware portions of the pulsed XEOL system are numbered for easy identification. The brass sample chamber, used to shield the operator from scattered x-rays, was redesigned for this system. All seams in the brass structure were fitted with right angle slots to eliminate streaming of scattered x-rays through conventional seams. A reproducible mount for the cryogenic vacuum shield was fitted on top of the chamber. A table, to which the chamber was securely fastened, was added to support a ball bushing and bearing assembly for easy insertion and extraction of the cryogenic system into and out of the vacuum shield. Figure 2 shows the cryogenic system removed from the vacuum shield. The table has three-dimensional adjustments to simplify optical alignment of the system. Optical alignment was performed using a continuous wave He-Ne laser with emission at 632.8 nm. (C. W. Radiation Inc. Mountain View, CA). The sides of the brass box are easily removed and

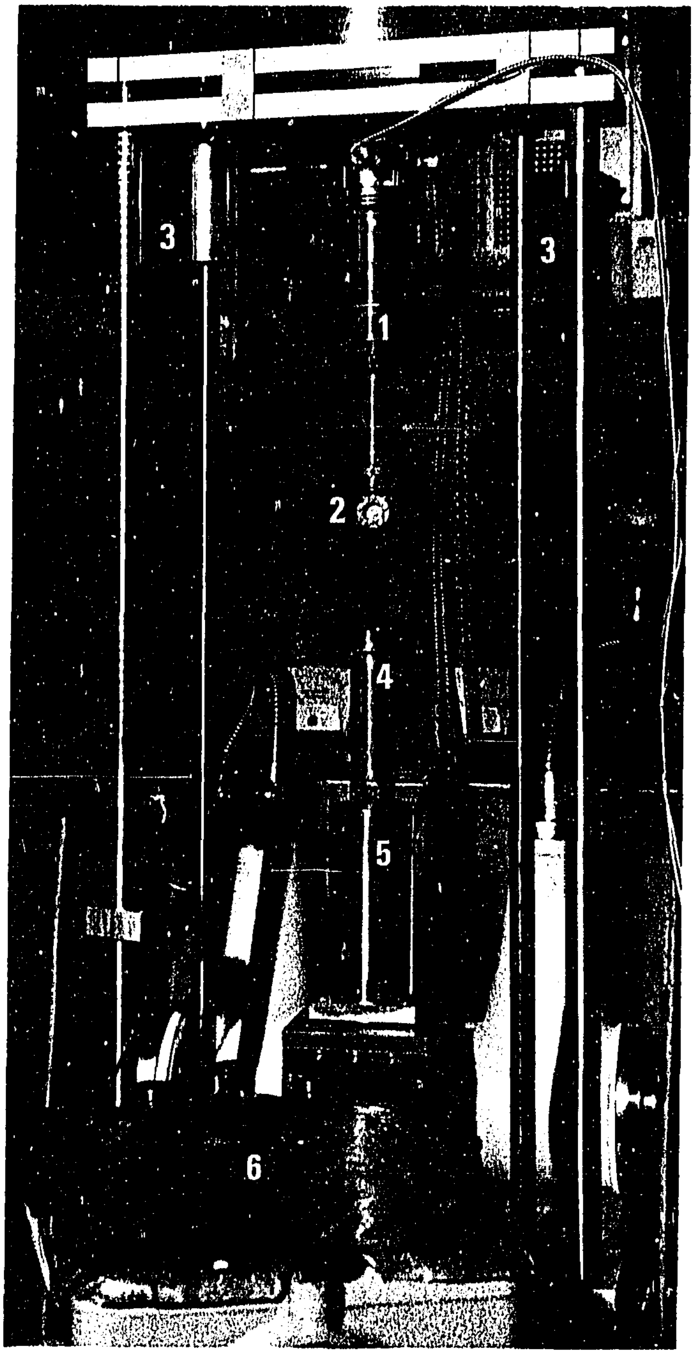

Figure 2. Photograph of the pulsed XEOL system with the cryostat removed from the vacuum shield. The numbered components are: 1. cryostat (cold end), 2. sample holder, 3. ball bushing and bearing assembly, 4. radiation shield, 5. vacuum shield and 6. monochromator.

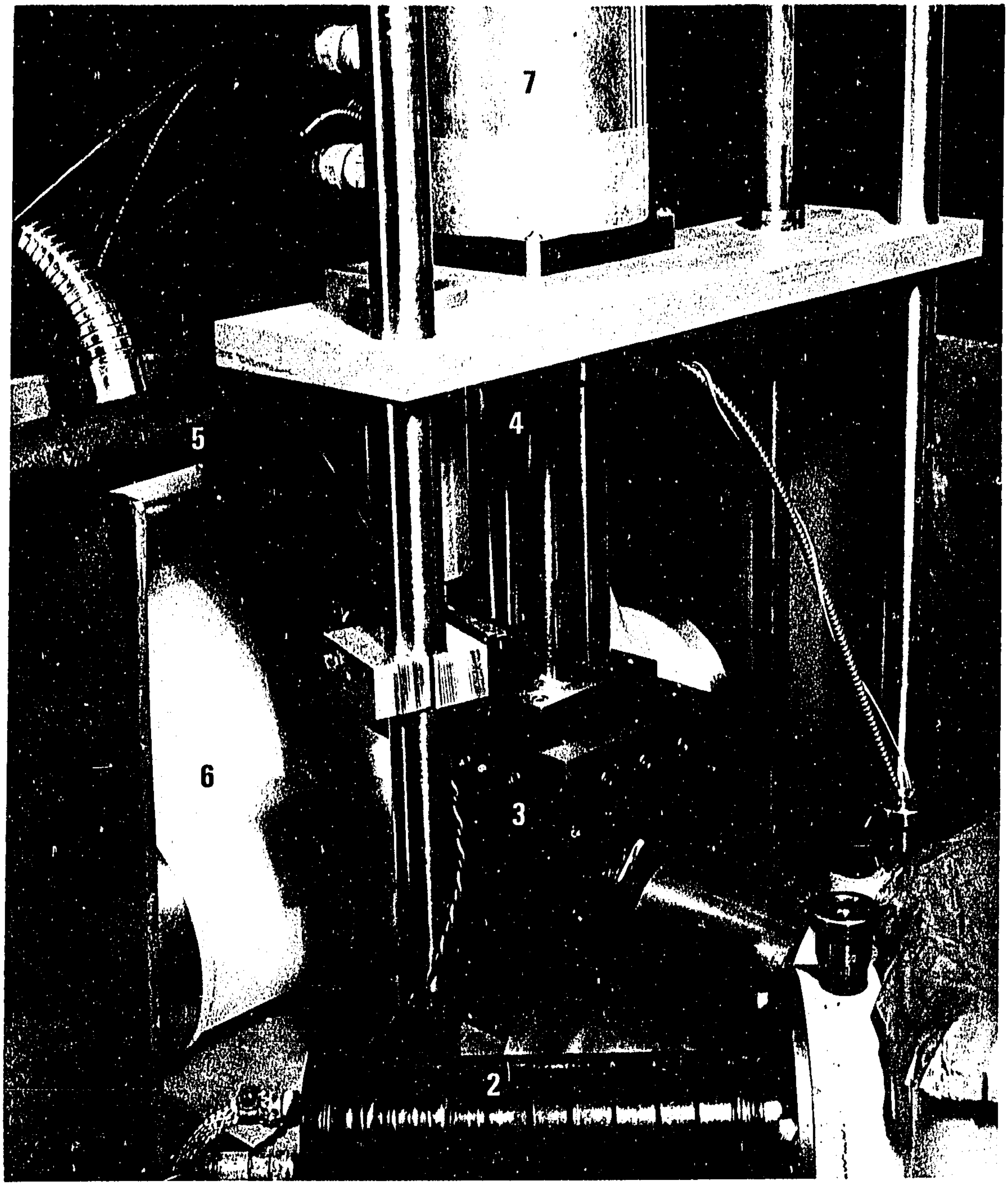

Figure 3. Photograph of the pulsed XEOL system with the cryostat inserted into the vacuum shield. The numbered components are: 1. monochromator, 2. photomultiplier tube in housing, 3. brass sample chamber, 4. vacuum shield, 5. vacuum line, 6. x-ray tube and 7. cryostat (mechanical end).

Table 1. Principal Components of Pulsed XEOL System

X-ray Sources	
DC x-ray power supply	Operated at 50 kV. and 40 mA. Water cooled Maximum 60 kV. 60 mA. (General Electric Corp., Milwaukee, WI Model XRD-6)
DC x-ray tube	Tungsten target Water cooled anode Emission of x-rays from 0.1 nm. to 0.02 nm. (General Electric Corp., Milwaukee, WI Model EA-75X)
Pulsed x-ray power supply	Medical x-ray unit Thyratron pulse circuits modified for computer control (Westinghouse Electric Corp., Greenville, PA)
Pulsed x-ray tube	Medical x-ray tube Operated at 60 kV. 100 mA. using large filament Rotating anode Conduction cooled (The Machlett Laboratories Inc., Stamford, CT)
Spectroscopic Equipment	
Monochromator	Scanning 0.3 meter Crossed Czerny Turner mount (McPherson Instrument Corp., Acton, MA, Model No. 218)
Detector	EMI 6256B photomultiplier S-13 response (EMI Gencom Inc., Plainview, NY)
High voltage power supply	Operated at 1200 VDC (NJE Corp., Kenilworth, NJ, Model S-325)

Table 1. (Continued)

External optics	Precision grade quartz lens 1 inch diameter 2 inch focal length (Corion Instrument Corp., Waltham, MA)
Amplifier	Fast current amplifier with adjustable rise time and zero suppression (Keithley Instruments, Cleveland, OH, Model 427)
Recorder	Two pen voltage recorder (Houston Instruments, Austin, TX, Model 5210-5)
Refrigeration and Vacuum Equipment	
Helium refrigerator	Helium refrigerant Temperature selectable from 10 K to 360 K with 1 degree resolution (Air Products and Chemicals Inc., Allentown, PA, Model CSA-202)
Diffusion pump	2 inch air cooled (NRC Equipment Co., Newton, MA)
Floor pump	(The Welch Scientific Co., Skokie, IL, Model 1397)
Vacuum gauge	(National Research Corp., Cambridge, MA)
Computer and Interfaces	
Computer	PDP8/E minicomputer (Digital Equipment Corp., Maynard, MA)
Control interface	See text
Data interface	(Heath Co., Benton Harbor, MI)

Table 1. (Continued)

Buffer	(Heath Co., Benton Harbor, MI)
Analog to Digital Converter	(Redcor Corp., Woodland Hills CA)
Teletype	(Teletype Corp., Skokie, IL, Model-33)

replaced to accommodate either a DC or pulsed x-ray tube. The x-ray tubes are positioned to minimize the distance from the anode to the vacuum, because air can severely attenuate the x-ray beam. Figure 3 shows the brass chamber with the pulsed x-ray tube attached and the refrigerator inserted.

The control interface was designed by G. Holland of Ames Laboratory Instrumentation Group and built by technicians in the same group. A simplified circuit diagram of the interface is presented in Figure 4. The interface instructions which control the operation of the x-ray source are indicated on the diagram. The flip flops are equivalent to toggle switches. The AND gates test two computer conditions before allowing pulses to reach the x-ray supply. A second circuit in the control interface generates timing pulses from the line voltage. The simplified circuit is drawn in Figure 5. The two operational amplifiers act as comparators. The voltage dividers, connected to the noninverting inputs, are used to fine tune the phase relationship between the x-ray

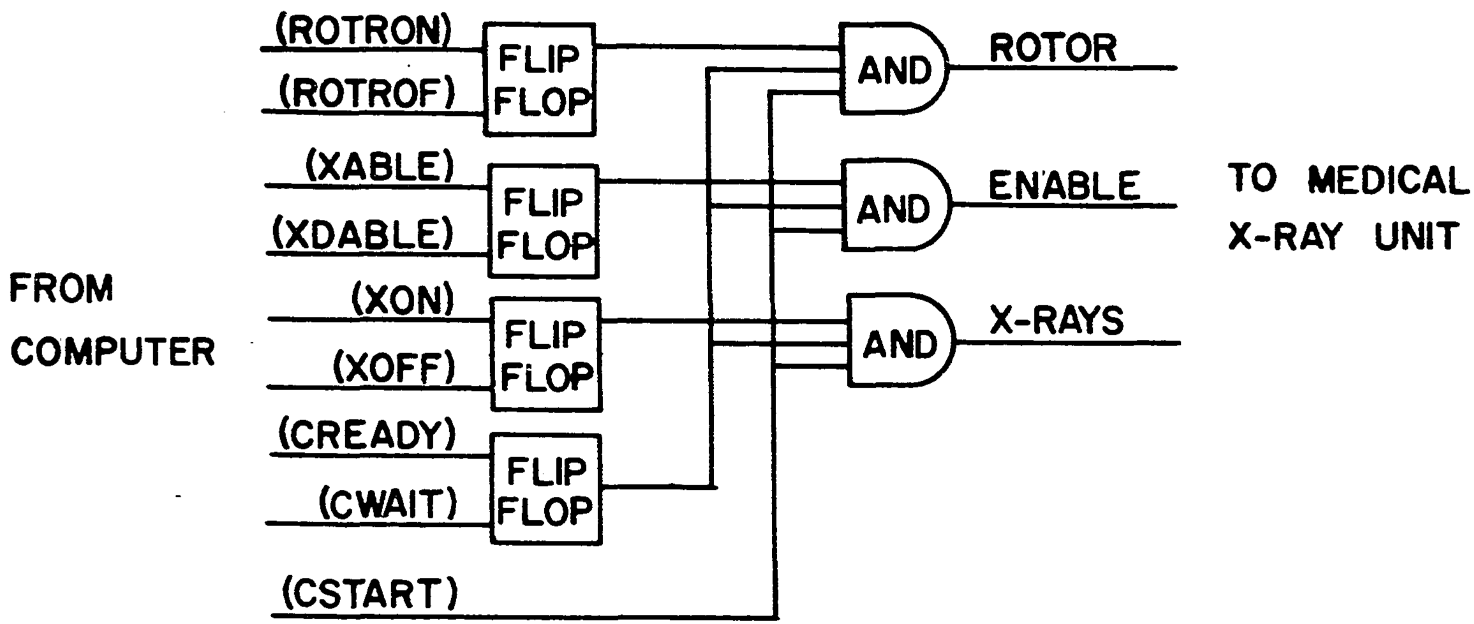

Figure 4. Simplified circuit diagram of the control interface. Interface commands are indicated in parentheses.

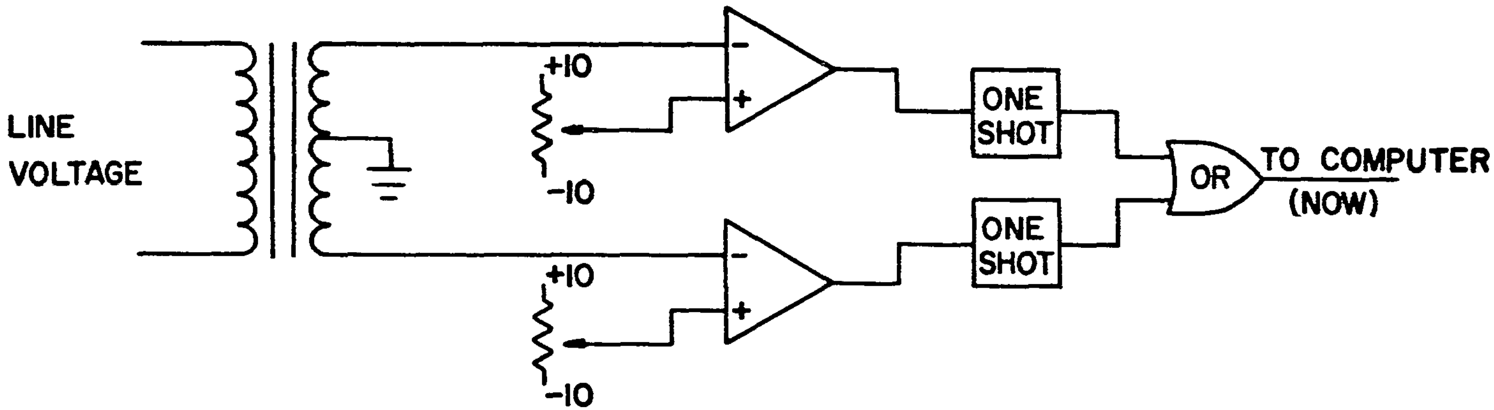

Figure 5. Simplified circuit diagram of the circuit used to generate timing reference pulses.

supply and the timing pulses. The gated integrator, also designed by G. Holland, is an operational amplifier with a feedback capacitor and several input resistors. The circuit board is contained in the control interface chassis. The simplified circuit is drawn in Figure 6. Three input resistances were included to attenuate the input voltage. The integrator is operated with two interface instructions shown on the diagram. All interface instructions, their octal values and functions are summarized in Table 2.

Table 2. Interface Instructions

Instruction	Octal Value	Function
CREADY	6337	Enable control interface
CREADY	6331	Open communication lines
CWAIT	6336	Close communication lines
NOW	6332	Timing pulse
ROTRON	6341	Turn rotor on
ROTROF	6342	Turn rotor off
XABLE	6343	Enable x-ray supply
XDABLE	6344	Disable x-ray supply
XON	6333	Turn x-rays on
XOFF	6334	Turn x-rays off
INBOX	6346	Initialize integrator
STBOX	6345	Start integrator
GETDAT	6354	Transfer data
STATOD	6455	Start A to D conversion
INATOD	6455	Initialize A to D converter

Computational Facilities

The data, produced by the pulsed XEOL system, is processed by PL/1 and FORTRAN IV programs. These programs are

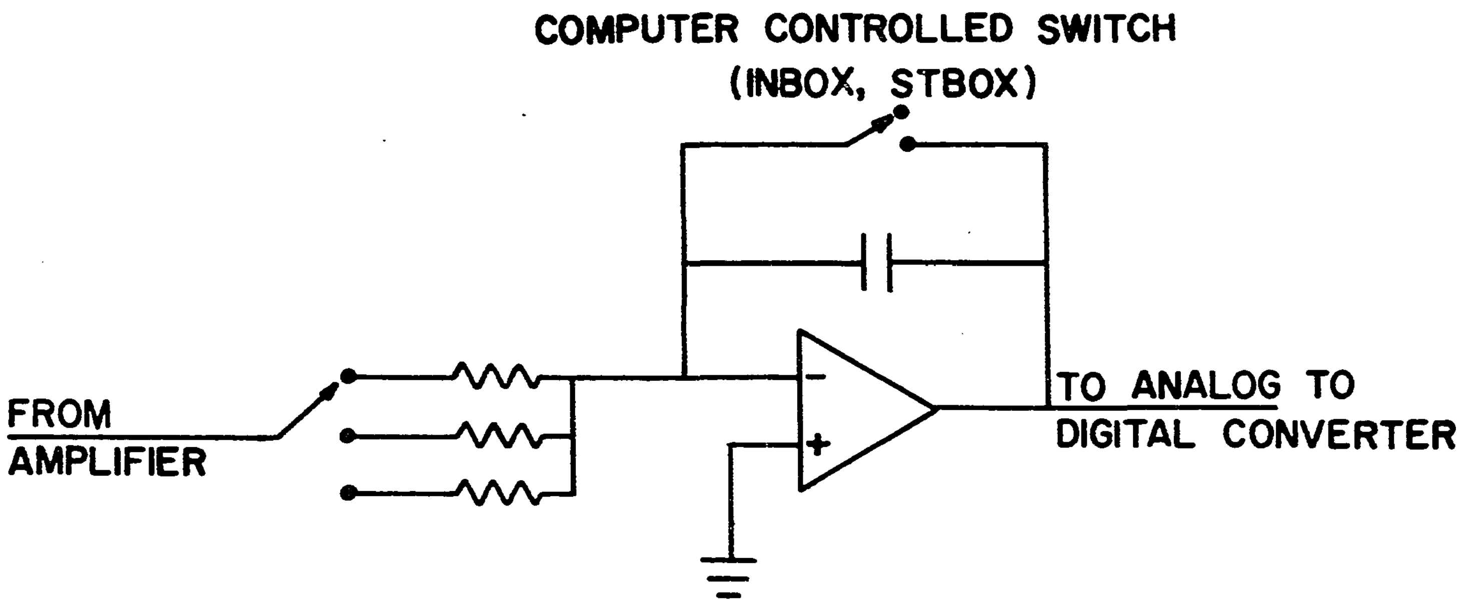

Figure 6. Simplified circuit diagram of the gated integrator. Control instructions are indicated in parentheses.

executed on the IBM 360/65 and ITEL AS/5 computers in the Iowa State University Computation Center. The PL/1 program was written to plot decay curve data using Simplotter (52) and to produce an input data set in the proper format for the FORTRAN IV program, called SMASH (53). SMASH was developed by the neutron activation analysis group at Ames Laboratory to separate complex decay curves and was modified for the present study to handle spectroscopic data. Listings of the PL/1 and SMASH programs appear in Appendix 1 and Appendix 2 respectively.

A conversational system, known as WYLBUR, makes operator interaction with the data processing system possible. WYLBUR was accessed over telephone lines located in our research area. A Decwriter II (Digital Equipment Corp. Maynard, MA) and Teletype (Teletype Corp., Skokie, IL, Model 35) were the devices used to communicate instructions to WYLBUR. WYLBUR is a text editing program with remote job entry and execute file capabilities supported by the Iowa State University Computation Center. The text editing features facilitate program writing and the remote job entry feature simplifies the debugging process. After the paper tape data set is transferred to the computer system, a WYLBUR execute file is used to generate a control data set for the PL/1 program and to create a system job composed of job control language, program listings and data. WYLBUR submits the job to the system and the results are printed in the computation center.

Another facility available at the Iowa State University Computation Center for displaying graphical data is Simplotter. Simplotter is a FORTRAN program, developed at Ames Laboratory, for general plotting requirements. Simplotter was used to display decay curves, calibration curves and other general data. A PL/1 program was written to access Simplotter directly to plot simple data sets while WYLBUR was used to generate the data set with the proper format. A listing of the WYLBUR execute file and PL/1 program is given in Appendix 3.

The computational facilities, available through the Iowa State University Computation Center, made the time resolution experiment possible. The separation of complex decay curves by a least squares method using a digital computer is a routine exercise. Without the least squares method we would have limited our resolution to simple two-component systems because graphical methods would have been employed. Our ability to use mathematical techniques, such as the SMASH routine, made it possible to extend time-resolved spectroscopy to mixtures with more than three components.

CHAPTER 3: PULSED XEOL SYSTEM

The pulsed x-ray excited optical luminescence system is shown as a block diagram in Figure 7. At the heart of the system is a dedicated minicomputer. The stringent timing requirements for x-ray pulse generation and the careful measurement of integration periods during data acquisition required the use of a dedicated computer. Human interaction with the system occurs at the teletype where input is typed at the keyboard and output is generated at the punch as paper tape. The assembly language program which generates the x-ray pulse, controls the data acquisition system and handles input and output information is listed in Appendix 4.

The computer interacts with the system through two interfaces. The data interface is used to transfer digital data from the analog-to-digital converter to the computer memory where it is stored until output is punched. The control interface connects the computer, the x-ray supply and the integrator. Timing reference pulses are produced in the control interface.

The excitation source in the luminescence system is a modified medical x-ray unit. The x-ray supply can produce a maximum voltage of 150 kV. across the x-ray tube and a maximum current of 300 mA. through the x-ray tube. The x-ray tube is a rotating anode, medical x-ray tube which is cooled by conduction.

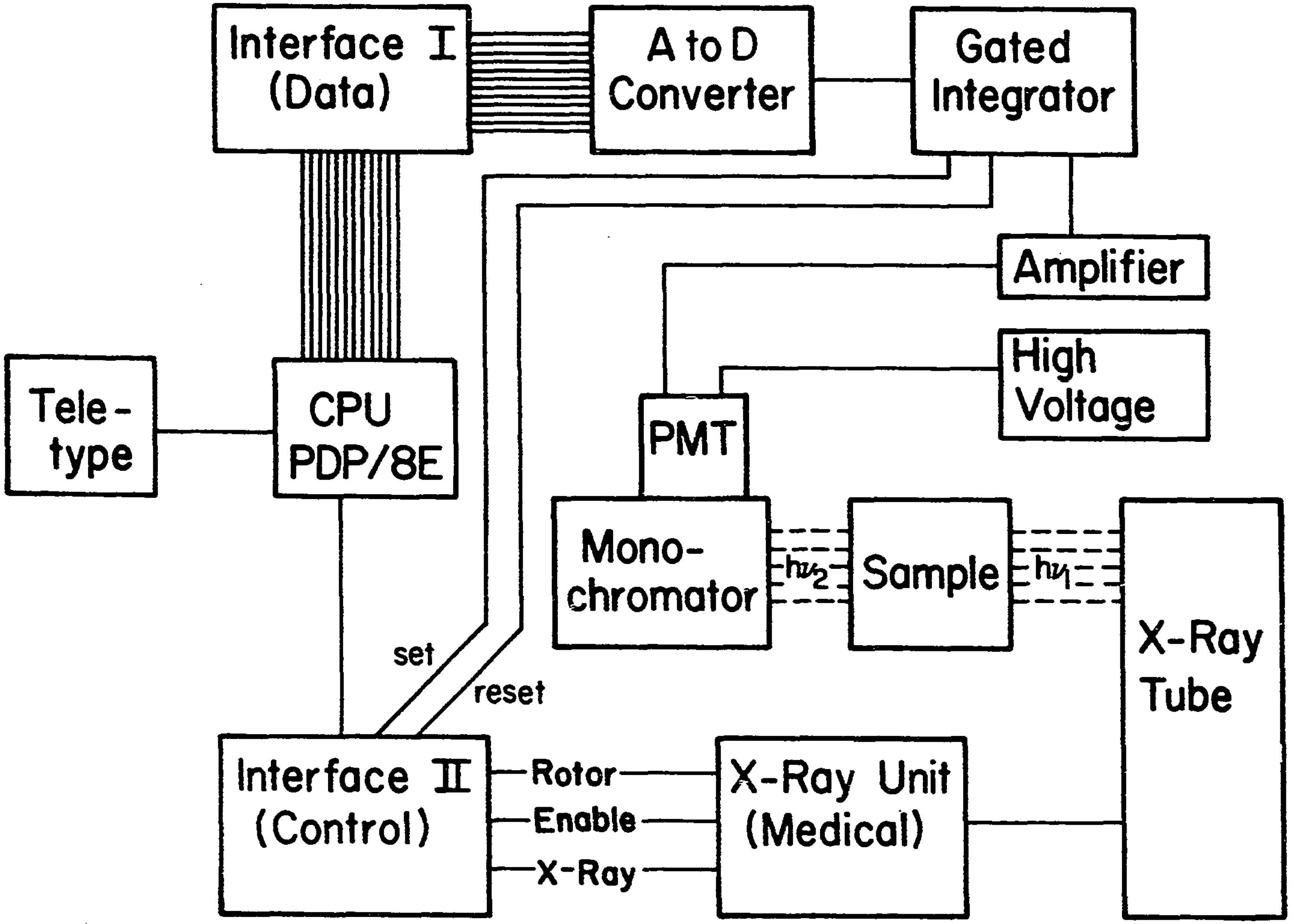

Figure 7. Block diagram of the pulsed x-ray excited optical luminescence system.

Three control signals are required to pulse the x-ray source. First, the rotating anode must be started. The rapid rate of rotation prevents excessive heating of localized areas of the anode surface and subsequent sputtering and pitting. Next the x-ray supply must be enabled. Under normal operation the enable function would produce x-rays. Finally, a gate pulse signals the power supply to release the thyratron switches and activate the x-ray tube for the duration of the pulse.

During the on period of the x-ray pulse, the sample, typically PAHs dissolved in n-heptane at 10 K, is excited. At termination of the x-ray pulse some initial activity exists and decays exponentially. The emission is collected by a lens, dispersed with a monochromator and detected by a photomultiplier tube. The photomultiplier tube current is amplified by a fast response (typically 1-10 msec.) current amplifier and a voltage signal results.

The gated integrator sums the voltage signal for a predetermined period and is reset. Prior to the reset command, the integrator output is sampled and an analog-to-digital conversion is performed. After the integrator is reset the process is repeated until the number of data points, specified by the operator, is obtained. The luminescent decay is characterized by the sequential data points. The timing relationship between the x-ray pulse and the integration of the voltage signal is precisely controlled by the minicomputer. The digital data are transferred to computer memory where luminescent decay from subsequent x-ray pulses can be added. The signal averaged data are punched on paper tape and analyzed on the Iowa State University Computation Center facilities.

In the following sections detailed explanations of the operation of different phases of the pulsed, x-ray excited, optical luminescence system are presented. The principles of x-ray pulse generation are outlined. The control of the sample temperature and the containment of the sample are described. The data acquisition options are presented and the section on data analysis follows the data after they are punched on paper tape to the final results. Finally, some consequences of the pulsing technique are discussed in the section on x-ray pulse characteristics.

X-ray Pulse Generation

The first attempt to produce an x-ray pulse involved a high voltage grid in the x-ray tube which could deflect the electron beam away from the anode. Before implementing the grid approach, the x-ray emission of the DC supply was characterized. A liquid scintillator was irradiated and the response was observed with an oscilloscope. A typical oscilloscope tracing is depicted in Figure 8. A full-wave

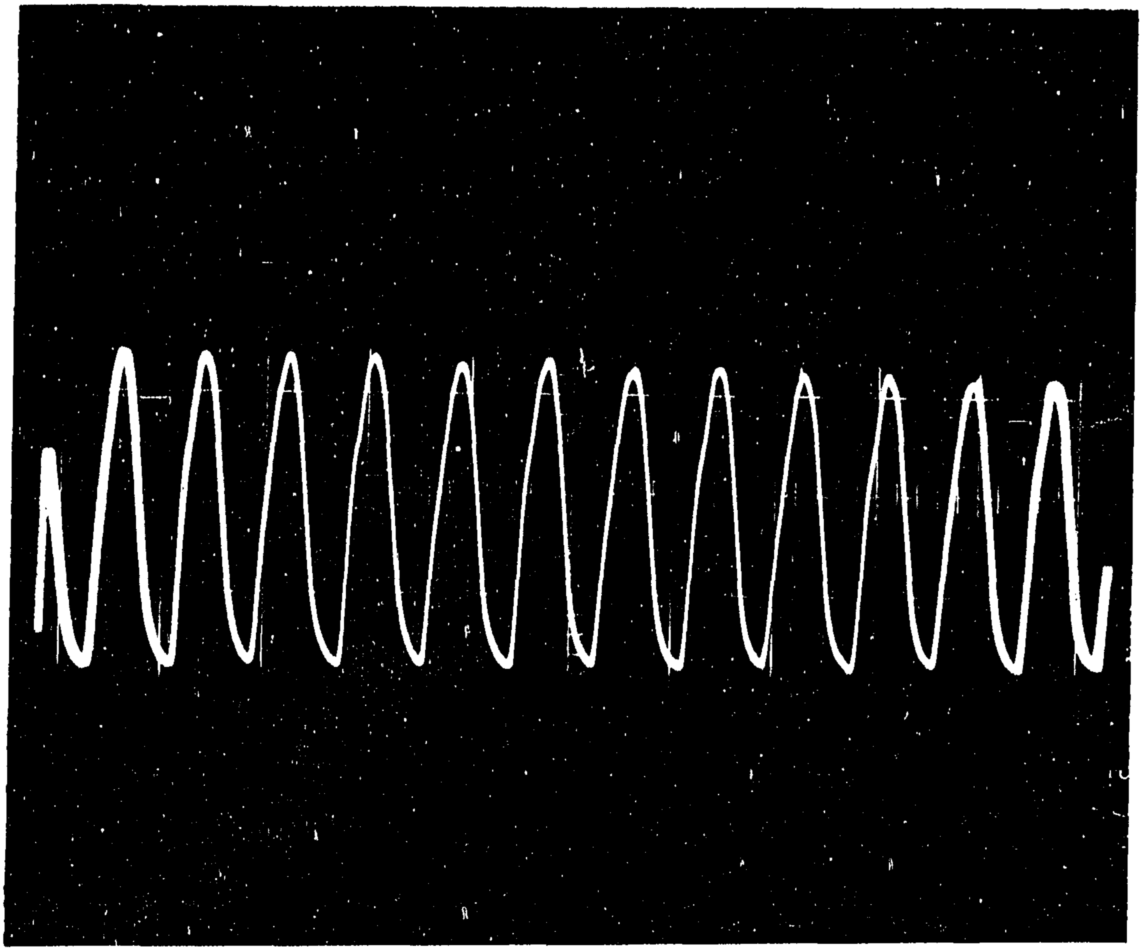

Figure 8. Oscilloscope tracing of the amplifier signal produced by a photomultiplier tube in response to a fast scintillator (perylene in n-heptane) excited by a DC x-ray source. Horizontal scale is 10 msec./cm. and vertical scale is 2 volts/cm.

rectified sine-wave with a frequency of 120 cycles per second was observed. The sine waveform and not a DC level was observed because manufacturers of x-ray equipment do not filter the voltage supply which powers the x-ray tube. The size of the capacitors and resistors that are required to filter kilovolt voltage levels are prohibitive. The switch-selectable voltages and currents on x-ray sources are root-mean-square values and represent the DC average of the waveform. The grid approach was abandoned and advantage was taken of the inherent pulsed nature of a DC x-ray supply. If the medical x-ray supply could be turned on at a zero point in the waveform and off at a later zero point, an x-ray pulse which is a multiple of 1/120th of a second in length could be produced.

To generate such an x-ray pulse required precise determination of zero points in voltage waveforms, such as the one shown in Figure 8. A computer was used to control the pulse generation. Because the computer could not monitor the voltage waveform of the medical x-ray unit directly, a virtual link between the computer and the x-ray unit was established with the control interface. The line voltage which powered the control interface was used to produce timing reference pulses every time the line voltage went to zero. Because the entire United States is on the same power grid the timing reference pulses differed from the zero points of the voltage waveform in the medical x-ray supply by a simple phase relationship. An oscilloscope was used to synchronize the timing reference pulses and the zero points in the voltage waveform with the phase adjustments in the control interface.

Normal operation of the medical unit required two steps to produce x-rays. After the thyratron switches were modified to function under computer control, three steps were required. The rotor had to be started, the x-ray unit had to be enabled, which produced x-rays in normal operation, and the thyratron switches had to be gated. The sequence of events in production of a typical x-ray pulse is shown in Figure 9. After the rotor was started and the x-ray unit was enabled, the computer start command enables the control interface. The computer ready command released the timing reference pulses. At the first zero point the x-rays were turned on and at the next zero point the x-rays were turned off. If a longer excitation period was required, the process was repeated until the number of waves, as specified by the operator, occurred. Variable length excitation periods from 1/120th of a second to several seconds could be produced. The maximum length of x-ray excitation period was limited by the voltage, current and time product which determined the electrical power the x-ray tube had to dissipate as heat.

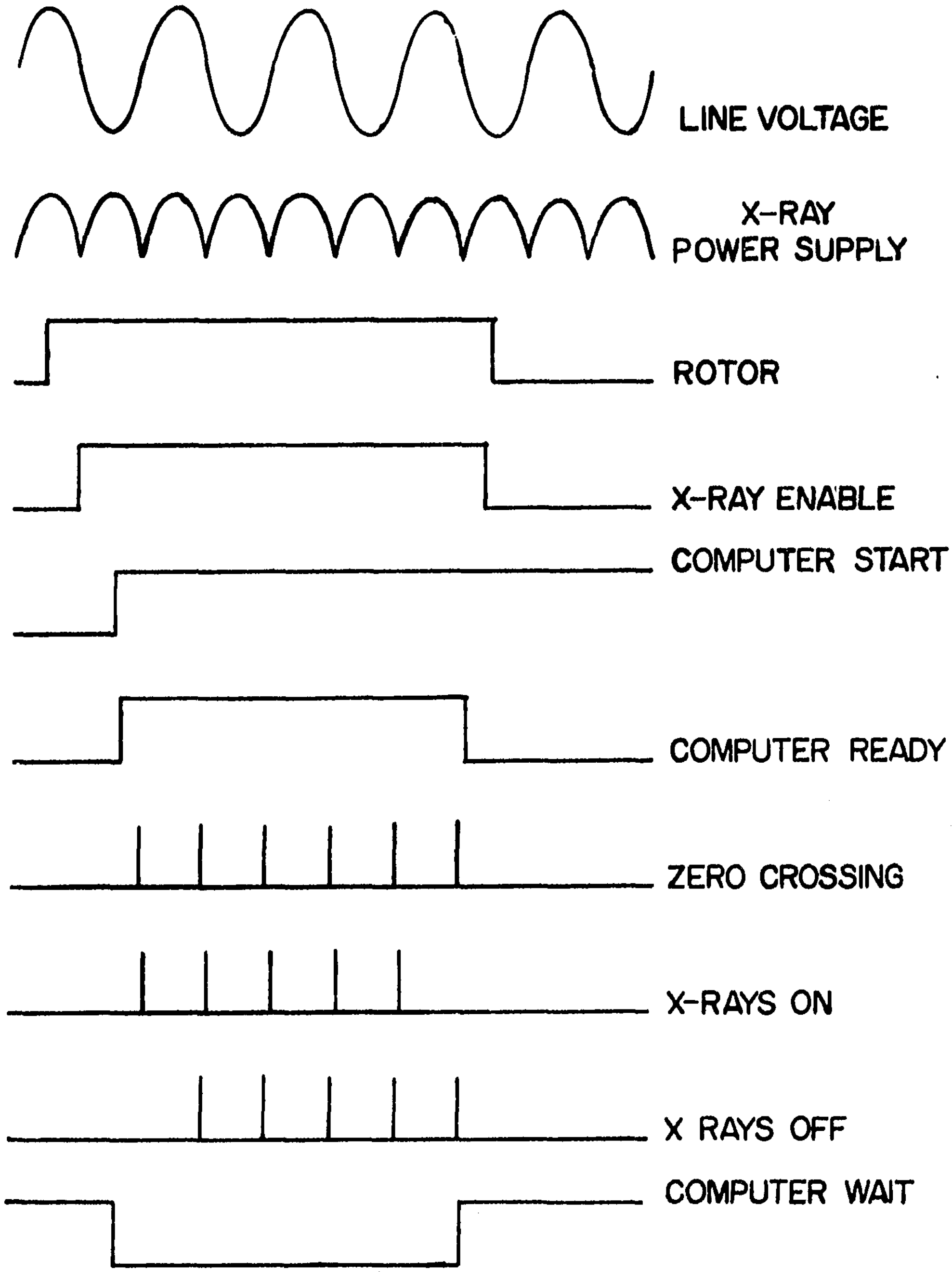

Figure 9. Timing diagram which illustrates the time relationship and sequence of events in the production of a typical x-ray pulse.

Refrigeration and Optical Systems

The pulsed XEOL system was developed to study a variety of samples over a large temperature range. A refrigeration system with the flexibility to study solids, liquids and gases at temperatures in the range from liquid helium to boiling water was desired. A helium refrigerator (see Table 1 for details) was purchased and incorporated in the pulsed XEOL system. The helium refrigerator was a two stage cryostat which worked on the Solvay process and provided the capability of examining the spectra of solids, liquids and gases at thumb-switch-selectable temperatures ranging from 10 to 360 K with 1 K resolution.

Unfortunately, the helium refrigerator presented its own problems. Because the vacuum used to insulate the cryostat from the surroundings prohibited the use of conventional XEOL sample handling techniques, a sample holder which could contain the sample in a vacuum, allow x-rays to irradiate the sample and transmit the optical radiation was designed. The materials problems encountered in designing the sample holder with the specifications mentioned above required a change from the conventional geometry used in an XEOL experiment.

The sample holder used in this study is sketched in Figure 10. The body of the sample holder was made of oxygen-free high conductivity (OFHC) copper. The quarter-twenty thread attaches the holder to the cryostat.

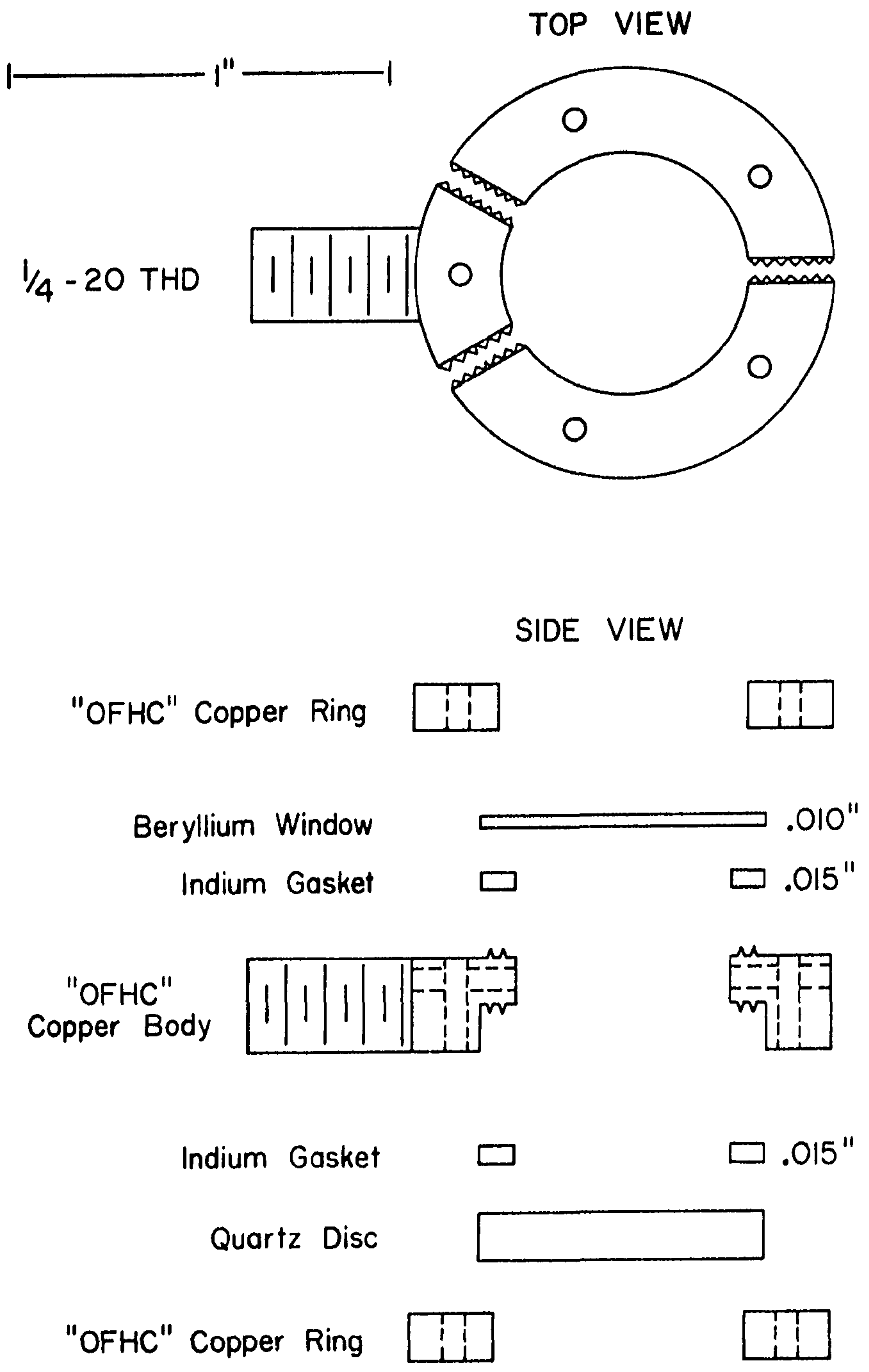

Figure 10. Sample holder used with the pulsed XEOL system. Main body and retaining rings were fabricated from oxygen free high conductivity copper.

An indium washer was placed between the cryostat and the holder to compensate for expansion and contraction effects and to insure that thermal contact was made between the cryostat and the sample holder. The sample was held between a beryllium window and a fused quartz disc. Both the window and the disc were sealed to the holder with OFHC copper retaining rings and indium gaskets. Indium gaskets were used because of the ductility of indium at 10 K. Also, 0.2 mm. (0.008 in.) indium gaskets replaced the thicker gaskets shown in Figure 10 because less indium was smeared into the sample holder. The sample was injected into the holder with a syringe through the filling ports. The ports were threaded and sealed with number two screws and indium gaskets. The holder was emptied by removing two of the three number two screws.

A "straight-through" geometry was used with the sample holder described above. The optical diagram is shown in Figure 11. Advantage was taken of the penetrating ability of x-ray radiation and the crossed Czerny-Turner mount of the monochromator. The x-ray cross section of capture for carbon and hydrogen is small so the x-ray beam is not significantly attenuated by a hydrocarbon sample, therefore, the x-ray beam and the luminescence proceed into the monochromator. At the collimating mirror the optical signal is reflected to the grating but the x-ray radiation passes through the mirror and is absorbed by the lead shielding which surrounds the

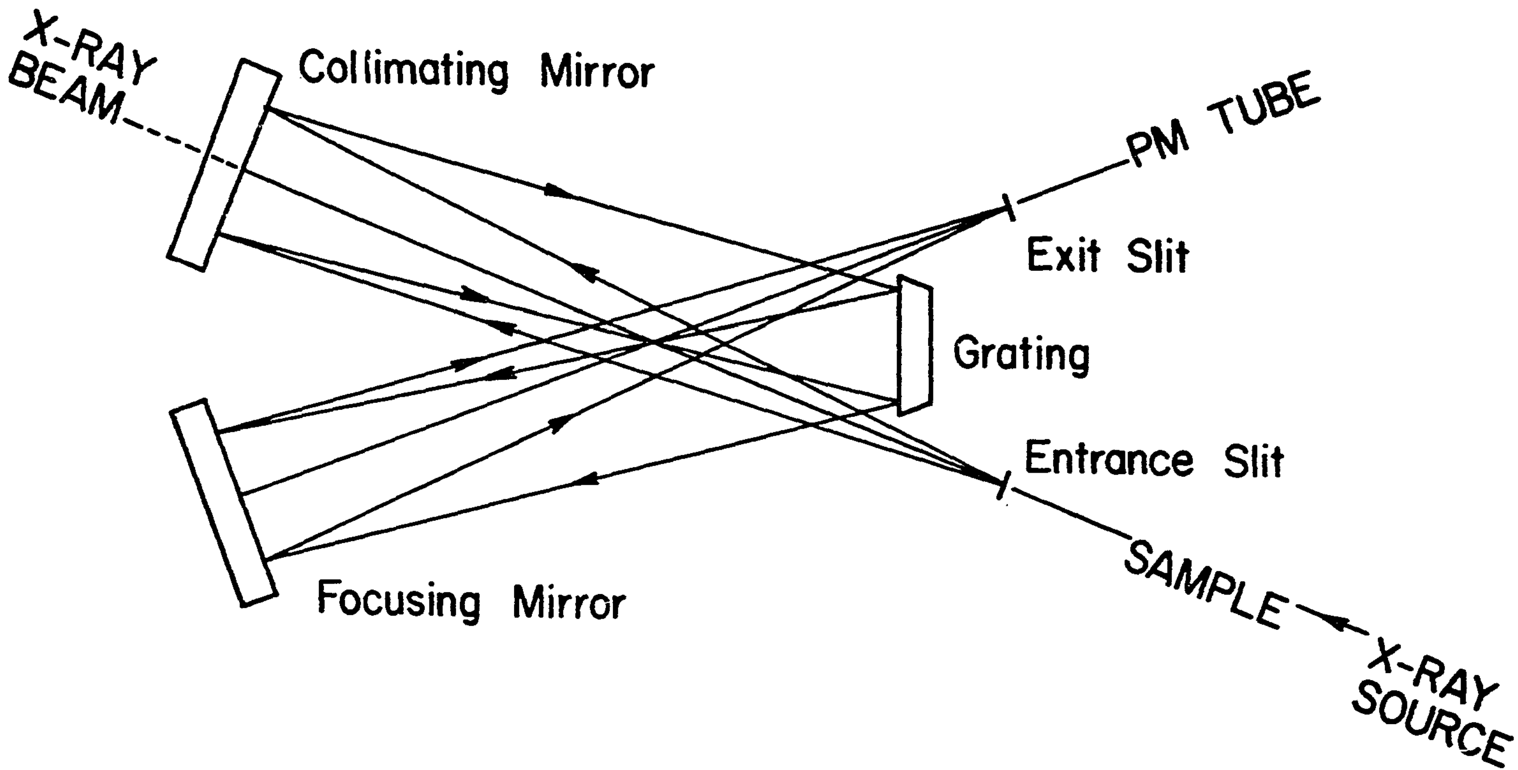

Figure 11. A schematic diagram of the optical system designed around the crossed Czerny-Turner mount of the McPherson monochromator used in the pulsed XEOL system.

monochromator. The optical signal is dispersed at the grating and proceeds to the photomultiplier tube where it is detected. Scattered x-ray radiation does not enter the photomultiplier tube to produce noise because the photomultiplier tube is positioned off the primary optical axis.

Data Acquisition System

The major objective for construction of the pulsed XEOL system was to obtain decay curve data. The large x-ray flux available with a pulsed source represents an advantage over the DC sources, hence a secondary objective was to obtain pseudo-DC data. The major instrumental components of the data acquisition system were the gated integrator, the analog-to-digital converter and the data interface. The heart of the system, however, was the software which controlled the gated integrator. The software was written to make the data acquisition system operate in one of two modes, a fast mode or a slow mode.

In the fast mode, pseudo-DC data was obtained. The fast mode was used to study fluorescent single component emission. The integrator was started at the zero point of the x-ray wave and reset at the next zero point. The luminescence produced by a single x-ray wave was integrated and the voltage output of the integrator was considered the average

DC level of the luminescence. To improve the signal-to-noise ratio and the statistical values of the data several successive waves could be integrated during an extended pulse and the data of several pulses could be summed to signal average the noise. A mean and standard deviation were calculated and used as an average DC value for subsequent analytical calculations.

In the slow mode, decay curve data were obtained. There were two algorithms for sampling an exponential decay. The first algorithm involved integration of the entire decay curve and periodic sampling of the integrator output. A numerical differentiation generated the original decay curve. The second algorithm divided the decay curve into equal time segments. Each time segment was integrated and the voltage output was plotted as a function of time to obtain the decay curve. The second approach was used because the individual integrations "signal averaged" the noise to a constant value which could be subtracted from each data point and enhanced signal-to-noise ratios as compared to the discrete sampling algorithm resulted.

Three integration periods (1000, 100 and 10 msec.) were programmed for the gated integrator, so that a large range of decay constants could be studied. The reset time of the integrator was 1 millisecond, hence a small percentage of the signal is lost. To illustrate, use of the 10 millisecond integration period means 10 percent of the signal was lost during the reset time whereas with the 1000 millisecond integration period, only 0.1 percent of the signal was lost. The same "real-time" must be integrated to obtain equivalent signal-to-noise ratios if different integration periods are used. For example, if 10 decay curves are summed using the 1000 millisecond integration period then 100 decay curves have to be summed using the 100 millisecond integration period and 1000 decay curves have to be summed using the 10 millisecond integration period to obtain equivalent signal-to-noise ratios.

In both modes the data acquisition system proceeded in several steps. The analog signal from the fast response current amplifier was integrated according to the algorithm of the mode. The integrator output was digitized by the analog-to -digital converter in 20 microseconds. The digitized signal was passed to the computer through the data interface in a parallel transmission. The data was temporarily stored in the computer until output was punched and then the paper tape was processed by the large computer system as described in the next section.

Data Analysis

The pulsed XEOL system generated large quantities of numerical data in either mode of operation. To process these data, sophisticated computational facilities were needed. Furthermore, the time resolution experiment was dependent on a numerical characterization of simple or complex decay curves. The statistical techniques needed to characterize the decay curves were ideally suited for computer analysis. For these reasons it was necessary to accumulate data with the minicomputer but process the data on a more sophisticated computer system.

The Iowa State University Computation Center operates an IBM 360/65 and an AS/5 computer system. PL/1 and FORTRAN IV are among the many languages supported by the system. An interactive system, known as WYLBUR, is also available. WYLBUR, PL/1 and FORTRAN IV were used extensively for the analysis of the numerical data.

The paper tape data set generated by the assembly language program contained control information used in the assembly language program and the numerical data collected from the experiment. The data set was transferred to the large computer and stored on disc. WYLBUR was used to construct a job which calculated the experimental results. If the fast mode was run the job contained only a PL/1 program which read the data from disc and calculated a mean and standard deviation. The results were printed with a data dump of the important control variables. If the slow mode was run, the job contained a PL/1 program and a modified FORTRAN IV program. The PL/1 program read the data from disc and plotted the decay curve using Simplotter. The data dump was generated and an output data set was created which was the input for the FORTRAN IV program, called SMASH. SMASH either calculated a decay curve by a direct-search method or used a linear least squares procedure to calculate initial activities of the luminescence. The results of the SMASH program were printed by the output routines contained within the program.

After the data analysis job was completed, the output was retrieved from the Iowa State University Computation Center. The results were extracted from the printed material. If wavelength or concentration plots were desired, another job could be created with a WYLBUR execute file and PL/1 program, which generated a computer plot with Simplotter. Analytical data were calculated with a hand calculator.

All the programs mentioned in this section are listed in Appendices 1-4. The PL/1 programs were written specifically for this study but the SMASH program was borrowed from the neutron activation analysis group and the input routine was modified to facilitate operation of the program. The job control language which regulates execution of the job is listed in Appendix 5. The WYLBUR execute file which created the job is listed in Appendix 6.

X-ray Pulse Characteristics

The method used to generate the x-ray pulse limited the range of the time resolution experiment. The limitation is manifest by a differential equation which relates the number of excited molecules as a function of time to a supply term and a depletion term. The relation is expressed in equation 1;

$$N' = S*F - k*N \qquad (1)$$

where N represents the number of excited molecules as a function of time, S is the cross section for capture of an x-ray photon, F is the driving function or functional form of the excitation source ($F=\sin(\omega t)$) and k is the decay constant of the excited molecule. The equation holds only while the x-ray pulse is active. The solution is given in equation 2;

$$N = S[k*\sin(\omega t)-\omega*\cos(\omega t)] / [k^2 + \omega^2] \qquad (2)$$

Three cases are considered to simplify the form of the solution. If $k>>\omega$, which corresponds to phosphorescent emission, then equation 3 results;

$$N = (S/\omega)\cos(\omega t) \qquad (3)$$

As the x-ray pulse ($\sin(\omega t)$) goes to zero, the number of excited molecules goes to a maximum and an initial activity exists after the x-ray pulse. If $k \ll \omega$, which corresponds to fluorescent emission, then equation 4 results;

$$N = (S/k)\sin(\omega t) \quad (4)$$

Now, as the x-ray pulse goes to zero so does the number of excited molecules and no initial activity exists after the x-ray pulse. Finally, if $k \approx \omega$ then no simplification of the equation is possible. Some initial activity does exist after the x-ray pulse but the decay is severely distorted by the shape of the excitation pulse. Fourier techniques are used to deconvolute the data and extract the decay curve.

To summarize the three cases, with the x-ray pulse used in the present study the time resolution experiment was limited to phosphorescent emission. Fluorescent emission could not be time resolved but was studied by observation of single component emission with the pseudo-DC mode. No intermediate decay curves were observed from the PAHs studied, but as the scope expands to include other types of organic compounds it will be necessary to develop the Fourier techniques to deconvolute the data.

CHAPTER 4: EXPERIMENTAL PROCEDURES

Preparation of Chemicals, Solvents and Solutions

All of the PAHs used in the XEOL study are listed in Table 3. The PAHs were purified by zone refining or vacuum sublimation as indicated in the table. The crude PAHs were sealed in a glass tube under a partial pressure of helium and melted before being zone refined. A minimum of five passes on a ten-stage zone refiner were used to purify the PAHs. The zone refined tubes were scratched with a file and broken in thirds. The top and bottom thirds of the tube were discarded and the middle third was retained. The PAHs were chipped and scraped from the glass tube when needed for solutions. To vacuum sublime coronene and benzo-ghi-perylene, the two compounds were sealed individually in a vacuum under a water-cooled glass probe. A mineral oil bath was used to sublime the PAHs which subsequently condensed on the glass probe. The glass probe was removed from the vacuum and the PAH was scraped from the surface and stored for later use. Vacuum sublimation was used because too little starting material was available for zone refining. Only naphthalene and fluorene were used as received.

On the basis of their XEOL spectra, seven of the PAHs were used as model compounds for the time resolution experiments. Triphenylene, coronene, chrysene, phenanthrene, fluoranthene, naphthalene and fluorene exhibited phosphorescent emission. Perylene and 3,4-benzopyrene were used as model compounds for the single component fluorescent experiments.

Table 3. Polynuclear Aromatic Hydrocarbons

Compound	Purity
Naphthalene	As received
Anthracene	Zone refined
Phenanthrene	Zone refined
1,2-Benzanthracene	Zone refined
Pyrene	Zone refined
Chrysene	Zone refined
Triphenylene	Zone refined
1,2,5,6-Dibenzanthracene	Zone refined
3,4-Benzopyrene	Zone refined
Perylene	Zone refined
Benzo-ghi-perylene	Vacuum sublimed
Coronene	Vacuum sublimed
Fluorene	As received
Fluoranthene	Zone refined

Three n-alkane solvents were used, n-hexane, n-heptane and n-octane. The solvents were distilled and passed through a cation exchange resin in the silver form to remove the last traces of aromatic impurities. A weak bond is formed between the silver cation and the pi bond of the aromatic system. If the price of the solvents should become prohibitive the purification procedure can be used to recycle the n-alkane solvents. Gas chromatographic analysis of the purified solvents revealed the only contaminants were trace amounts of isomeric aliphatic hydrocarbons.

Stock solutions of the PAHs were prepared in volumetric flasks from weighed quantities of purified PAHs. Concentrations ranged from 0.01 M to 0.0001 M. Solubility limited the maximum concentration for several PAHs. PAHs which dissolved slowly were equilibrated overnight or vigorously stirred by an ultrasonic cleaner. Concentrated stock solutions were prepared to minimize adsorption and decomposition effects commonly observed with very dilute solutions. All stock solutions were stored in the dark to avoid photodecomposition. Dilute solutions were prepared as needed on a day-to-day basis from the stock solutions. No successive dilutions were performed to minimize pipetting errors.

Time Resolved Spectroscopy

The principles of time resolved spectroscopy are based on the radiative lifetimes of excited molecules. The functional form of the time dependence of single component luminescence is given in equation 5:

$$I(t) = I(0)\exp(-kt) \qquad (5)$$

I(t) is the emitted intensity as a function of time, I(0) is the initial intensity at the termination of the excitation pulse, k is the decay constant of the excited species and t is the time. If many species are emitting simultaneously the time dependent intensity is expressed by equation 6:

$$I(t) = \sum_i I(0)_i \exp(-k_i t) \qquad (6)$$

The total intensity is the sum of the intensities of all the emitting species.

The time resolution experiment is divided into two phases. First, decay curves are obtained from the individual luminescent species and decay constants are determined by substitution of the data into equation 5. Second, decay curves from mixtures of luminescent species are collected. The decay constants, determined from single component decay curves, are substituted into equation 6 and the initial intensity of each component is calculated. Finally, the initial intensities are related to the concentration of the luminescent species in the sample.

To prepare either phase of the time resolution experiment the steps listed in Table 4 are performed. After the preparations are completed, the experiment is initiated by operator interaction with the minicomputer. The step by step operation of the minicomputer is described in Table 5.

After the experiment is completed and the paper tape data set is transferred to disc, WYLBUR is used to prepare a job which processes the data. If a decay constant is sought certain conventions are followed. A preliminary job is

Table 4. Stepwise Preparation of Pulsed XEOL System

1. Inject the sample into the holder and seal the holder with indium gaskets and number two screws (Approximately 1.0 ml. of sample is needed to fill the holder).
2. Attach the holder and radiation shield to the cryostat and insert the cyrostat into the vacuum shield.
3. Connect the vacuum line and pull a vacuum on the contents of the vacuum shield.
4. Start the refrigerator and wait for the sample to cool.
5. Turn on the medical x-ray unit and select the current and voltage for the x-ray pulse (typically 60 kV., 100 mA.).
6. Make certain the slits are opened (typically 1000 micrometers), the monochromator is tuned to zero order and the photomultiplier tube is on (typically 1200 volts).
7. Turn on the computer power key and the teletype.

created which generates a plot of the decay curve. An estimate of the half life is made from the decay curve by measuring the time the intensity drops to one half the initial value. The decay constant is equal to 0.693 divided by the half life. A second job is generated which contains SMASH. The estimate of the decay constant is input into SMASH as a negative number. The negative estimate signals SMASH to perform a direct search for the decay constant. The initial estimate is used to calculate a maximum value for the quality of fit. A search vector is followed and the value for the quality of fit is minimized as the search vector proceeds to the final value of the decay constant. At the completion of the calculation output is generated which lists the initial data and the calculated fit with the estimated decay constant and with the final decay constant.

Table 5. Minicomputer Operation

1. Load the assembly language program into memory if the program is not already present in memory (Consult the operations manual).

2. Depress all address switches and press the extended address load switch.

3. Load 200 octal into the address switches and press the address load switch.

4. Place the halt switch in the up position, press the clear switch and the continue switch (The telepype should print a message).

5. Enter the date and time as requested and answer subsequent questions. Typical answers are; Number of waves = 480, Number of passes = 10, Transient decay = 800, Number of data points = 100, Range code = 3. After the last question is answered the experiment will start automatically.

6. Turn the punch on and wait for the next question to be printed by the teletype.

7. After the experiment is completed depress the halt switch and tear the paper tape data set off the punch.

8. Roll the paper tape and submit it at the Iowa State University Computation Center for transfer to disc.

A complex decay curve can be time resolved with SMASH if different conventions are used. The same WYLBUR execute file is used to prepare the job. A decay constant, which has been determined from single component data, is entered for each species which contributed to the decay curve. All decay constants are entered as positive numbers. The positive decay constants signal SMASH to perform a linear least squares procedure to calculate the initial intensities of the various components. The quality of fit is calculated and if the value does not fall between specific limits, error messages are generated. The error messages indicate whether too many or too few decay constants were entered. The output contains the initial data and the calculated data. The initial intensities are listed with the corresponding decay constants.

The output produced by the job is retrieved from the ccmputation center and the calculated results are extracted from the printed matter and tabulated. If analytical results are sought the calculated results are normalized for amplifier gain and integrator input resistance. The normalization factors are listed in Table 6. After the results are normalized, calibration curves are plotted or unknown concentrations of PAH's are calculated.

Fluorescence Measurements

If fluorescent emission is measured the capacitor in the gated integrator is reduced by a factor of 60. Greater integrator sensitivity is needed because the integration

Table 6. Normalization Factors

Amplifier Gain	Input Resistor	Normalization Factor
1×10^8	50K ohms	1
	100K ohms	2
1×10^7	25K ohms	5
	50K ohms	10
	100K ohms	20
1×10^6	25K ohms	50
	50K ohms	100
	100K ohms	200

period is shortened to 1/120th of a second when single waves are integrated. After the integrator is modified the pulsed XEOL system is prepared as described in Table 4. The x-ray supply is adjusted to 90 kV. and 300 mA. because a shorter pulse is used for the fluorescence experiment and the x-ray tube can dissipate the heat. The experiment is initiated as described in Table 5 but different input is used. The fast mode is specified for the assembly language program and only the number of waves in the pulse and the number of passes are entered. Typically 40 waves and 20 passes are selected. The experiment begins after the last question is answered.

Even though computerized data analysis techniques exist for the fast mode, the techniques were not used. The data collected from fluorescent emission were analyzed with a programable calculator. If analytical results are desired the calculated results are normalized with the factors given in

Table 6. A mean and standard deviation were calculated from the signal averaged data obtained for each wave in the pulse. However, the data obtained from the first twenty waves were discarded because the x-ray flux produced by the x-ray tube is not stable immediately after the x-ray tube is turned on. The mean is used to profile emission bands, generate calibration curves and calculate unknown PAH concentrations.

CHAPTER 5: RESULTS AND DISCUSSION

Decay Constant Values

The first step in the time resolution experiment was the determination of decay constants of the phosphorescent PAHs. These constants were determined from the stock solutions prepared from purified PAH materials. Because the pulsed XEOL system was untested, a reproducibility study of the determination of several decay constants was performed. The five day stability of the system was measured for triphenylene, coronene, chrysene, phenanthrene and fluoranthene, and a mean was calculated from five values obtained on different days. The decay constants obtained on five different days for seven PAHs are listed in Table 7. Two of the values in the table were excluded from statistical calculations by the Dixon criterion. The excluded values resulted from an error in the search routine used by SMASH, because noise in the measurement system can cause a large spread in the data points which describe a decay curve, with the greatest spread late in the decay scheme, and a false minimum in the quality of fit can be sought by the search vector. The frequency of occurrence of the error in the search routine was governed by the signal-to-noise ratio of the data. The mean and percent relative standard deviation of each decay constant are summarized in Table 8.

Table 7. Five Day Determination of Decay Constants[1]

Compound	Day 1	Day 2	Day 3	Day 4	Day 5
Triphenylene	0.0696	0.0687	0.0688	0.0699	0.0689
Coronene	0.1160	0.1157	0.1165	0.1155	0.1169
Fluorene	0.1704	0.1690	0.1707	0.1704	0.1703
Phenanthrene	0.2775	0.2781	0.2460[2]	0.2736	0.2746
Naphthalene	0.3388	0.3483	0.3550	0.3385	0.2878[2]
Chrysene	0.3831	0.3809	0.3817	0.3849	0.3806
Fluoranthene	1.1231	1.1425	1.2067	1.0931	1.0222

[1]All quantities reported in sec^{-1}
[2]Values excluded by Dixon Criterion

Table 8. Decay Constant Statistics[1]

Compound	Mean Decay Constant	% RSD
Triphenylene	0.0692	0.77
Coronene	0.1161	0.50
Fluorene	0.1702	0.39
Phenanthrene	0.2760	0.79
Naphthalene	0.3452	2.3
Chrysene	0.3822	0.46
Fluoranthene	1.1175	6.0

[1]All quantities reported in sec^{-1}

If the decay constants are not independent of concentration, analytical applications of time resolved spectroscopy would be impossible. The concentration independent behavior of the decay constants had to be verified. Triphenylene, coronene, phenanthrene, chrysene and fluoranthene were selected for these verifications. The results are presented in Table 9. With the exception of the lowest concentration values for phenanthrene, chrysene and fluoranthene, the decay constants reported in Table 9 agreed with the values tabulated in Table 8. Therefore, the independent behavior of the decay constants with concentration was verified. The three values at the lowest concentration were severely distorted by a background luminescence. When the concentration dependence study was performed the background interference was not understood and no correction was made. The source and nature of the background luminescence will be discussed in the next section.

Table 9. Concentration Dependence of Decay Constants[1]

Compound	1 X 10^{-3}M	1 X 10^{-4}M	1 X 10^{-5}M	1 X 10^{-6}M
Triphenylene	0.0700	0.0705	0.0708	0.0715
Coronene	------	0.1171	0.1180	0.1182
Phenanthrene	0.2791	0.2770	0.2820	0.3037
Chrysene	0.3851	0.3879	0.3805	0.4950
Fluoranthene	1.2374	1.1924	0.9067	------

[1]All quantities reported in sec^{-1}

A comparison of the decay constants observed in this study with literature values is shown in Table 10. Examination of the tabulated values indicates XEOL-TRS and conventional methods give comparable results. The agreement between decay constants obtained from optical excitation and x-ray excitation helps to unravel the XEOL excitation mechanism. Normally, the decay constants of phosphorescent species in a highly ionized environment are significantly different from the decay constants of phosphorescenct species in a neutral environment. Thus, x-ray excitation as compared to optical excitation does not affect the environment of the excited species appreciably even though ionized intermediates are produced by x-ray interaction with matter. Finally, the results obtained from decay curves of individual PAHs are summarized as decay constants, lifetimes and half lives in Table 11. The decay constant and the lifetime are reciprocally related and the half life is 0.693 divided by the decay constant.

Mixture Analysis by Time Resolution

One advantage of time resolved spectroscopy was demonstrated by some early results obtained from simple two component systems. As a first example of the usefulness of time resolved spectroscopy, a mixture of triphenylene and phenanthrene was studied. On the right hand side of Figure 12 the DC spectra of triphenylene and phenanthrene are presented with the background trace and the DC spectrum of a mixture of the two compounds. The double lines which extend from the top spectrum to the bottom spectrum indicate the region of the

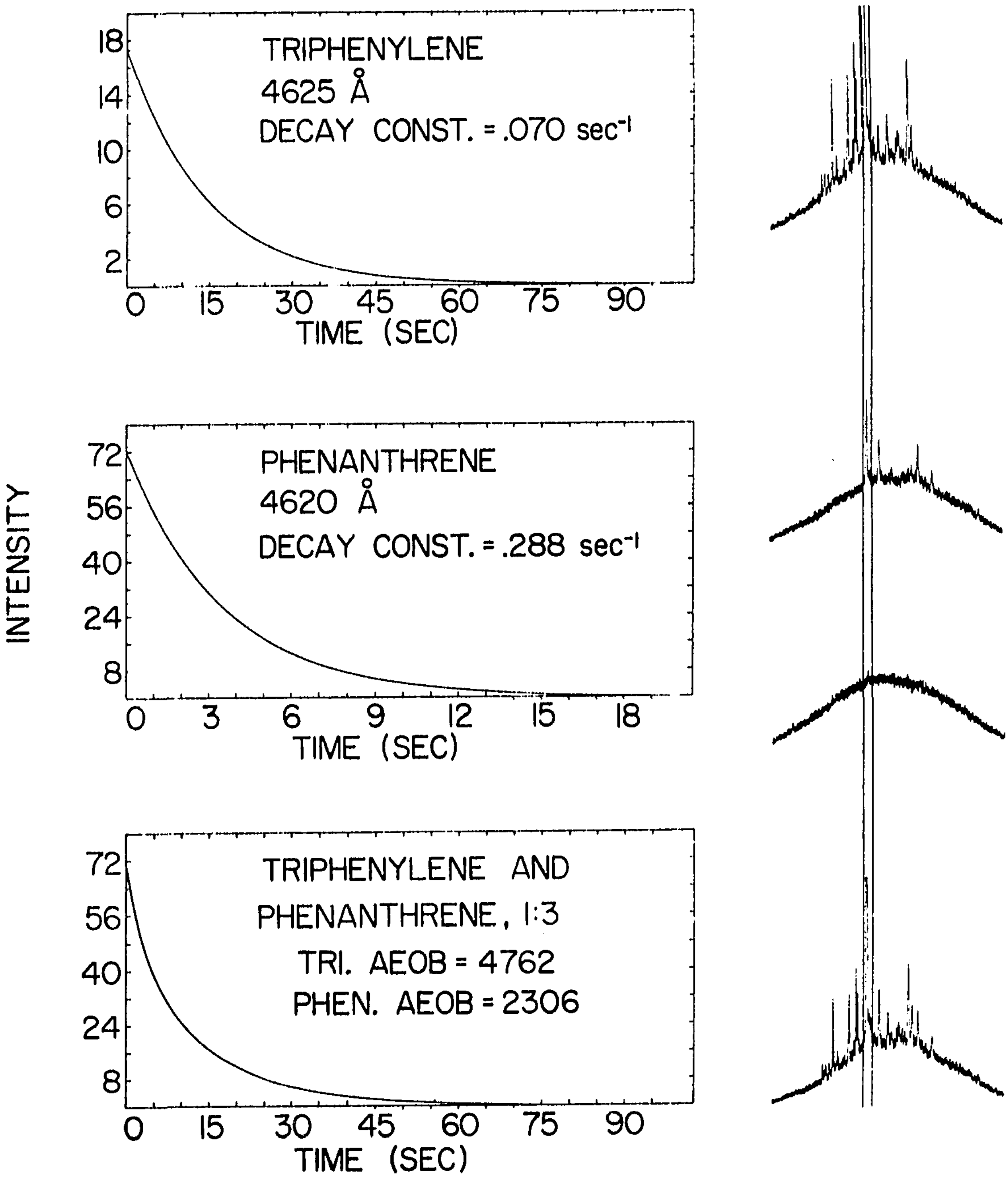

Figure 12. Time resolution of the phosphorescence emission from a mixture of triphenylene and phenanthrene in n-heptane by use of the pulsed XEOL technique.

Table 10. Comparison of XEOL and Published Decay Constants[1]

Compound	XEOL-TRS	Birks (26)	McClure (54)
Triphenylene	0.069	0.062	0.062
Coronene	0.12	0.11	0.11
Fluorene	0.17	0.20	0.20
Phenanthrene	0.28	0.29	0.30
Naphthalene	0.34	0.42	0.38
Chrysene	0.38	0.38	0.40
Fluoranthene	1.12	1.18	----

[1]All quantities reported in sec^{-1}

Table 11. Decay Constants, Lifetimes and Half Lives of PAHs

Compound	Decay Constant	Lifetime	Half Life
Triphenylene	0.069 sec^{-1}	14.5 sec	10.0 sec
Coronene	0.116 sec^{-1}	8.6 sec	6.0 sec
Fluorene	0.170 sec^{-1}	5.9 sec	4.1 sec
Phenanthrene	0.276 sec^{-1}	3.6 sec	2.5 sec
Naphthalene	0.345 sec^{-1}	2.9 sec	2.0 sec
Chrysene	0.382 sec^{-1}	2.6 sec	1.8 sec
Fluoranthene	1.118 sec^{-1}	0.89 sec	0.62 sec

spectra isolated by the monochromator. An obvious spectral interference is observed. On the left hand side of Figure 12 the decay curves for the individual compounds and the mixture are drawn. The decay constants used to time resolve the spectral interference are given on the top two plots and the initial intensities are summarized on the bottom plot. The nonzero initial intensities prove the spectral interference can be resolved temporally. A second example is presented in Figure 13 for the mixture of triphenylene and chrysene.

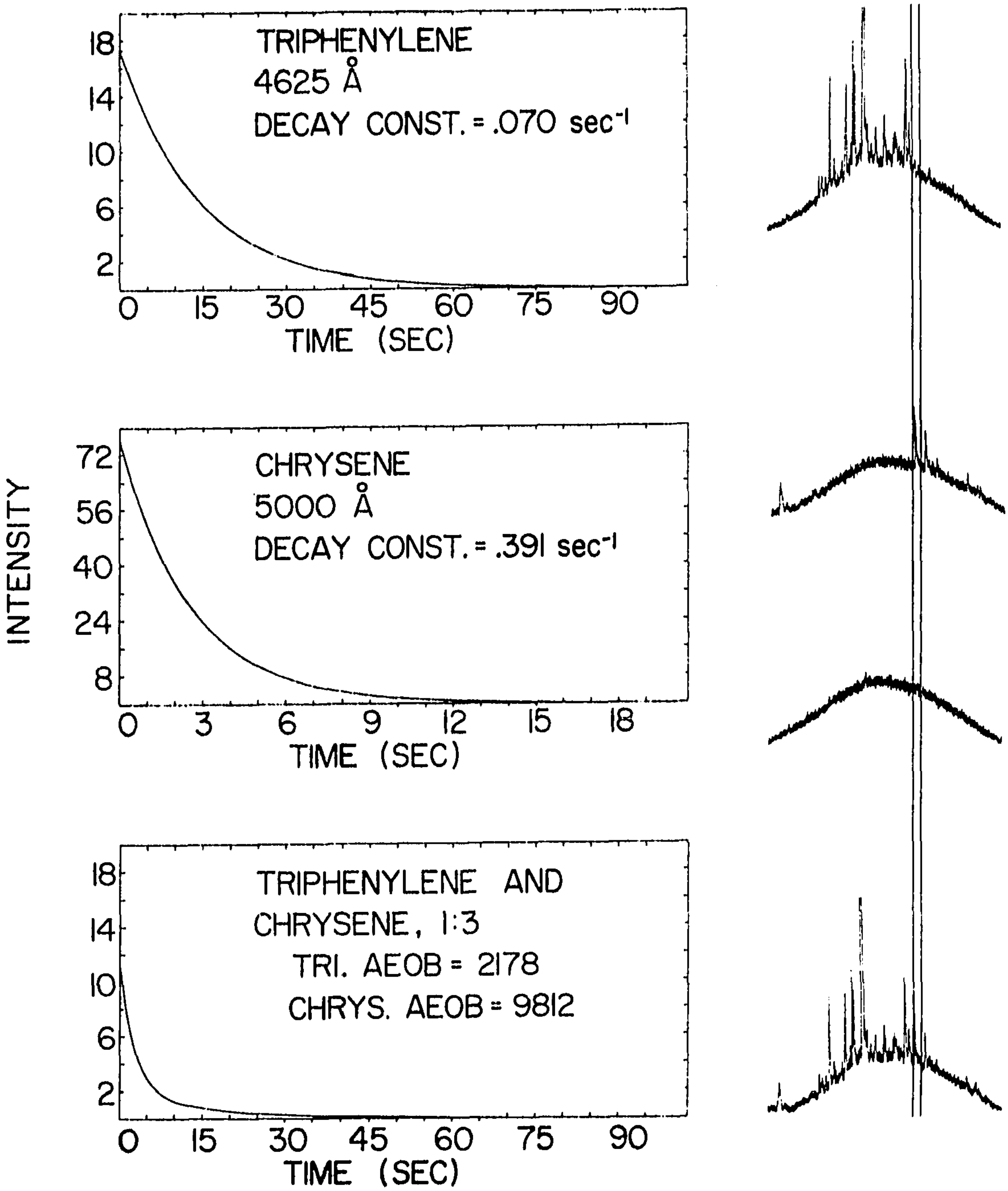

Figure 13. Time resolution of the phosphorescence emission from a mixture of triphenylene and chrysene in n-heptane by use of the pulsed XEOL technique.

To determine the problems encountered in the time resolution of more complex mixtures with the pulsed XEOL system, a five component system which contained triphenylene, coronene, chrysene, phenanthrene and fluoranthene was examined. The five PAHs were selected because their decay constants cover a large range of values with no overlap.

Even though the five components in the mixture share no common emission band and spectral interferences are not severe, a second advantage of time resolved spectroscopy was demonstrated when the five component mixture was time resolved. The individual lines in the emission bands of the PAHs were weak and analytical determinations based on emission of single lines lacked sensitivity. To demonstrate the improved sensitivity of PAH determination by time resolved spectroscopy the monochromator was tuned to zero order and the slits were opened to 1 millimeter. In this way all the light emitted by the sample proceeded through the monochromator unresolved. If the monochromator had not been an integral part of the pulsed XEOL system, only a lens and a mirror would have been used to transmit the optical signal to the photomultiplier tube. With the slits opened to 1 millimeter the optical throughput of the monochromator obviously increased and the sensitivity of the measurement improved. The amount of scattered radiation which reached the detector also increased as the slits were opened, but with time resolution only radiation which is characterized by a specific decay constant was detected. All other radiation produces a DC background which is removed by a simple subtraction.

Complex decay curves of several dilutions of the mixture were collected with the pulsed XEOL system. Each decay curve was time resolved and the results were normalized. Analytical calibration curves, both linear and logarithmic, for each component in the mixture were plotted and are drawn in Figures 14-18. Several unexpected features were observed for the logarithmic and linear plots of concentration versus intensity.

The first unexpected feature was the nonlinear behavior of the calibration curves. An approximate slope of one half was observed for the log plots, which indicated that the observed intensity was a function of the half power of concentration. Two explanations for the one half slope are possible. First, a half power rate expression could exist as an intermediate step in the kinetic scheme which describes the excitation mechanism. For example, a half power rate expression is observed for some free radical reactions (e.g. the formation of chlorine free radicals from molecular chlorine). Ionized species and free radicals are produced when x-rays interact with matter. The second possibility is based on the scattering of light within the translucent

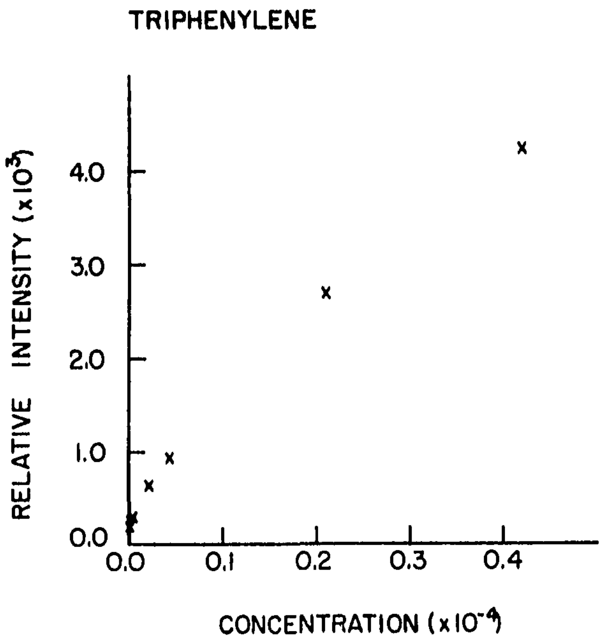

Figure 14a. Linear plot of intensity versus molar concentration for triphenylene.

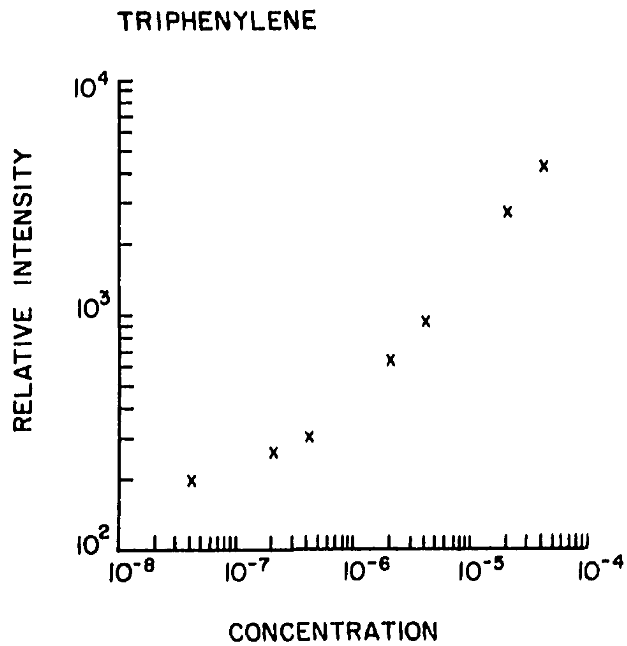

Figure 14b. Logarithmic plot of intensity versus molar concentration for triphenylene.

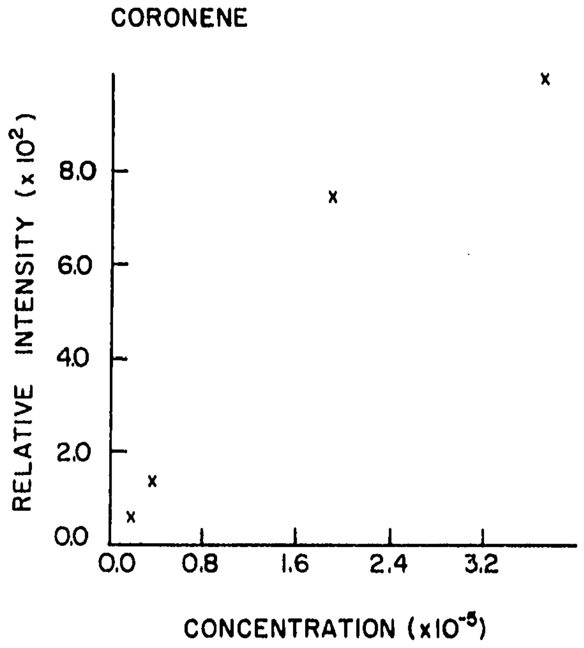

Figure 15a. Linear plot of intensity versus molar concentration for coronene.

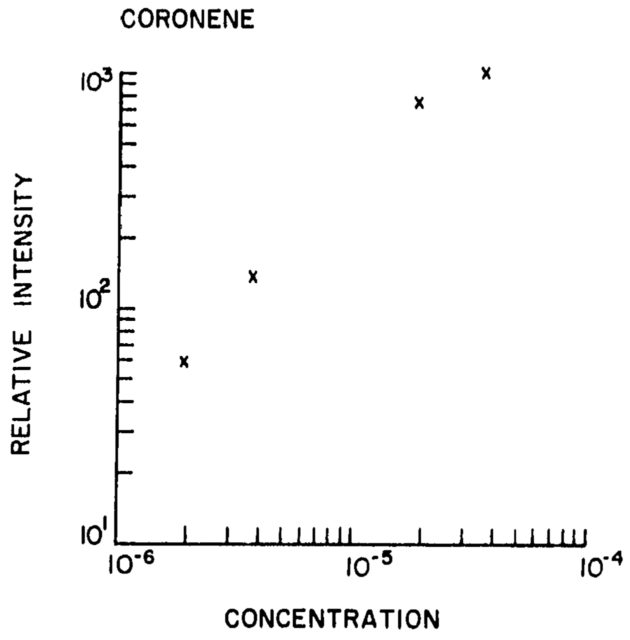

Figure 15b. Logarithmic plot of intensity versus molar concentration for coronene.

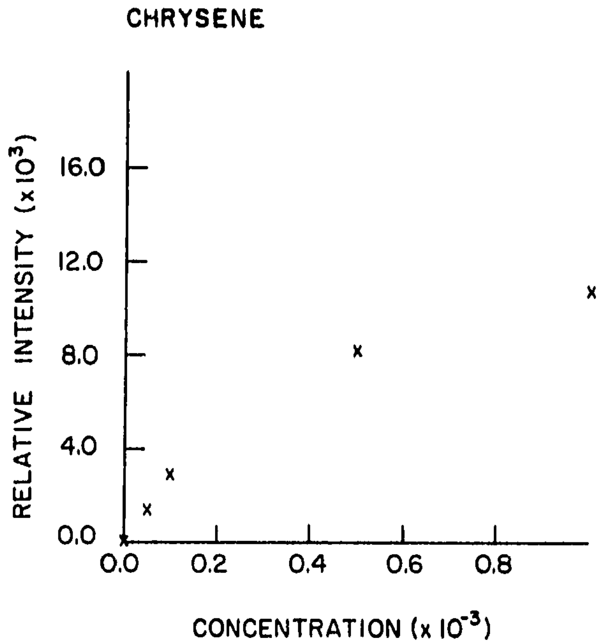

Figure 16a. Linear plot of intensity versus molar concentration for chrysene.

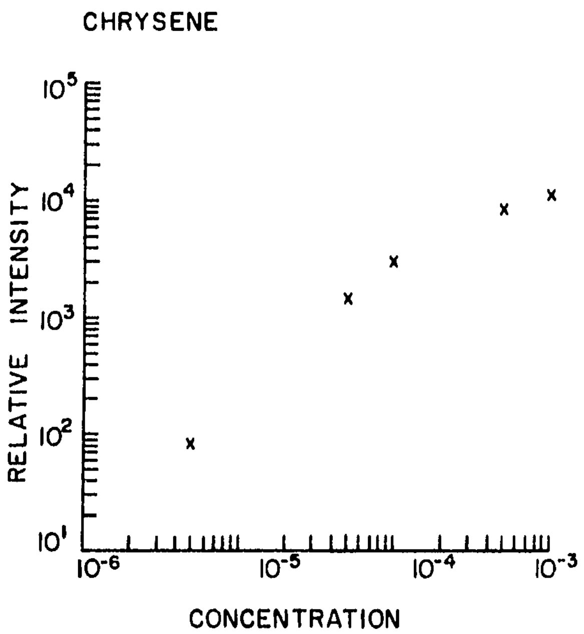

Figure 16b. Logarithmic plot of intensity versus molar concentration for chrysene.

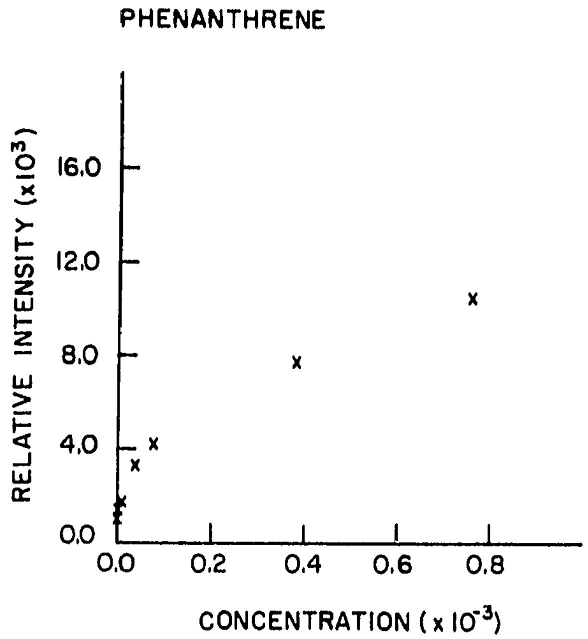

Figure 17a. Linear plot of intensity versus molar concentration for phenanthrene.

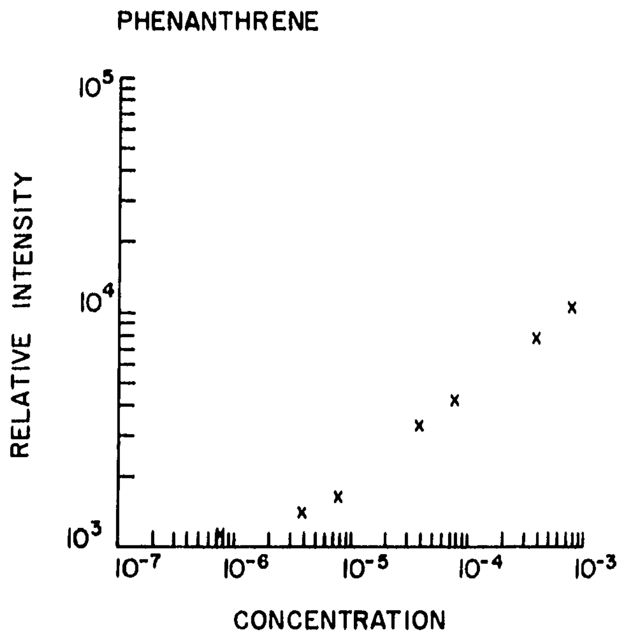

Figure 17b. Logarithmic plot of intensity versus molar concentration for phenanthrene.

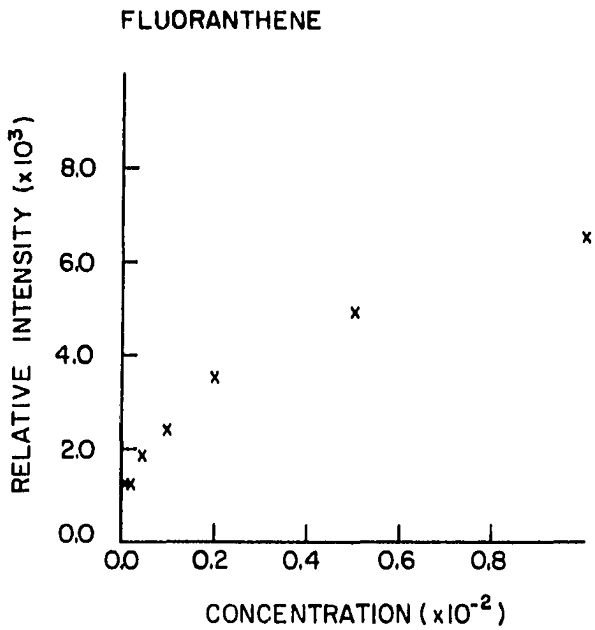

Figure 18a. Linear plot of intensity versus molar concentration for fluoranthene.

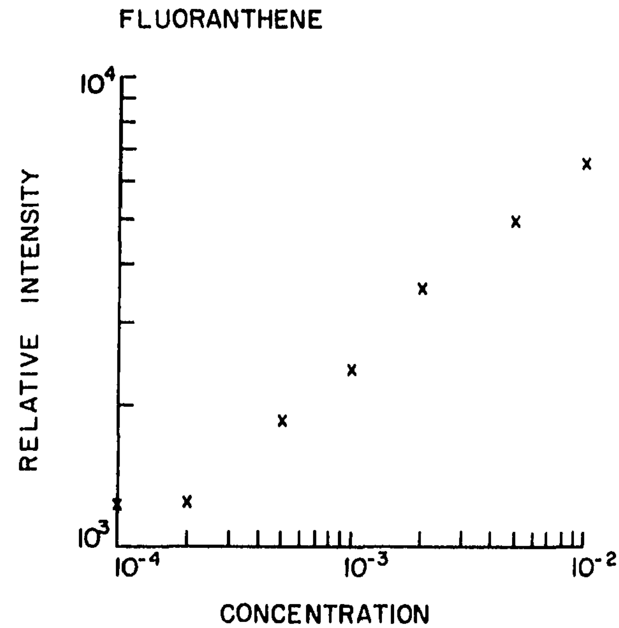

Figure 18b. Logarithmic plot of intensity versus molar concentration for fluoranthene.

sample. The emission of the sample originates from different depths within the sample and not just the sample surface. Formation of a microcrystalline snow when n-alkanes are frozen produced many reflective surfaces within the sample. Internal reflection and optical scattering reduced the probability of detection of a photon which originated in the interior of the sample as compared to a photon which originated on the surface of the sample. The relationship between concentration of luminescent species and the probability of detection of a photon emitted in the n-alkane snow as a function of distance from the surface of the sample must be considered. The functional behavior of the probability of detection as a function of distance from the surface of the sample could be responsible for the observed half power dependence of intensity on concentration. Escape depth considerations are common in many surface techniques and empirical functions have been used to make corrections for probabilities of escape for x-rays, photons and electrons (55). The answer to the question of which interpretation is correct, or if some other factors need to be considered could not be answered in the course of the present investigation.

The second unexpected feature was the flattening of the fluoranthene and triphenylene analytical calibration curves at low concentration. This flattening could be attributed to a background luminescence from the quartz window in the sample holder characterized by decay constants with values approximately equal to the decay constants for triphenylene and fluoranthene. The background luminescence of the quartz window at 10 K contains two slow components with decay constants 0.068 and 1.160 sec^{-1}. The second component was six times as intense as the first, hence a greater background effect was observed for fluoranthene as compared to triphenylene. The source of the background luminescence is defects and impurities in the quartz which become luminescent centers at low temperatures (56). Above 200 K no background luminescence is observed. Two possible solutions to this problem are considered in the next chapter.

Finally, the analytical calibration curves for coronene and chrysene flattened at high concentration. The observed behavior is not concentration quenching because singlet-triplet absorption is a forbidden process. The exact nature of the effect is not fully understood but energy transfer between luminescent species at high concentration and photochemical decomposition may be contributing to the observed behavior. Elucidation of photochemical processes in n-alkane systems induced by x-ray irradiation will be needed to understand the relationship between the observed intensity and high concentration of PAHs in the n-alkane snow.

To test the applicability of time resolved spectroscopy for analytical problems, three synthetic unknown PAH mixtures were prepared and analyzed. The analysis was performed in triplicate and the results are tabulated in Table 12. All the values in the table are reported in micrograms. The uncertainties range from a few percent to 20 percent relative. Values for coronene and chrysene are not reported for unknown No. 1 because the amount present was below the detection limit for that particular sample. The phenanthrene value for unknown No. 2 and the chrysene value for unknown No. 3 were low because of peculiarities in SMASH discussed earlier. Although the data in Table 12 are promising, additional development undoubtedly will be required before XEOL-TRS can make a major contribution to the determination of PAHs in complex mixtures.

Table 12. Analytical Data from XEOL-TRS Analysis[1] [2]

	Unknown No. 1		Unknown No. 2		Unknown No. 3	
Compound	Actual	Found	Actual	Found	Actual	Found
Triphenylene	0.57	0.64±0.05	2.0	1.9±0.2	5.7	5.7±0.9
Coronene	0.60	-----	3.0	3.0±0.3	6.0	5.4±2
Chrysene	5.7	-----	11	12±2	23	13±1
Phenanthrene	1.6	1.3±0.4	8.9	5.0±0.4	36	34±7
Fluoranthene	100	120±10	200	200±40	400	440±80

[1]All quantities reported in micrograms
[2]Analysis performed in triplicate

Single Component Analysis by Fluorescence

The pseudo-DC mode was used to measure fluorescent emission induced by the greater x-ray flux available from the medical x-ray supply. Wavelength profiles were obtained for 3,4-benzopyrene and perylene in the wavelength region around 427.5 nm. and 453.0 nm., respectively. Analytical calibration curves were plotted from normalized data obtained from the maxima of the wavelength profiles. The analytical calibration curves were used to analyze three synthetic unknowns. The third unknown contained both compounds whereas the other two unknowns contained only a single component. The analysis was performed in triplicate and the results are tabulated in Table 13. All values are reported in micrograms.

Table 13. Fluorescence Data from Pulsed XEOL Analysis[1 2]

Compound	Unknown No. 1 Actual	Unknown No. 1 Found	Unknown No. 2 Actual	Unknown No. 2 Found	Unknown No. 3 Actual	Unknown No. 3 Found
Perylene	2.5	1.6±0.8	---	-----	12.6	2.9±0.2
3,4-Benzopyrene	---	-----	2.3	2.2±0.6	3.2	2.5±2

[1]All quantities reported in micrograms
[2]Analysis performed in triplicate

The results are disappointing for the mixture and the uncertainties are unacceptable for all three unknowns. The large uncertainties are caused by the inability to reproducibly peak the monochromator on the maximum intensity wavelength of the emission band and the fluorescent background emitted by the sample holder. Location of the maximun intensity wavelength of the emission band was a long tedious process with the pseudo-DC excitation source as compared to the standard DC excitation source and an alternate approach was sought. Suggestions for the correction of these problems are discussed in the next chapter. The analysis of the mixture is further complicated by the suppression of 3,4-benzopyrene emission by perylene. Interferences of the type observed for unknown No. 3 are expected when fluorescence analysis is performed with PAHs because energy transfer processes play a major role in the excitation and deexcitation mechanisms of many PAH systems. After appropriate system improvements the XEOL technique could be applied to the fluorescent analysis of single component PAH systems. However, single component PAH analysis is not practical because PAHs occur in complex mixtures. Therefore, the use of internal reference compounds, prior isolation of PAHs by ring size and alkyl substitution or other innovative analytical approaches will be required before XEOL can be applied to the fluorescent analysis of PAHs.

Discussions and Conclusions

The results reported in this chapter demonstrate the feasibility of the XEOL-TRS technique for the analysis of simple mixtures of phosphorescent PAHs. The technique could obviously be applied to other organic phosphorescent systems. The present study is the first application of XEOL to organic systems and many basic principles were established. The use of low temperatures and unconventional geometries are two examples. Techniques for the determination of decay constants were developed. As the scope expands to other organic systems, Fourier techniques and phase resolution will be required to measure shorter decay constants. The examination of fluorescence produced with a high power x-ray pulse demonstrated the flexibility of the pulsed XEOL system to study fluorescence and phosphorescence. The combination of XEOL with conventional pulsed fluorescence techniques will expand the scope of the XEOL method. Finally, the temperature flexibility, supplied by the helium refrigerator employed in the pulsed XEOL system, makes possible the study of a wide range of solids, liquids and gases.

XEOL coupled with time resolved spectroscopy does not solve all the problems of PAH analysis. The technique in the present state of development does not compete with gas or liquid chromatography, GC-MS or conventional fluorescence techniques. The improvements discussed in the next chapter if implemented should improve the capabilities of the pulsed XEOL system. However, the true potential of the method as applied to PAH analysis will not be appreciated fully until a nanosecond width x-ray pulse is used for excitation. A synchrotron produces an intense x-ray pulse of nanosecond width which would eliminate the limitations imposed on the present study by the pulse characteristics. As time and space become available on national synchrotron facilities a proposal, based on the work presented here, should be prepared. The improved sensitivity and more general applicability of time resolved fluorescence as opposed to time resolved phosphorescence should be stressed. Interferences (e.g. the suppression of 3,4-benzopyrene emission by perylene) could be characterized by the pulsed XEOL system in the pseudo-DC mode prior to the synchrotron study. Even with ideal x-ray excitation sources and unlimited computational facilities the XEOL technique would not be the ultimate method for the analysis of PAH mixtures. The PAH problem is complex and many analytical techniques will be required to characterize natural and man made mixtures of PAHs.

CHAPTER 6: MISCELLANEOUS OBSERVATIONS AND FUTURE WORK

The work reported earlier (13,45), combined with the results presented in this dissertation, is the first application of XEOL to an organic system. Furthermore, the use of a pulsed x-ray excitation source is a novel approach to XEOL. These two facts suggest the scope of application for XEOL coupled with conventional luminescent methods is very broad and requires additional investigation.

Before new applications of XEOL are considered, modifications of the pulsed XEOL system are described in the following section. Implementation of the modifications would eliminate many of the problems encountered in the PAH study. In the next section the effects of solvent composition are discussed and suggestions are presented for the enhancement of the sensitivity of the PAH analysis by XEOL. Finally, XEOL results obtained from novel systems are presented in the last section and new applications of XEOL to analytical problems are indicated.

Pulsed XEOL System Modifications

The major problem encountered in the analysis of PAHs with the pulsed XEOL system was the background luminescence emitted by the quartz window in the sample holder. To correct the problem, the quartz window can be replaced by a window composed of a different material or removed completely.

Several window materials were tested to eliminate the background luminescence but no suitable substitute was found. Single crystal quartz was not available when the other materials were tested. A sample of single crystal quartz should be obtained and tested as a substitute window material.

An alternate approach to eliminate the background luminescence from the quartz window in the sample holder involved deposition of the sample on a cold beryllium disk from a flowing gas stream. A doughnut-shaped manifold with twelve directional ports was designed. At the present time deposition techniques are being developed. The major problems that need to be solved are improved vacuum control, measurement and control of sample deposition and efficient vaporization and transport methods for the PAH material. After the problems are solved, many interesting experiments are possible, in particular, x-ray generation of reactive species and photochemical reactions. The deposition of gaseous samples on a cold surface opens the realm of matrix isolation to study by the XEOL technique.

Another problem, encountered in the fluorescence study, was the inability to reproducibly position the monochromator at a specific wavelength. Mechanical play in the wavelength counter and large temperature variations in the laboratory contributed to the problem. To correct the difficulty software should be developed to calculate a polynomial fit from discrete data points which characterize the profile of the emission band. A numerical differentiation of the polynomial produces the derivative of the emission band shape. The wavelength of maximum intensity is equal to one of the roots of the polynomial expression which represents the derivative set equal to zero. The maximum intensity is calculated by substitution of the wavelength of maximum intensity into the original polynomial. These numerical methods eliminate the need to position the monochromator reproducibly because only the relative positions of the data points with respect to one another are required. The relative positions can be accurately determined by use of a computer-controlled stepper motor to position the monochromator at the discrete wavelengths in the profile of the emission band. The software and interface needed to operate a stepper motor by computer control were developed by D. Kalnicky (57) and are available in the laboratory. A stepper motor should be purchased and mounted on the monochromator and modifications of software for use of the stepper motor should be started.

In addition to the modifications described in the preceding paragraphs, optimization of the x-ray pulse characteristics is imperative. The trade offs between voltage, current, and pulse duration of the x-ray pulse should be studied. Figures 19-21 are plots of intensity versus current, voltage and pulse duration. A factor of two increase in current or pulse duration doubles the measured intensity but an approximate fifty percent increase in voltage produces an equivalent enhancement. Optimization of PAH analysis with respect to the three pulse parameters, within the limits determined by the energy the x-ray tube must dissipate as heat, should enhance the sensitivity and lower the detection limits of the XEOL technique.

Solvent Composition

The host matrix or solvent composition for an organic system, e.g. PAHs in n-alkane solvents, is an important factor in all XEOL experiments. The host matrix has to interact with the primary x-ray radiation and support energy transfer processes which excite the guest species. Very few host matrices exhibit XEOL emission from guest species. A better understanding of the excitation processes in those matrices which exhibit XEOL emission should be developed in the near future. The results of a study of the excitation mechanism for PAHs in n-alkanes in particular, will assist in the prediction of new organic systems which will exhibit XEOL emission. The importance of solvent composition for the PAH study is demonstrated by two probing experiments.

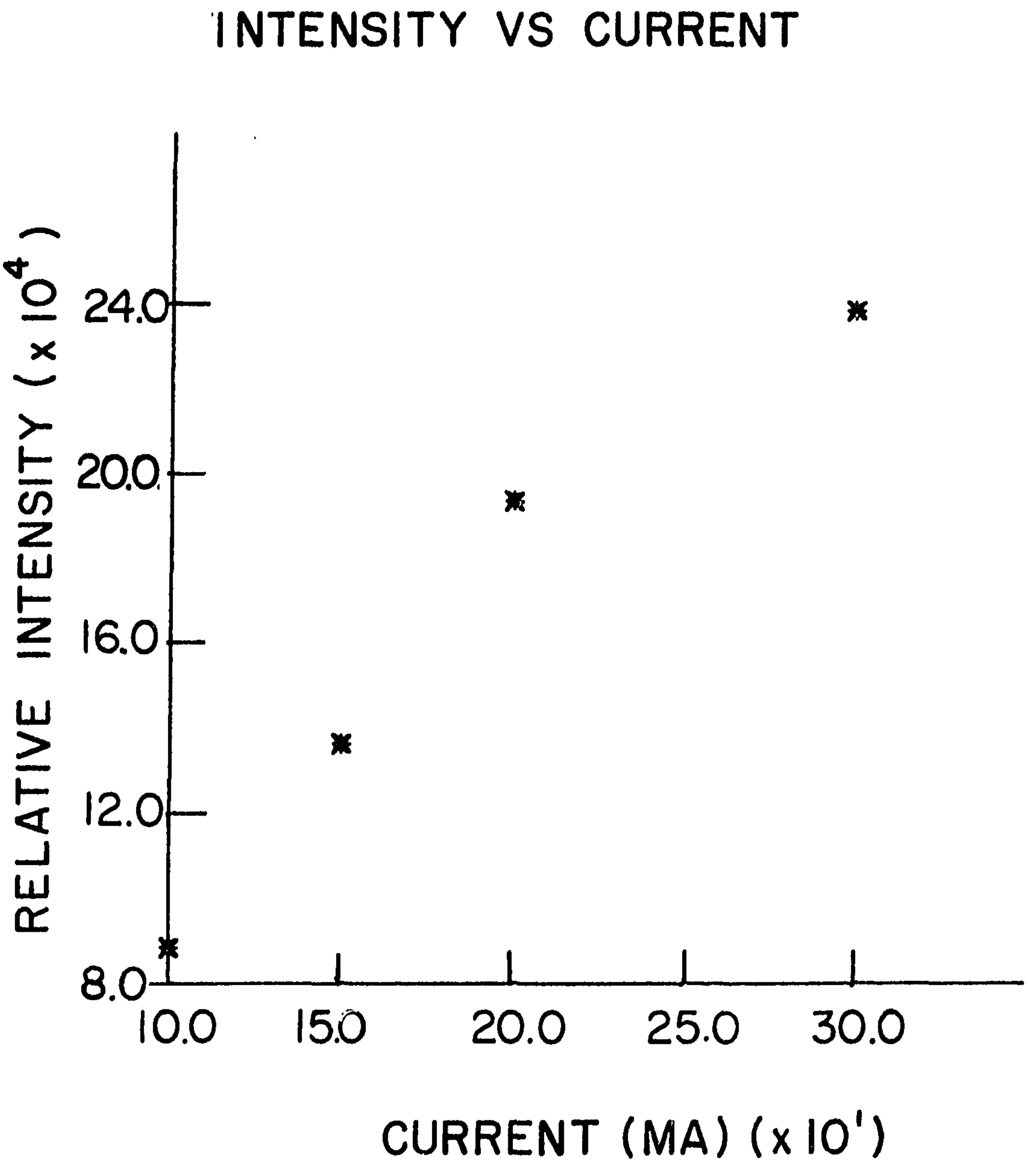

Figure 19. Measured intensity as a function of the current of the electron beam used to produce the x-ray pulse.

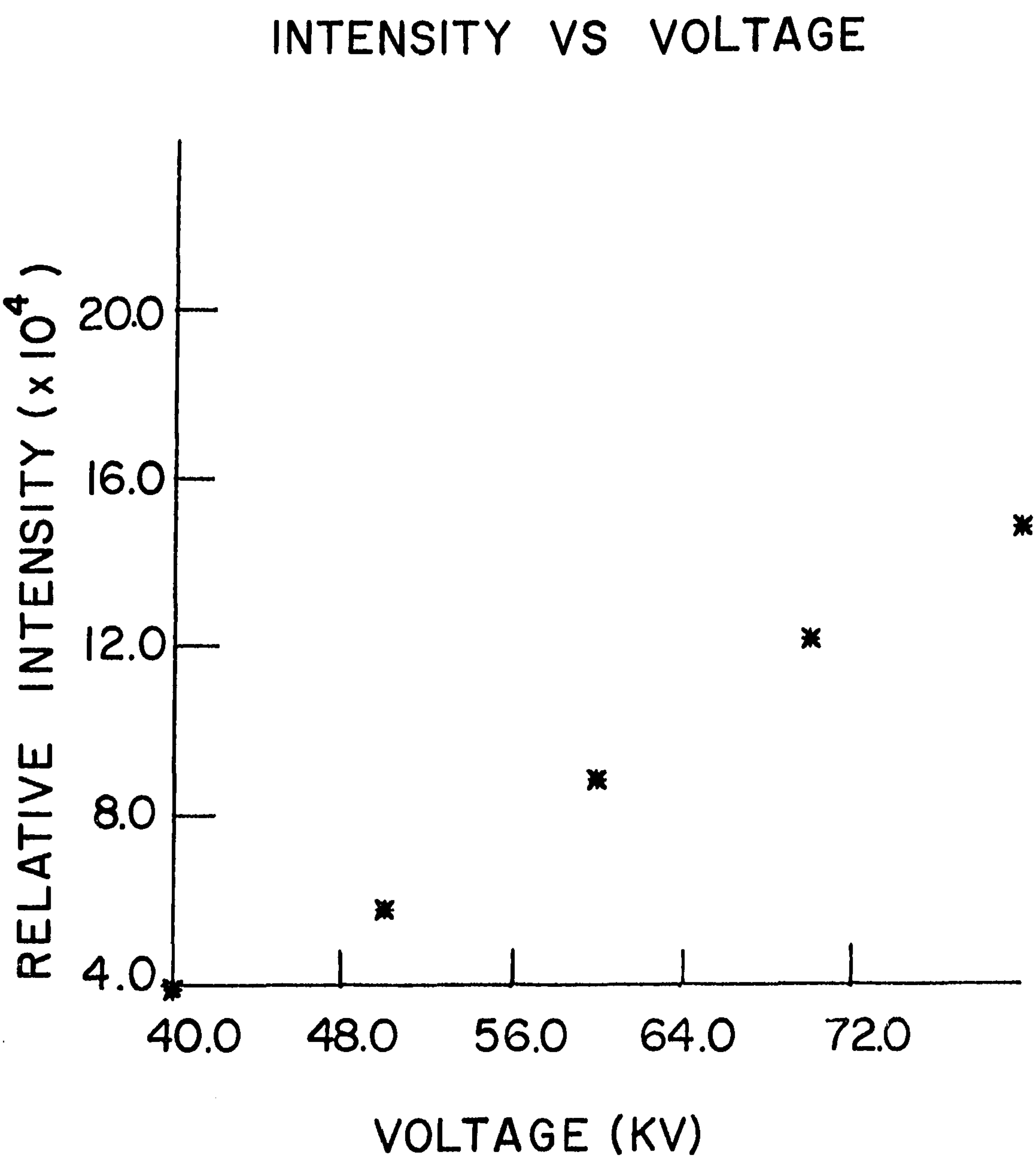

Figure 20. Measured intensity as a function of the acceleration voltage experienced by the electron beam used to produce the x-ray pulse.

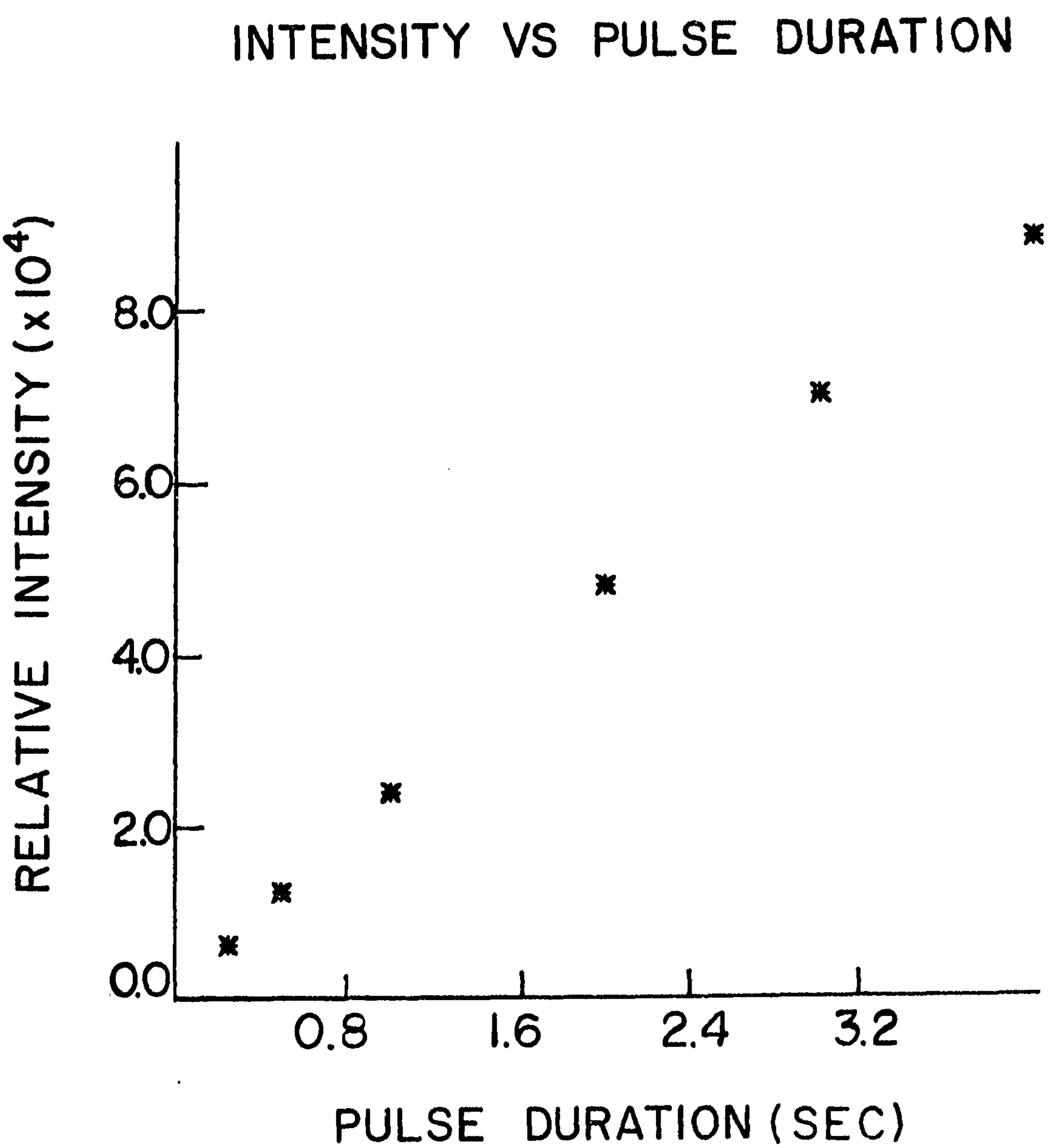

Figure 21. Measured intensity as a function of the duration of the x-ray pulse.

The first experiment examined the effect of n-alkane chain length on the structure of the XEOL spectrum. Anthracene and 3,4-benzopyrene were examined in n-hexane, n-heptane and n-octane. The three anthracene spectra are presented in Figures 22-24. The emission band for anthracene in n-hexane is broad and structureless whereas in n-heptane several sharp lines are observed and in n-octane a weak band is observed. A different effect is observed for 3,4-benzopyrene as shown in Figures 25-27. The structure of the emission sharpens and the intensity increases as the chain length increases. Similar solvent effects are observed for all the PAHs studied. These solvent effects and others previously observed for UV excitation of n-alkane-PAH systems (35,58-61) need to be investigated so that the analysis of PAHs by the XEOL technique can be optimized.

A second probing experiment on solvent composition involved the introduction of a heavy atom to the n-alkane-PAH system by addition of iodobutane or tetra-n-butyllead to the solvent. Addition of a heavy atom to the solvent induces the external heavy atom effect in PAH systems (62-64). The increase of the spin-orbit coupling of excited singlet and triplet states results in an increase in the rate of intersystem crossing between singlet and triplet states and thus enhanced phosphorescence emission. Analytical applications of the external heavy atom effect in UV excited,

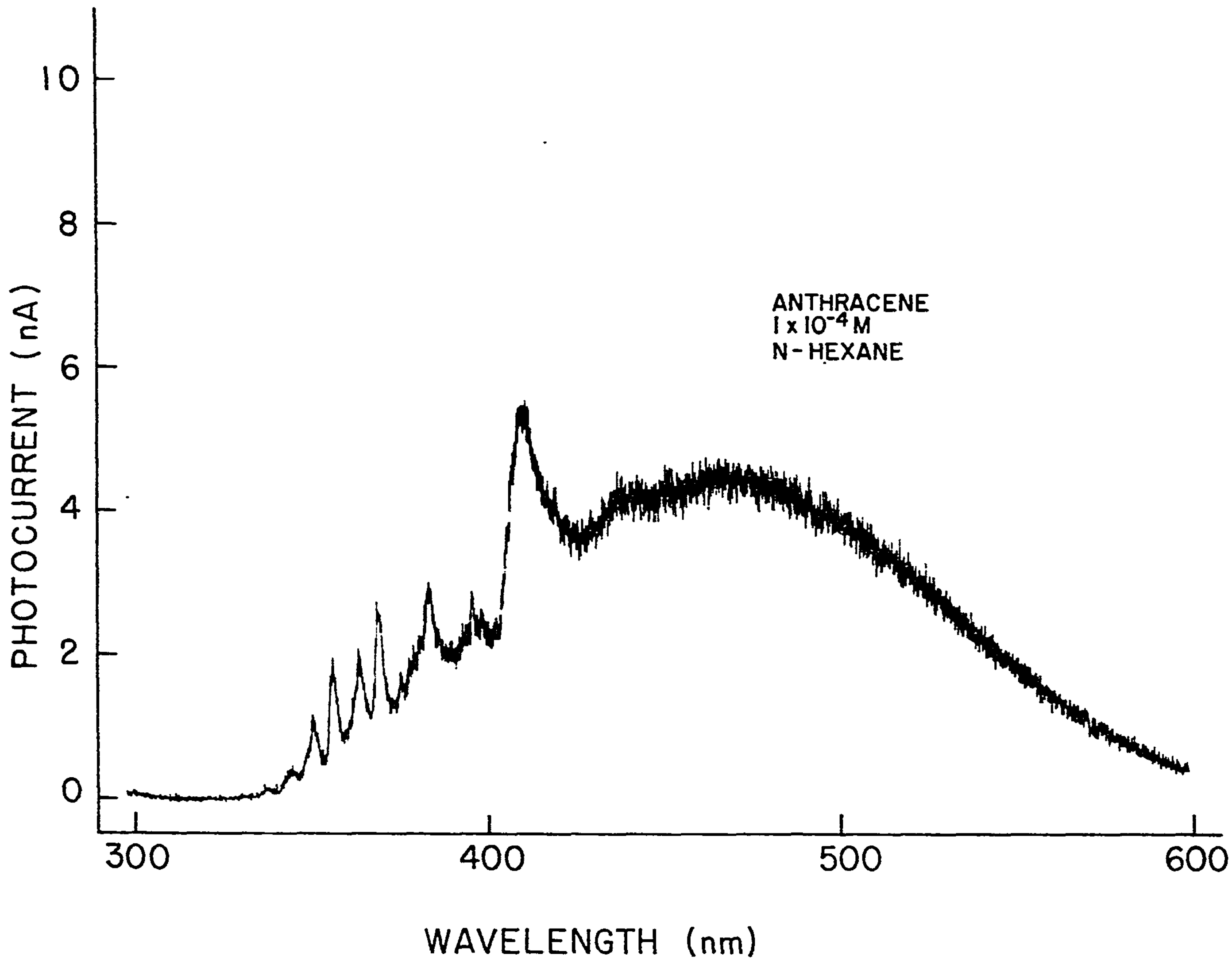

Figure 22. XECL spectrum of anthracene in n-hexane at a concentration of 1 X 10^{-4} M.

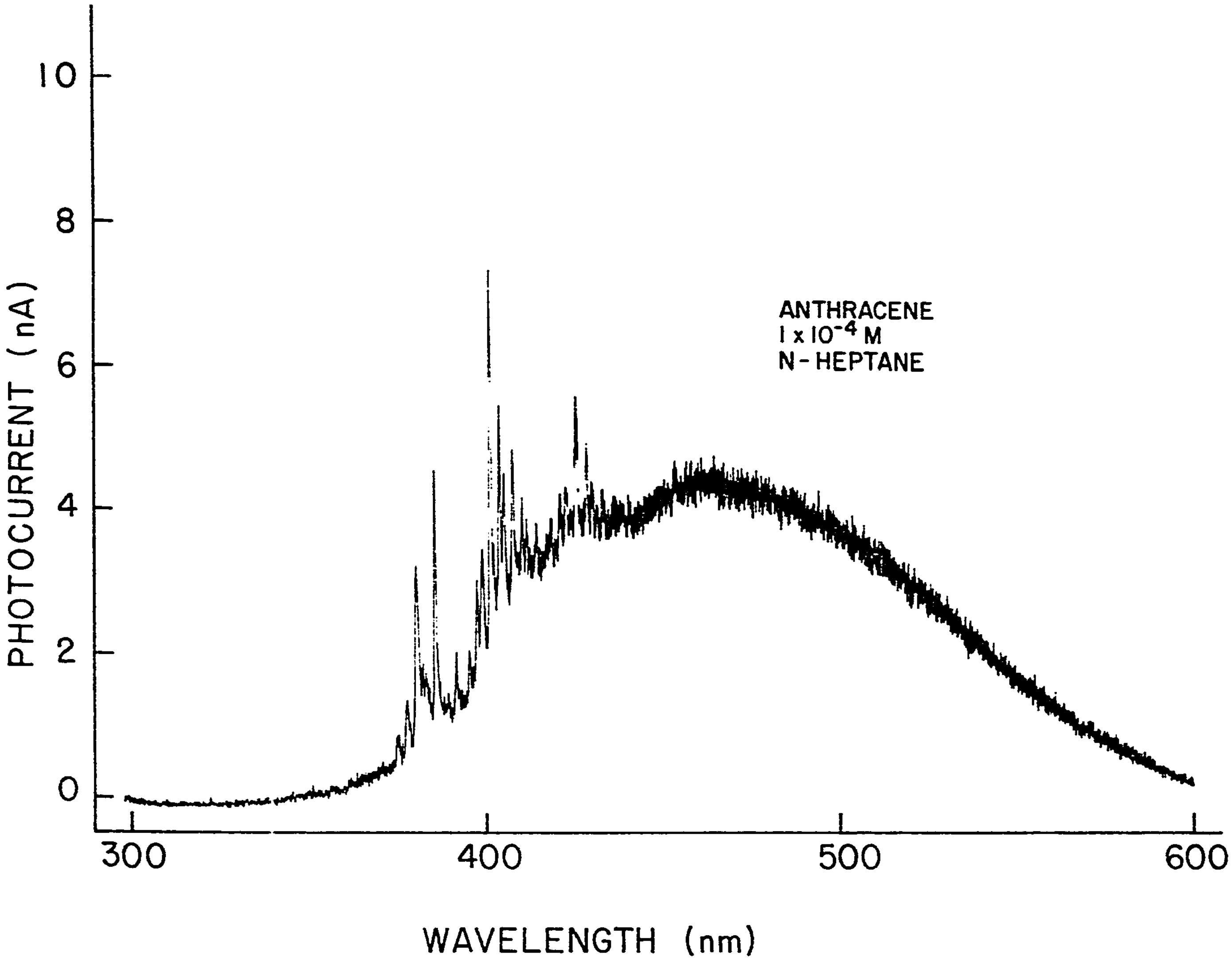

Figure 23. XECL spectrum of anthracene in n-heptane at a concentration of 1 X 10^{-4} M.

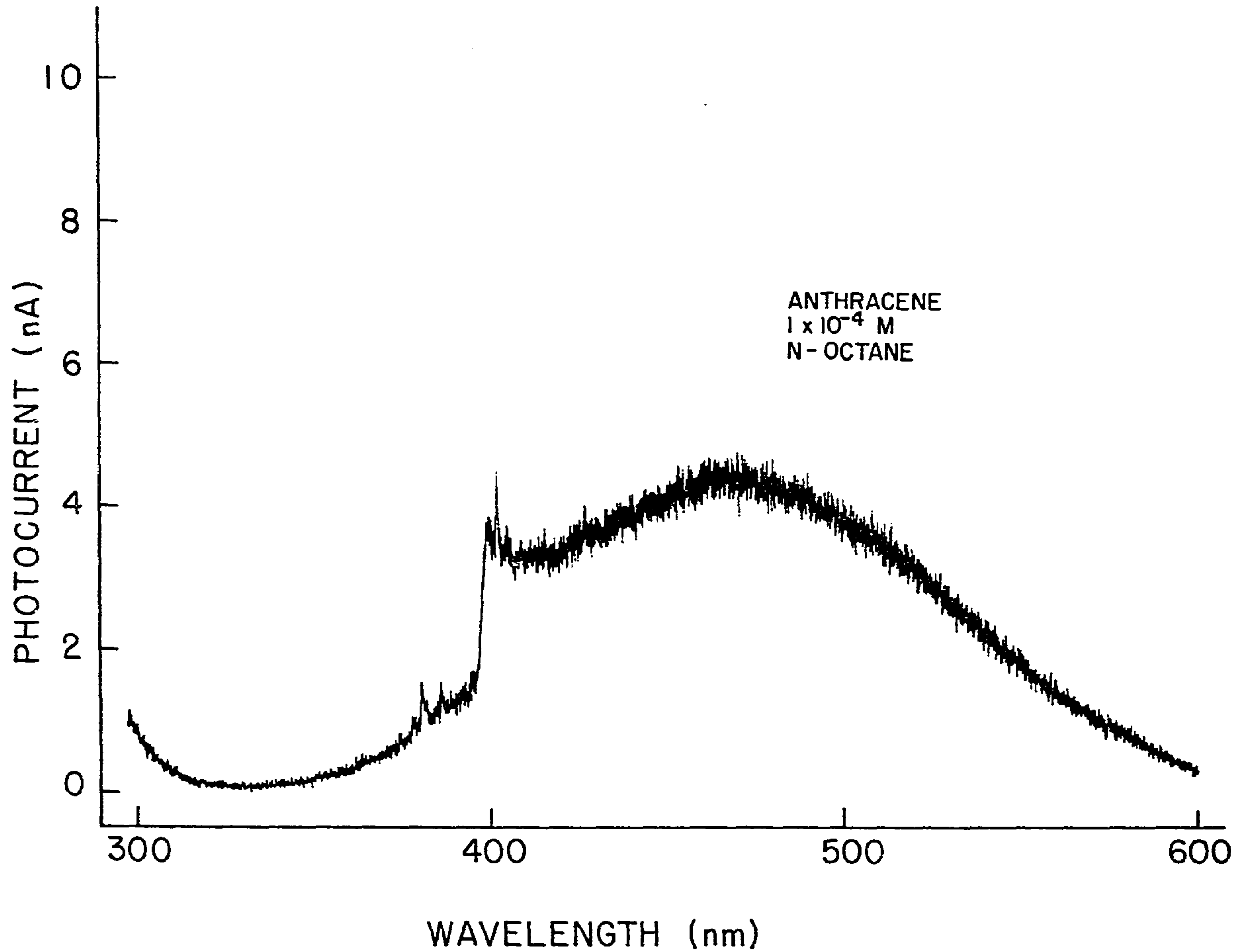

Figure 24. XECL spectrum of anthracene in n-octane at a concentration of 1 X 10^{-4} M.

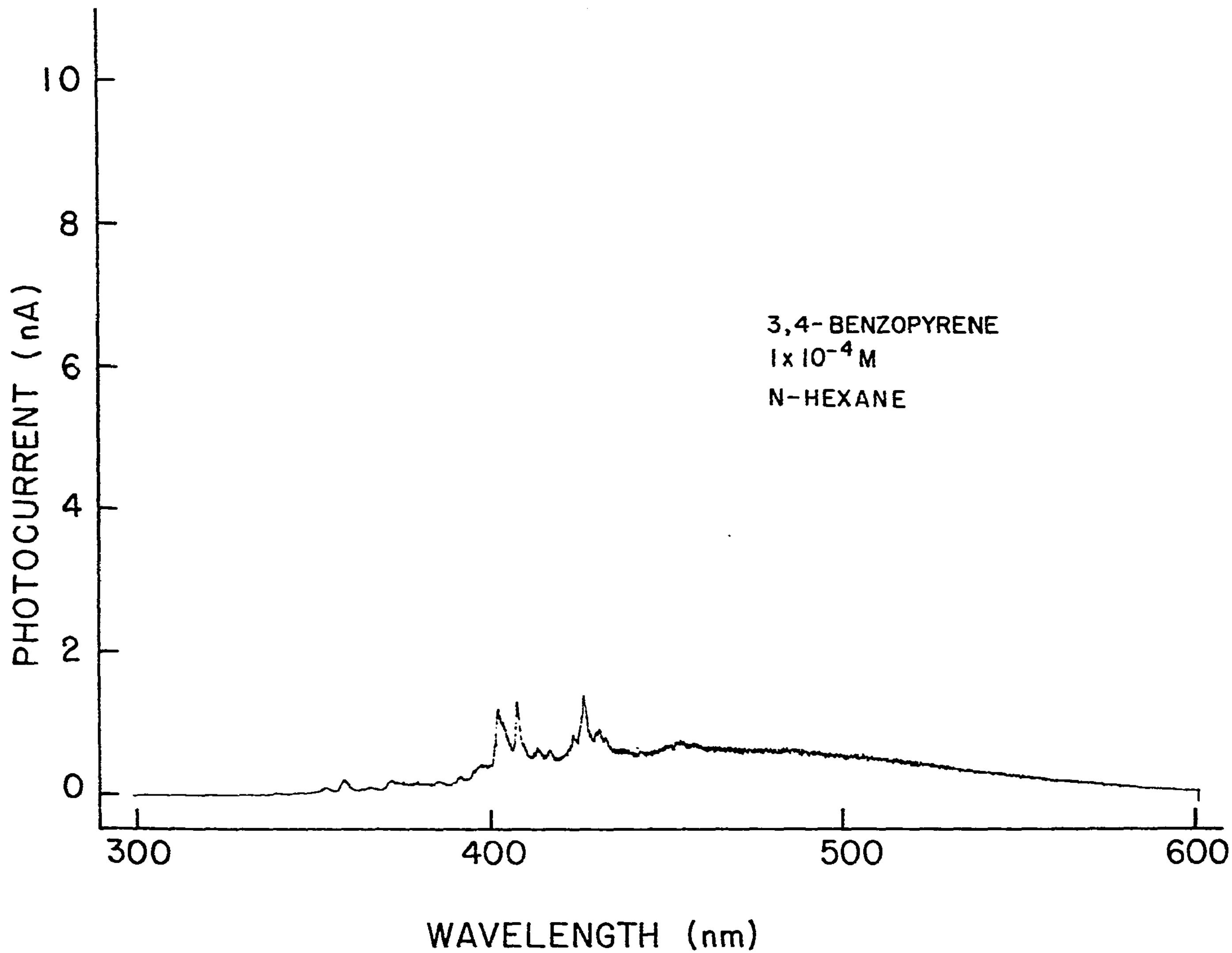

Figure 25. XECL spectrum of 3,4-benzopyrene in n-hexane at a concentration of 1 X 10^{-4} M.

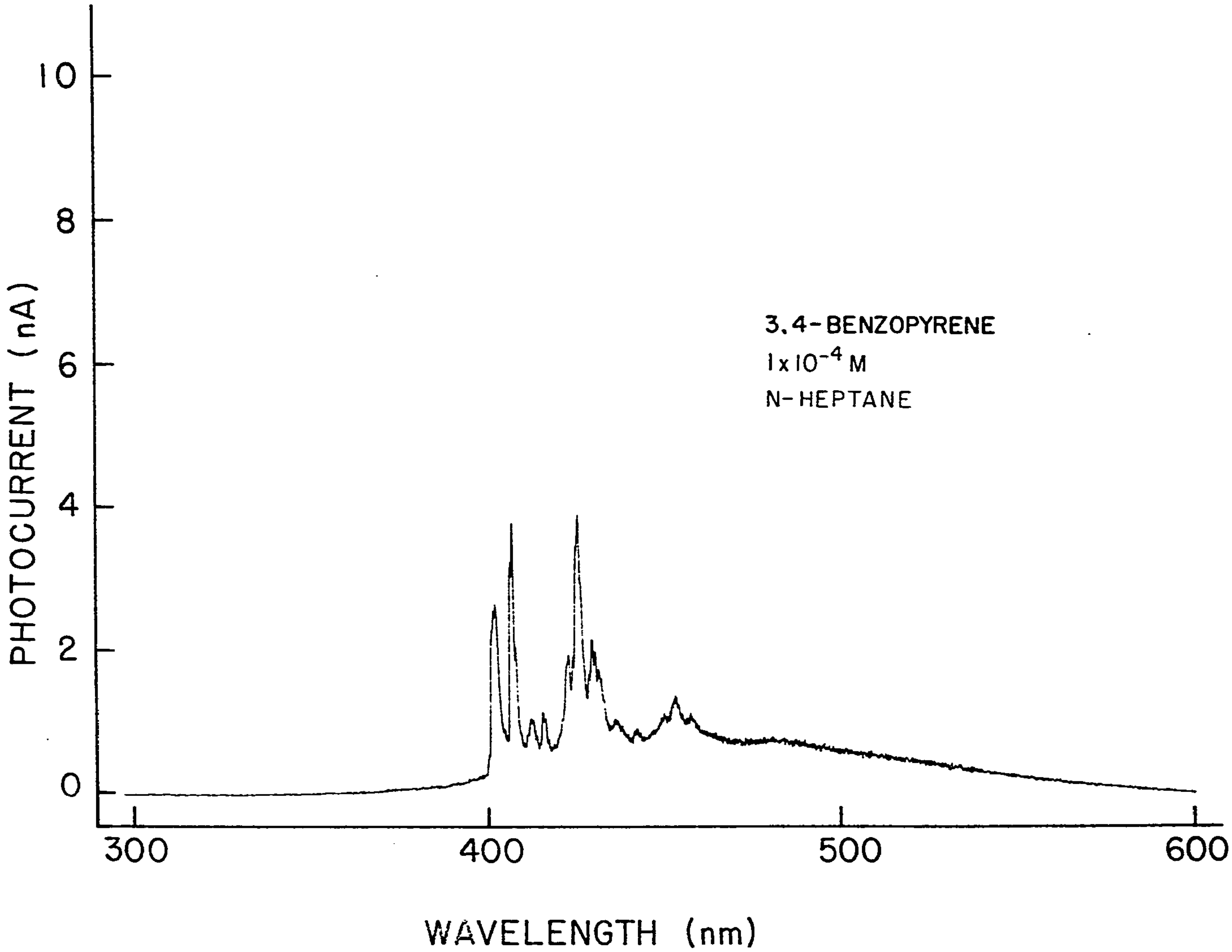

Figure 26. XECL spectrum of 3,4-benzopyrene in n-heptane at a concentration of 1 X 10^{-4} M.

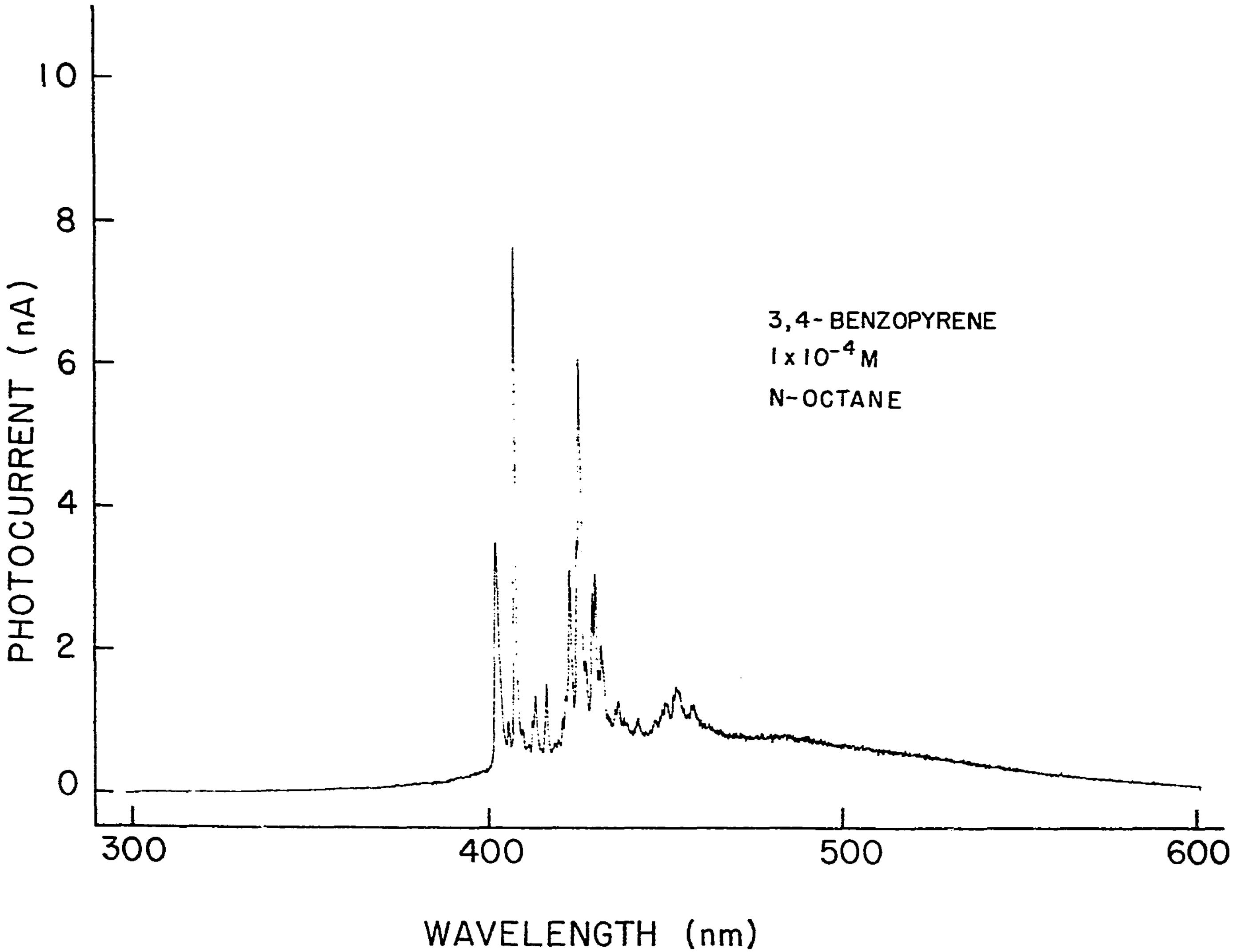

Figure 27. XECL spectrum of 3,4-benzopyrene in n-octane at a concentration of 1 X 10^{-4} M.

PAH systems are numerous (65-67). Furthermore, the x-ray capture cross section of an atom increases with atomic number (47). Therefore, the addition of a heavy atom to the solvent results in a host with a large x-ray capture cross section and a second enhancement of the luminescence emission should result with the XEOL technique. The heavy atom host captures more x-ray photons than a hydrocarbon host and the energy of the x-ray beam is more efficiently converted to electronic excitation energy for the PAH guest molecules.

No effect was observed for iodobutane but an enhancement was observed for tetra-n-butyllead. Table 14 summarizes the effect of tetra-n-butyllead on five PAHs at a concentration of 10 microliters of tetra-n-butyllead per 1 milliliter of n-heptane. The results indicate improved detection limits could be achieved with the addition of a heavy atom to the solvent. Future experiments should be scheduled to study the effect of heavy atom concentration on the signal and decay constant of the analyte. Also, the optimum concentration of heavy atom and the optimum heavy atom need to be determined.

Other Systems Amenable to Study by XEOL

An obvious application of the XEOL study of PAHs is the characterization of fuel oils by the PAH fraction as described by the U. S. Coast Guard (68). Fuel oil samples were collected and XEOL spectra were obtained. The initial

Table 14. External Heavy Atom Effect on PAH Emission

Compound	Conc.	Signal Without Heavy Atom	Signal With Heavy Atom	Percent Increase
Fluoranthene	$1X10^{-2}M$	8642	76050	780%
Chrysene	$1X10^{-3}M$	13019	21060	62%
Phenanthrene	$1X10^{-3}M$	31484	47200	50%
Triphenylene	$1X10^{-3}M$	88157	123700	40%
Coronene	$1X10^{-4}M$	8454	9360	11%

results were not competitive with the U. S. Coast Guard results, hence the fuel oil samples are being stored until the instrumental modifications have been completed. After the modifications are tested, the fuel oil samples will be characterized by XEOL spectra and complex decay curves. Characterization of fuel oils by complex decay curves will be one more method of identification necessary to fingerprint fuel oil spills and stock supplies of fuel oils.

XEOL emission from the final system considered was discovered by accident. The first experiments performed with the gas manifold involved the co-deposition of argon and PAHs on the beryllium disc to take advantage of the large x-ray capture cross section of argon as compared to carbon and hydrogen. A routine examination of a "pure" argon deposit revealed a complex spectrum, as shown in Figure 28. The many lines and bands are characteristic of nitrogen, oxygen and other gaseous impurities in argon. Possible analytical applications for the determination of these gases in argon

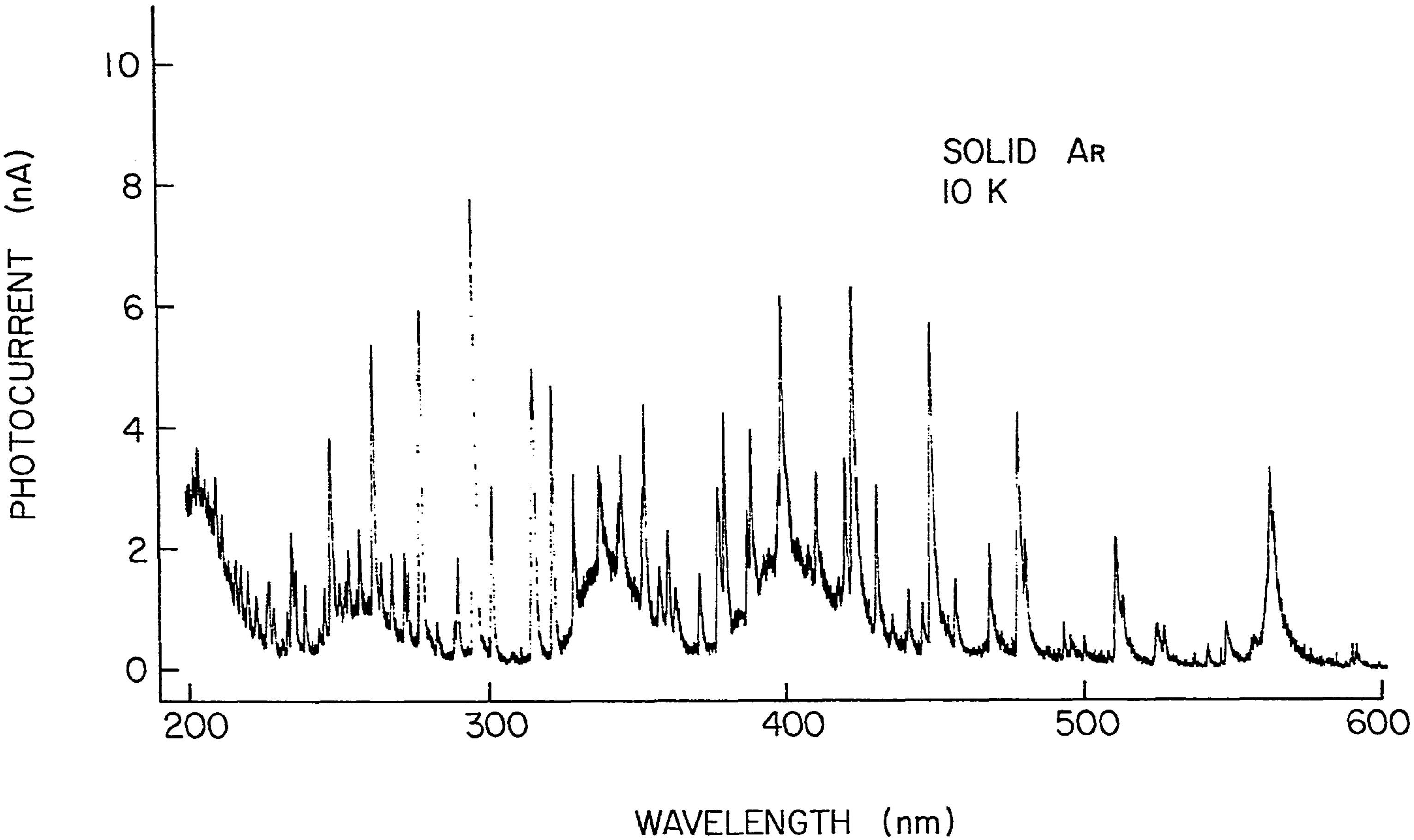

Figure 28. XECL spectrum of solid argon deposited on a beryllium window at 10 K from a flowing gas stream.

should be investigated.

In Figures 29 and 30 the spectra of krypton and xenon are shown. The broad bands in the short wavelength region suggest that these materials may be better suited as hosts for PAHs and other luminescent organic molecules. This possibility is being investigated. The origins of the other lines in the two spectra are unknown but trace gaseous impurities are the most likely sources.

The combination of rare gases and hydrocarbons, both aliphatic and aromatic, opens many avenues of research for the XEOL technique in the pulsed and DC modes. The many matrices with varying degrees of heavy atom concentration, structural peculiarities and x-ray capture cross sections should supply ideal XEOL environments for many different types of organic analytes.

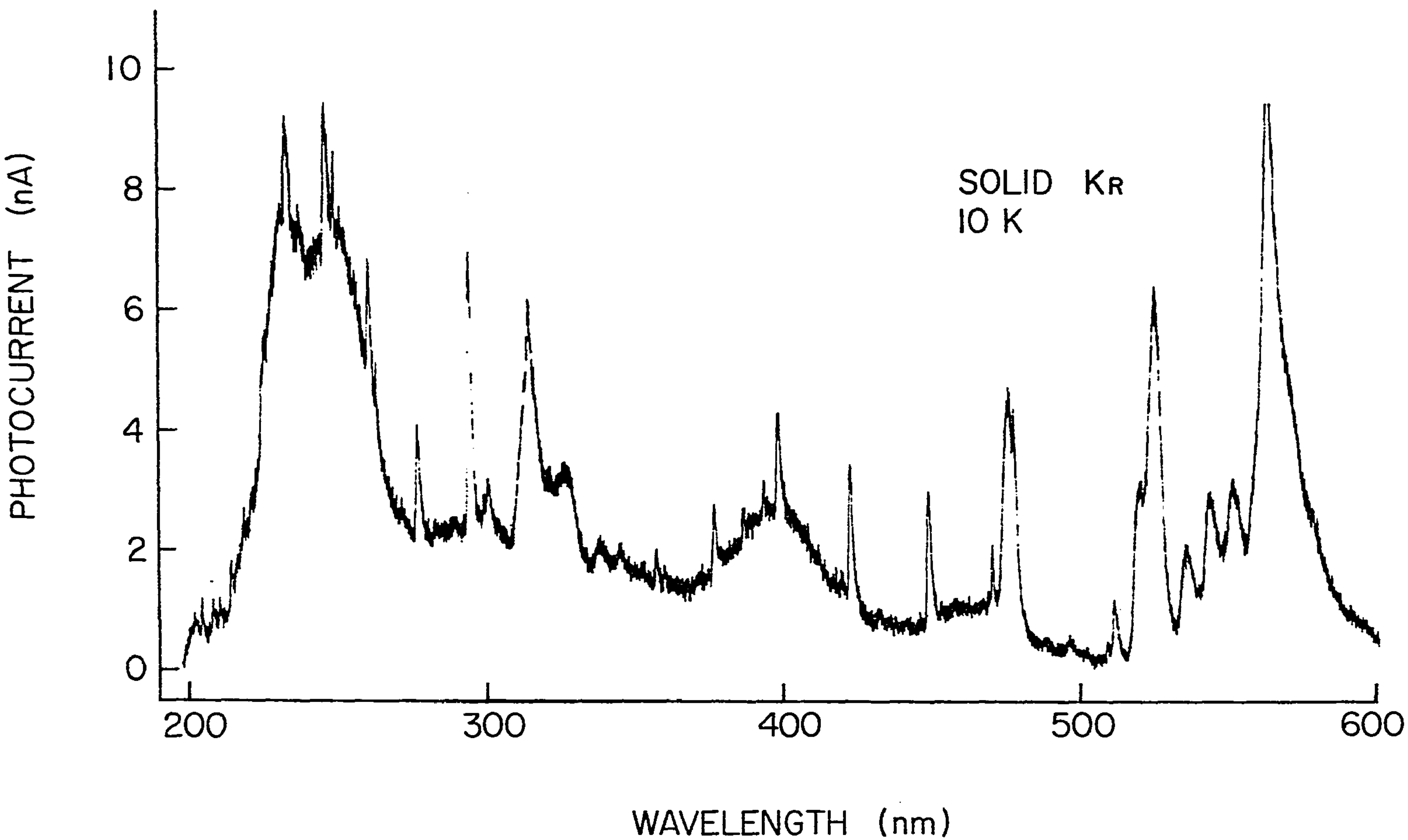

Figure 29. XECL spectrum of solid krypton deposited on a beryllium window at 10 K from a flowing gas stream.

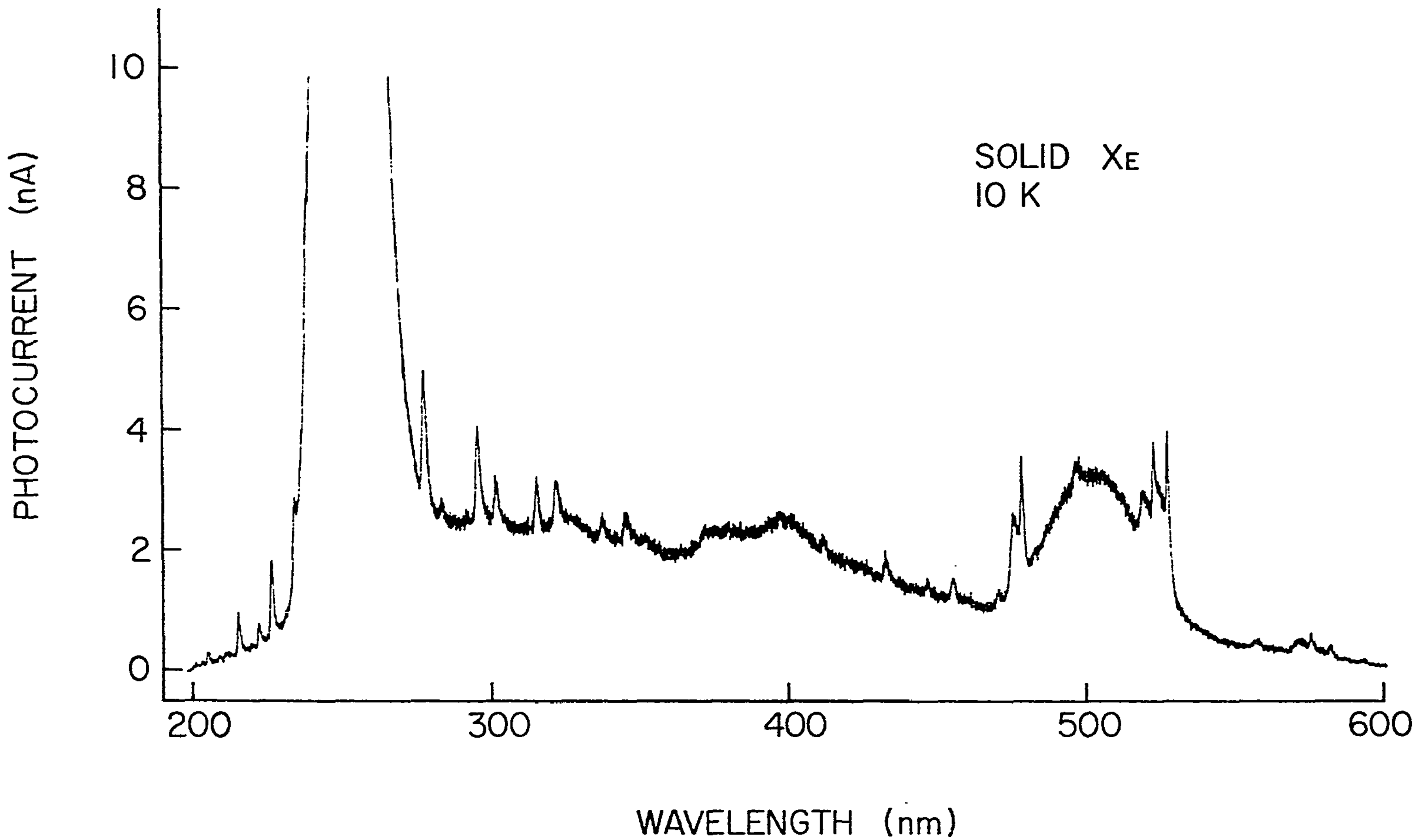

Figure 30. XECL spectrum of solid xenon deposited on a beryllium window at 10 K from a flowing gas stream.

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APPENDIX 1: TRS3

TRS3 is the PL/1 program which reads the experimental data from disc and generates the output data set which is the input data for SMASH. The PL/1 program translates data from a format specified by the assembly language program which runs on the PDP8/E minicomputer to data in the proper format for SMASH. Execution of TRS3 is the first major step in the job which calculates experimental results. TRS3 is run automatically by the WYLBUR execute file which appears in Appendix 6. The operation of TRS3 is controlled by a group of input variables which specify the number of experiments which were performed and the mode of the pulsed XEOL system employed for each experiment. If the slow mode is specified TRS3 plots the decay curve with Simplotter. Simplotter is accessed by the CALL GRAPH and CALL GRAPHS statements which appear in the listing. A CALL ORIGIN statement, one of the Simplotter options, is used to move the position of the graph on the paper on which the graph is plotted. A listing of the source statements of TRS3 is given on the following pages.

```
 (STRG,SUBRG):
CORE: PROCEDURE OPTIONS (MAIN);
      DCL GRAPH ENTRY (FIXED BIN, (*) FLOAT, (*) FLOAT,
              FIXED BIN, FIXED BIN, FLOAT, FLOAT, FLOAT,
              FLOAT, FLOAT, FLOAT, CHAR(20), CHAR(20),
              CHAR(20), CHAR(20));
      DCL GRAPHS ENTRY (FIXED BIN, (*) FLOAT, (*) FLOAT,
              FIXED BIN, FIXED BIN, CHAR(20));
      DCL ORIGIN ENTRY (FLOAT,FLOAT,FIXED BIN);
      DCL IN FILE INPUT;
      DCL OUT FILE OUTPUT ENVIRONMENT (CONSECUTIVE);
      DCL OPTION(50) FIXED;
      DCL (REJECT, INPUT) CHAR(80);
      DCL (X1(POINTS), Y1(POINTS), CORRECT(POINTS),
              ADDRESS(POINTS)) FLOAT CONTROLLED;
      DCL (SUMSQR(POINTS),VAR(POINTS)) FLOAT CONTROLLED;
      DCL (LAB1, LAB2) CHAR(20);
      DCL COMP(NCOMP) FLOAT CONTROLLED;
      DCL (DATE, TIME) CHAR(6);
      DCL (RUNS, PASSES, NUMWAV, POINTS) FIXED BIN;
      DCL (HEAD, XLAB, YLAB, GLAB, DATLAB) CHAR(80);
      CALL ORIGIN (0.0,1.0,1);
      GET FILE (IN) LIST (RUN);
      DO I=1 TO RUN;
              GET FILE (IN) LIST (OPTION(I));
      END;
      RUNCNT=RUN;M=1;
GETIN:GET EDIT (REJECT) (COL(1),A(70)) COPY;
      GET EDIT (INPUT) (COL(1),A(63)) COPY;
      GET STRING (INPUT) EDIT (DATE,TIME,RUNS,NUMWAV,
              PASSES,POINTS,LUMIN) (A(6),X(2),A(4),
              X(2),5(F(5),X(2)));
      IF LUMIN=1 THEN
              GET STRING (INPUT) EDIT (DELTIM,RANGE)
              (X(49),2(F(5),X(2)));
      J=1;
      ALLOCATE Y1(POINTS);
INDAT:GET EDIT (INPUT) (COL(1),A(70)) COPY;
      DO I=1 TO 7;
              GET STRING (SUBSTR(INPUT,(10*I-9),8)) EDIT
              (Y1(J)) (F(8));
              IF J=POINTS THEN GO TO ENDIN;
              J=J+1;
      END;
      IF J¬=POINTS+1 THEN GO TO INDAT;
ENDIN:RUNCNT=RUNCNT-1;
      J=1;
      Y1=-Y1;
      ALLOCATE CORRECT(POINTS);
      ALLOCATE ADDRESS(POINTS);
```

```
CORIN:GET EDIT (INPUT) (COL(1),A(70)) COPY;
      DO I=1 TO 5;
              GET STRING (SUBSTR(INPUT,(14*I-13),14)) EDIT
              (CORRECT(J),ADDRESS(J)) (2(F(5),X(2)));
              IF CORRECT(J)=0 THEN GO TO CORR;
              J=J+1;
      END;
      IF CORRECT(J-1)¬=0 THEN GO TO CORIN;
CORR: ALLOCATE SUMSQR(POINTS);
      J=1;
INSQR:GET EDIT (INPUT) (COL(1),A(70)) COPY;
      DO I=1 TO 7;
              GET STRING (SUBSTR(INPUT,(10*I-9),8)) EDIT
              (SUMSQR(J)) (F(8));
              IF J=POINTS THEN GO TO ENDSQR;
              J=J+1;
      END;
      IF J¬=POINTS+1 THEN GO TO INSQR;
ENDSQR:DO I=1 TO POINTS;
      IF CORRECT(I)=0 THEN GO TO ENDIT;
      SUMSQR(ADDRESS(I))=SUMSQR(ADDRESS(I))+
              CORRECT(I)*16777216;
      END;
 ENDIT:FREE CORRECT;
      FREE ADDRESS;
      IF LUMIN=0 THEN GO TO FAST;
      ALLOCATE VAR(POINTS);
      VAR=ABS(SUMSQR-Y1**2/PASSES)/(PASSES-1);
      FREE SUMSQR;
      CHECK=999;
      DO I=1 TO POINTS;
              IF VAR(I)¬=0 THEN CHECK=MIN(CHECK,VAR(I));
      END;
      DO I=1 TO POINTS;
              IF VAR(I)=0 THEN VAR(I)=CHECK;
      END;
      Y1=Y1/PASSES;
      ALLOCATE X1(POINTS);
      X1(1)=0;
      IF RANGE=1 THEN RANVAL=0.01;
              ELSE IF RANGE=2 THEN RANVAL=0.1;
              ELSE RANVAL=1;
      DO I=2 TO POINTS;
              X1(I)=X1(I-1)+RANVAL;
      END;
      GET FILE (IN) EDIT (LAB1,LAB2) (COL(1),2(A(20)));
      CALL ORIGIN (11.0,0.0,1);
      CALL GRAPH (POINTS,X1,Y1,1,7,9,7,0,0,0,0,
              'TIME  (SEC)','INTENSITY',LAB1,LAB2);
      CALL GRAPHS (POINTS,X1,Y1,0,121,DATE||'  '||TIME);
```

```
       IF OPTION(M)=1 THEN GO TO SMASH;
 DUMP: PUT PAGE;
       PUT SKIP LIST ('TRS2 DATA DUMP');
       PUT SKIP LIST ('DATE',DATE,'TIME',TIME,'RUN NO.',
               RUNS);
       PUT SKIP LIST ('NUMBER OF PASSES',PASSES,
               'NUMBER OF XRAY WAVES',NUMWAV);
       IF LUMIN=0 THEN GO TO CONT1;
       PUT SKIP LIST ('TRANSIENT DECAY TIME (USEC)',(DELTIM*
               5+10),'INTEGRATION TIME (MSEC)',(10**RANGE));
       PUT SKIP;
       PUT SKIP LIST ('THE TIME VALUES ARE:');
       PUT SKIP LIST (X1);
 CONT1:PUT SKIP;
       PUT SKIP LIST ('THE INTENSITY VALUES ARE:');
       PUT SKIP LIST (Y1);
       PUT SKIP;
       PUT SKIP LIST ('THE VARIANCE VALUES ARE:');
       PUT SKIP LIST (VAR);
       PUT PAGE;
       M=M+1;
       IF RUNCNT¬=0 THEN GO TO GETIN;
       PUT FILE (OUT) SKIP;
       GO TO STOP;
 SMASH:AVE=0;IFIRST=0;DEADT=0.0;SIGMAB=0.0;
       DO I=1 TO 10;
               AVE=AVE+Y1(POINTS+1-I);
       END;
       BACKGR=AVE/10;
       GET FILE (IN) EDIT (ISMASH) (COL(1),F(2));
       DO I=1 TO ISMASH;
               GET FILE (IN) EDIT (NCOMP,INPU,IPLOT)
               (COL(1),3(F(5)));
               PUT FILE (OUT) EDIT (NCOMP,POINTS,IFIRST,
               INPU,DEADT,BACKGR,SIGMAB,IPLOT)
               (COL(1),4(F(5)),3(F(12,3)),X(19),F(5));
               GET FILE (IN) EDIT (HEAD) (COL(1),A(80));
               PUT FILE (OUT) EDIT (HEAD) (COL(1),A(80));
               IF IPLOT=0 THEN GO TO CONT3;
               GET FILE (IN) EDIT (XLAB,YLAB,GLAB,DATLAB)
               (COL(1),4(A(20)));
               PUT FILE (OUT) EDIT (XLAB,YLAB,GLAB,DATLAB)
               (COL(1),4(A(20)));
 CONT3:        ALLOCATE COMP(NCOMP);
               GET FILE (IN) EDIT (COMP) ((NCOMP)(F(10,3)));
               PUT FILE (OUT) EDIT (COMP) (COL(1),(NCOMP)
               (F(10,3)));
               FREE COMP;
               IF INPU<0 THEN GO TO CONT4;
               PUT FILE (OUT) EDIT (Y1) (COL(1),6 E(12,5));
```

```
               PUT FILE  (OUT) EDIT (X1)  (COL(1),6 E(12,5));
               PUT FILE  (OUT) EDIT (VAR)  (COL(1),6 E(12,5));
CCNT4:END;
      GO TO DUMP;
FAST: AVE=SUM(Y1)/POINTS;
      VARI=0;
      DO I=1 TO PCINTS;
               VARI=VARI+((Y1(I)-AVE)**2);
      END;
      VARI=VARI/(POINTS-1);
      STAND=SQRT(VARI);
      PUT SKIP LIST ('THE AVERAGE VALUE IS:',AVE);
      PUT SKIP LIST ('THE STANDARD DEVIATION IS:',STAND);
      PUT SKIP;
      GO TO DUMP;
STOP: END CORE;
```

APPENDIX 2: SMASH

SMASH is a FORTRAN IV program which determines decay constants for single component decay curves and initial intensities for each component in a multiple component decay curve. The operation of SMASH is described elsewhere (53). Several modifications were made on the input routines and declaration statements to facilitate the execution of the program for the analysis of spectroscopic data. SMASH is the second major step in the job which calculates experimental results. A listing of SMASH with the modifications appears on the following pages.

```
C
C     SMASH, A PROGRAM FOR THE ANALYSIS OF DECAY CURVES,
C     BY P.J.M. KORTHOVEN AND F.S. CARLSEN
C
      CALL SMASH1
      STOP
      END
      SUBROUTINE SMASH1
      DIMENSION IPAR(10),SSIZE(10),X(10),Y(10)
      REAL LAMBDA(10)
      COMMON NSTEPS,NCOMP,FIT2,IFIRST,SSIZE,LAMBDA,ORFIT,
     1NVAR,FIT1
    1 NSTEPS=0
      KOUNT=0
      CALL SMINP1
      IF (NCOMP) 2,63,2
    2 ICONV=NVAR*400
    3 KOUNT=KOUNT+1
      DO 4 I=1,NCOMP
    4 IPAR(I)=0
      IA=0
      IB=0
      CALL SMFIT1
      FIT1=FIT2
      IF (NVAR) 6,5,6
    5 IFIRST=0
    6 IF (IFIRST) 10,7,10
    7 CALL SMOUT1(1)
      IFIRST=1
      IF (NVAR) 8,1,8
    8 IF (KOUNT-1) 10,9,10
    9 ORFIT=FIT2
   10 TEMFIT=FIT2
   11 FIT1=TEMFIT
C
C     INITIAL SEARCH
C
      DO 25 I=1,NCOMP
      X(I)=LAMBDA(I)
      IF (SSIZE(I)) 13,12,13
   12 IPAR(I)=0
      GO TO 25
   13 LAMBDA(I)=LAMBDA(I)+SSIZE(I)
      CALL SMFIT1
      IF (NSTEPS-ICONV) 14,14,62
   14 IF (FIT2-FIT1) 15,20,20
   15 IF (IPAR(I)-2) 16,17,16
   16 IPAR(I)=0
   17 IF (ABS(FIT2-FIT1)-0.000001) 19,18,18
   18 IB=1
```

```
      IPAR(I)=1
   19 FIT1=FIT2
      GO TO 25
   20 LAMBDA(I)=X(I)-SSIZE(I)
      CALL SMFIT1
      IF (NSTEPS-ICONV) 21,21,62
   21 IF (FIT2-FIT1) 22,23,23
   22 SSIZE(I)=-SSIZE(I)
      GO TO 15
   23 LAMBDA(I)=X(I)
      IF (IPAR(I)-2) 24,25,24
   24 IPAR(I)=0
   25 CONTINUE
C
C     END INITIAL SEARCH
C
   26 DO 27 I=1,NCOMP
      IF (IPAR(I)-1) 27,38,27
   27 CONTINUE
      IF (IB) 28,33,28
   28 DO 32 I=1,NCOMP
      IF (IPAR(I)-2) 30,29,30
   29 SSIZE(I)=SSIZE(I)*0.2
      IPAR(I)=0
   30 IF (ABS(SSIZE(I))-0.00002*LAMBDA(I)) 31,32,32
   31 SSIZE(I)=0.0
   32 CONTINUE
      IB=0
      GO TO 58
   33 DO 34 I=1,NCOMP
      IF (ABS(SSIZE(I))-0.00002*LAMBDA(I)) 34,34,35
   34 CONTINUE
      IF (ABS(FIT1-FIT2)-0.000001) 61,3,3
   35 DO 37 I=1,NCCMP
      SSIZE(I)=SSIZE(I)*0.2
      IF (ABS(SSIZE(I))-0.00002*LAMBDA(I)) 36,37,37
   36 SSIZE(I)=0.0
   37 CONTINUE
      GO TO 58
C
C     ADJUST PARAMETERS FOR THE SELECTED SEARCH
C
   38 TEMFIT=FIT1
      DO 43 I=1,NCOMP
      TEMP=LAMBDA(I)
      IF (IPAR(I)-1) 40,39,40
   39 LAMBDA(I)=LAMBDA(I)*2.0-X(I)
   40 X(I)=TEMP
      IF (IA-1) 41,43,41
   41 IPAR(I)=0
```

```
      IF (SSIZE(I)) 42,43,42
   42 IPAR(I)=1
   43 CONTINUE
      CALL SMFIT1
      IF (NSTEPS-ICONV) 44,44,62
   44 IF (FIT2-FIT1) 45,46,46
   45 FIT1=FIT2
C
C     SELECTED SEARCH
C
   46 DO 54 I=1,NCOMP
      IF (IPAR(I)-1) 54,47,54
   47 Y(I)=LAMBDA(I)
      LAMBDA(I)=LAMBDA(I)+SSIZE(I)
      CALL SMFIT1
      IF (NSTEPS-ICONV) 48,48,62
   48 IF (FIT2-FIT1) 53,49,49
   49 LAMBDA(I)=Y(I)-SSIZE(I)
      CALL SMFIT1
      IF (NSTEPS-ICONV) 50,50,62
   50 IF (FIT2-FIT1) 51,52,52
   51 SSIZE(I)=-SSIZE(I)
      GO TO 53
   52 LAMBDA(I)=Y(I)
      IPAR(I)=2
      GO TO 54
   53 IA=1
      IB=1
      FIT1=FIT2
   54 CONTINUE
C
C     END SELECTED SEARCH
C
      IF (FIT1-TEMFIT) 38,55,55
   55 DO 57 I=1,NCCMP
      IF (IPAR(I)-1) 57,56,57
   56 IPAR(I)=2
   57 LAMBDA(I)=X(I)
      IA=0
      GO TO 11
   58 IF (FIT2-TEMFIT) 10,59,59
   59 DO 60 I=1,NCCMP
   60 LAMBDA(I)=X(I)
      GO TO 11
   61 CALL SMOUT1 (0)
      GO TO 1
   62 CALL SMOUT1 (-1)
      GO TO 1
   63 STOP
      END
```

```
C
C     SUBROUTINE INPUT
C
      SUBROUTINE SMINP1
      DIMENSION IDENT(20),HALFL(10),SSIZE(10),XLAB(5),
     1YLAB(5),DATLAB(5),GLAB(5),TM(1000),RATE(1000),
     2DIFF(1000),ACALC(1000),A0(10),C(10,10),P(1000,10),
     3BGRND(1000),SIGMBG(1000),RAVAR(1000),DFIT(10),
     4VAR(1000),COUNTS(1000),DELTAT(1000),WDIFF(1000),
     5X(10),HL(10)
      REAL LAMBDA(10)
      INTEGER DF
      COMMON NSTEPS,NCOMP,FIT2,IFIRST,SSIZE,LAMBDA,ORFIT,
     1IDENT,TM,RATE,VAR,XLAB,YLAB,GLAB,DATLAB,IPLOT,COUNTS,
     2ACALC,DIFF,DF,HL,A0,C,P,WDIFF,KS,DEADT,BACKGR,SIGMAB,
     3RAVAR,IWRIT,FIT1,NVAR,DELTAT,NP,HALFL,TO
      NVAR=0
      READ (5,101) NCOMP,NP,IFIRST,INPU,DEADT,BACKGR,SIGMAB,
     1IDUAL,IPLOT
  101 FORMAT (4I5,3F12.3,14X,2I5)
      IF (IPLOT) 116,115,116
  116 CALL ORIGIN (0.0,0.0,0)
      CALL ORIGIN (0.0,1.0,1)
  115 IF (NCOMP) 102,145,102
  102 READ (5,103) (IDENT(I),I=1,20)
  103 FORMAT (20A4)
      IF (IPLOT) 104,105,104
  104 READ (5,103) XLAB,YLAB,GLAB,DATLAB
  105 READ (5,106) (HALFL(I),I=1,NCOMP)
  106 FORMAT (8F10.3)
      IF (INPU) 129,112,111
  111 NCOMP=0
      GO TO 145
  112 READ (5,126) (COUNTS(I),I=1,NP)
      READ (5,126) (TM(I),I=1,NP)
      READ (5,126) (VAR(I),I=1,NP)
  126 FORMAT (6E12.5, 8X)
  113 DO 127 I=1,NP
      RATE(I)=COUNTS(I)-BACKGR
      RAVAR(I)=RATE(I)/VAR(I)
      DELTAT(I)=TM(I)
  127 CONTINUE
      DO 128 I=2,NP
  128 TM(I)=TM(I)-TM(1)
      TO=TM(1)
      TM(1)=0.0
  129 DO 130 I=1,NCOMP
      IF (HALFL(I)) 220,230,220
  230 LAMBDA(I)=0.0
      GO TO 130
```

```
  220 LAMBDA(I)=ABS(HALFL(I))
  130 CONTINUE
      IF (NCOMP-1) 107,107,108
  108 XN=0.0
      IWRIT=1
      CALL SMFIT1
      FIT1=FIT2
      DO 131 I=1,NCOMP
      X(I)=LAMBDA(I)
      IF (HALFL(I)) 132,136,136
  132 XX=LAMBDA(I)*0.05
      LAMBDA(I)=LAMBDA(I)+XX
      CALL SMFIT1
      IF (FIT2-FIT1) 133,134,134
  134 LAMBDA(I)=LAMBDA(I)-2.0*XX
      CALL SMFIT1
      IF (FIT2-FIT1) 133,136,136
  133 DFIT(I)=FIT1-FIT2
      GO TO 135
  136 DFIT(I)=XN-1.0
  135 LAMBDA(I)=X(I)
  131 CONTINUE
      DO 140 I=1,NCOMP
      K=NCOMP-1
      DO 140 J=1,K
      IF (DFIT(J)-DFIT(J+1)) 141,140,140
  141 SWAP=DFIT(J)
      DFIT(J)=DFIT(J+1)
      DFIT(J+1)=SWAP
      SWAP=LAMBDA(J)
      LAMBDA(J)=LAMBDA(J+1)
      LAMBDA(J+1)=SWAP
      SWAP=HALFL(J)
      HALFL(J)=HALFL(J+1)
      HALFL(J+1)=SWAP
  140 CONTINUE
  107 IWRIT=0
      NSTEPS=0
      DO 142 I=1,NCOMP
      IF (HALFL(I)) 143,144,144
  143 SSIZE(I)=0.05*LAMBDA(I)
      NVAR=NVAR+1
      GO TO 142
  144 SSIZE(I)=0.0
  142 CONTINUE
  145 RETURN
      END
C
C     SUBROUTINE FIT
C
```

```
      SUBROUTINE SMFIT1
      DIMENSION TM(1000),P(1000,10),V(10),RATE(1000),
     1A0(10),ACALC(1000),DIFF(1000),HL(10),IDENT(20),
     2YLAB(5),GLAB(5),DATLAB(5),COUNTS(1000),DELTAT(1000),
     3HALFL(10),RAVAR(1000),CC(10,10),PAR(10),WDIFF(1000),
     4XLAB(5),SSIZE(10),VAR(1000),C(10,10)
      REAL LAMBDA(10)
      INTEGER DF
      COMMON NSTEPS,NCOMP,FIT2,IFIRST,SSIZE,LAMBDA,ORFIT,
     1IDENT,TM,RATE,VAR,XLAB,YLAB,GLAB,DATLAB,IPLOT,CCUNTS,
     2ACALC,DIFF,DF,HL,A0,C,P,WDIFF,KS,DEADT,BACKGR,SIGMAB,
     3RAVAR,IWRIT,FIT1,NVAR,DELTAT,NP,HALFL,TO
      NSTEPS=NSTEPS+1
      IF (NSTEPS-1) 700,701,700
  701 DO 702 I=1,NCOMP
  702 PAR(I)=1.0E60
  700 DO 2031 J=1,NCOMP
      IF (PAR(J)-LAMBDA(J)) 300,2031,300
  300 DO 203 I=1,NP
      DECAYF=-LAMBDA(J)*TM(I)
      IF (ABS(DECAYF)-50.0) 202,201,201
  201 P(I,J)=0.0
      GO TO 203
  202 P(I,J)=EXP(DECAYF)
  203 CONTINUE
 2031 CONTINUE
      DO 204 I=1,NCOMP
      IF (PAR(I)-LAMBDA(I)) 320,204,320
  320 V(I)=0.0
      DO 204 K=1,NP
      V(I)=V(I)+P(K,I)*RAVAR(K)
  204 CONTINUE
      DO 2051 I=1,NCOMP
      DO 2051 J=1,NCOMP
      IF (PAR(I)-LAMBDA(I)) 2205,2206,2205
 2206 IF (PAR(J)-LAMBDA(J)) 2205,2207,2205
 2207 C(I,J)=CC(I,J)
      GO TO 2051
 2205 C(I,J)=0.0
      DO 205 K=1,NP
      C(I,J)=C(I,J)+P(K,I)*P(K,J)/VAR(K)
  205 CC(I,J)=C(I,J)
 2051 CONTINUE
      DO 2500 I=1,NCOMP
 2500 PAR(I)=LAMBDA(I)
      CALL SMATNV (C,NCOMP,DETERM)
      DO 206 I=1,NCCMP
      A0(I)=0.0
      DO 206 J=1,NCOMP
  206 A0(I)=A0(I)+C(I,J)*V(J)
```

```
      RS=0.0
      DO 208 I=1,NP
      ACALC(I)=0.0
      DO 207 J=1,NCOMP
  207 ACALC(I)=ACALC(I)+P(I,J)*A0(J)
      DIFF(I)=RATE(I)-ACALC(I)
      RS=RS+DIFF(I)**2/VAR(I)
  208 CONTINUE
      DF=NP-NCOMP
      XDF=DF
      FIT2=SQRT(RS/XDF)
      IF (IWRIT) 217,751,217
  751 DO 211 I=1,NCOMP
      IF (LAMBDA(I)) 210,209,210
  209 HL(I)=0.0
      GO TO 211
  210 HL(I)=LAMBDA(I)
  211 CONTINUE
      IF (NSTEPS-1) 215,212,215
  212 IF (IFIRST) 213,217,213
  213 WRITE (6,214) (I,I=1,NCOMP)
  214 FORMAT (1H1,5H STEP,6X,3HFIT,9X,9(1H-,I1,1H-,8X),1H-,
     1I2,1H-/1H0)
  215 WRITE (6,216) NSTEPS,FIT2,(HL(I),I=1,NCOMP)
  216 FORMAT (I5,F13.6,9F11.4,F12.4)
  217 RETURN
      END
C
C     SUBROUTINE MATINV
C
      SUBROUTINE SMATNV (A,N,DETERM)
      DIMENSION A(10,10),PIVOT(10),INDEX(10,2),IPIVOT(10)
      EQUIVALENCE (IROW,JROW),(ICOLUM,JCOLUM),(AMAX,T,SWAP)
C
C     INITIALIZATION
C
      DETERM=1.0
      DO 301 J=1,N
  301 IPIVOT(J)=0
      DO 314 I=1,N
C
C     SEARCH FOR PIVOT ELEMENT
C
      AMAX=0.0
      DO 306 J=1,N
      IF (IPIVOT(J)-1) 302,306,302
  302 DO 305 K=1,N
      IF (IPIVOT(K)-1) 303,305,318
  303 IF (ABS(AMAX)-ABS(A(J,K))) 304,305,305
  304 IROW=J
```

```
      ICOLUM=K
      AMAX=A(J,K)
  305 CONTINUE
  306 CONTINUE
      IPIVOT(ICOLUM)=IPIVOT(ICOLUM)+1
C
C     INTERCHANGE ROWS TO PUT PIVOT ELEMENT ON DIAGONAL
C
      IF (IROW-ICOLUM) 307,309,307
  307 DETERM=-DETERM
      DO 308 L=1,N
      SWAP=A(IROW,L)
      A(IROW,L)=A(ICOLUM,L)
  308 A(ICOLUM,L)=SWAP
  309 INDEX(I,1)=IROW
      INDEX(I,2)=ICOLUM
      PIVOT(I)=A(ICOLUM,ICOLUM)
      DETERM=DETERM*PIVOT(I)
C
C     DIVIDE PIVOT ROW BY PIVOT ELEMENT
C
      A(ICOLUM,ICOLUM)=1.0
      DO 310 L=1,N
  310 A(ICOLUM,L)=A(ICOLUM,L)/PIVOT(I)
C
C     REDUCE NON-PIVOT ROWS
C
  311 DO 314 L1=1,N
      IF (L1-ICOLUM) 312,314,312
  312 T=A(L1,ICOLUM)
      A(L1,ICOLUM)=0.0
      DO 313 L=1,N
  313 A(L1,L)=A(L1,L)-A(ICOLUM,L)*T
  314 CONTINUE
C
C     INTERCHANGE COLUMNS
C
      DO 317 I=1,N
      L=N+1-I
      IF (INDEX(L,1)-INDEX(L,2)) 315,317,315
  315 JROW=INDEX(L,1)
      JCOLUM=INDEX(L,2)
      DO 316 K=1,N
      SWAP=A(K,JROW)
      A(K,JROW)=A(K,JCOLUM)
      A(K,JCOLUM)=SWAP
  316 CONTINUE
  317 CONTINUE
  318 RETURN
      END
```

```
C
C     SUBROUTINE OUTPUT
C
      SUBROUTINE SMOUT1(ICASE)
      DIMENSION DATLAB(5),A0(10),P(1000,10),SAZERO(10),
     1IDENT(20),SRELAT(10),WDIFF(1000),HALFL(10),HL(10),
     2DELTAT(1000),COUNTS(1000),RATE(1000),ACALC(1000),
     3XLAB(5),YLAB(5),GLAB(5),THALFL(10),TEMPHL(5),
     4SSIZE(10),TM(1000),CORR(10),DIFF(1000),VAR(1000),
     5AZERO(10),C(10,10)
      REAL LAMBDA(10),LOGACT(1000),LOGFC(1000)
      INTEGER DF
      COMMON NSTEPS,NCOMP,FIT2,IFIRST,SSIZE,LAMBDA,ORFIT,
     1IDENT,TM,RATE,VAR,XLAB,YLAB,GLAB,DATLAB,IPLOT,COUNTS,
     2ACALC,DIFF,DF,HL,A0,C,P,WDIFF,KS,DEADT,BACKGR,SIGMAB,
     3HALFL,TO,DELTAT,NP,FIT1,NVAR
      EQUIVALENCE (LOGACT(1),WDIFF(1)),(LOGFC(1),ACALC(1))
      DO 400 I=1,NP
  400 TM(I)=TM(I)+TO
      DO 401 I=1,NCOMP
      CORR(I)=EXP(TO*LAMBDA(I))
      AZERO(I)=A0(I)*CORR(I)
      SAZERO(I)=SQRT(C(I,I))*CORR(I)*FIT1
  401 SRELAT(I)=SAZERO(I)/AZERO(I)*100.0
      IPERC1=0
      IPERC2=0
      IPERC3=0
      DO 406 I=1,NP
      VAR(I)=SQRT(VAR(I))
      WDIFF(I)=DIFF(I)/VAR(I)
      IWDIFF=IABS(IFIX(WDIFF(I)))+1
      IF (ABS(WDIFF(I))-3.0) 402,403,403
  402 GO TO (406,404,405),IWDIFF
  403 IPERC3=IPERC3+1
      GO TO 406
  404 IPERC1=IPERC1+1
      GO TO 406
  405 IPERC2=IPERC2+1
  406 CONTINUE
      PERC1=FLOAT(IPERC1+IPERC2+IPERC3)/FLOAT(NP)*100.0
      PERC2=FLOAT(IPERC2+IPERC3)/FLOAT(NP)*100.0
      PERC3=FLOAT(IPERC3)/FLOAT(NP)*100.0
      WRITE (6,407) (IDENT(I),I=1,20)
  407 FORMAT (1H1,20A4)
      IF (ICASE) 408,410,414
  408 WRITE (6,409) NSTEPS
  409 FORMAT (86H THE SOLUTION IS NOT YET REACHED, OUTPUT IS
     1CALCULATED WITH THE PARAMETER VALUES AFTER,I5,6H STEPS
     2/1H0)
      GO TO 412
```

```
410 WRITE (6,411)
411 FORMAT (45H RESULTS OBTAINED WITH FINAL PARAMETER
   1VALUES/1H0)
412 WRITE (6,413) NP,NSTEPS,NCOMP,PERC1,NVAR,DF,PERC2,
   2BACKGR,SIGMAB,PERC3,DEADT,ORFIT,FIT1
413 FORMAT (15X,16HINPUT QUANTITIES,50X,17HOUTPUT QUANTITI
   1ES//12X,23HNUMBER OF DATA POINTS =,I5,56X,17HNUMBER OF
   2 STEPS =,I5/13X,22HNUMBER OF COMPONENTS =,I5,23X,50HPE
   3RCENTAGE OF POINTS DEVIATING MORE THAN 1 SIGMA =,F8.2/
   44X,31HNUMBER OF VARIABLE DECAY CONS =,I5,34X,28H(THEOR
   5ETICAL VALUE = 31.74 ) /15X,20HDEGREES OF FREEDOM =,I5
   6,23X,50HPERCENTAGE OF POINTS DEVIATING MORE THAN 2 SIG
   7MA =,F8.2/7X,28HBACKGROUND (COUNTS/MINUTE) =,F9.1,30X,
   828H(THEORETICAL VALUE =  4.56 )/1H ,34HSIGMA BACKGROUN
   9D (COUNTS/MINUTE) =,F7.1,21X,50HPERCENTAGE OF POINTS D
   8EVIATING MORE THAN 3 SIGMA =,F8.2/8X,27HDEAD TIME (MIC
   7RO SECONDS) =,F7.1,32X,29H(THEORETICAL VALUE = 0.26 )
   6//21X,14HORIGINAL FIT =,F14.6,53X,11HFINAL FIT =,F14.6
   5//1H0)
    IF (ICASE) 445,548,417
445 WRITE (6,447)
447 FORMAT (1H0/58X,17H*****WARNING*****/51X,30H*****CHECK
   1 YOUR ESTIMATES*****/1H0/1H0)
    GO TO 448
548 NEG=0
    DO 442 I=1,NCOMP
    IF (AZERO(I)) 443,443,442
443 NEG=1
442 CONTINUE
    IF (NEG-1) 438,460,460
460 WRITE (6,444)
444 FORMAT (1H0/58X,17H*****WARNING*****/38X,56H*****THE N
   1UMBER OF COMPONENTS IS PROBABLY TOO LARGE*****/1H0)
    GO TO 448
438 IF (FIT2-2.0) 448,439,439
439 WRITE (6,440)
440 FORMAT (1H0/58X,17H*****WARNING*****/38X,56H*****THE N
   1UMBER OF COMPONENTS IS PROBABLY TOO SMALL*****/1H0)
    GO TO 448
414 WRITE (6,415)
415 FORMAT (48H RESULTS OBTAINED WITH ORIGINAL PARAMETER
   1VALUES/1H0)
    DO 416 I=1,NCOMP
    TEMPHL(I)=HL(I)
    THALFL(I)=HALFL(I)
    HALFL(I)=ABS(HALFL(I))
416 HL(I)=0.0
    FIT1=FIT2
    NV=NVAR
    NVAR=0
```

```
      ORFIT=0.0
      GO TO 412
  417 IF (NV) 448,449,448
  449 IF (FIT1-2.0) 448,450,450
  450 WRITE (6,447)
  448 IF (ICASE) 420,420,418
  418 NVAR=NV
  420 WRITE (6,421)
  421 FORMAT (1H0,22X,9HCOMPONENT,8X,8HORIGINAL,9X,5HFINAL,9
     1X,8HACTIVITY,9X,5HSIGMA,9X,5HSIGMA/39X,9HDECAY CON,7X,
     29HDECAY CON,8X,6HAT EOB,8X,8HABSOLUTE,7X,8HRELATIVE//)
      WRITE (6,422) (I,HALFL(I),HL(I),AZERO(I),SAZERO(I),
     1SRELAT(I),I=1,NCOMP)
  422 FORMAT (22X,I5,F21.4,F16.4,F16.3,F14.3,F13.3)
      WRITE (6,423)
  423 FORMAT (1H0///1H0)
  424 WRITE (6,425)
  425 FORMAT (8X,7HMIDTIME, 7X,4HTIME,10X,8HORIGINAL,8X,9HCO
     1RRECTED,8X,5HSIGMA,8X,10HCALCULATED,9X,8HABSOLUTE,11X,
     210HDIFFERENCE/9X,5HCOUNT,6X,8HINTERVAL,10X,4HDATA,13X,
     34HRATE,11X,4HRATE,11X,4HRATE,11X,10HDIFFERENCE,8X,13H(
     4SIGMA UNITS)/1H0)
      WRITE (6,426) (I,TM(I),DELTAT(I),COUNTS(I),RATE(I),
     1VAR(I),ACALC(I),DIFF(I),WDIFF(I),I=1,NP)
  426 FORMAT (I4,F10.6,F12.6,F18.1,F17.1,F14.1,F16.1,
     1F18.1,F18.3)
  427 DO 428 I=1,NP
  428 VAR(I)=VAR(I)**2
      IF (IPLOT) 429,432,431
  429 DO 430 I=1,NP
      IF (RATE(I)) 461,461,462
  461 RATE(I)=1.0
  462 LOGACT(I)=ALOG10(RATE(I))
      IF (ACALC(I)) 463,463,464
  463 ACALC(I)=1.0
  464 LOGFC(I)=ALOG10(ACALC(I))
  430 CONTINUE
      CALL ORIGIN (11.0,0.0,1)
      CALL GRAPH (NP,TM,LOGACT,3,7,9.,-7.,0,0,0,0,XLAB,YLAB,
     1GLAB,DATLAB)
      CALL GRAPH (NP,TM,LOGFC,3,2,0,0,0,0,0,0,0,0,0,0)
      GO TO 432
  431 CALL ORIGIN (11.0,0.0,1)
      CALL GRAPH (NP,TM,RATE,3,7,9.,7.,0,0,0,0,XLAB,YLAB,
     1GLAB,DATLAB)
      CALL GRAPH (NP,TM,ACALC,3,2,0,0,0,0,0,0,0,0,0,0)
  432 IF (ICASE) 437,437,433
  433 DO 419 I=1,NCOMP
      HL(I)=TEMPHL(I)
  419 HALFL(I)=THALFL(I)
```

```
      IF (NVAR) 434,437,434
  434 WRITE (6,435) (I,I=1,NCOMP)
  435 FORMAT (1H1,5H STEP,6X,3HFIT,9X,9(1H-,I1,1H-,8X),1H-,
     1I2,1H-/1H0)
      WRITE (6,436) NSTEPS,FIT2,(HL(I),I=1,NCOMP)
  436 FORMAT (I5,F13.6,9F11.4,F12.4)
  437 DO 446 I=1,NP
  446 TM(I)=TM(I)-TO
      RETURN
      END
```

APPENDIX 3: GENPLOT

GENPLOT, a utility program for the generation of plots of general data, is a combination of a WYLBUR execute file and a PL/1 program. The execute file requests input information and data from the operator. The PL/1 program accesses Simplotter with CALL GRAPH and CALL GRAPHS statements. Logarithmic or linear plots can be generated. Several data sets can be plotted on the same graph and several graphs can be plotted at one time.

GENPLOT was used to plot calibration curves, decay curves, current, voltage and time relationships and other general data. The program was written to plot general data sets with many options of Simplotter available. Increased use of GENPLOT for examination of data trends and shapes of curves should be encouraged. The listing of the program follows on subsequent pages.

```
10   SET EXEC NOL TERSE
20   SET ESC :
25   CLR TEXT
30   COPY 700/761 EXEC TO 1
40   REA VAL N0 PRO 'NUMBER OF GRAPHS ?  '
50   CH '###' TO ':N0' N
55   SET VAL W0=100
60   SET VAL N1=0
70   SET VAL N1=N1+1
80   IF (N1 GT N0) EXEC 550
90   REA VAL N2 PRO 'NUMBER OF PLOTS ON GRAPH :N1 ?  '
100  :W0 :N2
101  SET VAL W0=W0+1
110  SET VAL N3=0
130  REA STR S0 PRO 'X-AXIS LABEL ?  '
140  :W0 ':S0'
145  SET VAL W0=W0+1
150  REA STR S0 PRO 'Y-AXIS LABEL ?  '
160  :W0 ':S0'
165  SET VAL W0=W0+1
170  REA STR S0 PRO 'GRAPH LABEL ?  '
180  :W0 ':S0'
181  SET VAL W0=W0+1
182  REA STR S0 PRO 'LIN=LINEAR OR LOG=LOGARITHMIC PLOT ? '
183  :W0 ':S0'
190  SET VAL W0=W0+1
200  SET VAL N3=N3+1
210  IF (N3 GT N2) EXEC 70
220  REA VAL N4 PRO 'HOW MANY POINTS IN PLOT :N3 ?  '
230  REA VAL N5 PRO 'ENTER A NUMBER BETWEEN 1-13 !  '
240  SET VAL S0=N4||' '||N5
250  :W0 :S0
260  SET VAL W0=W0+1
270  SET VAL N5=0
274  COMM ENTER X VALUES ONE AT A TIME
275  SET VAL S1=''
280  SET VAL N5=N5+1
285  IF (N5 GT N4) EXEC 340
300  REA STR S0 PRO 'X(:N5)= '
310  SET VAL S1=S1||' '||S0
320  IF (SIZE(S1) LE 60) EXEC 280
330  EXEC 500 SAVE
333  IF (N5 EQ N4) EXEC 360
335  EXEC 275
340  :W0 :S1
350  SET VAL W0=W0+1
360  SET VAL N5=0
364  COMM ENTER Y VALUES ONE AT A TIME
365  SET VAL S1=''
370  SET VAL N5=N5+1
```

```
375    IF (N5 GT N4) EXEC 430
390    REA STR S0 PRO 'Y(:N5)= '
400    SET VAL S1=S1||' '||S0
410    IF (SIZE(S1) LE 60) EXEC 370
420    EXEC 500 SAVE
423    IF (N5 EQ N4) EXEC 450
425    EXEC 365
430    :W0 :S1
440    SET VAL W0=W0+1
450    REA STR S0 PRO 'DATA LABEL ?  '
460    :W0 ':S0'
470    SET VAL W0=W0+1
480    EXEC 200
500    :W0 :S1
510    SET VAL W0=W0+1
520    EXEC RETURN
550    COMM TO PLOT DATA TYPE EXEC NEXT
560    EXEC PAUSE
570    COPY 800/805 EXEC TO L+1
600    RUN UNN
610    EXEC PAUSE
700    //A411GJO JOB A0099,GJO,TIME=(,29)
701    //S1 EXEC PL1LFCG,PARM.PL1L='A,X,NEST',REGION.GO=128K
702    //PL1L.SYSIN DD *
703     PLOT:PROC OPTIONS (MAIN);
704     DCL GRAPH ENTRY(FIXED BIN,(*) FLOAT,(*) FLOAT,FIXED
705     BIN,FIXED BIN,FLOAT,FLOAT,FLOAT,FLOAT,FLOAT,FLOAT,
706     CHAR(20),CHAR(20),CHAR(20),CHAR(20));
707     DCL GRAPHS ENTRY (FIXED BIN,(*) FLOAT,(*) FLOAT,FIXED
708     BIN,FIXED BIN,CHAR(20));
709     DCL LETTRS ENTRY (FLOAT,FLOAT,FLOAT,CHAR(80),FLOAT,
709.5   FIXED BIN);
710     DCL ORIGIN ENTRY (FLOAT,FLOAT,FIXED BIN);
711     DCL (XLAB,YLAB,GLAB,DATLAB) CHAR(20) VARYING;
712     DCL (STRING) CHAR (3);
713     CALL ORIGIN (0.0,3.0,1);
714     DO I=1 TO ###;
715     CALL ORIGIN (8.5,0.0,1);
716     CALL ORIGIN (1.0,-1.5,6);
717     GET LIST (IPLOT);
718     GET LIST (XLAB,YLAB,GLAB);
719     GET LIST (STRING);
720     GET LIST (NPOINTS,ISYM);
721     PLOT1:BEGIN;
722     DCL (X(NPOINTS),Y(NPOINTS)) FLOAT;
723     GET LIST (X);
724     GET LIST (Y);
725     GET LIST (DATLAB);
726     IF STRING='LOG' THEN DO;
727     X=LOG10(X);
```

```
Y=LOG10(Y);
END;
IF STRING='LOG' THEN DO;
I5=-5;
XYSF=0.5;
END;
ELSE DO;
I5=5;
XYSF=0.0;
END;
CALL GRAPH (NPOINTS,X,Y,ISYM,7,I5,I5,XYSF,0.0,XYSF,
0.0,';',';',';',DATLAB);
CALL LETTRS (0.0,5.5,0.2,GLAB,0.0,80);
CALL LETTRS ((5-(LENGTH(XLAB)/5))/2,-1.0,0.2,XLAB,
0.0,20);
CALL LETTRS (-1.0,(5-(LENGTH(YLAB)/5))/2,0.2,YLAB,
90.0,20);
END PLOT1;
IF IPLOTS=1 THEN GO TO STOP;
DO J=2 TO IPLOT;
GET LIST (NPOINTS,ISYM);
PLOTS:BEGIN;
DCL (X(NPOINTS),Y(NPOINTS)) FLOAT;
GET LIST (X);
GET LIST (Y);
GET LIST (DATLAB);
IF STRING='LOG' THEN DO;
X=LOG10(X);
Y=LOG10(Y);
END;
CALL GRAPHS (NPOINTS,X,Y,ISYM,107,DATLAB);
END PLOTS;
END;
END;
STOP:END PLOT;
//GO.SYSIN DD *
//GO.FT14F001 DD DSN=&SM,UNIT=SCRTCH,DISP=(NEW,PASS),
// SPACE=(800,(120,15)),DCB=(RECFM=VS,LRECL=796,
// BLKSIZE=800)
/*
//SMPLTTR EXEC PLOT,PLOTTER=INCRMNTL,FORM=W
/*
//
```

APPENDIX 4: TRSGJO

TRSGJO is an assembly language program which runs on the PDP8/E minicomputer. TRSGJO controls the x-ray pulse generation, data acquisition and format of the paper tape data set of the pulsed XEOL system. The assembly language program is composed of several subroutines. Many of the subroutines are utilities for accepting input from the keyboard or paper tape reader, generating output on the teletype or paper tape punch or performing simple numerical operations. The subroutines which contain interface instructions control the x-ray supply or gated integrator. The program, in compiled form, appears on the following pages.

```
              / TRSGJO
              / OESTREICH 5-20-77

        0000  FIELD 0

        0000  *0

        0020  *20

00020   7402            HLT
00021   0000  CNTR1,    0
00022   0000  CNTR2,    0
00023   3777  ISTORE,   3777
00024   0000  P,        0
00025   0000  PASSES,   0
00026   0000  SUM2,     0
00027   0000  NUMWAV,   0
00030   0000  DELTIM,   0
00031   0000  PUN1,     0
00032   0000  RUNCNT,   0
00033   0000  LUMIN,    0
00034   0000  DATPOT,   0
00035   0000  RANGE,    0
00036   0000  N,        0
00037   0000  SUM,      0
00040   0000  DELRAN,   0
00041   0000  TEMPST,   0
00042   0000            0
00043   0000  CNT1,     0
00044   0000  CNT2,     0
00045   0000  HIGH,     0
00046   0000  LOW,      0

        0200  *200

00200   7300  START,    CLA CLL          /CLEAR LINK & LINK
00201   6046            TLS              /RAISE TTY PRINT FLAG
00202   4577            JMS I  DATTIM    /INPUT DATE & TIME
00203   4576  RESET,    JMS I  RESET1    /RESET ROUTINE
00204   4231  PASS,     JMS SET1         /SET WORKING VARIABLES
00205   4575            JMS I  PREP      /ROTOR ON & ENABLE
00206   1033            TAD LUMIN
00207   7650            SNA CLA
00210   4304            JMS BOMB2        /XRAYS FAST
00211   4254            JMS BOMB         /X-RAYS SLOW
00212   4574            JMS I  SUMDAT
00213   4573            JMS I  SUMSQR    /SUM SQUARES
00214   2024            ISZ P            /TEST PASS COUNT
00215   5204            JMP PASS
```

```
0C216  4572            JMS I  DATOUT
0C217  7200            CLA
00220  1377            TAD (MSG15-1    /ANOTHER RUN ?
0C221  3017            DCA 17
00222  4571            JMS I  MESAGE
00223  4570            JMS I  NUMGET   /GET ANSWER
00224  7640            SZA CLA
00225  5203            JMP RESET
00226  4567            JMS I  ENDFIL
0C227  4566            JMS I  CRLF
00230  7402            HLT

00231  0000  SET1,     0               /SET WORKING VARIABLES
0C232  7200            CLA
00233  1023            TAD ISTORE      /SET STORAGE POINTER
0C234  3010            DCA 10
00235  1033            TAD LUMIN       /FAST OR SLOW
0C236  7650            SNA CLA
00237  5251            JMP POINTS      /FAST, GO BOMB
00240  7340            CLA CLL CMA     /SLOW, SET OTHERS
00241  1034            TAD DATPOT      /DATA POINT COUNTER
0C242  3037            DCA SUM
0C243  7340            CLA CLL CMA
00244  1010            TAD 10
00245  3010            DCA 10
0C246  1034            TAD DATPOT      /DATA REFERENCE
00247  3026            DCA SUM2
0C250  5631            JMP I SET1
00251  1027  POINTS,   TAD NUMWAV
0C252  3026            DCA SUM2
00253  5631            JMP I SET1

00254  0000  BOMB,     0               /BCMB ROUTINE
0C255  6337            CSTART          /CCNTROLLER STARTS
00256  1027            TAD NUMWAV      /# OF WAVES
0C257  3036            DCA N
00260  6331            CREADY          /COMPUTER READY
0C261  6332            NOW             /ZERO CROSSING OF WAVE
00262  5261            JMP .-1
0C263  6333  MULTI,    XON             /TURN XRAY ON
00264  7346            CLA CLL CMA RTL
0C265  4565            JMS I  DEL      /5 USEC * AC DELAY
0C266  6332            NOW             /INDICATES X-RAY OFF
0C267  5266            JMP .-1
00270  6334            XOFF            /HOLDS X-RAYS OFF
CC271  7346            CLA CLL CMA RTL
0C272  4565            JMS I  DEL      /5 USEC * AC DELAY
0C273  2036            ISZ N           /ANOTHER WAVE ?
00274  5263            JMP MULTI       /YES, REPEAT PROCESS
0C275  6336            CWAIT           /NO, RESET NOW PULSE
```

```
00276  6344            XDABLE              /XRAY DISABLE
00277  6342            ROTROF              /TURN ROTOR OFF
00300  1030            TAD DELTIM          /TRANSIENT DELAY
00301  4565            JMS I  DEL          /5 USEC * AC DELAY
00302  4564            JMS I  DATA         /COLLECT DATA
00303  5654            JMP I BOMB

00304  0000  BOMB2,    0                   /BCMB ROUTINE FAST
00305  6337            CSTART              /CONTROLLER START
00306  1027            TAD NUMWAV
00307  3036            DCA N
00310  6331            CREADY              /COMPUTER READY
00311  6332            NOW
00312  5311            JMP .-1
00313  6333  MULT,     XON                 /TURN XRAY ON
00314  1376            TAD (-1440
00315  4565            JMS I  DEL          /5 USEC * AC DELAY
00316  6345            STBOX               /START INTEGRATOR
00317  6332            NOW
00320  5317            JMP .-1
00321  6334            XOFF                /HOLD XRAY OFF
00322  1376            TAD (-1440
00323  4565            JMS I  DEL          /5 USEC * AC DELAY
00324  6455            STATOD              /START A TO D
00325  7346            CLA CLL CMA RTL
00326  4565            JMS I  DEL          /5 USEC * AC DELAY
00327  6354            GETDAT              /GET DATA POINT
00330  6346            INBOX               /RESET INTEGRATOR
00331  3410            DCA I 10
00332  6332            NOW
00333  5332            JMP .-1
00334  7346            CLA CLL CMA RTL
00335  4565            JMS I  DEL          /5 USEC * AC DELAY
00336  2036            ISZ N               /MORE WAVES ?
00337  5313            JMP MULT            /YES, BOMB
00340  6336            CWAIT               /NO, RESET
00341  6344            XDABLE              /DISABLE XRAY
00342  6342            ROTROF              /TURN ROTOR OFF
00343  2304            ISZ BOMB2
00344  5704            JMP I BOMB2

00376  6340
00377  3206

       0400  * 400

00400  0000  MESAGE,   0                   /MESSAGE ROUTINE
00401  7300  ENT10,    CLA CLL
00402  1241            TAD LIT1
00403  3240            DCA BYTCNT
```

```
00404  1417           TAD I 17
00405  3246           DCA STOR1
00406  1246           TAD STOR1
00407  7002           BSW             /BYTE SWAP
00410  0242  ENT11,   AND LIT2        /CHECK FOR TERMINATOR
00411  7440           SZA             /ZERO IN AC ?
00412  5214           JMP .+2         /NO; CONTINUE
00413  5600           JMP I MESAGE    /YES; END MESSAGE
00414  1243           TAD LIT3
00415  7500           SMA
00416  5221           JMP .+3
00417  1244           TAD LIT4
00420  5222           JMP .+2
00421  1245           TAD LIT5
00422  3247           DCA STOR2
00423  1247           TAD STOR2       /CHECK FOR CRLF
00424  1250           TAD MDOLAR
00425  7640           SZA CLA         /IS THE CHARACTER A $
00426  5231           JMP .+3         /NO; PRINT IT
00427  4566           JMS I  CRLF     /YES; CRLF
00430  5233           JMP .+3
00431  1247           TAD STOR2
00432  4563           JMS I  TYPEIT
00433  2240           ISZ BYTCNT      /GET NEXT CHARACTER
00434  5236           JMP .+2
00435  5201           JMP ENT10
00436  1246           TAD STOR1
00437  5210           JMP ENT11
00440  0000  BYTCNT,  0
00441  7776  LIT1,    7776
00442  0077  LIT2,    0077
00443  7745  LIT3,    7745
00444  0333  LIT4,    0333
00445  0233  LIT5,    0233
00446  0000  STOR1,   0
00447  0000  STOR2,   0
00450  7534  MDOLAR,  -244

00451  0000  NUMGET,  0               /NO INTERPRETER ROUTINE
00452  7300           CLA CLL
00453  3323           DCA DIGITS
00454  1324           TAD DIGLOC
00455  3010           DCA DIGPTR
00456  3325           DCA TEMP
00457  4562  GETDIG,  JMS I READ      /READ CHARACTER
00460  3325           DCA TEMP
00461  1325           TAD TEMP        /CHECK FOR ERASE
00462  1326           TAD MSLASH      /KEY (SLASH)
00463  7650           SNA CLA         /IS CHAR A SLASH ?
00464  5311           JMP ERROR       /YES; REPEAT ENTRY
```

```
00465  1325            TAD TEMP         /NO; TEST FOR TERMINAL
00466  1327            TAD RETURN       /RETURN CHARACTER
00467  7650            SNA CLA          /IS IT A RETURN ?
00470  5316            JMP CLEAR        /YES; EXIT THIS ROUTINE
00471  1325            TAD TEMP         /NO; CHECK FOR
00472  1377            TAD (-260        /OCTAL INPUT
00473  7510            SPA              /IS CHAR < 260 ?
00474  5311            JMP ERROR        /YES; GO TO ERROR
00475  1330            TAD MNINE        /NO; SUBTRACT 9 DECIMAL
00476  7740            SMA SZA CLA      /IS CHAR > 271 ?
00477  5311            JMP ERROR        /YES; GO TO ERROR
00500  1325            TAD TEMP         /NO; GET THE CHAR
00501  3410            DCA I DIGPTR
00502  2323            ISZ DIGITS       /INCREMENT DIGIT COUNT
00503  7300            CLA CLL
00504  1323            TAD DIGITS       /CHECK DIGIT COUNT
00505  1376            TAD (-4
00506  7740            SMA SZA CLA      /DIGITS <= 4 ?
00507  5311            JMP ERROR        /NO; GO TO ERROR BRANCH
00510  5257            JMP GETDIG
00511  4566  ERROR,    JMS I  CRLF      /CRLF
00512  1322            TAD MQM          /GET ?
00513  7041            CIA
00514  4563            JMS I  TYPEIT    /PRINT THE ?
00515  5252            JMP NUMGET+1     /DISREGARD BAD ENTRY
00516  7300  CLEAR,    CLA CLL
00517  4331            JMS CONVRT       /CONVERT TO OCTAL
00520  5651            JMP I NUMGET
00521  0000  MDIGIT,   0
00522  7501  MQM,      -277
00523  0000  DIGITS,   0
00524  0567  DIGLOC,   567
00525  0000  TEMP,     0
00526  7521  MSLASH,   -257
00527  7555  RETURN,   -223
00530  7767  MNINE,    -11
       0010            DIGPTR=10

00531  0000  CONVRT,   0                /CONVERT ASCII TO OCTAL
00532  7300            CLA CLL
00533  1323            TAD DIGITS       /SET DIGIT COUNTER
00534  7041            CIA
00535  3321            DCA MDIGIT
00536  1324            TAD DIGLOC       /SET POINTER
00537  3010            DCA DIGPTR
00540  3325            DCA TEMP         /ZERO TEMPORARY STORAGE
00541  1325  PACK,     TAD TEMP         /LOAD PARTIAL NUMBER
00542  7106            CLL RTL          /MULTIPLY BY 10
00543  1325            TAD TEMP
00544  7004            RAL
```

```
00545  3325          DCA TEMP
00546  1410          TAD I DIGPTR    /ADD NEXT STORED DIGIT
00547  1377          TAD (-260       /SUBTRACT 260
00550  1325          TAD TEMP        /ADD TO PARTIAL NUMBER
00551  3325          DCA TEMP        /STORE PARTIAL NUMBER
00552  2321          ISZ MDIGIT      /ALL DIGITS DONE ?
00553  5341          JMP PACK        /NO; GET ANOTHER
00554  1325          TAD TEMP        /YES; GET PACKED NUMBER
00555  5731          JMP I CONVRT

       0570  *570

00570  0000          0
00571  0000          0
00572  0000          0
00573  0000          0

00576  7774
00577  7520

       0600  * 600

00600  0000  SDPRNT, 0
00601  7300          CLA CLL
00602  1600          TAD I SDPRNT    /PICK UP ADDRESS OF
00603  3303          DCA SDGET       /HIGH ORDER WORD
00604  6211          CDF 10
00605  1703          TAD I SDGET     /GET HIGH ORDER WORD
00606  7700          SMA CLA         /IS IT NEGATIVE ?
00607  1272          TAD SDPLUS      /NO, GENERATE SPACE
00610  1273          TAD SDMNS       /YES, GENERATE MINUS
00611  1377          TAD (260
00612  4563          JMS I  TYPEIT   /TYPE IT OUT
00613  1703          TAD I SDGET     /GET HIGH ORDER WORD
00614  7510          SPA             /IS IT POSITIVE ?
00615  7060          CMA CML         /NO, COMPLEMENT IT
00616  3275          DCA SDHIGH      /STORE POSITIVE WORD
00617  2303          ISZ SDGET
00620  1703          TAD I SDGET     /PICK UP LOW ORDER WORD
00621  6201          CDF 00
00622  7430          SZL             /IS LINK SET ?
00623  7141          CMA CLL IAC     /YES, TWO'S COMPLEMENT
00624  7430          SZL             /DID AC OVERFLOW
00625  2275          ISZ SDHIGH      /YES, CORRECT HIGH WORD
00626  3276          DCA SDLOW       /STORE LOW ORDER WORD
00627  1270          TAD SDLOOP      /INITIALIZE COUNTER=7
00630  3274          DCA SDCNT
00631  1271          TAD SDADDR      /INITIALIZE POINTER TO
00632  3304          DCA SDPTR       /TABLE OF POWERS OF TEN
00633  2200          ISZ SDPRNT      /INDEX RETURN LINKAGE
```

```
00634  1704  SDARND, TAD I SDPTR     /PICK UP POWER OF TEN
00635  2304          ISZ SDPTR       /FOR USE IN SUBSTRACT
00636  3277          DCA SDHSUB
00637  1704          TAD I SDPTR
00640  2304          ISZ SDPTR
00641  3300          DCA SDLSUB
00642  7100  SDDO,   CLL             /DOUBLE PRECISION
00643  1300          TAD SDLSUB      /SUBTRACTION
00644  1276          TAD SDLOW
00645  3302          DCA SDTEML
00646  7004          RAL
00647  1277          TAD SDHSUB
00650  1275          TAD SDHIGH
00651  7510          SPA             /DID IT UNDERFLOW ?
00652  5260          JMP SDOUT       /NO, COUNT IS DONE
00653  2301          ISZ SDBOX       /YES, COUNT NOT DONE
00654  3275          DCA SDHIGH      /DEPOSIT HIGH ORDER
00655  1302          TAD SDTEML      /PORTION RESTORE LOW
00656  3276          DCA SDLOW       /ORDER PORTION
00657  5242          JMP SDDO        /GO BACK AND SUBTRACT
00660  7200  SDOUT,  CLA
00661  1301          TAD SDBOX       /PICK UP DIGIT
00662  1377          TAD (260
00663  4563          JMS I  TYPEIT   /TYPE IT OUT
00664  3301          DCA SDBOX       /INITIALIZE DIGIT TO 0
00665  2274          ISZ SDCNT       /HAVE WE TYPED 7 DIGITS
00666  5234          JMP SDARND      /NO, DETERMINE NEXT
00667  5600          JMP I SDPRNT    /YES, END ROUTINE
00670  7771  SDLOOP, -7              /COUNT OF 7 DIGITS
00671  0705  SDADDR, SDCONL          /ADDRESS OF POWERS
00672  7763  SDPLUS, -15             /'SPACE' GENERATOR
00673  7775  SDMNS,  -3              /'MINUS' GENERATOR
00674  0000  SDCNT,  0               /STORAGE LOCATIONS
00675  0000  SDHIGH, 0
00676  0000  SDLOW,  0
00677  0000  SDHSUB, 0
00700  0000  SDLSUB, 0
00701  0000  SDBOX,  0
00702  0000  SDTEML, 0
00703  0000  SDGET,  0
00704  0000  SDPTR,  0
00705  7413  SDCONL, 7413            /TABLE OF POWERS OF TEN
00706  6700          6700            /-1,000,000
00707  7747          7747            /-100,000
00710  4540          4540
00711  7775          7775            /-10,000
00712  4360          4360
00713  7777          7777            /-1,000
00714  6030          6030
00715  7777          7777            /-100
```

```
00716  7634            7634
00717  7777            7777         /-10
00720  7766            7766
00721  7777            7777         /-1
00722  7777            7777

00723  0000  SSPRNT,   0
00724  7100            CLL
00725  7510            SPA          /IS IT POSITIVE ?
00726  7061            CML CMA IAC  /NO, SET LINK
00727  3370            DCA SSVAL    /STORE NUMBER
00730  3366            DCA SSBOX    /SET LOCATION TO ZERO
00731  1365            TAD SSCNTR   /INITIALIZE COUNTER=4
00732  3367            DCA SSCNT
00733  1362            TAD SSADDR   /INITIALIZE INSTRUCTION
00734  3343            DCA SSXYZ+1  /TO GET FIRST 10
00735  1363            TAD SSPLUS   /GET CODE TO TYPE +
00736  7430            SZL          /IS NUMBER NEGATIVE ?
00737  1364            TAD SSMNS    /YES, CHANGE CODE TO -
00740  1377            TAD (260
00741  4563            JMS I  TYPEIT  /TYPE IT OUT
00742  1370  SSXYZ,    TAD SSVAL    /PICK UP NUMBER
00743  1371            TAD SSCON    /SUBSTRACT POWER OF TEN
00744  7510            SPA          /IS RESULT NEGATIVE ?
00745  5351            JMP .+4      /YES, INDEXING FINISHED
00746  2366            ISZ SSBOX    /NO, INDEX DIGIT LOCA.
00747  3370            DCA SSVAL    /STORE REMAINDER SSVAL
00750  5342            JMP SSXYZ    /CONTINUE SUBSTRACTING
00751  7200            CLA
00752  1366            TAD SSBOX    /GET THE DIGIT NUMBER
00753  1377            TAD (260
00754  4563            JMS I  TYPEIT  /TYPE IT OUT
00755  3366            DCA SSBOX    /DIGIT COUNTER=0
00756  2343            ISZ SSXYZ+1  /GET POWER OF TEN
00757  2367            ISZ SSCNT    /TYPED FOUR DIGITS
00760  5342            JMP SSXYZ    /NO, CONTINUE
00761  5723            JMP I SSPRNT /YES, RETURN
00762  1371  SSADDR,   TAD SSCON    /TO GET FIRST POWER
00763  7760  SSPLUS,   -20          /'SPACE' GENERATOR
00764  0015  SSMNS,    15           /'MINUS' GENERATOR
00765  7774  SSCNTR,   -4           /COUNT OF 4 DIGITS
00766  0000  SSBOX,    0            /STORAGE REGISTERS
00767  0000  SSCNT,    0
00770  0000  SSVAL,    0
00771  6030  SSCON,    6030         /-1000
00772  7634            7634         /-100
00773  7766            7766         /-10
00774  7777            7777         /-1

00777  0260
```

```
        1000    * 1000

01000   0000    ENDFIL, 0               /PUNCH TRAILER
01001   7200            CLA
01002   3031            DCA PUN1
01003   1377            TAD (204
01004   4264            JMS TYPEIT
01005   1376            TAD (-36
01006   3021            DCA CNTR1
01007   1375            TAD (377
01010   4264            JMS TYPEIT
01011   2021            ISZ CNTR1
01012   5207            JMP .-3
01013   1374            TAD (-372
01014   3021            DCA CNTR1
01015   4264            JMS TYPEIT
01016   2021            ISZ CNTR1
01017   5215            JMP .-2
01020   5600            JMP I ENDFIL

01021   0000    DEL,    0               /DEL ROUTINE
01022   3021            DCA CNTR1
01023   7000            NOP
01024   2021            ISZ CNTR1
01025   5223            JMP .-2
01026   5621            JMP I DEL

01027   0000    LEADER, 0               /PUNCH LEADER
01030   1374            TAD (-372
01031   3021            DCA CNTR1
01032   4264            JMS TYPEIT
01033   2021            ISZ CNTR1
01034   5232            JMP .-2
01035   1376            TAD (-36
01036   3021            DCA CNTR1
01037   1375            TAD (377
01040   4264            JMS TYPEIT
01041   2021            ISZ CNTR1
01042   5237            JMP .-3
01043   5627            JMP I LEADER

01044   0000    SPACE,  0               /PUNCH TWO SPACES
01045   7200            CLA
01046   1373            TAD (240
01047   4264            JMS TYPEIT
01050   1373            TAD (240
01051   4264            JMS TYPEIT
01052   5644            JMP I SPACE
```

```
01053  0000  ENDREC, 0             /PUNCH END RECORD CHAR.
01054  7200          CLA
01055  1372          TAD (223
01056  4264          JMS TYPEIT
01057  1375          TAD (377
01060  4264          JMS TYPEIT
01061  1375          TAD (377
01062  4264          JMS TYPEIT
01063  5653          JMP I ENDREC

01064  0000  TYPEIT, 0             /TTY PRINT ROUTINE
01065  6041          TSF
01066  5265          JMP .-1
01067  6046          TLS
01070  7300          CLA CLL
01071  5664          JMP I TYPEIT

01072  0000  CRLF,   0             /CRLF ROUTINE
01073  7300          CLA CLL
01074  1371          TAD (215
01075  4264          JMS TYPEIT
01076  1370          TAD (212
01077  4264          JMS TYPEIT
01100  5672          JMP I CRLF

01101  0000  READ,   0             /KEYBOARD READ ROUTINE
01102  6031          KSF
01103  5302          JMP .-1
01104  7300          CLA CLL
01105  6036          KRB
01106  6046          TLS
01107  5701          JMP I READ

01170  0212
01171  0215
01172  0223
01173  0240
01174  7406
01175  0377
01176  7742
01177  0204

       1200  *1200

01200  0000  DST,    0             /DOUBLE PRECISION STORE
01201  3222          DCA ACC       /SAVE AC
01202  6214          RDF           /SAVE DATA FIELD
01203  1220          TAD KCDF
01204  3211          DCA CHG       /GENERATE CDF INSTRUCT.
01205  6201          CDF 00
```

```
01206  1600            TAD I DST        /GET STORAGE ADDRESS
01207  3221            DCA ARG
01210  2200            ISZ DST          /SET RETURN ADDRESS
01211  0000  CHG,      0                /CHANGE DATA FIELD BACK
01212  1222            TAD ACC          /RECOVER AC
01213  3621            DCA I ARG        /STORE HIGH ORDER WORD
01214  2221            ISZ ARG
01215  7701            ACL              /LOAD AC FROM MQ
01216  3621            DCA I ARG        /STORE LOW ORDER  WORD
01217  5600            JMP I DST
01220  6201  KCDF,     CDF
01221  0000  ARG,      0
01222  0000  ACC,      0

01223  0000  DCM,      0                /DOUBLE PRECISION
01224  7100            CLL              /COMPLEMENT
01225  7040            CMA              /SET AC TO 7777
01226  7521            SWP
01227  7041            CIA              /NEGATE MQ CONTENTS
01230  7521            SWP
01231  7430            SZL              /CHECK FOR OVERFLOW
01232  7001            IAC
01233  5623            JMP I DCM

01234  0000  DAD,      0                /DOUBLE PRECISION ADD
01235  3222            DCA ACC          /SAVE AC
01236  6214            RDF              /SAVE DATA FIELD
01237  1220            TAD KCDF
01240  3245            DCA CHANG
01241  6201            CDF 00
01242  1634            TAD I DAD        /GET ADDRESS OF
01243  3221            DCA ARG          /STORED VALUES
01244  2234            ISZ DAD          /SET RETURN ADDRESS
01245  0000  CHANG,    0                /CHANGE DATA FIELD BACK
01246  1621            TAD I ARG        /GET HIGH ORDER STORED
01247  3262            DCA HIGHT        /VALUE AND SAVE
01250  2221            ISZ ARG
01251  7100            CLL
01252  7521            SWP              /LOAD MQ INTO AC
01253  1621            TAD I ARG        /GET LOW ORDER  STORED
01254  7521            SWP              /LOW ORDER SUM IN MQ
01255  7430            SZL              /WAS THERE A CARRY ?
01256  7101            IAC CLL          /YES, INCREMENT AC
01257  1222            TAD ACC          /NO, ADD HIGH ORDER
01260  1262            TAD HIGHT
01261  5634            JMP I DAD        /RETURN
01262  0000  HIGHT,    0

01263  0000  SUMDAT,   0                /SUM DATA
01264  7200            CLA
```

```
01265  1023           TAD ISTORE      /FIND DATA
01266  3010           DCA 10
01267  3306           DCA MSHPNT      /SET MSH POINTER
01270  3310           DCA MSHPNT+2
01271  1026           TAD SUM2
01272  3021           DCA CNTR1       /DATA COUNTER
01273  7621   SUMLUP, CAM
01274  1410           TAD I 10        /GET FIRST VALUE
01275  7500           SMA             /IS IT NEGATIVE ?
01276  5303           JMP ADD1        /NO, ADD IT
01277  7041           CIA             /YES, MAKE IT POSITIVE
01300  7521           SWP             /PUT IN MQ
01301  4223           JMS DCM         /MAKE IT NEGATIVE
01302  7410           SKP
01303  7521   ADD1,   SWP             /PUT IN MQ
01304  6211           CDF 10
01305  4234           JMS DAD         /DCUBLE PRECISION ACD
01306  0000   MSHPNT, 0
01307  4200           JMS DST         /DCUBLE PRECISION STOPE
01310  0000   DUMMY,  0
01311  6201           CDF 00
01312  2306           ISZ MSHPNT      /SET NEW ADDRESS
01313  2306           ISZ MSHPNT
01314  2310           ISZ MSHPNT+2
01315  2310           ISZ MSHPNT+2
01316  2021           ISZ CNTR1       /ALL DATA SUMMED ?
01317  5273           JMP SUMLUP      /NO, NEXT VALUE
01320  7300           CLA CLL         /YES, DELAY
01321  1033           TAD LUMIN       /DELAY TEST
01322  7650           SNA CLA         /FAST OR SLOW ?
01323  5347           JMP STDEL       /FAST, DELAY
01324  1035           TAD RANGE       /SLOW, TEST
01325  7041           CIA
01326  7001           IAC
01327  7450           SNA             /10 MSEC RANGE ?
01330  5342           JMP TESTA       /YES, TEST TWO
01331  7001           IAC             /NO, 100 MSEC RANGE ?
01332  7640           SZA CLA
01333  5663           JMP I SUMDAT    /NC, FORGET DELAY
01334  1034           TAD DATPOT      /YES, TEST TWO
01335  7041           CIA
01336  0377           AND (7400
01337  7640           SZA CLA
01340  5663           JMP I SUMDAT
01341  5347           JMP STDEL
01342  1034   TESTA,  TAD DATPOT
01343  7041           CIA
01344  0376           AND (4000
01345  7640           SZA CLA
01346  5663           JMP I SUMDAT
```

```
01347  1375   STDEL,   TAD (-3720        /STANDARD DELAY
01350  3022            DCA CNTR2
01351  1375   DELMIN,  TAD (-3720
01352  4565            JMS I  DEL        /5 USEC * AC DELAY
01353  2022            ISZ CNTR2
01354  5351            JMP DELMIN
01355  5663            JMP I SUMDAT      /END

01375  4060
01376  4000
01377  7400

       1400   *1400

01400  0000   DATOUT,  0                 /PUNCH GENERAL DATA
01401  7200            CLA
01402  1031            TAD PUN1
01403  7650            SNA CLA
01404  4561            JMS I  LEADER     /PUNCH LEADER
01405  2031            ISZ PUN1
01406  4566            JMS I  CRLF
01407  4560            JMS I  ENDREC
01410  1377            TAD (-6
01411  3021            DCA CNTR1
01412  1376            TAD (PNTDAT
01413  3013            DCA 13
01414  1413            TAD I 13
01415  4563            JMS I  TYPEIT
01416  2021            ISZ CNTR1
01417  5214            JMP .-3
01420  4557            JMS I  SPACE
01421  1413            TAD I 13
01422  1413            TAD I 13
01423  7200            CLA
01424  1375            TAD (-4
01425  3021            DCA CNTR1
01426  1413            TAD I 13
01427  4563            JMS I  TYPEIT
01430  2021            ISZ CNTR1
01431  5226            JMP .-3
01432  4557            JMS I  SPACE
01433  1032            TAD RUNCNT
01434  4556            JMS I  SSPRNT
01435  4557            JMS I  SPACE
01436  1027            TAD NUMWAV
01437  7041            CIA
01440  4556            JMS I  SSPRNT
01441  4557            JMS I  SPACE
01442  1025            TAD PASSES
01443  7041            CIA
```

```
01444  4556           JMS I  SSPRNT
01445  4557           JMS I  SPACE
01446  1026           TAD SUM2
01447  7041           CIA
01450  4556           JMS I  SSPRNT
01451  4557           JMS I  SPACE
01452  1033           TAD LUMIN
01453  4556           JMS I  SSPRNT
01454  4557           JMS I  SPACE
01455  1033           TAD LUMIN
01456  7650           SNA CLA
01457  5267           JMP CONTIN
01460  1030           TAD DELTIM
01461  7041           CIA
01462  4556           JMS I  SSPRNT
01463  4557           JMS I  SPACE
01464  1035           TAD RANGE
01465  4556           JMS I  SSPRNT
01466  4557           JMS I  SPACE
01467  4566  CONTIN,  JMS I  CRLF
01470  4560           JMS I  ENDREC
01471  4555           JMS I  PUNCH
01472  4554           JMS I  PUNSQR
01473  5600           JMP I DATOUT     /END

01474  0000  PUNCH,   0                /SUMMED DATA OUTPUT
01475  7200           CLA
01476  3305           DCA ADR
01477  1026           TAD SUM2
01500  3021           DCA CNTR1
01501  1374  LOP,     TAD (-7
01502  3022           DCA CNTR2
01503  7200  INLOP,   CLA
01504  4553           JMS I  SDPRNT
01505  0000  ADR,     0
01506  4557           JMS I  SPACE
01507  2305           ISZ ADR
01510  2305           ISZ ADR
01511  2021           ISZ CNTR1
01512  5314           JMP .+2
01513  5321           JMP ENDTAP
01514  2022           ISZ CNTR2
01515  5303           JMP INLOP
01516  4566           JMS I  CRLF
01517  4560           JMS I  ENDREC
01520  5301           JMP LOP
01521  4566  ENDTAP,  JMS I  CRLF
01522  4560           JMS I  ENDREC
01523  1373           TAD (5777        /OVERLOAD OUTPUT
01524  3010           DCA 10
```

```
01525  3305            DCA ADR
01526  2305            ISZ ADR
01527  1026            TAD SUM2
01530  3021            DCA CNTR1
01531  1372            TAD (-5
01532  3022            DCA CNTR2
01533  7200  LOPIN,    CLA
01534  1410            TAD I 10
01535  7450            SNA
01536  5352            JMP POL
01537  4556            JMS I  SSPRNT
01540  4557            JMS I  SPACE
01541  1305            TAD ADR
01542  4556            JMS I  SSPRNT
01543  4557            JMS I  SPACE
01544  2022            ISZ CNTR2
01545  5352            JMP POL
01546  4566            JMS I  CRLF
01547  4560            JMS I  ENDREC
01550  1372            TAD (-5
01551  3022            DCA CNTR2
01552  2305  POL,      ISZ ADR
01553  2021            ISZ CNTR1
01554  5333            JMP LOPIN
01555  7200            CLA
01556  4556            JMS I  SSPRNT
01557  4557            JMS I  SPACE
01560  4556            JMS I  SSPRNT
01561  4557            JMS I  SPACE
01562  4566            JMS I  CRLF
01563  4560            JMS I  ENDREC
01564  5674            JMP I PUNCH

01572  7773
01573  5777
01574  7771
01575  7774
01576  1711
01577  7772

       1600  *1600

01600  0000  RESET1,   0                 /RESET FOR RUN
01601  2032            ISZ RUNCNT        /SET RUN COUNTER
01602  7200            CLA
01603  1377            TAD (MSG03-1      /REPEAT RUN
01604  3017            DCA 17
01605  4571            JMS I  MESAGE
01606  4570            JMS I  NUMGET     /GET ANSWER
01607  7650            SNA CLA           /REPEAT ?
```

```
01610  4552            JMS I  MESSY     /NO, PRINT MESSAGES
01611  1025            TAD PASSES       /YES, RESET VARIABLES
01612  3024            DCA P
01613  3021            DCA CNTR1        /ZERO FIELD 1
01614  6211            CDF 10
01615  3421   ZLOOP,   DCA I CNTR1
01616  2021            ISZ CNTR1
01617  5215            JMP ZLOOP
01620  6201            CDF 00
01621  1376            TAD (3777        /ZERO OVERLOAD
01622  3010            DCA 10
01623  1375            TAD (-3000
01624  3021            DCA CNTR1
01625  3410            DCA I 10
01626  2021            ISZ CNTR1
01627  5225            JMP .-2
01630  5600            JMP I RESET1

01631  0000   PREP,    0                /ROTOR ON & ENABLE
01632  6341            ROTRON           /TURN ROTOR ON
01633  7200            CLA
01634  1374            TAD (-764        /DELAY 5 SEC
01635  3022            DCA CNTR2
01636  1373   RLOOP,   TAD (-3720
01637  4565            JMS I  DEL       /5 USECD * AC DELAY
01640  2022            ISZ CNTR2
01641  5236            JMP RLOOP
01642  6343            XABLE            /ENABLE X-RAYS
01643  1372            TAD (-6          /DELAY 60 MSEC
01644  3022            DCA CNTR2
01645  1373   XLOOP,   TAD (-3720
01646  4565            JMS I  DEL       /5 USEC * AC DELAY
01647  2022            ISZ CNTR2
01650  5245            JMP XLOOP
01651  6455            INATOD           /INITIALIZE A TO D
01652  6346            INBOX            /INITIALIZE INTEGRATOR
01653  5631            JMP I PREP       /END

01654  0000   DATTIM,  0                /DATE & TIME ROUTINE
01655  1371            TAD (MSG01-1
01656  3017            DCA 17
01657  4571            JMS I  MESAGE    /PRINT MESSAGE
01660  7200            CLA
01661  1372            TAD (-6
01662  3021            DCA CNTR1        /SET DIGIT COUNTER
01663  1310            TAD DATPNT       /GET STORAGE LOCATION
01664  3311            DCA PNTDAT
01665  4562   DNEXT,   JMS I  READ      /GET DIGIT
01666  3711            DCA I PNTDAT     /STORE DIGIT
01667  2311            ISZ PNTDAT       /RESET STORAGE LOCATION
```

```
01670  2021           ISZ CNTR1         /MORE DIGITS ?
01671  5265           JMP DNEXT         /YES, GET DIGIT
01672  1370           TAD (MSG02-1      /NO, GET TIME
01673  3017           DCA 17
01674  4571           JMS I  MESAGE     /PRINT MESSAGE
01675  7200           CLA
01676  1367           TAD (-4
01677  3021           DCA CNTR1         /SET DIGIT COUNTER
01700  1320           TAD TIMPNT        /GET STORAGE LOCATION
01701  3321           DCA PNTTIM
01702  4562  TNEXT,   JMS I  READ       /GET DIGIT
01703  3721           DCA I PNTTIM      /STORE DIGIT
01704  2321           ISZ PNTTIM        /RESET
01705  2021           ISZ CNTR1         /MORE DIGITS ?
01706  5302           JMP TNEXT         /YES, GET DIGIT
01707  5654           JMP I DATTIM      /NO, END ROUTINE
01710  1712  DATPNT,  DATPNT+2
01711  0000  PNTDAT,  0
01712  0000           0                 /STORAGE OF DATE
01713  0000           0
01714  0000           0
01715  0000           0
C1716  0000           0
01717  0000           0
01720  1722  TIMPNT,  TIMPNT+2
01721  0000  PNTTIM,  0
01722  0000           0                 /STORAGE OF TIME
01723  0000           0
01724  0000           0
01725  0000           0

01767  7774
01770  3006
01771  2777
01772  7772
01773  4060
01774  7014
C1775  5000
01776  3777
01777  3020

       2000  *2000

02000  0000  MESSY,   0                 /INFORMATION INPUT
02001  1377           TAD (MSG04-1      /GET # OF WAVES
02002  3017           DCA 17
02003  4571           JMS I  MESAGE
02004  4570           JMS I  NUMGET     /GET ANSWER
02005  7041           CIA
02006  3027           DCA NUMWAV
```

```
02007  1376           TAD (MSG05-1     /# OF PASSES
02010  3017           DCA 17
02011  4571           JMS I  MESAGE
02012  4570           JMS I  NUMGET    /GET ANSWER
02013  7041           CIA
02014  3025           DCA PASSES
02015  1375           TAD (MSG06-1     /FAST OR SLOW ?
02016  3017           DCA 17
02017  4571           JMS I  MESAGE
02020  4570           JMS I  NUMGET    /GET ANSWER
02021  3033           DCA LUMIN
02022  1033           TAD LUMIN
02023  7650           SNA CLA
02024  5600           JMP I MESSY
02025  1374           TAD (MSG07-1     /TRANSIENT DECAY
02026  3017           DCA 17
02027  4571           JMS I  MESAGE
02030  4570           JMS I  NUMGET    /GET ANSWER
02031  7041           CIA
02032  3030           DCA DELTIM
02033  1373           TAD (MSG08-1     /# DATA POINTS
02034  3017           DCA 17
02035  4571           JMS I  MESAGE
02036  4570           JMS I  NUMGET    /GET ANSWER
02037  7041           CIA
02040  3034           DCA DATPOT
02041  1372           TAD (MSG09-1     /RANGE CODE
02042  3017           DCA 17
02043  4571           JMS I  MESAGE
02044  4570           JMS I  NUMGET    /GET ANSWER
02045  3035           DCA RANGE
02046  1035           TAD RANGE
02047  1255           TAD PTR
02050  3254           DCA TEMPER
02051  1654           TAD I TEMPER
02052  3040           DCA DELRAN
02053  5600           JMP I MESSY
02054  0000  TEMPER,  0
02055  2055  PTR,     PTR
02056  2217           DEL1
02057  2223           DEL2
02060  2233           DEL3

02172  3162
02173  3152
02174  3116
02175  3070
02176  3056
02177  3041
```

```
        2200   *2200

02200   0000   DATA,   0                 /DATA ROUTINE
02201   6455           STATOD            /START A TO D
02202   7346           CLA CLL CMA RTL
02203   4565           JMS I  DEL        /5 USEC * AC DELAY
02204   6354           GETDAT            /GET DATA POINT
02205   6346           INBOX             /INITIAL INTEGRATOR
02206   3410           DCA I 10          /STORE DATA
02207   2037           ISZ SUM           /MORE DATA ?
02210   5212           JMP .+2           /YES, GET IT
02211   5600           JMP I DATA        /NO, STOP
02212   1377           TAD (-276
02213   4565           JMS I  DEL        /5 USEC * AC DELAY
02214   6345           STBOX             /START INTEGRATOR
02215   4440           JMS I DELRAN      /DELAY RANGE VALUE
02216   5201           JMP DATA+1

02217   0000   DEL1,   0                 /10 MSEC DELAY
02220   1376           TAD (-3405
02221   4565           JMS I  DEL
02222   5617           JMP I DEL1

02223   0000   DEL2,   0                 /100 MSEC DELAY
02224   1375           TAD (-5
02225   3022           DCA CNTR2
02226   1374           TAD (213
02227   4565           JMS I  DEL
02230   2022           ISZ CNTR2
02231   5226           JMP .-3
02232   5623           JMP I DEL2

02233   0000   DEL3,   0                 /1 SEC DELAY
02234   1373           TAD (-62
02235   3022           DCA CNTR2
02236   1372           TAD (147
02237   4565           JMS I  DEL
02240   7000           NOP
02241   2022           ISZ CNTR2
02242   5236           JMP .-4
02243   5633           JMP I DEL3

02244   0000   UDPRNT, 0
02245   7300           CLA CLL
02246   1644           TAD I UDPRNT      /PICK UP ADDRESS OF
02247   3331           DCA UDGET         /HIGH ORDER WORD
02250   6211           CDF 10
02251   1731           TAD I UDGET       /PICK UP BOTH WORDS FOR
02252   3323           DCA UDHIGH        /USE IN SUBROUTINE
02253   2331           ISZ UDGET
```

```
02254  1731            TAD I UDGET
02255  3324            DCA UDLOW
02256  6201            CDF 00
02257  1320            TAD UDLOOP      /INITIALIZE COUNTER
02260  3322            DCA UDCNT
02261  1321            TAD UDADDR      /INITIALIZE TO TABLE OF
02262  3332            DCA UDPTR       /POWERS OF TEN
02263  2244            ISZ UDPRNT      /SET RETURN ADDRESS
02264  1732  UDARND,   TAD I UDPTR     /PICK UP FIRST POWER
02265  2332            ISZ UDPTR       /FOR USE IN SUBTRACTION
02266  3325            DCA UDHSUB
02267  1732            TAD I UDPTR
02270  2332            ISZ UDPTR
02271  3326            DCA UDLSUB
02272  7100  UDDO,     CLL             /DOUBLE PRECISION SUB
02273  1326            TAD UDLSUB
02274  1324            TAD UDLOW
02275  3330            DCA UDTEML
02276  7004            RAL
02277  1325            TAD UDHSUB
02300  1323            TAD UDHIGH
02301  7420            SNL             /DID IT OVERFLOW ?
02302  5310            JMP UDOUT       /NO, COUNT IS DONE
02303  2327            ISZ UDBOX       /YES, CONTINUE
02304  3323            DCA UDHIGH      /SAVE REMAINDER
02305  1330            TAD UDTEML
02306  3324            DCA UDLOW
02307  5272            JMP UDDO
02310  7200  UDOUT,    CLA
02311  1327            TAD UDBOX       /GET DIGIT
02312  1371            TAD (260
02313  4563            JMS I  TYPEIT   /TYPE IT
02314  3327            DCA UDBOX
02315  2322            ISZ UDCNT       /MORE DIGITS ?
02316  5264            JMP UDARND      /YES, GET NEXT
02317  5644            JMP I UDPRNT    /NO, DONE
02320  7770  UDLOOP,   -10
02321  2333  UDADDR,   UDCONL
02322  0000  UDCNT,    0
02323  0000  UDHIGH,   0
02324  0000  UDLOW,    0
02325  0000  UDHSUB,   0
02326  0000  UDLSUB,   0
02327  0000  UDBOX,    0
02330  0000  UDTEML,   0
02331  0000  UDGET,    0
02332  0000  UDPTR,    0
02333  3166  UDCONL,   3166            /POWERS OF TEN
02334  4600            4600            /-10,000,000
02335  7413            7413            /-1,000,000
```

```
02336  6700           6700
02337  7747           7747             /-100,000
02340  4540           4540
02341  7775           7775             /-10,000
02342  4360           4360
02343  7777           7777             /-1000
02344  6030           6030
02345  7777           7777             /-100
02346  7634           7634
02347  7777           7777             /-10
02350  7766           7766
02351  7777           7777             /-1
02352  7777           7777

02371  0260
02372  0147
02373  7716
02374  0213
02375  7773
02376  4373
02377  7502

       2400   *2400

02400  0000   SQR,    0                /SQUARE ROUTINE
02401  1600           TAD I SQR        /GET DATA ADDRESS
02402  3273           DCA ARGU
02403  2200           ISZ SQR          /SET RETURN ADDRESS
02404  1673           TAD I ARGU       /GET DATA POINT
02405  7041           CIA              /MAKE IT POSITIVE
02406  3274           DCA STORE        /STORE TEMPORAILY
02407  1274           TAD STORE
02410  3275           DCA TEST         /SET TEST VALUE
02411  7001           IAC
02412  3276           DCA MASK         /SET MASK TO ONE
02413  1377           TAD (-14         /SET BIT COUNTER
02414  3044           DCA CNT2
02415  3045           DCA HIGH
02416  3046           DCA LOW
02417  1275   TESTBT, TAD TEST
02420  0276           AND MASK         /CHECK FOR BIT TRUE
02421  7740           SZA CLA CLL      /TRUE ?
02422  5235           JMP ADD          /YES, ADD PARTIAL PROD.
02423  1276   RETUR,  TAD MASK         /RESET MASK
02424  7104           RAL CLL
02425  3276           DCA MASK
02426  2044           ISZ CNT2         /MORE BITS ?
02427  5217           JMP TESTBT       /YES, TEST NEXT
02430  1046           TAD LOW          /NO, LOAD RESULT IN
02431  7521           SWP              /MQ AND AC
```

```
02432  7200            CLA
02433  1045            TAD HIGH
02434  5600            JMP I SQR          /END
02435  1044  ADD,      TAD CNT2           /DETERMINE WHICH BIT
02436  1376            TAD (14            /WAS BEING TESTED
02437  7140            CMA CLL
02440  3043            DCA CNT1
02441  1274            TAD STORE
02442  3041            DCA TEMPST
02443  3042            DCA TEMPST+1
02444  2043  REDO,     ISZ CNT1           /SET VALUE OF
02445  5247            JMP .+2            /PARTIAL PRODUCT
02446  5262            JMP DADSTP         /ADD PARTIAL PRODUCT
02447  1042            TAD TEMPST+1
02450  7004            RAL
02451  3042            DCA TEMPST+1
02452  1041            TAD TEMPST
02453  7004            RAL
02454  3041            DCA TEMPST
02455  7420            SNL                /CHECK FOR OVERFLOW
02456  5244            JMP REDO           /NO, CONTINUE
02457  2042            ISZ TEMPST+1       /YES, INCREMENT MSD
02460  7100            CLL
02461  5244            JMP REDO
02462  1041  DADSTP,   TAD TEMPST         /DOUBLE PRECISION ADD
02463  7521            SWP
02464  7200            CLA
02465  1042            TAD TEMPST+1
02466  4551            JMS I  DAD         /ADD ROUTINE
02467  0045            HIGH
02470  4550            JMS I  DST         /STORE ROUTINE
02471  0045            HIGH
02472  5223            JMP RETUR
02473  0000  ARGU,      0
02474  0000  STORE,     0
02475  0000  TEST,      0
02476  0000  MASK,      0

02477  0000  SUMSQR,    0                 /SUM OF SQUARES
02500  7300            CLA CLL
02501  1375            TAD (4000          /STORAGE ADDRESS
02502  3317            DCA MSHSQR
02503  1375            TAD (4000
02504  3321            DCA MSHSQR+2
02505  1375            TAD (4000          /RESET DATA LOCATOR
02506  3314            DCA DATLOC
02507  1026            TAD SUM2           /GET # DATA POINTS
02510  3021            DCA CNTR1
02511  1374            TAD (6000          /OVERFLOW COUNTERS
02512  3022            DCA CNTR2
```

```
02513  4200  SQRSUM, JMS SQR         /SQUARE VALUE
02514  4000  DATLOC, 4000
02515  6211          CDF 10
02516  4551          JMS I  DAD      /DOUBLE PRECISION ADD
02517  0000  MSHSQR, 0
02520  4550          JMS I  DST      /DOUBLE PRECISION STORE
02521  0000  DUMB,   0
02522  6201          CDF 00
02523  7430          SZL             /TEST, OVERFLOW
02524  2422          ISZ I CNTR2     /YES, INCREMENT COUNTER
02525  7100          CLL
02526  2022          ISZ CNTR2       /RESET ADDRESS
02527  2314          ISZ DATLOC
02530  2317          ISZ MSHSQR
02531  2317          ISZ MSHSQR
02532  2321          ISZ MSHSQR+2
02533  2321          ISZ MSHSQR+2
02534  2021          ISZ CNTR1       /MORE DATA ?
02535  5313          JMP SQRSUM      /YES, SQUARE & ADD
02536  5677          JMP I SUMSQR    /NO, RETURN

02537  0000  PUNSQR, 0               /SUMMED SQUARES OUTPUT
02540  7200          CLA
02541  1375          TAD (4000
02542  3351          DCA ADRSQR
02543  1026          TAD SUM2
02544  3021          DCA CNTR1
02545  1373  LOPSQR, TAD (-7
02546  3022          DCA CNTR2
02547  7200  INSQR,  CLA
02550  4547          JMS I  UDPRNT
02551  0000  ADRSQR, 0
02552  4557          JMS I  SPACE
02553  2351          ISZ ADRSQR
02554  2351          ISZ ADRSQR
02555  2021          ISZ CNTR1
02556  5360          JMP .+2
02557  5365          JMP ENDSQR
02560  2022          ISZ CNTR2
02561  5347          JMP INSQR
02562  4566          JMS I  CRLF
02563  4560          JMS I  ENDREC
02564  5345          JMP LOPSQR
02565  4566  ENDSQR, JMS I  CRLF
02566  4560          JMS I  ENDREC
02567  5737          JMP I PUNSQR

02573  7771
02574  6000
02575  4000
```

```
02576   0014
02577   7764

        3000   *3000

03000   4424   MSG01,   TEXT /$TODAYS DATE /
03001   1704
03002   0131
03003   2340
03004   0401
03005   2405
03006   4000
03007   4040   MSG02,   TEXT /  TIME (MILITARY) /
03010   2411
03011   1505
03012   4050
03013   1511
03014   1411
03015   2401
03016   2231
03017   5140
03020   0000
03021   4422   MSG03,   TEXT /$REPEAT PREVIOUS RUN 1-YES,
03022   0520                  0-NO /
03023   0501
03024   2440
03025   2022
03026   0526
03027   1117
03030   2523
03031   4022
03032   2516
03033   4061
03034   5531
03035   0523
03036   5440
03037   6055
03040   1617
03041   4000
03042   4416   MSG04,   TEXT /$NUMBER OF WAVES IN BOMB /
03043   2515
03044   0205
03045   2240
03046   1706
03047   4027
03050   0126
03051   0523
03052   4011
03053   1640
03054   0217
```

```
03055  1502
03056  4000
03057  4040  MSG05,   TEXT /  NUMBER OF PASSES /
03060  1625
03061  1502
03062  0522
03063  4017
03064  0640
03065  2001
03066  2323
03067  0523
03070  4000
03071  4406  MSG06,   TEXT /$FAST OR SLOW LUMINESCENCE
03072  0123                0-FAST, 1-SLOW /
03073  2440
03074  1722
03075  4023
03076  1417
03077  2740
03100  1425
03101  1511
03102  1605
03103  2303
03104  0516
03105  0305
03106  4060
03107  5506
03110  0123
03111  2454
03112  4061
03113  5523
03114  1417
03115  2740
03116  0000
03117  4424  MSG07,   TEXT /$TRANSIENT DECAY 5.0 USEC-CNT
03120  2201                INITIAL OFFSET 12.6 USEC /
03121  1623
03122  1105
03123  1624
03124  4004
03125  0503
03126  0131
03127  4065
03130  5660
03131  4025
03132  2305
03133  0355
03134  0316
03135  2440
03136  1116
```

```
03137  1124
03140  1101
03141  1440
03142  1706
03143  0623
03144  0524
03145  4061
03146  6256
03147  6640
03150  2523
03151  0503
03152  4000
03153  4443  MSG08,   TEXT /$# DATA POINTS /
03154  4004
03155  0124
03156  0140
03157  2017
03160  1116
03161  2423
03162  4000
03163  4040  MSG09,   TEXT /  RANGE CODE 1-10, 2-100, 3-1000
03164  2201                MSEC /
03165  1607
03166  0540
03167  0317
03170  0405
03171  4061
03172  5561
03173  6054
03174  4062
03175  5561
03176  6060
03177  5440
03200  6355
03201  6160
03202  6060
03203  4015
03204  2305
03205  0340
03206  0000
03207  4403  MSG15,   TEXT /$CONTINUE RUNS 1-YES, 0-NO /
03210  1716
03211  2411
03212  1625
03213  0540
03214  2225
03215  1623
03216  4061
03217  5531
03220  0523
```

```
03221   5440
03222   6055
03223   1617
03224   4000

        6345          STBOX=6345
        6455          STATOD=6455
        6354          GETDAT=6354
        6346          INBOX=6346
        6455          INATOD=6455
        6344          XDABLE=6344
        6342          ROTROF=6342
        6337          CSTART=6337
        6331          CREADY=6331
        6332          NOW=6332
        6333          XON=6333
        6334          XOFF=6334
        6336          CWAIT=6336
        6343          XABLE=6343
        6341          ROTRON=6341
        7701          ACL=7701
        7621          CAM=7621

            $

00147   2244
00150   1200
00151   1234
00152   2000
00153   0600
00154   2537
00155   1474
00156   0723
00157   1044
00160   1053
00161   1027
00162   1101
00163   1064
00164   2200
00165   1021
00166   1072
00167   1000
00170   0451
00171   0400
00172   1400
00173   2477
00174   1263
00175   1631
00176   1600
00177   1654
```

ACC	1222
ACL	7701
ADD	2435
ADD1	1303
ADR	1505
ADRSQR	2551
ARG	1221
ARGU	2473
BCMB	0254
BCMB2	0304
BYTCNT	0440
CAM	7621
CHANG	1245
CHG	1211
CLEAR	0516
CNTR1	0021
CNTR2	0022
CNT1	0043
CNT2	0044
CONTIN	1467
CONVRT	0531
CREADY	6331
CRLF	1072
CSTART	6337
CWAIT	6336
DAD	1234
DADSTP	2462
DATA	2200
DATLOC	2514
DATOUT	1400
DATPNT	1710
DATPOT	0034
DATTIM	1654
DCM	1223
DEL	1021
DELMIN	1351
DELRAN	0040
DELTIM	0030
DEL1	2217
DEL2	2223
DEL3	2233
DIGITS	0523
DIGLOC	0524
DIGPTR	0010
DNEXT	1665
DST	1200
DUMB	2521
DUMMY	1310
ENDFIL	1000
ENDREC	1053
GETDAT	6354
GETDIG	0457
HIGH	0045
HIGHT	1262
INATOD	6455
INBOX	6346
INLOP	1503
INSQR	2547
ISTORE	0023
KCDF	1220
LEADER	1027
LIT1	0441
LIT2	0442
LIT3	0443
LIT4	0444
LIT5	0445
LOP	1501
LOPIN	1533
LOPSQR	2545
LOW	0046
LUMIN	0033
MASK	2476
MDIGIT	0521
MDOLAR	0450
MESAGE	0400
MESSY	2000
MNINE	0530
MQM	0522
MSG01	3000
MSG02	3007
MSG03	3021
MSG04	3042
MSG05	3057
MSG06	3071
MSG07	3117
MSG08	3153
MSG09	3163
MSG15	3207
MSHPNT	1306
MSHSQR	2517
MSLASH	0526
MULT	0313
MULTI	0263
N	0036
NOW	6332
NUMGET	0451
NUMWAV	0027
P	0024
PACK	0541
PASS	0204
PREP	1631
PTR	2055
PUNCH	1474
PUNSQR	2537
PUN1	0031
RANGE	0035
READ	1101
REDO	2444
RESET	0203
RESET1	1600
RETUR	2423
RETURN	0527
RLOOP	1636
ROTROF	6342
ROTRON	6341
RUNCNT	0032
SDADDR	0671
SDARND	0634
SDBOX	0701
SDCNT	0674
SDCONL	0705
SDDO	0642
SDGET	0703
SDHIGH	0675
SDHSUB	0677
SDLOOP	0670
SDLOW	0676
SDLSUB	0700
SDMNS	0673
SDOUT	0660
SDPLUS	0672
SDPRNT	0600
SDPTR	0704
SDTEML	0702
SET1	0231
SPACE	1044
SQR	2400
SQRSUM	2513
SSADDR	0762
SSBOX	0766
SSCNT	0767
SSCNTR	0765
SSCON	0771
SSMNS	0764
SSPLUS	0763
SSPRNT	0723
SSVAL	0770
SSXYZ	0742
START	0200
STATOD	6455
SUM	0037
SUMDAT	1263
SUMLUP	1273
SUMSQR	2477
SUM2	0026
TEMP	0525
TEMPER	2054
TEMPST	0041
TEST	2475
TESTA	1342
TESTBT	2417
TIMPNT	1720
TNEXT	1702
TYPEIT	1064
UDADDR	2321
UDARND	2264
UDBOX	2327
UDCNT	2322
UDCONL	2333
UDDO	2272
UDGET	2331
UDHIGH	2323
UDHSUB	2325
UDLOOP	2320
UDLOW	2324
UDLSUB	2326
UDOUT	2310
UDPRNT	2244
UDPTR	2332
UDTEML	2330
XABLE	6343
XDABLE	6344
XLOOP	1645
XOFF	6334
XON	6333
ZLOOP	1615

ENDSQR	2565	PASSES	0025	STBOX	6345
ENDTAP	1521	PNTDAT	1711	STDEL	1347
ENT10	0401	PNTTIM	1721	STORE	2474
ENT11	0410	POINTS	0251	STOR1	0446
ERROR	0511	POL	1552	STOR2	0447

ERRORS DETECTED: 0
LINKS GENERATED: 0

APPENDIX 5: JCL

JCL is the acronym for job control language. The listing which follows contains all the JCL statements required to run the job which calculates the experimental results. The sections where data and program source decks belong are indicated in the listing. The WYLBUR execute file, EXECTRS3 (see Appendix 6), moves the the proper data sets to the indicated positions when the job is created. The statements in the listing are applicable only to the Iowa State University Computation Center and are subject to change as system changes are implemented.

```
   1 //A411GJO JOB A0099,GJO,TIME=(1,59)
   2 /*JOBPARM  LINES=10
   3 //S1 EXEC PGM=IEBGENER
   4 //SYSPRINT DD SYSOUT=A
   5 //SYSIN DD DUMMY
   6 //SYSUT2 DD DSN=&CARDS1,UNIT=DISK,DISP=(NEW,PASS),
   7 // SPACE=(3520,(5,5),RLSE),DCB=(RECFM=FB,LRECL=80,
   8 // BLKSIZE=3520)
   9 //SYSUT1 DD *
     Control Variables
 180 /*
 801 //S2 EXEC PL1LFCLG,PARM.PL1L='A,X,NEST',REGION.GO=160K
 802 //PL1L.SYSIN DD *
     TRS3 Source Deck
 803 /*
 804 //GO.SYSIN DD DSN=CPS07.A0986.GJO1,DISP=SHR
 805 //IN       DD DSN=&CARDS1,DISP=(OLD,DELETE)
 807 //OUT      DD DSN=CPS07.A0986.GJO2,UNIT=DISK,
 808 // VOL=SER=RJEPAK,DISP=(NEW,KEEP,DELETE),SPACE=(3520,
 809 // (5,5)),DCB=(RECFM=FB,LRECL=80,BLKSIZE=3520)
 810 //GO.FT14F001 DD DSN=&SM,UNIT=SCRTCH,DISP=(NEW,PASS),
 811 // SPACE=(800,(120,15)),DCB=(RECFM=VS,LRECL=796,
 812 // BLKSIZE=800)
 813 //SIMPLTTR EXEC PLOT,PLOTTER=INCRMNTL,FORM=W
 814 //S3 EXEC FORTG,REGION.GO=160K,TIME.GO=(2,00)
 815 //FORT.SYSLIN DD DISP=(OLD,PASS)
 816 //FORT.SYSIN DD *
     SMASH Source Deck
 817 //LKED.SYSLMOD DD DSN=&GOSET2(GO)
 818 //GO.FT05F001 DD DSN=CPS07.A0986.GJO2,DISP=SHR,
 819 // VOL=SER=RJEPAK,UNIT=2314
 820 //GO.FT06F001 DD SYSOUT=A
 821 //GO.FT14F001 DD DSN=&SM2,UNIT=SCRTCH,DISP=(NEW,PASS),
 822 // SPACE=(800,(120,15)),DCB=(RECFM=VS,LRECL=796,
 823 // BLKSIZE=800)
 824 //SIMPLTTR EXEC PLOT,PLOTTER=INCRMNTL,FORM=W
 825 //PLOT.FT14F001 DD DSN=&SM2
 998 /*
 999 //
1000
```

APPENDIX 6: EXECTRS3

EXECTRS3 is a WYLBUR execute file which creates the job which calculates the experimental results. The execute file starts with the JCL statements (Appendix 5), copies TRS3 (Appendix 1) and SMASH (Appendix 2) to the appropriate lines and interrogates the operator for input information. After the job is created the execute file submits the job to the ccmputer system for execution and erases the original input data set in preparation for the next use of the execute file. The WYLBUR statements which make up the execute file are listed on the following pages.

```
 10 SET EXEC NOL TER
 20 SET ESC :
 40 SET VOL CAT
 50 USE #JCL CLR
 60 COPY ALL FROM #TRS3 TO 802.001
 70 SCR $CPS07.A0986.GJO2 ON RJEPAK
 80 COMM HOW MANY RUNS?
 90 INS 11 UNN
100 REA VAL NO USING 11
110 COPY 1000 TO 12
120 SET VAL W0=12
130 SET VAL W1=13
140 SET VAL N1=0
150 SET VAL N1=N1+1
160 REA STR S0 PRO 'IS RUN :N1 FAST OR SLOW?  '
170 SET VAL N9=2*:N1
180 IF (S0 EQ 'FAST') EXEC 400
190 REA STR S0 PRO 'WILL SMASH BE RUN?  '
200 IF (S0 EQ 'NO') CH :N9/:N9 TO 0 IN :W0 N
210 COPY 1000 TO :W1
220 REA STR S1 PRO 'GRAPH LABEL RUN :N1?  '
230 CH 1/20 TO ':S1' IN :W1 N
240 REA STR S1 PRO 'DATA LABEL RUN :N1?  '
250 CH 21/40 TO ':S1' IN :W1 N
260 SET VAL W1=W1+1
270 IF (S0 EQ 'YES') EXEC 450 SAVE
280 IF (N1 LT N0) EXEC 150
290 COMM TO RUN JOB TYPE EXEC NEXT
300 EXEC PAUSE
310 IF (N2 NE 1) DEL 813/822
320 IF (N2 EQ 1) COPY ALL FROM #SMASH TO 816.001
350 RUN 1/999 UNN
351 SCR $CPS07.A0986.GJO3
360 EXEC PAUSE
400 CH :N9/:N9 TO 0 IN :W0 N
410 EXEC 280
450 REA VAL N8 PRO '#SMASHES RUN :N1?  '
460 COPY 1000 TO :W1
470 CH 1 TO :N8 IN :W1 N
480 SET VAL W1=W1+1
490 SET VAL N2=1
500 CH :N9/:N9 TO 1 IN :W0 N
510 SET VAL N3=0
520 SET VAL  N3=N3+1
530 IF (N3 GT N8) EXEC RETURN
540 COPY 1000 TO :W1
550 IF (N3 EQ 1) CH 10/10 TO 0 IN :W1 N
560 IF (N3 NE 1) CH 9/10 TO -1 IN :W1 N
570 REA STR S1 PRO 'HOW MANY COMPONENTS SMASH :N3?  '
580 CH 5/5 TO ':S1' IN :W1 N
```

```
590 REA STR S1 PRO 'GRAPHS SMASH :N3?  '
600 IF (S1 EQ 'YES') EXEC 630
610 CH 15/15 TO 0 IN :W1 N
620 EXEC 660
630 REA STR S1 PRO 'LIN=LINEAR, LOG=SEMILOG  '
640 IF (S1 EQ 'LIN') CH 15/15 TO 1 IN :W1 N
650 IF (S1 EQ 'LOG') CH 14/15 TO -1 IN :W1 N
660 SET VAL W2=W1
670 SET VAL W1=W1+1
680 REA STR S1 PRO 'PRINTED OUTPUT HEADING?  '
690 COPY 1000 TO :W1
700 CH 1/80 TO ':S1' IN :W1 N
710 SET VAL W1=W1+1
720 REA VAL W9 USING :W2 COLS 15/15
730 IF (W9 EQ 0) EXEC 840
740 COPY 1000 TO :W1
750 REA STR S1 PRO 'X-AXIS LABEL?  '
760 CH 1/20 TO ':S1' IN :W1 N
770 REA STR S1 PRO 'Y-AXIS LABEL?  '
780 CH 21/40 TO ':S1' IN :W1 N
790 REA STR S1 PRO 'GRAPH LABEL?  '
800 CH 41/60 TO ':S1' IN :W1 N
810 REA STR S1 PRO 'DATA LABEL?  '
820 CH 61/80 TO ':S1' IN :W1 N
830 SET VAL W1=W1+1
840 COPY 1000 TO :W1
850 SET VAL N4=0
860 REA VAL N5 USING :W2 COL 5/5
870 SET VAL N4= N4+1
880 SET VAL N6=N4*10-9
890 SET VAL N7=N4*10
900 REA STR S1 PRO 'DECAY CONSTANT FOR COMPONENT :N4  '
910 CH :N6/:N7 TO ':S1' IN :W1 N
920 IF (N4 LT N5) EXEC 870
930 SET VAL W1=W1+1
940 EXEC 520
```