Department Of

Physics

Grambling State University

Grambling, Louisiana

INTRODUCTION

The final technical report on the Nuclear Quardupole Resonance Studies sponsored by NASA at Grambling State University is presented in three separate sections: Part I describes the instrumentation, consisting of the development and assembly of the Nuclear Quadrupole Resonance Spectrometer. Part II presents (a) the types of experiments carried out so far by the principal investigator, along with several undergraduate students, over a period of 5 years, and (b) a discussion of the results. Part III presents the theoretical studies on the solid state crystalline electrostatic fields, field gradients and antishielding factors.

Background

A modest start of the NQR project at Grambling State University was made in late 1970, with a grant made by the Research Corporation ($7,480) to the principal investigator. Since the funds were not sufficient to obtain the complete spectrometer, our efforts were confined to building a simple super-regenerative type of oscillator, and computation of antishielding factors in simple systems; thus, providing research training to the participating undergraduate students.

With the aid of the National Aeronautics and Space Administration (NASA) grant, we have been able to establish a complete Nuclear Quadrupole Resonance Spectroscopy facility at Grambling State University and provide training in research to the participating undergraduate students. The main function of the department being undergraduate education, every effort was made to structure the project activity to achieve this objective. Appendix A shows the list of student participants in the project.

INSTRUMENTATION

The main reason for initiating the Nuclear Quadrupole Resonance project at Grambling State University is its inherent amenability for undergraduate comprehension. Both the theoretical physics needed and the experimental techniques involved are fairly simple and appropriate for undergraduate research exposure and introducing them to the power of physics in solving specific problems.

It was very succinctly expressed by J.A.S. Smith[1] that the simplest and cheapest radio frequency spectrometer for chlorine nuclear quardupole resonance is relatively easy to build, but extremely difficult to control. The first circuit we attemped is a super regenerative oscillator system similar to that described by Dean and Pollack[2] and Smith.[1] Figures 1 & 2 show the schematic of the circuit and Plates I & II are pictures of the unit built by the participating undergraduate students here. A simple Heath Kit assembled radio was used to determine the frequency of the SRO and the receiver was calibrated with W.W.V. standard frequency broadcasts. For this purpose a simple antenna was erected on top of the Carver Hall building in which the Physics Department is housed. The sensitivity of the unit was so limited that it has been possible to observe a 0.5 cm peak above the noise level for the NQR resonance signal of chlorine in paradichlorobenzene only. Due to the inherent difficulty associated with the SRO system for accurate frequency determination, our attempts to study lattice effects with this unit proved unsuccessful.

Plate III shows the commercially produced marginal oscillator unit obtained from the Research Education Systems Company of Lexington, Massachuetts and our interfacing module. The oscillator served as a very good piece of demonstration equipment for oscilloscope display of Cl signals in $KClO_3$ and PCl_2 O, etc. Several modifications were made in the circuit to enable the recording of the signals on a chart recorder. Among these the most important introduction was

SUPER-REGENERATIVE
N.Q.R OSCILLATOR

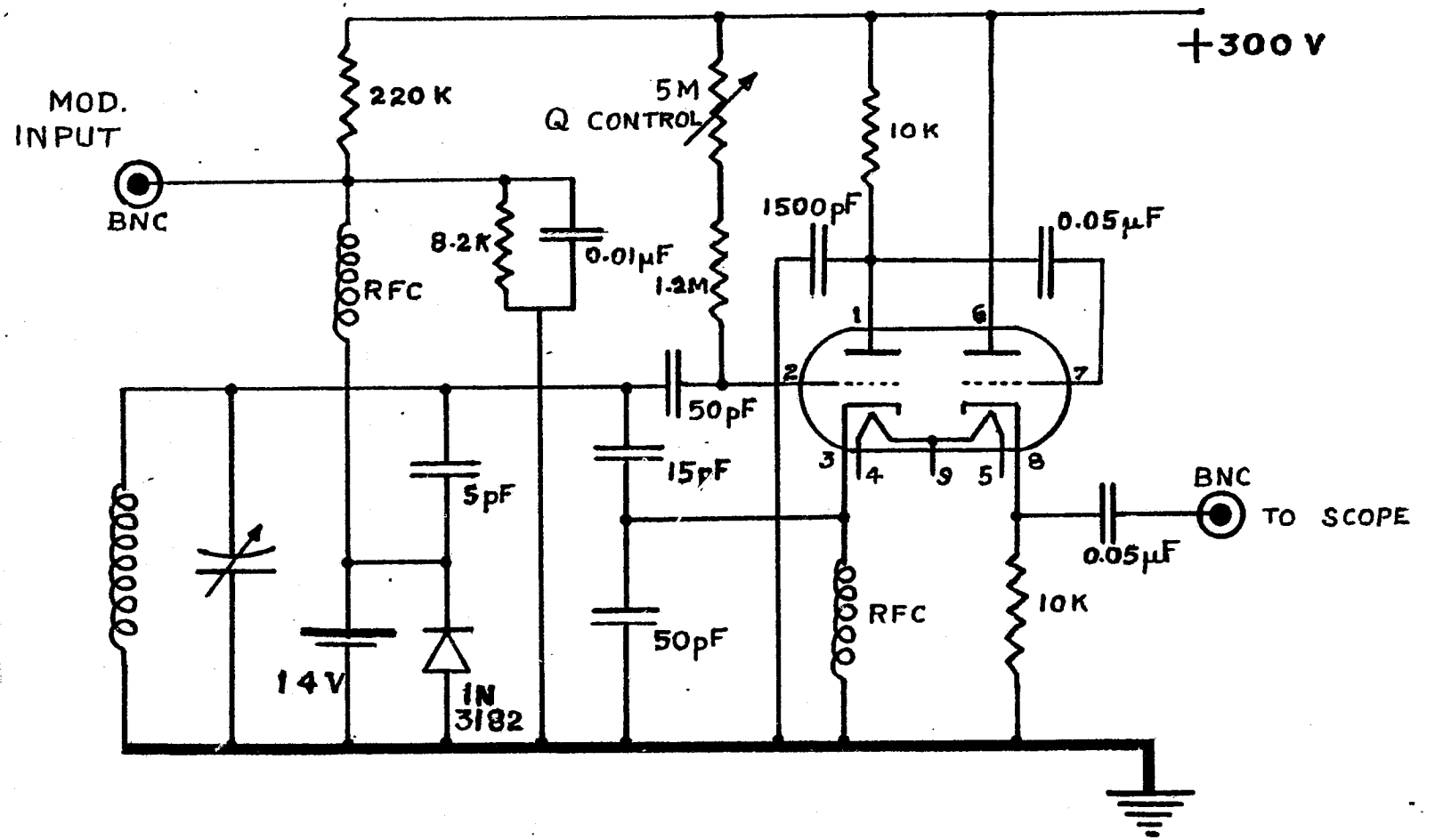
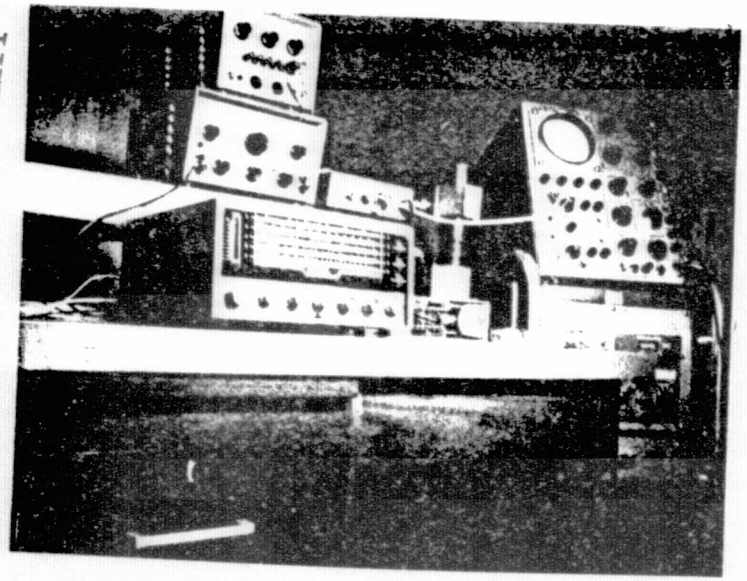
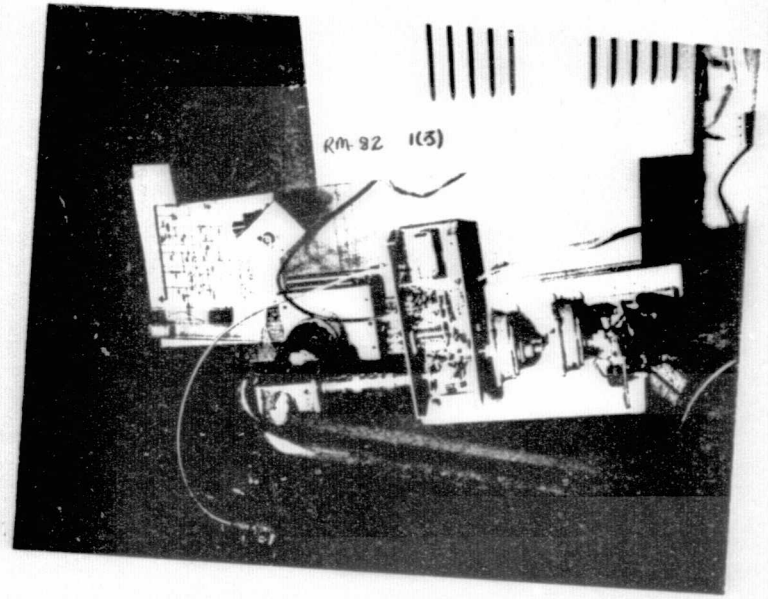


PLATE I

FIRST SUPER-REGENERATIVE NQR OSCILLATOR AND SPECTROMETER SYSTEM
DEVELOPED IN OUR LABS



1. Front View



2. Top View

SELF-QUENCHING
F E T OSCILLATOR

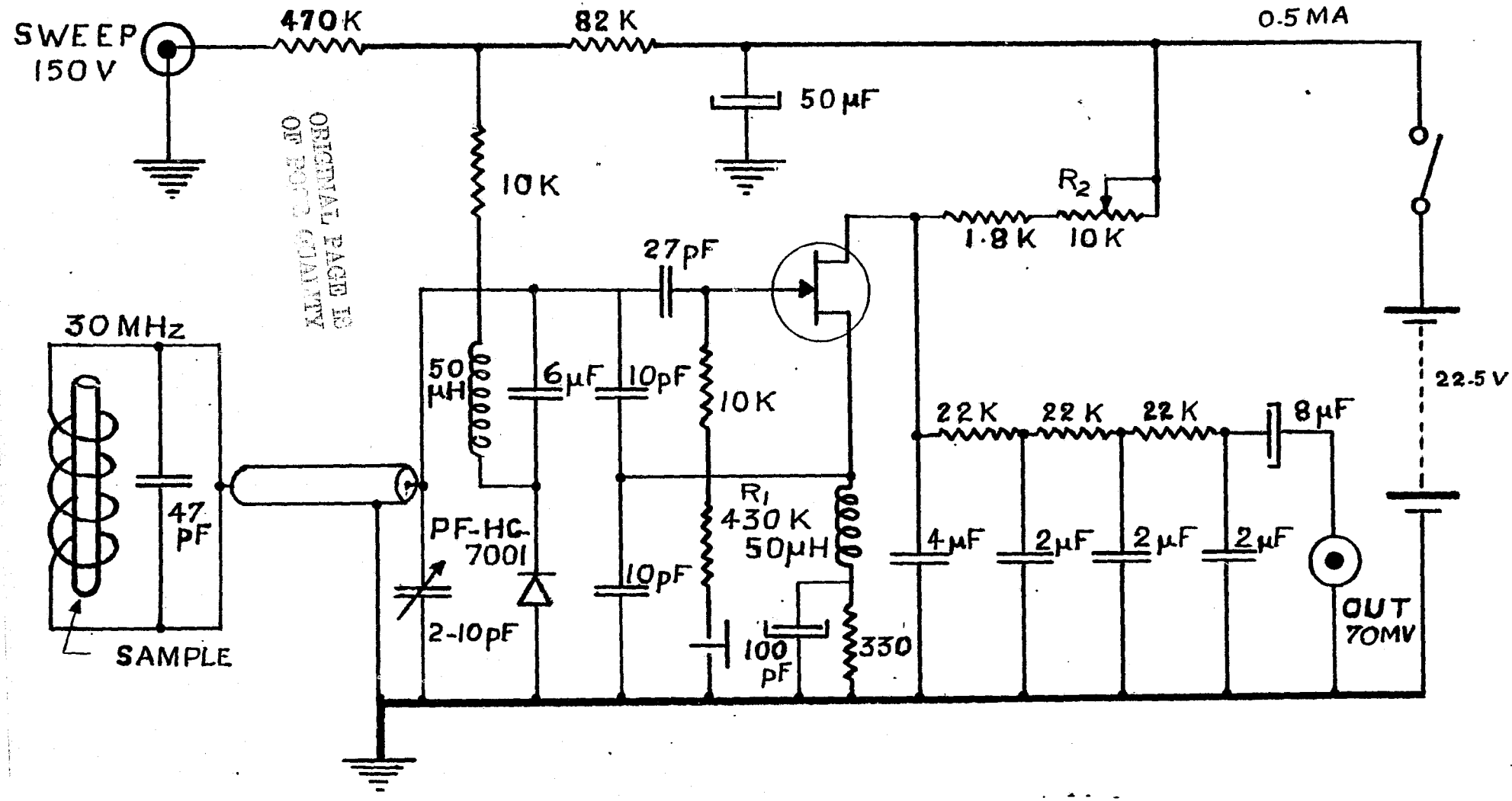
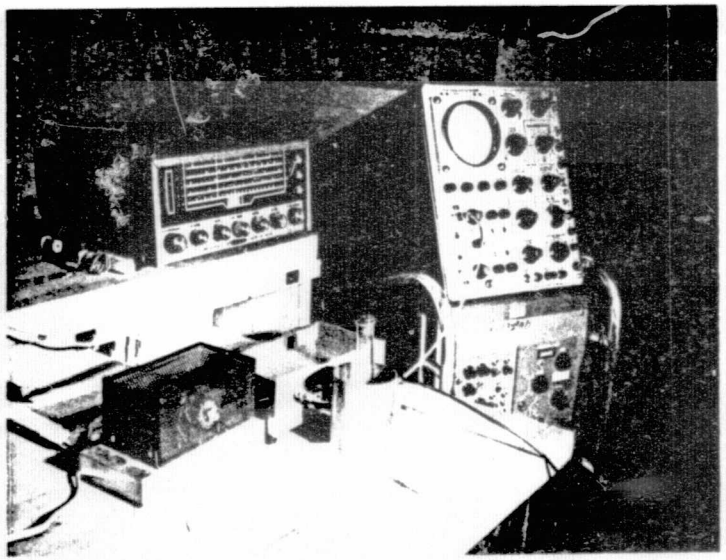


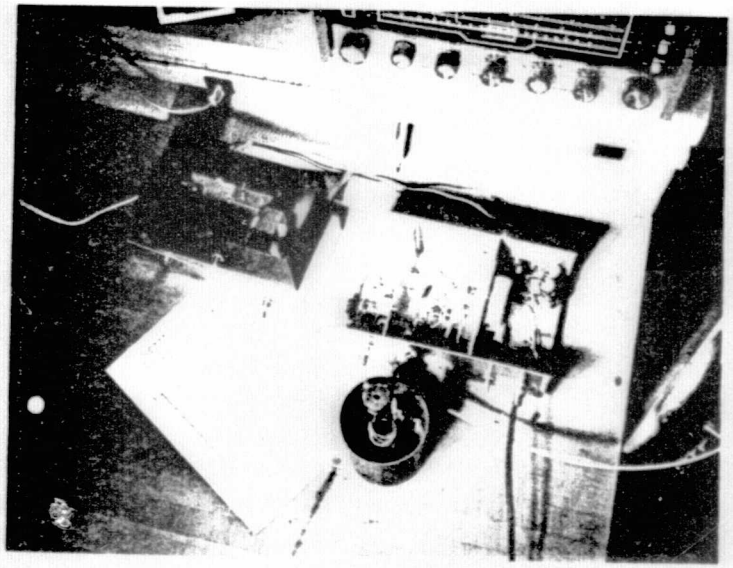
PLATE II

SELF QUENCHED NQR SYSTEM

(Constructed by Participant Students' F.E.T. Oscillator)



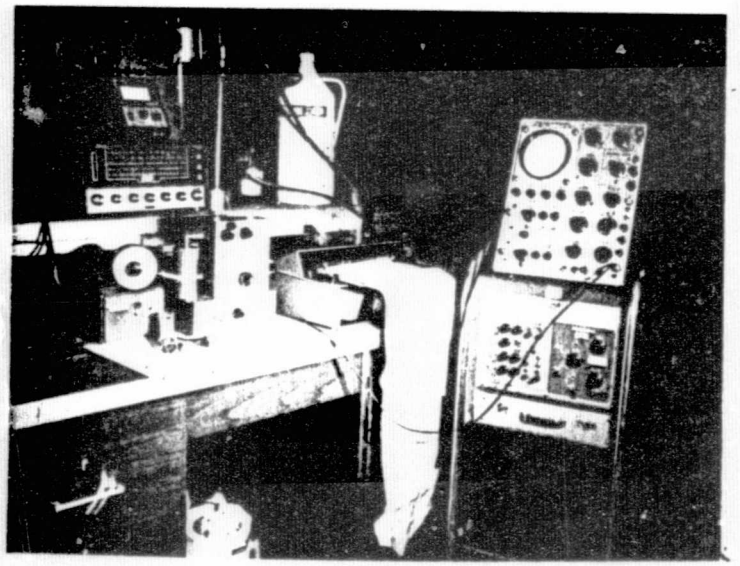
1. Front View



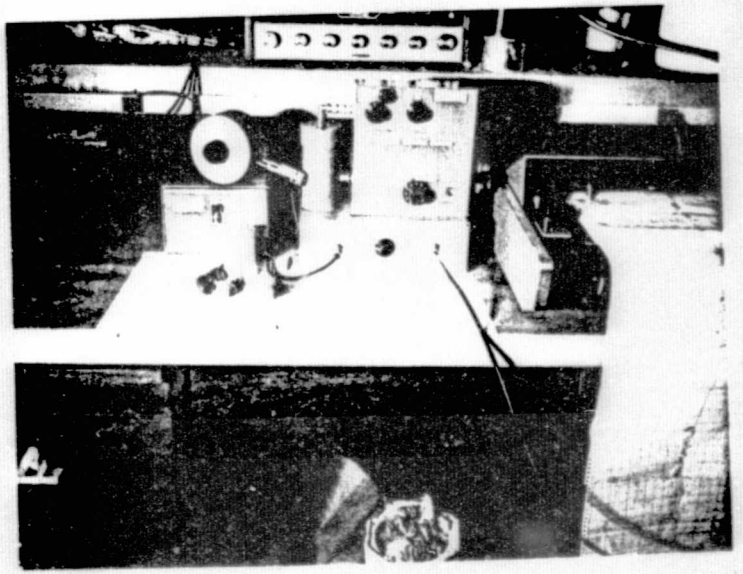
2. Top View

PLATE III

RESEARCH SYSTEMS MARGINAL OSCILLATOR AND SPECTROMETER ASSEMBLY



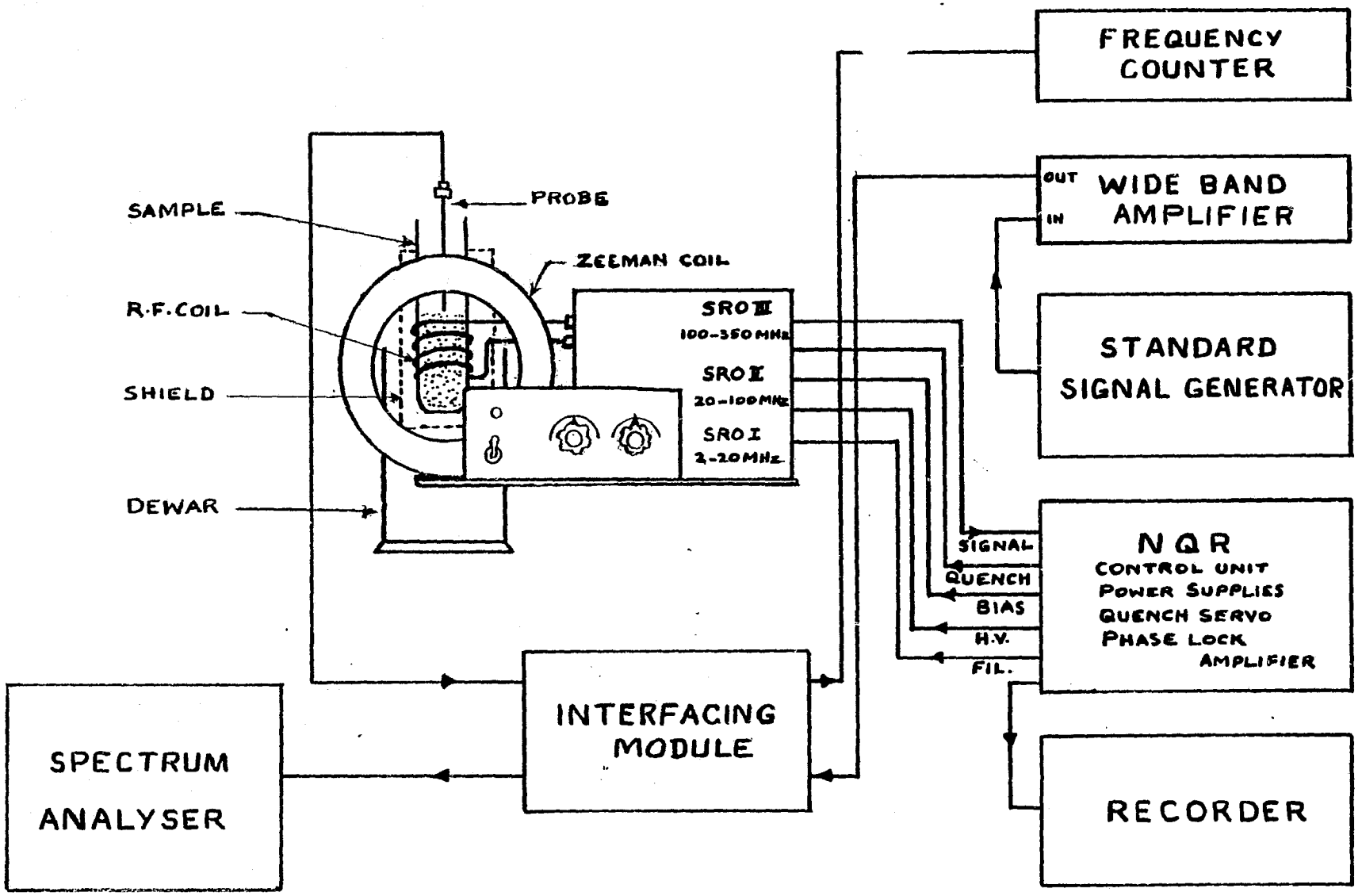
1. Complete Assembly



2. Oscillator and Interfacing Module Only

the interfacing circuitory to monitor the ramp of the frequency sweep diode externally from the sawtooth voltage output of an oscilloscope. This provided considerable control on the sweep rate and signal could be simultaneously recorded on a chart recorder and displayed on the screen of the long persistance scope. This system with its limited capabilities proved useful for a detailed study of the line shapes; if the frequency is already known and the absorption signals are strong such as in the chlorates of sodium and potassium, copperoxide, paradichlorobenzene, etc.

Since the major aim of the project has been to study the semimetallic environments by NQR techniques we obtained the most sensitive automatic super-regenerative scanning spectrometer from Wilks Scientific Company. Plate IV shows the current arrangement of the spectrometer facility. Figure III is a block diagram of the complete system, showing the main spectrometer and the auxiliary facilities. Though most of the units were commercially obtained except for the zone melting heater, procuring the units, housing, assembling and putting into operation has been a valuable experience to the participants. This phase of the project while being most strenuous and time-consuming has been rewarding to the participating undergraduate students; in that they had the first hand exposure and experience of establishing research facilities. Grambling State University being mainly an undergraduate teaching institution, was not equipped until recently for undertaking research-type of investigations. The National Aeronautics and Space Administration grant has been of immense value in establishing these basic facilities, in addition to the main Nuclear Quardupole Resonance Spectroscopy facility. Plates V and VI show the auxiliary facilities developed during the course of the projects.

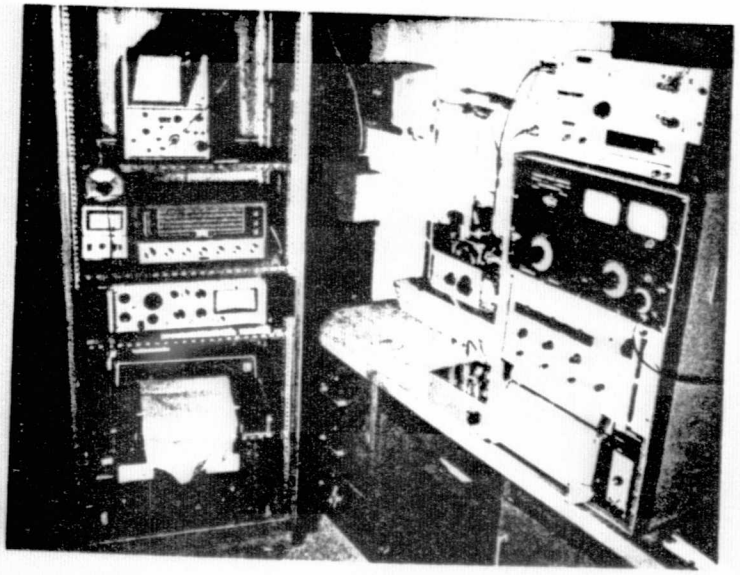


NQR SPECTROMETER SYSTEM

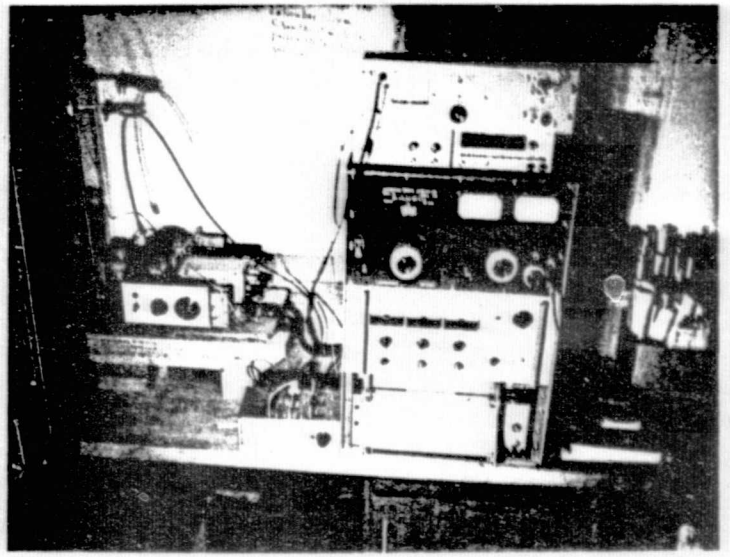
BLOCK DIAGRAM

PLATE IV

NUCLEAR QUADRUPOLE RESONANCE SPECTROMETER SYSTEM



1. Complete System with Spectrum Analyzer and Lock in Facilities



2. WILKS Scientific Control Unit, S.R.O. and Interfacing Module

EXPERIMENTAL STUDIES

The electrostatic field gradient "q" ($q = \partial^2 V / \partial Z^2$) being a classical quantity presents no conceptual problems to the undergraduate student and can be directly obtained from an analysis of the NQR spectrum. A knowledge of "q" reveals the nature and extent of intra- and intermolecular interactions in solids. As such our main objective has been to change the solid state electronic charge distribution in a controlled manner, and study the microscopic effects on the electrostatic field gradient at the site of the quadrupole nucleus by analyzing its NQR spectrum.

This environmental effect is considered to be of importance in semi-metallic structures such as Antimony, Indium, Gallium, etc., because even minute impurity addition alters the conduction properties in a marked fashion, and the conduction electrons provide appreciable contribution to the electrostatic field gradient.[3,4] Alterations in the valence/conduction electron charge distributions can be produced by:

(1) Chemical bond formations with the neighboring atoms in different compounds.

(2) Addition of impurities to the host lattice.

(3) Perturbutions of lattice charges due to electrical conduction.

(4) Temperature and pressure effects.

Results and Discussion

To acquaint the student participants with the operation of the spectrometer and provide training in the techniques of frequency measurement, the NQR spectra of several known compounds were repeated as a preliminary training and the frequency measurement accuracy assessed, before they attempted search runs on new compounds. Table II is a listing of the typical measurements that were repeated by several students to gain practice.

Table II

	Compound		Measured Frequency	Litereative Value[5]
1.	$AsCl_3$	As	76.2 ± 0.2 MHz	76.4
		Cl^{35}	24.8 ± 0.2	24.5
2.	As_2O_3	As	108.2 ± 0.4	108.6
3.	Sb_2O_3	Sb^{121}	82.2 ± 0.2	82.6
		Sb^{123}	50.2 ± 0.2	50.2
4.	$SbCl_3$	Cl^{35}	20.6 ± 0.2	20.4
5.	$C_6H_4Cl_2$	Cl^{35}	34.2 ± 0.1	34.3
6.	$NaClO_3$	Cl^{35}	29.9 ± 0.1	29.9
7.	$KClO_3$	Cl^{35}	28.1 ± 0.1	28.1
8.	Cu_2O	Cu^{63}	26.1 ± 0.1	26.0
		Cu^{65}	24.0 ± 0.1	24.1

These lines, particularly those of chlorine and copper served as test spectra and reference standards for all other investigations.

New Compounds Studied

Several intermetallic compounds of the p-block (III - VI) elements such as selenides, tellurides, sulfides and oxides of Indium, Arsenic, Antimony and Bismuth, have been investigated during the course of the project and detailed discussions of the results reported in the earlier interim semiannual reports.[6] Typical recorder runs of the spectra in traditional compounds and lattice effect studies are presented in Appendix B. Table III is a listing of the several compounds investigated in our laboratory.

Table III

	Compounds		Remarks	Reference
1.	As_2O_5		Multiplet lines* 20 - 60 MHz	6
2.	As_2S_2		Broad/Weak signals 50 - 60 MHz	6
3.	As_2Te_3		115.9 $\pm$ 0.5 MHz	7
4.	As_2Se_3		Weak lines 70 - 80 MHz	6
5.	Bi_2O_3 (Bismite Form)		No Signal (previous data exists)	9,8
6.	Bi_2S_3		Broad signal* 60 - 65 MHz	6,8
7.	Bi_2Te_3		No Signals Scan 10 - 150 MHz	9
8.	Bi		No Signals Scan 10 - 150 MHz	9,8
9.	Sb_2O_5		Weak multiplets* 50 - 100 MHz	6
10.	Sb_2S_5		Weak multiplets* 20 - 80 MHz	6
11.	Sb_2Te_3	Sb^{121} Sb^{123}	82.8 $\pm$ 0.2 50.1 $\pm$ 0.2	7
12.	In_2S_3		Weak multiplets 5 - 50 MHz	
13.	In Se		Weak multiplets 5 - 50 MHz	6
14.	In_2O_3		Weak Signals* 5 - 20 MHz	6
15.	Ga_2O_3		No Signal Scan 5 - 25 MHz	6

*Several search runs were made on these samples at lower temperatures and a note is under preparation presenting the data.

Studies on Doped Samples

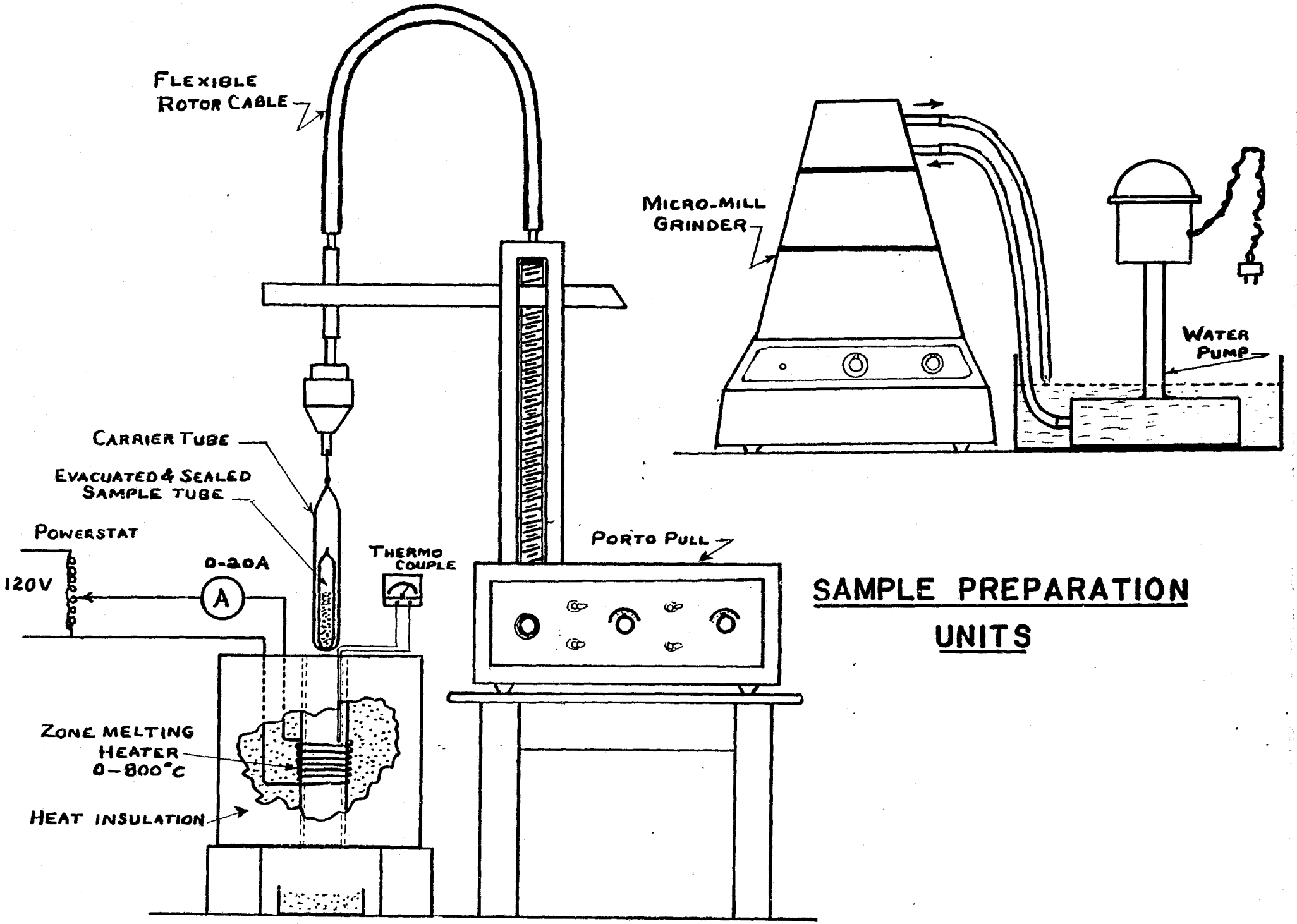
Since the earlier studies in Antimony and Indium clearly indicated[3,4] that conduction electrons provide appreciable contribution to the field gradient at the nuclear site, we have devoted considerable time and energy to investigate this feature, with no commensurate returns. Of the group of elements of interest: Indium, Antimony, Bismuth and Gallium, only Antimony was amenable for investigation on our spectrometer. Indium resonances exist below 10 MHz where our system sensitivity and reliability proved to be very low. Several trials on Bismuth both here and in the NQR Laboratories of Queen Elizabeth College, University of London, indicated no signals even at liquid nitrogen temperature. Our studies in Antimony and Gallium were encouraging in that signals of desirable strength could be observed when sufficient care in the sample preparation and operation of the spectrometer were exercised. We confined most of our studies to Antimony alone because of the high cost of pure Gallium. The fact that the signals lie in the 10 MHz region; where the spectrometer operating conditions are not at their best; and the preparation of doped samples involved a tedious and time-consuming process, impeded the progress of our studies severely. The results of our investigation were presented[10] at the Fifty-First Louisiana Academy of Sciences meeting and summarized below.

The presence of an impurity in the proximity of a quadrupole nucleus changes the electrostatic field gradient at the nuclear site normally due to its different size and charge. In addition, we expected it could also alter the conduction electron distribution in the neighborhood of the resonating nucleus and cause a frequency shift. As such we have chosen three types of impurity elements to be doped in the host lattice of Antimony. They are Cadmium, Indium and Bismuth.

Bi in Sb: Concentration range 0.01 to 1 percent by weight. Since both Bi and Sb have similar outer shell electronic structures namely 6 S^2 6 P^3 and 5 S^2 5 P^3, there should be only size effect and if any a minor perturbation in the conduction electron distribution. We also expected that since Bi and Sb have similar crystal structure the added impurity atoms would occupy preferred interstitial lattice site causing a splitting of the NQR line. At 1 percent concentration the lines were completely wiped out while at 0.01 there was a decrease in the intensity of the signal associated by a broadening of the line. To find out the limiting point of impurity concentration for an observable signal, samples with 0.5, 0.2, 0.1, 0.05 and 0.02 percent Bi were investigated. The signals became gradually broader and weaker up to 0.1 and disappeared at 0.2 percent concentration. This result indicates there occurred a rapid distribution of field gradients as the number of impurity centers increased; and no additional information could be obtained regarding the perturbations in the extra ionic electron distribution.

In in Sb: Concentrations of impurity studied 0.005, 0.01, 0.02, 0.05, 0.1. Since the electronic structure of In is 5 S^2 5P the size effect should be minimal and the charge effect should be the dominant factor. The results of our study are interesting in that the signals disappeared even at a small concentration as low as 0.02% compared with that of 0.2% for Bismuth impurity. This makes us believe that the Indium impurity might behave like an acceptor in the Antimony lattice marked by influencing the EFG at Sb site. Up to 0.01 percent concentration there seems to be a shift of 0.2 MHz associated with a slight drop in intensity and broadening of the signal. The frequency shift was the same both at 0.005 and 0.01 percent Indium.

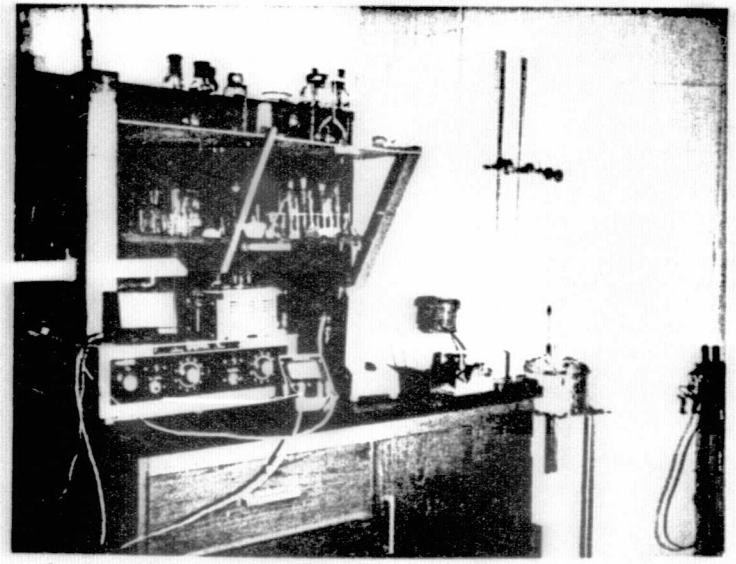
Cd in Sb: Concentration range studied 0.005, 0.01, 0.1, 0.5, 1 percent by weight. Since electronic structure of Cadmium is 5 S^2, we expected both the



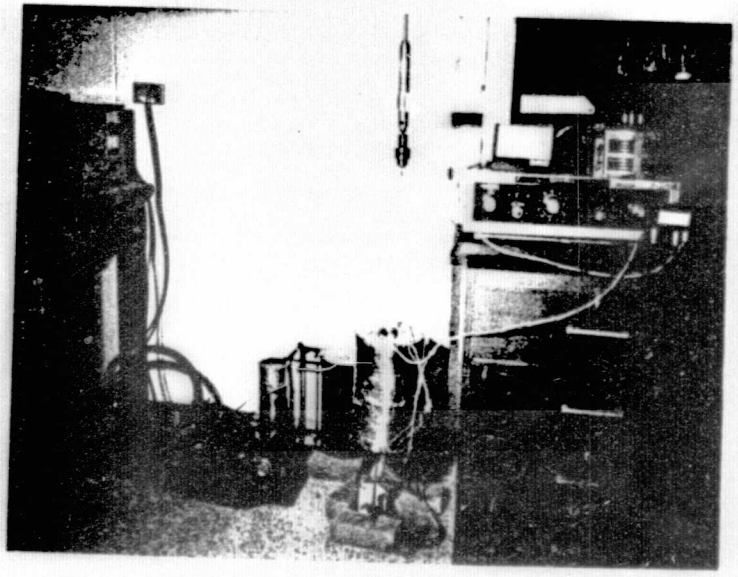
SAMPLE PREPARATION UNITS

PLATE V

SAMPLE PREPARATION FACILITY



1. Crystal Pullers and Micro-Mill Grinder



2. Zone Melting and Annealing Heating Units

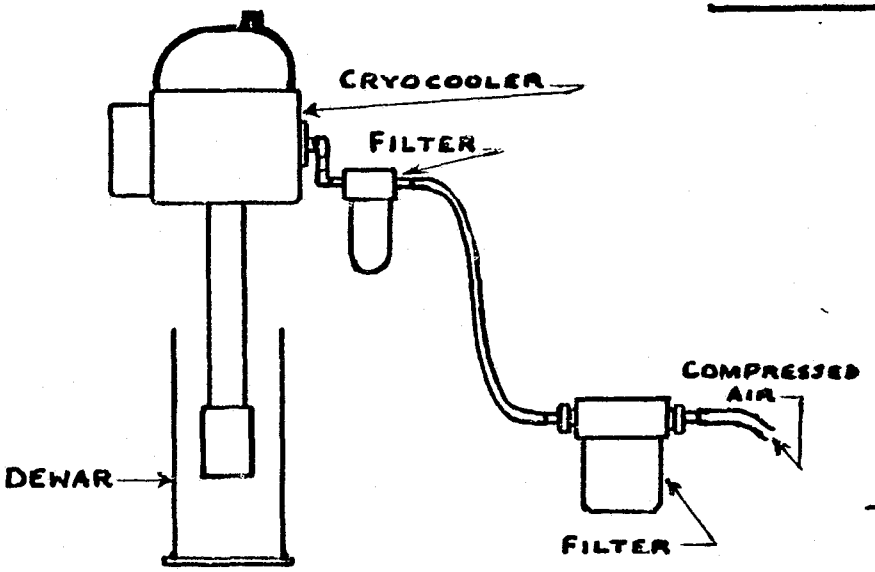
charge and size effects must be minimal. But to our surprise signals disappeared at even the lowest concentration of 0.005 percent. It is not known whether occurrance of a compound formation is the reason for this feature.

Sample Preparation Techniques

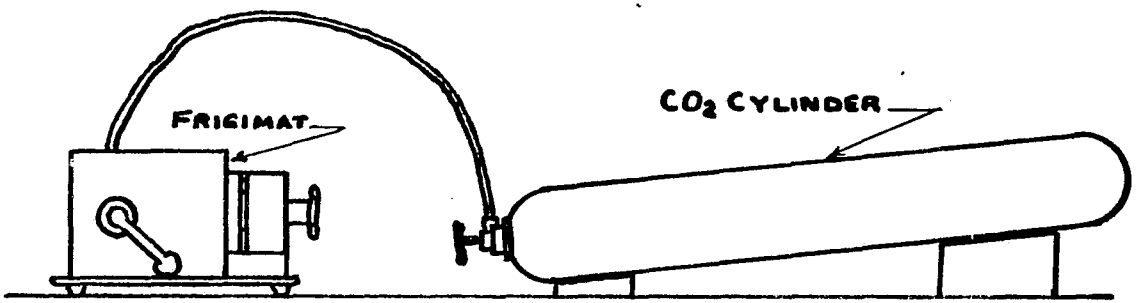
It is appropriate on my part to inject a statement of caution in the analysis of our observations. As mentioned earlier Antimony signals in the pure metal itself are not strong and are very sensitive to the annealing state of the sample and operating conditions of the spectrometer. Plates V and VI show our sample preparation arrangment.[6] After mixing the desired amounts of impurity and Antimony, the sample is loaded in a Vycor tubing and evacuated, dried and sealed. The sealed tube is lowered in a carrier tube which was slowly passed through the hot zone several times (5 - 6) up and down. The hot zone of the heater is about 1", at a maximum temperature of about 800°C. This zone levelling process is expected to uniformly distribute the impurity in the host lattice. The sample comes out as a solid rod which was pulverized by the micromild and sifted to a fineness of 350 mesh powder. Then the powdered sample is again loaded in a glass tube and annealed under vacuum at a temperature of 550°C, before using for NQR scanning.

Every concentration for each impurity-type sample was made following the above tedious procedure. Now the disappearance of a signal or the converse, leaves doubt in one's mind, whether doping took place at all; if one observes the signal; and whether the small changes observed or the disappearances could be due to the annealing and stress status of the sample. Being concerned with these questions our desire to publish the data is quenched. Our discussion of the doubts with professionals in the field added to further futile pursuits at lower temperatures. One assuring factor that emerged out of our low temperature

LOW TEMPERATURE FACILITIES

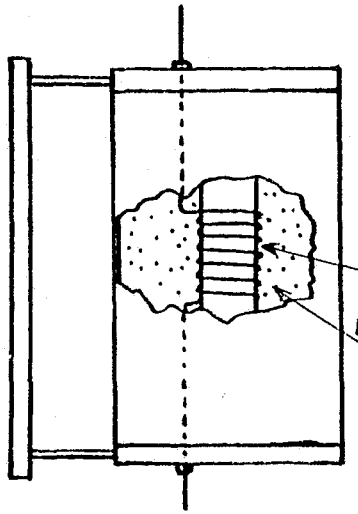


CRYOCOOLER

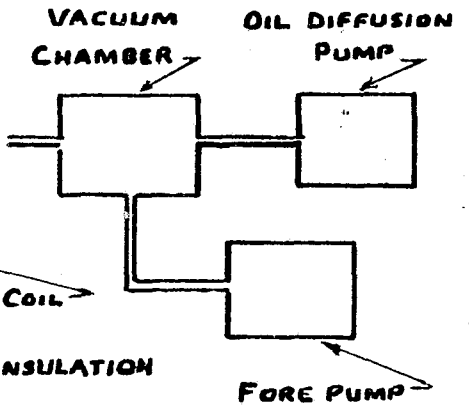


DRY ICE MAKER

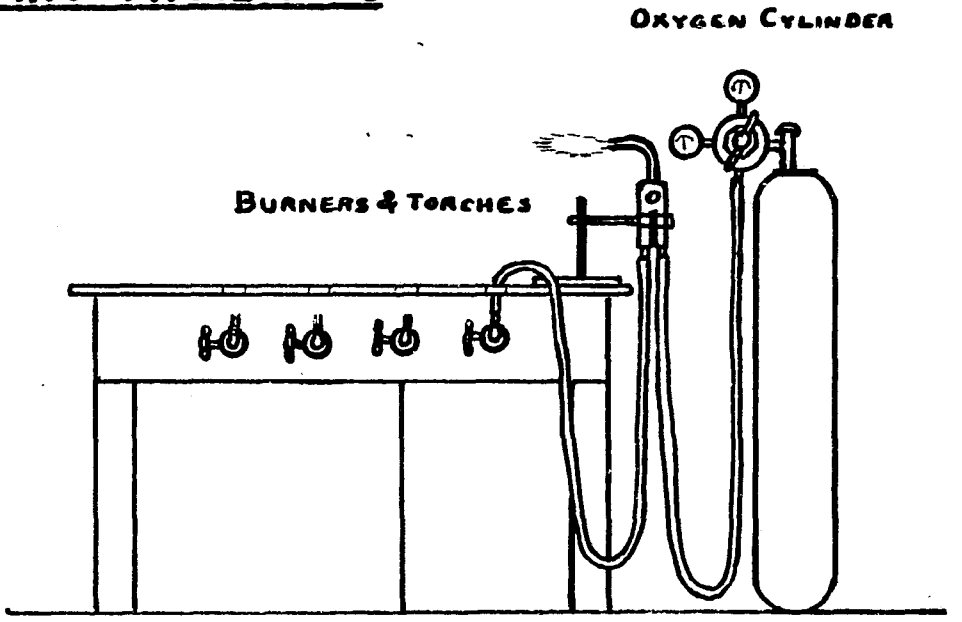
VACUUM AND GLASS-BLOWING FACILITIES



ANNEALING



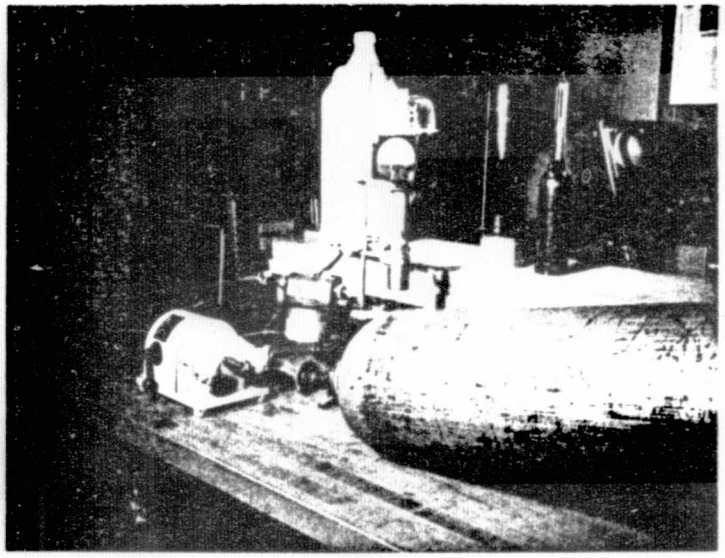
VACUUM



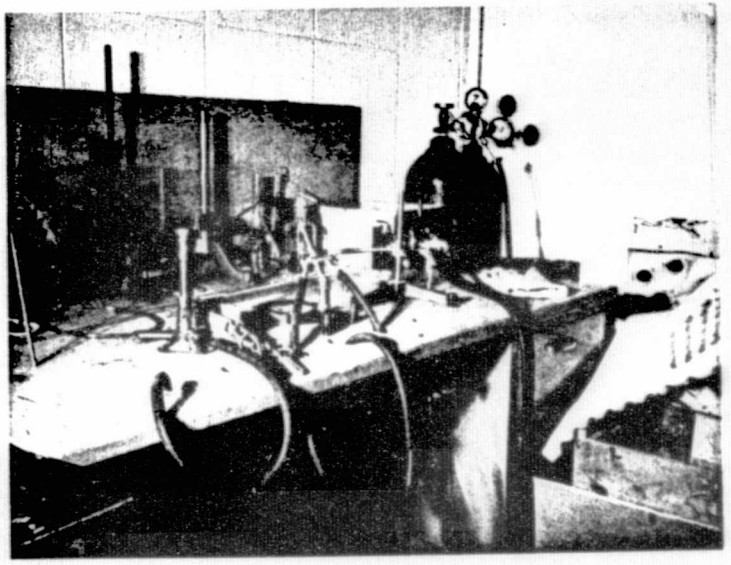
GLASS-BLOWING

PLATE VI

LOW TEMPERATURE AND GLASSBLOWING FACILITIES



1. Dry Ice Maker and Cryo Cooler



2. Glass Blowing Table

studies, is that the signals were reproducible in a similar fashion in all our samples. Still the sample effect remains a questionable factor.

Lattice Effects: The general objective being the investigation of the effect of the environmental charge distribution; a special study was carried in similar lines to those of Baer and Dean[11], using the Cl nucleus in $P Cl_2 \phi$, and $K Cl O_3$ in the host lattice of the piezo electric environment of Rochelle salt, water and paraffin wax.[12]

A novel study was carried out by us for the first time by passing an electric current through the solid sample. The results are interesting and show a shift of the order of 50 KHz when a current of about 50 ma was passed through the sample.[10] Appendix B shows the actual recorded spectra at liquid nitrogen temperatures. Though one can phonomenologically understand the shift as due to the changes in conduction electron contribution to EFG, no rigorous band theory explanation is possible at this time.

Effect of Pressure: Several interesting investigations were carried out by the principal investigator in collaboration with Professor J.A.S. Smith, Professor of Chemistry, University of London, during the period January - August, 1976; on the effect of high pressures (5 - 35 K bars) on the NQR spectra. So far, the pressure effect studies were confined only to low pressures below 5 K bars.[13,15] The studies at high pressures were made possible by the NASA grant to the principal investigator and the British Reserach Council grant for work at Standard Telecommunication Labs (STL-Harlow Essex) using their tetrahedron anvil press facilities. Since our studies being the first of their kind, several experimental design studies had to be made to couple the RF oscillator sample coil with the spectrometer.[8] Various sample coils (7 mm dia., 7 mm long) were fitted in pyrophyllite tetrahedron and coupled to the oscillator by a 50 ohm miniature coaxial cable. With this arrangement paradichlorobenzene

signals could be observed up to 10 tons including the $\alpha - \gamma$ phase transistion. Above 10 tons the signals weakened rapidly and completely disappeared at 30 tons. A probe into the reasons included a study of the quality factor of the coil which rapidly dropped to a value of 10 - 12 at a pressure of about 10 K-bar. Further studies indicated that in the anvil press system of SRC high pressure gradients[14] will be generated across the sample unlike in the hydrostatic (Bridgeman type) systems.

The second stage of investigations at STL (S.R.C. Essex) involved modification of the piston cylinder apparatus which can give pressures up to 15 K-bar to be compatible with the Queen Elizabeth College (University of London, England) spectrometer. Using 1:1 mixture of castor oil and amyl alcohol as a transmission fluid, several runs were made on molecular solids such as paradichlorobenzene, and addition compound of chloroanil with bis-8-hydroquinolinato palladium. These runs could be made successfully up to pressures of 15 K bars though there occurred considerable deterioration of signal strength.

The operation of the SRC high pressure unit involved considerable manpower and technical requirements. These constraints allowed only quick and short scans on the doped samples of Sb. Sb signals being weak in the beginning, rapidly disappeared as the pressure reached a value of 3 tons. To study the pressure effects in ionic solids where strong signals are observable, a preliminary search was carried out in the following minerals borrowed from the British Science Museum. The plan was to study them first at dry ice temperatures in the piston cylinder apparatus without applying pressure and reinvestigate those that seem potential samples for high pressure work.

1.	Grpiment	As_2S_3	72 - 75 MHz	Weak signal
2.	Arsenolite	As_4O_6	Signals beyond the range	
3.	Clauditite	As_4O_6	Signals beyond the range	

4.	Bismite	Bi_2O_3	35 - 70 MHz	Fairly good signals
5.	Sillinite	Bi_2O_3	40 - 60 MHz	Fairly good signals
6.	Senarmonite	Sb_2O_3	50 MHz	Weak signals
7.	Vallentinite	Sb_2O_3	68 MHz	Weak signals
8.	Stibinite	Sb_2S_3	30 - 45 MHz	Good signals

Based on these studies it was planned to reinvestigate the spectra of Bismite, Sillinite and Stibinite samples with the collaboration of Prof. Smith and Mr. M. K. Sabir when future time allocations become available at the SRC facility.

THEORETICAL STUDIES

This phase of the project has been one of the most rewarding activities of the program in that it made possible esoteric theoretical studies from journals to the classroom investigations. Two projects were introduced for upper level physics students elucidating the applications of basic principles of electrostatics[16] to the electrostatic fields and field gradients in solid state. Both the theoretical and experimental projects developed based on the NASA program are included in Appendix A following the list of student participants.

Our theoretical studies were mainly concerned in developing a comprehensive computer program for a self consistant estimation of electrostatic field gradients in ionic solids. The computational details of the program were presented in an earlier report[13] and the actual program (computer output) is given in Appendix C.

Starting with the basic crystal structure data the system locates all the ions in the solid, a desired number of unit cells away in all the three directions, from the lattice site of interest. After establishing the nearest neighbor ions, fields and field gradients at these sites are computed in a self

consistant way assigning the induced quadrupole and dipole moments for these lattice points. The program treats each lattice site as a multipole consisting of charge dipole and quadrupole moments, and evaluates these values in a self consistant manner. The program is successfully applied to verify the previous calculations in Al_2O_3.[18] The usefulness of this program is enhanced since different sections of it can be separated as subroutines to perform different operations. The program is used (a) to illustrate the solid state lattice structure and unit cell composition and nature graphically from the standard x-ray data; (b) to make a simple point charge estimation of electric fields in gases and solids; (c) to estimate induced dipole moments in solids and gases; (d) to evaluate antishielding factors; (e) to solve simultaneous equations (La. Tech program); and (f) to carry out tensor coordinate transformations.

The second aspect of our theoretical studies consisted of developing numerical solutions for the secular equations for the pure quadrupole interaction Hamiltonian. Using the Newton Raphson[19] iteration process, energy factors (multiples of the quadrupole coupling constant e^2Qq) were computed numerically for values of the asymmetry parameter η from 0 to 1 in steps of 0.01. The iteration process was continued until the successive values of the energy factors lie within 1×10^{-4}. The tables can be readily used for the analysis of the NQR spectra of nuclei with spin values I = 5/2, 7/2 and 9/2. Such tables as far as we know are available for I = 5/2 only in the Oak Ridge National Laboratory reports.[20] The reference tables developed by us are presented in detail in an earlier report[6] and the program details are given in Appendix D.

General Conclusions and Comments

The National Aeronautics and Space Administration grant NGR 19-011-016, along with the four other projects previously sponsored by NASA had the most positive impact on the academic standing and reputation of the Physics Department

at Grambling State University. It has helped immensely in establishing the Nuclear Quadrupole Resonance research facility for undergraduate research participation. Starting at a point where routine classroom experimental facilities were constrained, the general laboratory facilities have expanded to (a) high and low temperature generation and measurement facility; (b) facilities for radio frequency generation and measurement with the modern spectrum analyzers, precision frequency counters and standard signal generators; (c) vacuum and glass blowing facilities; and (d) miscellaneous electronic and machine shop facilities. (Plates IV, V & VI)

Since the NQR project was started from scratch, it provided a wide variety of learning experiences to a number of student participants. The details of student activities are presented in Appendix A. Though considerable student effort and time were dedicated to the establishment of the experimental facilities, the project studies yielded notable theoretical and experimental results leading to the following publications. It has been a most rewarding experience for the two physics majors, Mr. Eddie R. Wallace and Mr. Michael Coleman, who presented papers both at the national and international conferences.

(1) A.N. Murty, E.R. Wallace* and N. Gajendar. "Estimation of the Antishielding Factors of Certain Group III and V Elements," Proc. 45th La. Acad. Sci. and La. Phys. Teacher Conference 1973 (Abs)

(2) A.N. Murty. "NQR Spectra of the Tellurides of Arsenic and Antimony," Proc. Third International Symposium on NQR, Tampa, Florida 86, 1975 (Abs)

(3) A.N. Murty, Michael Coleman*. "Lattice Effects on the NQR Spectrum of Antimony." Proc. 51st La. Acad. Sci. and La. Phys. Teacher Conference, 1977 (Abs.)

(4) A.N. Murty and Michael Coleman*. "Lattice Effects on the Pure NQR Spectra." Proc. Third International Symposium on NQR, Tampa, Florida 114, 1975 (Abs)

(5) A.N. Murty and M. Balaram. "Self Consistant Estimation of Electrostatic Field Gradients in the Trioxides of Arsenic and Antimony and Bismuth." (In preparation)

(6) A.N. Murty. "NQR Signals in Certain Group III and V Compounds." (In preparation)

Nuclear Quadrupole Resonance spectroscopy though attractive due to its relatively least sophistication in instrumentation as compared to the sister branches of radio frequency spectroscopy such as microwave spectroscopy nuclear magnetic resonance, electron spin resonance, etc. is seriously handicapped due to the limitations on the accuracy and sensitivity of the spectrometer as well as the meagerness of the information yield. Even using the best commercially available spectrometers both here (our spectrometer system made by Wilks Scientific) and in England (University of London system made by Decca Radar Corporation) it has not been possible to make unambiguous determinations of small frequency shifts as encountered due to impurities and electric field effects in the range of (2 - 20 KHz); nor retrieve signals in metallic samples such as Bismuth or the natural minerals discussed earlier. However NQR proved to be a most powerful educational tool in elucidating solid state electrostatic forces in simple ionic solids. The instructional projects developed by us for classroom use are presented in Appendix A.

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APPENDIX A

EDUCATIONAL AND INSTRUCTIONAL YIELDS OF NASA-NQR PROJECT

Educational Impact of the Nuclear Quadrupole Resonance Project
Undergraduate Research Participation Training

The following students were supported by the NASA NGR-19-011-016 grant and previous Research Corporation grant and received training.

	Name	Learning Activity
1.	Eddie Ray Wallace	Computation of field gradients in diatomic molecules
2.	William Morris	Electronic circuits
3.	Stonewall Hunter	Electronic circuits and hardware
4.	Alan Kennedy	Hardware assembly and installation
5.	Rosemary Kline	Laboratory organization
6.	Israel Hall	Hardware assembly and installation
7.	Nathaniel Paul	Electronic circuits design and construction
8.	Ronnie Blake	Glass blowing-Sample preparation
9.	Therone Baker	Glass blowing-Sample preparation
10.	Clarence Hubbard	High temperature heater construction
11.	Jerry Gray	Electronic circuits construction
12.	Alvin Kennedy	Vacuum system, glass blowing-sample preparation
13.	Michael Coleman	Spectrum scanning analysis--sample preparation
14.	Dorothy Phillips	Spectrum scanning, record keeping
15.	Roy Jopes	Lattice effects, spectrum scanning
16.	Robert Lyons	Low temperature system
17.	Fred Gordon	Computer programs
18.	Shasti B.N.	Literature survey--data computation
19.	Frederick Wilson	Spectrum scanning

In addition to these direct participants, regular upperclassmen in physics worked on the following topics that have been developed from the NASA project studies.

PROJECTS IN PHYSICS

Physics 420-421

The objective of this course is to provide the upper level physics majors with an opportunity to plan and carry out simple projects under the guidance of the instructor in charge with minimum help. As such the emphasis is not on conducting an experiment with specific instruction and arriving at an acceptable result as accurately as possible, but to pursue the activity with ingenuity and skill and evaluate the result with a critical analysis. The activity may involve:

(1) development and assembling the needed units;

(2) "make-do" with minor modifications of the available units;

(3) utilizing modern systems consisting of several units and comprehend the techniques of using standard equipment with the aid of instruction manuals, etc.; and

(4) repeating the published work in standard journals of physics and acquire the techniques of research and publication, with a view to achieve the project objectives.

PROJECTS

I. Derive the general expressions for obtaining the electrostatic fields and field gradients due to a monopole, dipole and quadrupole.

REF: 1. Electromagnetic Fields and Waves by Lorrain and Carson

II. Develop a computer program to calculate the dipole moments of diatomic molecules from structural data.

REF: 1. "Binding Energy and Dipole Moments of Alkali Halide Molecules" by Edmund S. Rittner. J. Chem. Phys. 19, 1050 (1951).

2. "Dipole Moments of Alkali Halide Molecules by the Molecular Beam Electric Resonance Method" by A.J. Herbert, F.J. Lovas, C.A. Melenders, et. al. J. Chem. Phys. 48, 284 (1968).

3. "Electronic Polarizabilities of Ions" by J.R. Tessman, A.H. Kahn. Phys. Rev. 92, 890 (1953).

III. Develop a computer program to evaluate the electrostatic field gradients in gaseous diatomic molecules at the positive ion sites.

REF: 1. "Antishielding and Polarizabilities in Alkali Halide Gases" by Gerald Burns. Phys. Rev. 115, 357 (1959).

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IV. Observe the Nuclear Quadrupole Resonance signals in paradichlorobenzene and potassium chlorate and determine the frequency using the Spectrum Analyser.

REF: WILKS NQR SPECTROMETER Instruction Manual

V. Study the frequency shift of the NQR signal in $NaClO_3$ as a function of temperature.

REF: Research Systems NQR Oscillator Manual

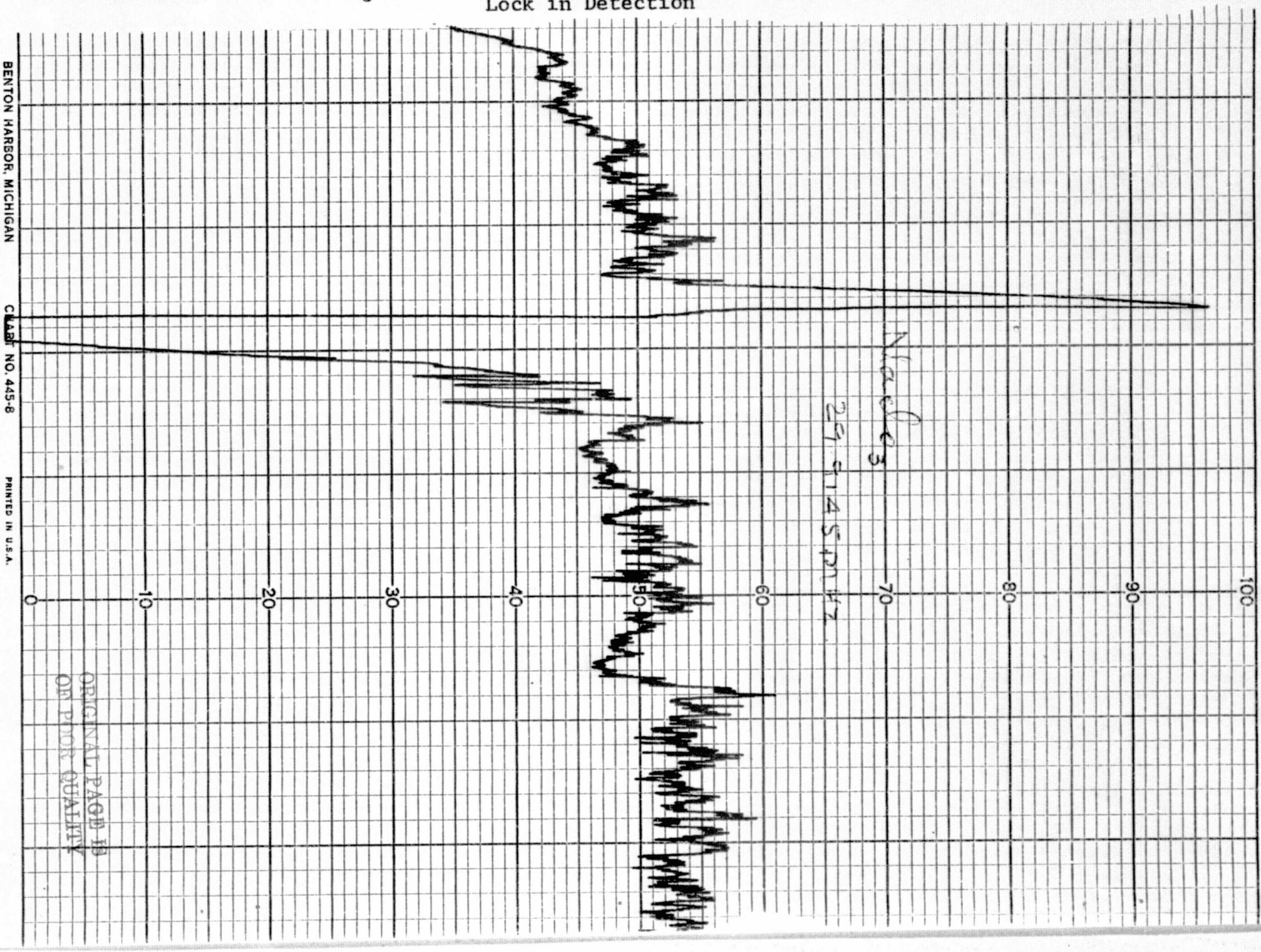
VI. Determine the frequencies of Bismuth NQR signals in $BiCl_3$ and obtain the asymmetry parameter value by assigning the spectrum using the frequency ratio tables.

REF: Third Semi-Annual Status Report, NASA Project NGR-19-011-016, 8-74.

APPENDIX B

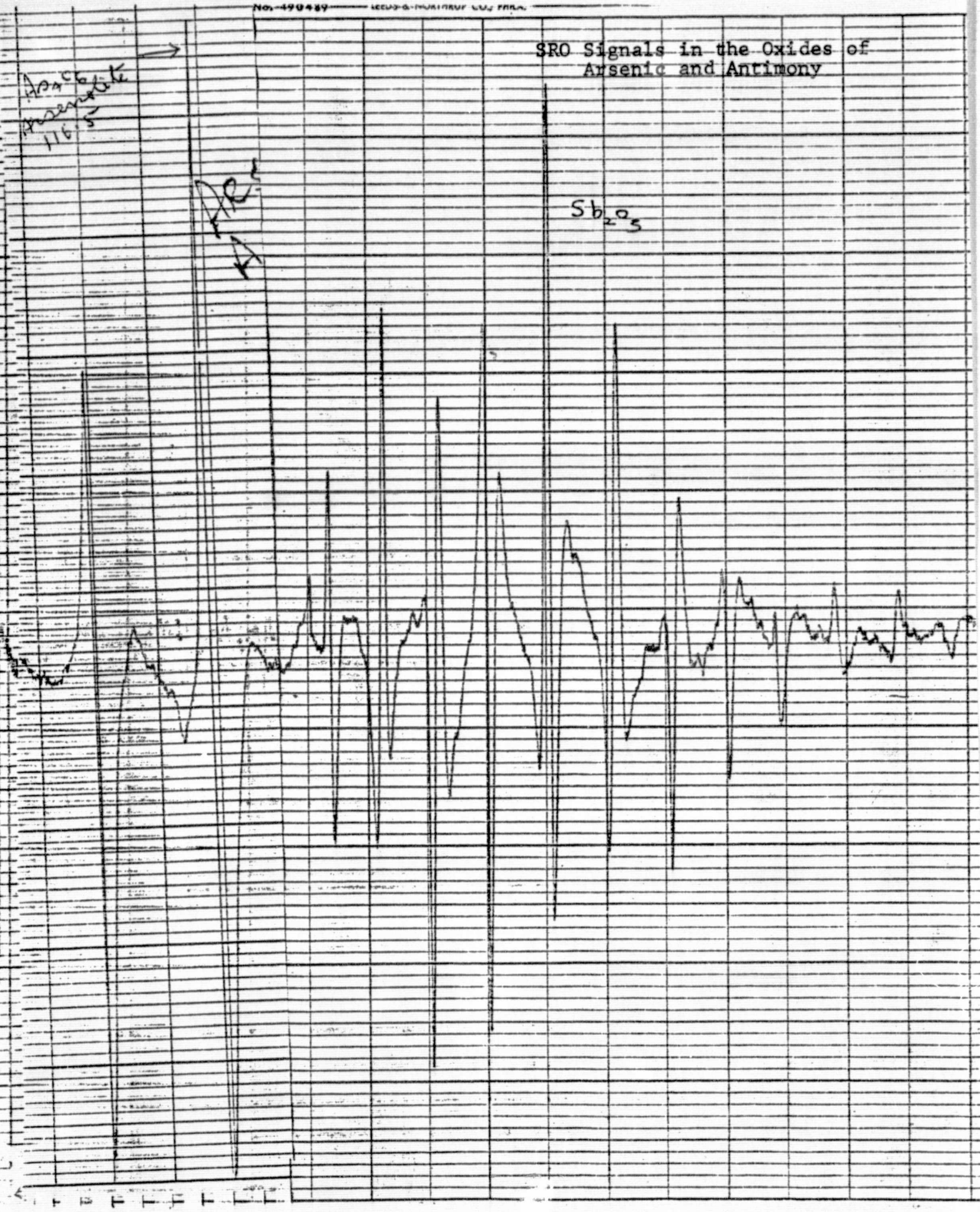
TYPICAL RECORDER OUTPUTS OF NQR SPECTRA

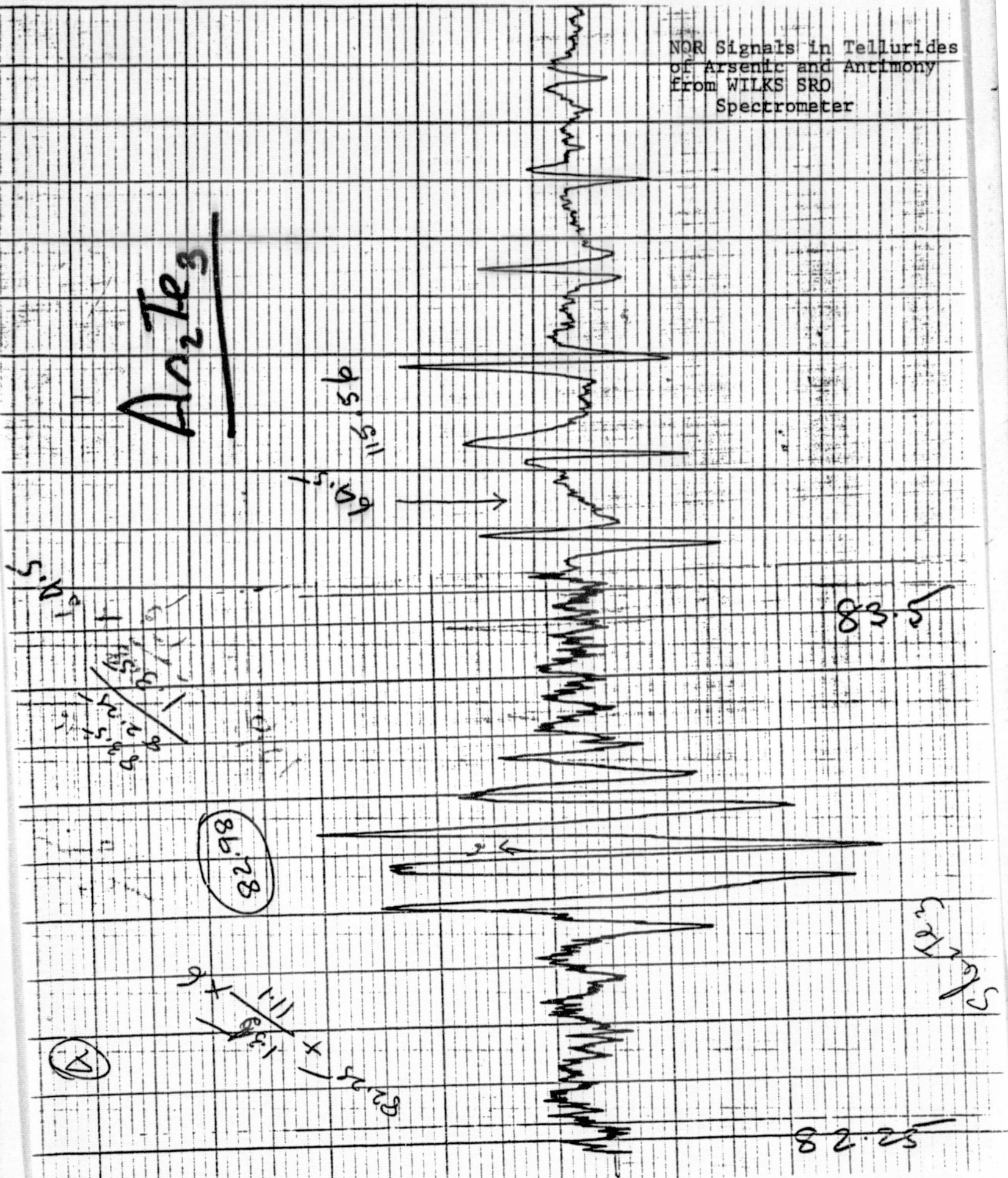
$NaClO_3$ Signal from Research Systems Marginal Oscillator Unit Using Lock in Detection

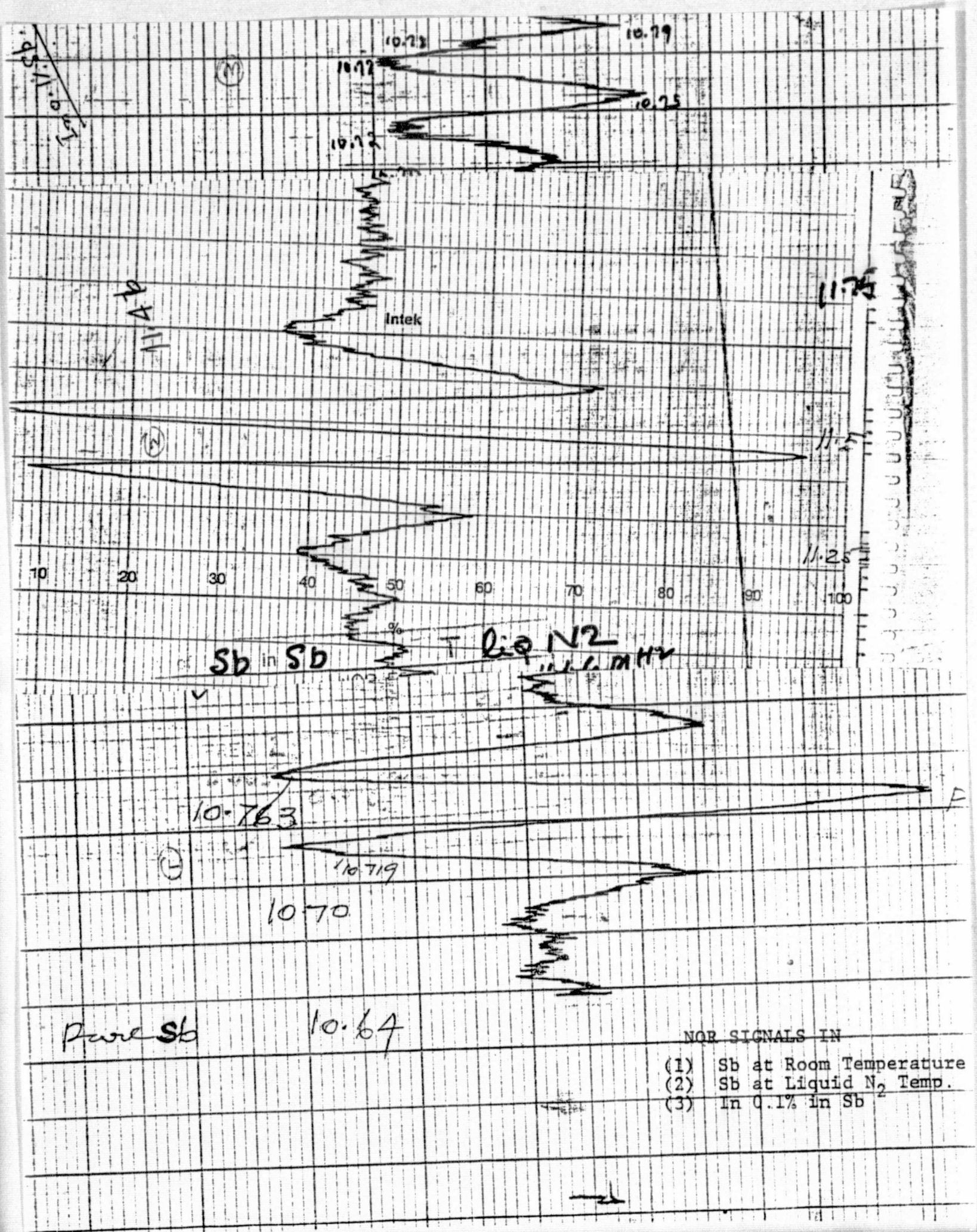


BENTON HARBOR, MICHIGAN CHART NO. 445-B PRINTED IN U.S.A.

SRO Signals in the Oxides of Arsenic and Antimony





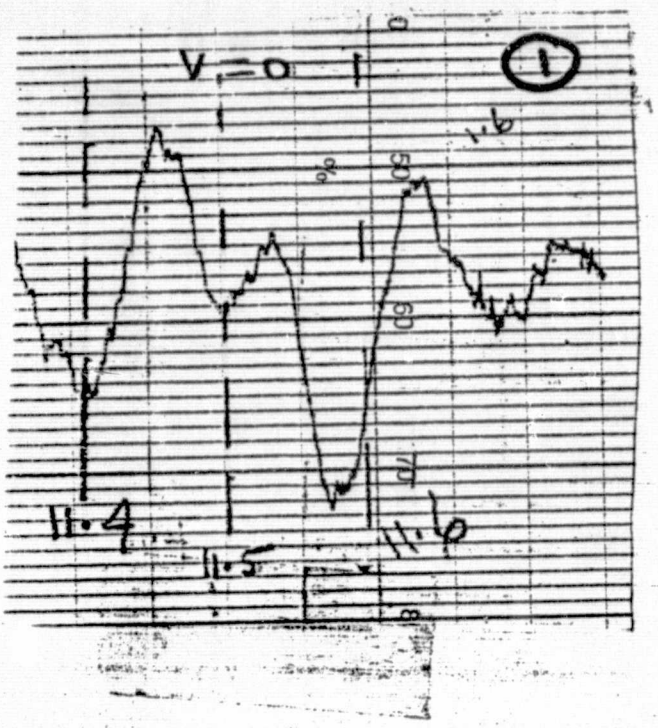


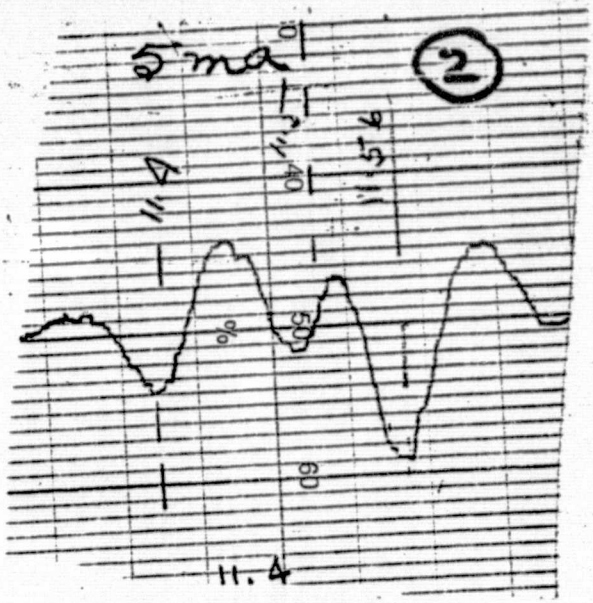
NOR SIGNALS IN

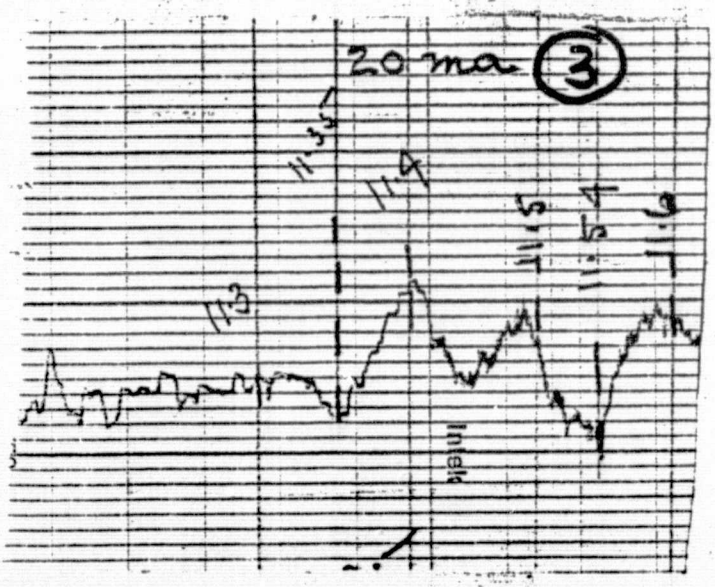
(1) Sb at Room Temperature
(2) Sb at Liquid N_2 Temp.
(3) In 0.1% in Sb

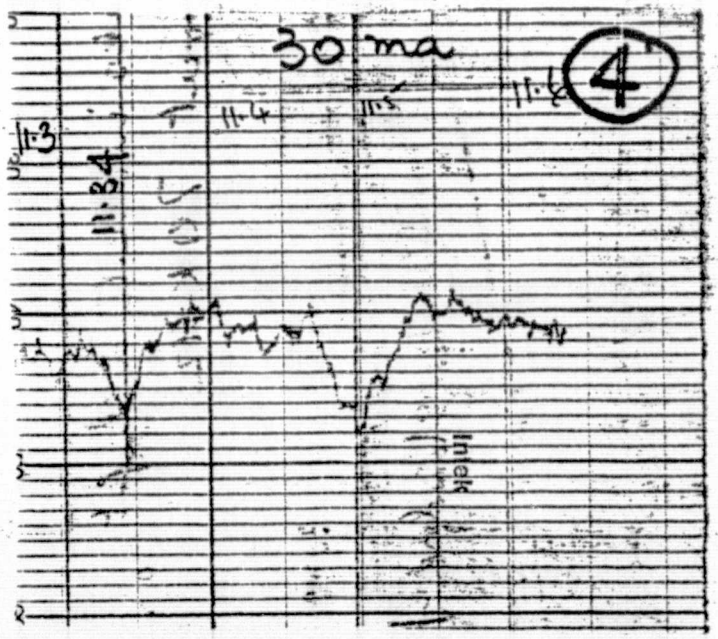
Sample Sb. liq N_2 Temp.

Line Broadening and Frequency Shift due to Conduction Current Increase









APPENDIX C

COMPUTER PROGRAM FOR SELF CONSISTANT ESTIMATION OF ELECTROSTATIC FIELD GRADIENTS

```
      C
      C
      C     A. N. MURTY, PHYSICS DEPARTMENT
      C
      C     PROGRAM FOR SELF CONSISTANT ESTIMATION OF ELECTROSTATIC FIELDS
      C     AND FIELD GRADIENTS IN IONIC SOLIDS
      C
0001        DIMENSION XO(1250),YO(1250),ZO(1250),TYPEO(1250),NATO(1250),
           1XR(1250),YR(1250),ZR(1250),RR(1250),TYPE(1250),NAT(1250),
           2NUM(1250),A(4,4),D(10),V(10,1),T(9,10),C(9,10),TC(9,9),ALPHA(9),
           3CH(9,1)
0002        S1(F1)=-F1/R3
0003        S2(F1,F2)=(-3.*F1*F2)/R5
0004        S3(F1)=(R2-3.*F1*F1)/R5
0005        S4(F1,F2)=(3.*F1*(R2-5.*F2*F2)/R5)/R2
0006        S5(F1,F2)=(3.*F1*(3.*R2-5.*F2*F2)/R5)/R2
0007        S6(F1)=5.*F1/R2
0008        S7(F1)=1.-7.*F1*F1/R2
0009        S8(F1)=((3.*F1*F1)/R5)/R2
0010        S9(F1)=3.-7.*F1*F1/R2
0011        S13(F1,F2)=(3./R5/R4)*((R2-5.*F1*F1)*(R2-5.*F2*F2)
           1+10.*F1*F1*F2*F2)
0012        S14(F1,F2)=(1.5/R2/R5)*((1.-7.*F1*F1/R2)*
           1(R2-5.*F2*F2)+2.*F1*F1)
0013        S15(F1)=(1.5/R2/R5)*((1.-7.*F1*F1/R2)*
           1(3.*R2-5.*F1*F1)-4.*F1*F1)
0014        ELECH=4.8
0015        JK=63
      C     JK SPECIFIES THE LATTICE AT WHICH FIELDS AND FIELD GRADIENTS
      C     ARE COMPUTED.
0016        M=0
0017        READ(5,10)NC,AC,BC,CC,AD,AG
      C     READS THE NUMBER OF ATOMS AND THE DIMENSIONS OF THE UNIT CELL AND
      C     POLARISABILITY VALUES.
0018        H=0.5
0019        F=0.866
0020        A(1,3)=0.0
0021        A(2,3)=0.0
0022        A(3,1)=0.0
0023        A(3,2)=0.0
0024        A(3,3)=1.0
0025        DO 3 L= 1,NC
0026        READ(5,2)U,VV,W,ATOM,NATOM
      C     READS THE CRYSTALLINE POSITION COORDINATES OF ALL THE ATOMS IN THE
      C     GIVEN UNIT CELL ALONG WITH THEIR IDENTIFICATION NUMBERS
0027        U1=U-3.
0028        DO 3 I=1,5
0029        U1=U1+1.
0030        V1=VV-3.
0031        DO 3 J=1,5
0032        V1=V1+1.
0033        W1=W-3.
0034        DO 3 K=1,5
0035        W1=W1+1.
0036        CA=AD*U1
0037        CB=BC*V1
```

```
0038              CC=CO*W1
0039              M=M+1
0040              NATO(M)=NATOM
0041              TYPEO(M)=ATOM
0042              XO(M)=0.268*(CA+CB-2.0*CC)
0043              YO(M)=0.464*(CA-CB)
0044              ZO(M)=0.644*(CA+CB+CC)
0045            3 CONTINUE
                C     STARTING FROM THE GIVEN UNIT CELL LOCATES ALL ATOMS IN THE LATTICE
                C     2 UNIT CELLS AWAY IN ALL THE THREE CRYSTALLINE AXES DIRECTIONS,
                C     CONVERTS THEM INTO CARTESIAN COORDINATES AND STORES IN THE XO,YO,
                C     ZO, COLUMN MATRICES.
0046              NT=NO*125
0047            5 DO 4 J=1,NT
0048              XR(J)=XO(JK)-XO(J)
0049              YR(J)=YO(JK)-YO(J)
0050              ZR(J)=ZO(JK)-ZO(J)
0051              TYPE(J)=TYPEO(J)
0052              NAT(J)=NATO(J)
0053              NUM(J)=J
0054              X2=XR(J)*XR(J)
0055              Y2=YR(J)*YR(J)
0056              Z2=ZR(J)*ZR(J)
0057            4 RR(J)=SQRT(X2+Y2+Z2)
0058              K=NT
0059              KM1=K-1
0060              DO 9 N=1,KM1
0061              NP1=N+1
0062              M=N
0063              DO 11 J=NP1,K
0064              IF(RR(M)-RR(J))11,11,12
0065           12 M=J
0066           11 CONTINUE
0067              RT=RR(N)
0068              RR(N)=RR(M)
0069              RR(M)=RT
0070              XT=XR(N)
0071              XR(N)=XR(M)
0072              XR(M)=XT
0073              YT=YR(N)
0074              YR(N)=YR(M)
0075              YR(M)=YT
0076              ZT=ZR(N)
0077              ZR(N)=ZR(M)
0078              ZR(M)=ZT
0079              TYPET=TYPE(N)
0080              TYPE(N)=TYPE(M)
0081              TYPE(M)=TYPET
0082              NATT=NAT(N)
0083              NAT(N)=NAT(M)
0084              NAT(M)=NATT
0085              NUMT=NUM(N)
0086              NUM(N)=NUM(M)
0087              NUM(M)=NUMT
0088            9 CONTINUE
0089              WRITE(6,20)NT,TYPE(NT),NAT(NT),XR(NT),YR(NT),ZR(NT),RR(NT),M
```

```
      C     TAKING THE JK ATOM AS ORIGIN COORDINATES DISTANCES OF ALL THE
      C     ATOMS IN THE LATTICE RELATIVE TO THE JK ATOM, ARE COMPUTED AND
      C     STORED IN THE XR,YR,ZR,RR COLUMN MATRICES IN ASCENDING ORDER OF
      C     DISTANCE.
0090     70 DO 13 I=1,9
0091        DO 13 J=1,10
0092     13 T(I,J)=0.0
0093        DO 14 L=1,NT
0094        X=XR(L)
0095        Y=YR(L)
0096        Z=ZR(L)
0097        R=RR(L)
0098        NSITE=NAT(L)
0099        IF(R.EQ.0.0) GO TO 14
0100        R2=R*R
0101        R3=R2*R
0102        R4=R2*R2
0103        R5=R3*R2
0104        IF(NSITE-1)18,18,19
      C     DEPENDING ON THE NATURE OF THE ATOM ITS IONIC CHARGE IS ASSIGNED
0105     18 CP=-2.*ELECH
0106        GO TO 21
0107     19 CP=3.*ELECH
0108     21 C(1,1)=S1(X)*CP
0109        C(2,1)=S1(Y)*CP
0110        C(3,1)=S1(Z)*CP
0111        C(4,1)=-S3(X)*CP
0112        C(5,1)=-S3(Y)*CP
0113        C(6,1)=-S3(Z)*CP
0114        C(7,1)=-S2(X,Y)*CP
0115        C(8,1)=-S2(Y,Z)*CP
0116        C(9,1)=-S2(Z,X)*CP
      C     COMPUTES THE CHARGE CONTRIBUTIONS TO THE FIELDS AND FIELD GRADIENTS
0117        IF(NSITE-1)22,22,23
0118     22 IF(TYPE(L).EQ.11.) GO TO 60
0119        IF(TYPE(L).EQ.12) GO TO 62
0120        IF(TYPE(L).EQ.13.) GO TO 63
0121        IF(TYPE(L).EQ.14.) GO TO 64
0122        IF(TYPE(L).EQ.15.) GO TO 65
0123        IF(TYPE(L).EQ.16.) GO TO 66
      C     CHOOSES PROPER COORDINATE TRANSFORMATION MATRIX FOR THE DIPOLE AND
      C     QUADRUPOLE MOMENTS OF THE POLARISABLE ATOMS IN THE LATTICE FOR
      C     COMPUTING FIELDS AND FIELD GRADIENTS AT THE JK IONIC SITE.
0124     62 A(1,1)=-H
0125        A(1,2)=F
0126        A(2,1)=-F
0127        A(2,2)=-H
0128        GO TO 60
0129     63 A(1,1)=-H
0130        A(1,2)=-F
0131        A(2,1)=F
0132        A(2,2)=-H
0133        GO TO 60
0134     64 A(1,1)=-1.0
0135        A(1,2)=0.0
0136        A(2,1)=0.0
```

```
0137            A(2,2)=-1.0
0138            GO TO 60
0139         65 A(1,1)=H
0140            A(1,2)=-F
0141            A(2,1)=F
0142            A(2,2)=H
0143            GO TO 60
0144         66 A(1,1)=H
0145            A(1,2)=F
0146            A(2,1)=-F
0147            A(2,2)=H
0148         60 DO 39 J=1,3
0149            A(4,J)=A(1,J)
0150         39 A(J,4)=A(J,1)
0151            A(4,4)=A(1,1)
0152         50 P1=2.5/R2
0153            P2=P1*S7(X)
0154            P3=P1*S7(Y)
0155            P4=P1*S7(Z)
0156            P5=P1*S9(X)
0157            P6=P1*S9(Y)
0158            P7=P1*S9(Z)
0159            C(1,2)=S3(X)
0160            C(2,2)=S2(X,Y)
0161            C(3,2)=S2(Z,X)
0162            C(4,2)=-S5(X,X)
0163            C(5,2)=-S4(X,Y)
0164            C(6,2)=-S4(X,Z)
0165            C(7,2)=-S4(Y,X)
0166            C(8,2)=-S6(Z)*C(2,2)
0167            C(9,2)=-S4(Z,X)
0168            C(1,3)=C(2,2)
0169            C(2,3)=S3(Y)
0170            C(3,3)=S2(Y,Z)
0171            C(4,3)=C(7,2)
0172            C(5,3)=-S5(Y,Y)
0173            C(6,3)=-S4(Y,Z)
0174            C(7,3)=C(5,2)
0175            C(8,3)=-S4(Z,Y)
0176            C(9,3)=C(8,2)
0177            C(1,4)=C(3,2)
0178            C(2,4)=C(3,3)
0179            C(3,4)=S3(Z)
0180            C(4,4)=C(9,2)
0181            C(5,4)=C(8,3)
0182            C(6,4)=-S5(Z,Z)
0183            C(7,4)=C(8,2)
0184            C(8,4)=C(6,3)
0185            C(9,4)=C(6,2)
0186            C(1,5)=-0.5*C(4,2)
0187            C(2,5)=-0.5*C(4,3)
0188            C(3,5)=-0.5*C(4,4)
0189            C(4,5)=S15(X)
0190            C(5,5)=S14(Y,X)
0191            C(6,5)=S14(Z,X)
0192            C(7,5)=P5*C(1,3)
```

```
0193              C(8,5)=P2*C(2,4)
0194              C(9,5)=P5*C(1,4)
0195              C(1,6)=-0.5*C(5,2)
0196              C(2,6)=-0.5*C(5,3)
0197              C(3,6)=-0.5*C(8,3)
0198              C(4,6)=S14(X,Y)
0199              C(5,6)=S15(Y)
0200              C(6,6)=S14(Z,Y)
0201              C(7,6)=P6*C(1,3)
0202              C(8,6)=P6*C(2,4)
0203              C(9,6)=P3*C(1,4)
0204              C(1,7)=-0.5*C(6,2)
0205              C(2,7)=-0.5*C(6,3)
0206              C(3,7)=-0.5*C(6,4)
0207              C(4,7)=S14(X,Z)
0208              C(5,7)=S14(Y,Z)
0209              C(6,7)=S15(Z)
0210              C(7,7)=P4*C(1,3)
0211              C(8,7)=P7*C(2,4)
0212              C(9,7)=P7*C(1,4)
0213              C(1,8)=-C(7,2)
0214              C(2,8)=-C(5,2)
0215              C(3,8)=-C(8,2)
0216              C(4,8)=2.*C(7,5)
0217              C(5,8)=2.*C(7,6)
0218              C(6,8)=2.*C(7,7)
0219              C(7,8)=S13(X,Y)
0220              C(8,8)=2.*C(9,6)
0221              C(9,8)=2.*C(8,5)
0222              C(1,9)=-C(9,3)
0223              C(2,9)=-C(5,4)
0224              C(3,9)=-C(6,3)
0225              C(4,9)=2.*C(8,5)
0226              C(5,9)=2.*C(8,6)
0227              C(6,9)=2.*C(8,7)
0228              C(7,9)=2.*C(9,6)
0229              C(8,9)=S13(Y,Z)
0230              C(9,9)=C(6,8)
0231              C(1,10)=2.*C(3,5)
0232              C(2,10)=C(1,9)
0233              C(3,10)=2.*C(1,7)
0234              C(4,10)=2.*C(9,5)
0235              C(5,10)=C(7,9)
0236              C(6,10)=2.*C(9,7)
0237              C(7,10)=C(4,9)
0238              C(8,10)=C(6,8)
0239              C(9,10)=S13(Z,X)
                C     COMPUTATION OF THE COEFFICIENTS ( C MATRIX) OF DI (DIPOLE MOMENT
                C     COMPONENTS) AND QIJ (QUADRUPOLEMENT COMPONENTS) TO (VI AND VIJ IS)
                C     FIELDS AND FIELD GRADIENTS
                C     COMPLETED AND STARTS STORING IN THE T-MATRIX.
0240              IF (TYPE(L).NE.11.) GO TO 61
0241              DO 16 I=1,9
0242              DO 16 J=1,10
0243           16 T(I,J)=T(I,J)+C(I,J)
0244              GO TO 14
```

```
0245          61 DO 71 I=1,9
0246          71 T(I,1)=T(I,1)+C(I,1)
0247             DO 72 I=1,9
0248             DO 72 M=1,3
0249             DO 72 N=1,3
0250          72 T(I,M+1)=T(I,M+1)+A(M,N)*C(I,N+1)
0251             DO 73 I=1,9
0252             DO 73 M=1,3
0253             DO 73 N=1,3
0254          73 T(I,M+4)=T(I,M+4)+A(M,N)*A(M,N)*C(I,N+4)
0255             DO 74 I=1,9
0256             DO 74 M=1,3
0257             DO 74 N=1,3
0258          74 T(I,M+4)=T(I,M+4)+A(M,N)*A(M,N+1)*C(I,N+7)
0259             DO 75 I=1,9
0260             DO 75 M=1,3
0261             DO 75 N=1,3
0262          75 T(I,M+7)=T(I,M+7)+2.0*A(M,N)*A(M+1,N)*C(I,N+4)
0263             DO 76 I=1,9
0264             DO 76 M=1,3
0265             DO 76 N=1,3
0266          76 T(I,M+7)=T(I,M+7)+(A(M,N)*A(M+1,N+1)+A(M+1,N)*A(M,N+1))*C(I,N+7)
0267             GO TO 14
0268          23 DO 25 I=1,9
0269          25 T(I,1)=T(I,1)+C(I,1)
0270          14 CONTINUE
0271             WRITE(6,200)
0272             DO 26 I=1,9
0273          26 WRITE(6,300) (T(I,J),J=1,10)
0274             IF(JK.EQ.813) GO TO 33
0275             DO 80 I=1,3
0276          80 ALPHA(I)=-AO
0277             DO 81 I=4,9
0278          81 ALPHA(I)=AQ
0279             DO 77 I=1,9
0280          77 CH(I,1)=T(I,1)
0281             DO 78 I=1,9
0282             DO 78 J=1,9
0283          78 TC(I,J)=-T(I,J+1)*ALPHA(J)
0284             DO 79 I=1,9
0285             DO 79 J=1,9
0286          79 IF(I.EQ.J)TC(I,J)=TC(I,J)+1.
0287             CALL SIMQ(TC,CF,9,KS)
0288             IF(KS.EQ.0) GO TO 82
0289             WRITE(6,90)KS
0290             GO TO 36
0291          82 WRITE(6,100) (CH(I,1),I=1,9)
0292             DO 83 J=1,9
0293             V(J,1)=CH(J,1)
0294          83 D(J+1)=ALPHA(J)*V(J,1)
0295             D(1)=1.0
0296             WRITE (6,120)
0297          42 WRITE(6,35) (D(L),L=1,10)
0298             WRITE(6,55)AO,AQ
0299          33 DO 34 I=1,9
0300             IF (I.EQ.1) WRITE(6,130)
```

```
0301            VC=T(I,1)*D(1)
0302            VDX=T(I,2)*D(2)
0303            VDY=T(I,3)*D(3)
0304            VDZ=T(I,4)*D(4)
0305            VD=VDX+VDY+VDZ
0306            VQXX=T(I,5)*D(5)
0307            VQYY=T(I,6)*D(6)
0308            VQZZ=T(I,7)*D(7)
0309            VQXY=T(I,8)*D(8)
0310            VQYZ=T(I,9)*D(9)
0311            VQZX=T(I,10)*D(10)
0312            VQ=VQXX+VQYY+VQZZ+VQXY+VQYZ+VQZX
0313            V(I,1)=VC+VD+VQ
0314         34 WRITE(6,45)VC,VDX,VDY,VDZ,VD,VQXX,VQYY,VQZZ,VQXY,VQYZ,VQZX,
               1VQ,V(I,1)
0315            IF(JK.EQ.813) GO TO 36
0316            JK=813
0317            GO TO 5
0318         36 STOP
0319          2 FORMAT(3F11.8,F4.0,I2)
0320         10 FORMAT(I5,5F7.3)
0321         15 FORMAT(10F7.3)
0322         40 FORMAT(20X,F7.4,/)
0323         20 FORMAT(8X,I4,2X,F4.0,2X,I2,4(3X,F8.3),I9)
0324         30 FORMAT(8X,I4,2X,F4.0,2X,I2,3(3X,F8.3))
0325         35 FORMAT(6X,10(4X,F8.3))
0326         45 FORMAT(///,13(2X,F8.3))
0327         55 FORMAT(30X,2F15.2)
0328         90 FORMAT(10X,I2)
0329        100 FORMAT(8X,9(4X,F8.3),//)
0330        200 FORMAT(50X,20H** T  M  A  T  R  I  X **,//)
0331        300 FORMAT(8X,10(4X,F8.3),//)
0332        120 FORMAT(50X,22H** MULTIPOLE MOMENTS**,//)
0333        130 FORMAT(50X,31H** FIELDS AND FIELD GRADIENTS**,//)
0334            END
```

```
      C                                                                      SIMQ  10
      C     ------------------------------------------------------------------SIMQ  20
      C                                                                      SIMQ  30
      C        SUBROUTINE SIMQ                                               SIMQ  40
      C                                                                      SIMQ  50
      C        PURPOSE                                                       SIMQ  60
      C           OBTAIN SOLUTION OF A SET OF SIMULTANEOUS LINEAR EQUATIONS, SIMQ  70
      C           AX=B                                                       SIMQ  80
      C                                                                      SIMQ  90
      C        USAGE                                                         SIMQ 100
      C           CALL SIMQ(A,B,N,KS)                                        SIMQ 110
      C                                                                      SIMQ 120
      C        DESCRIPTION OF PARAMETERS                                     SIMQ 130
      C           A - MATRIX OF COEFFICIENTS STORED COLUMNWISE.  THESE ARE    SIMQ 140
      C               DESTROYED IN THE COMPUTATION.  THE SIZE OF MATRIX A IS  SIMQ 150
      C               N BY N.                                                SIMQ 160
      C           B - VECTOR OF ORIGINAL CONSTANTS (LENGTH N). THESE ARE      SIMQ 170
      C               REPLACED BY FINAL SOLUTION VALUES, VECTOR X.           SIMQ 180
      C           N - NUMBER OF EQUATIONS AND VARIABLES. N MUST BE .GT. ONE.  SIMQ 190
      C           KS - OUTPUT DIGIT                                          SIMQ 200
      C                0 FOR A NORMAL SOLUTION                               SIMQ 210
      C                1 FOR A SINGULAR SET OF EQUATIONS                     SIMQ 220
      C                                                                      SIMQ 230
      C        REMARKS                                                       SIMQ 240
      C           MATRIX A MUST BE GENERAL.                                  SIMQ 250
      C           IF MATRIX IS SINGULAR , SOLUTION VALUES ARE MEANINGLESS.   SIMQ 260
      C           AN ALTERNATIVE SOLUTION MAY BE OBTAINED BY USING MATRIX    SIMQ 270
      C           INVERSION (MINV) AND MATRIX PRODUCT (GMPRD).               SIMQ 280
      C                                                                      SIMQ 290
      C        SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                 SIMQ 300
      C           NONE                                                       SIMQ 310
      C                                                                      SIMQ 320
      C        METHOD                                                        SIMQ 330
      C           METHOD OF SOLUTION IS BY ELIMINATION USING LARGEST PIVOTAL SIMQ 340
      C           DIVISOR. EACH STAGE OF ELIMINATION CONSISTS OF INTERCHANGINGSIMQ 350
      C           ROWS WHEN NECESSARY TO AVOID DIVISION BY ZERO OR SMALL     SIMQ 360
      C           ELEMENTS.                                                  SIMQ 370
      C           THE FORWARD SOLUTION TO OBTAIN VARIABLE N IS DONE IN       SIMQ 380
      C           N STAGES. THE BACK SOLUTION FOR THE OTHER VARIABLES IS      SIMQ 390
      C           CALCULATED BY SUCCESSIVE SUBSTITUTIONS. FINAL SOLUTION     SIMQ 400
      C           VALUES ARE DEVELOPED IN VECTOR B, WITH VARIABLE 1 IN B(1),  SIMQ 410
      C           VARIABLE 2 IN B(2),......, VARIABLE N IN B(N).             SIMQ 420
      C           IF NO PIVOT CAN BE FOUND EXCEEDING A TOLERANCE OF 0.0,     SIMQ 430
      C           THE MATRIX IS CONSIDERED SINGULAR AND KS IS SET TO 1. THIS  SIMQ 440
      C           TOLERANCE CAN BE MODIFIED BY REPLACING THE FIRST STATEMENT. SIMQ 450
      C                                                                      SIMQ 460
      C     ------------------------------------------------------------------SIMQ 470
      C                                                                      SIMQ 480
0001        SUBROUTINE SIMQ(A,B,N,KS)                                        SIMQ 490
0002        DIMENSION A(1),B(1)                                              SIMQ 500
      C                                                                      SIMQ 510
      C        FORWARD SOLUTION                                              SIMQ 520
      C                                                                      SIMQ 530
0003        TOL=0.0                                                          SIMQ 540
0004        KS=0                                                             SIMQ 550
0005        JJ=-N                                                            SIMQ 560
```

```
0006            DO 65 J=1,N                                                  SIMQ 570
0007            JY=J+1                                                       SIMQ 580
0008            JJ=JJ+N+1                                                    SIMQ 590
0009            BIGA=0                                                       SIMQ 600
0010            IT=JJ-J                                                      SIMQ 610
0011            DO 30 I=J,N                                                  SIMQ 620
                C                                                            SIMQ 630
                C       SEARCH FOR MAXIMUM COEFFICIENT IN COLUMN             SIMQ 640
                C                                                            SIMQ 650
0012            IJ=IT+I                                                      SIMQ 660
0013            IF(ABS(BIGA)-ABS(A(IJ))) 20,30,30                            SIMQ 670
0014         20 BIGA=A(IJ)                                                   SIMQ 680
0015            IMAX=I                                                       SIMQ 690
0016         30 CONTINUE                                                     SIMQ 700
                C                                                            SIMQ 710
                C       TEST FOR PIVOT LESS THAN TOLERANCE (SINGULAR MATRIX) SIMQ 720
                C                                                            SIMQ 730
0017            IF(ABS(BIGA)-TOL) 35,35,40                                   SIMQ 740
0018         35 KS=1                                                         SIMQ 750
0019            RETURN                                                       SIMQ 760
                C                                                            SIMQ 770
                C       INTERCHANGE ROWS IF NECESSARY                        SIMQ 780
                C                                                            SIMQ 790
0020         40 I1=J+N*(J-2)                                                 SIMQ 800
0021            IT=IMAX-J                                                    SIMQ 810
0022            DO 50 K=J,N                                                  SIMQ 820
0023            I1=I1+N                                                      SIMQ 830
0024            I2=I1+IT                                                     SIMQ 840
0025            SAVE=A(I1)                                                   SIMQ 850
0026            A(I1)=A(I2)                                                  SIMQ 860
0027            A(I2)=SAVE                                                   SIMQ 870
                C                                                            SIMQ 880
                C       DIVIDE EQUATION BY LEADING COEFFICIENT               SIMQ 890
                C                                                            SIMQ 900
0028         50 A(I1)=A(I1)/BIGA                                             SIMQ 910
0029            SAVE=B(IMAX)                                                 SIMQ 920
0030            B(IMAX)=B(J)                                                 SIMQ 930
0031            B(J)=SAVE/BIGA                                               SIMQ 940
                C                                                            SIMQ 950
                C       ELIMINATE NEXT VARIABLE                              SIMQ 960
                C                                                            SIMQ 970
0032            IF(J-N) 55,70,55                                             SIMQ 980
0033         55 IQS=N*(J-1)                                                  SIMQ 990
0034            DO 65 IX=JY,N                                                SIMQ1000
0035            IXJ=IQS+IX                                                   SIMQ1010
0036            IT=J-IX                                                      SIMQ1020
0037            DO 60 JX=JY,N                                                SIMQ1030
0038            IXJX=N*(JX-1)+IX                                             SIMQ1040
0039            JJX=IXJX+IT                                                  SIMQ1050
0040         60 A(IXJX)=A(IXJX)-(A(IXJ)*A(JJX))                              SIMQ1060
0041         65 B(IX)=B(IX)-(B(J)*A(IXJ))                                    SIMQ1070
                C                                                            SIMQ1080
                C       BACK SOLUTION                                        SIMQ1090
                C                                                            SIMQ1100
0042         70 NY=N-1                                                       SIMQ1110
0043            IT=N*N                                                       SIMQ1120
```

```
0044          DO 80 J=1,NY                                          SIMQ1130
0045          IA=IT-J                                               SIMQ1140
0046          IB=N-J                                                SIMQ1150
0047          IC=N                                                  SIMQ1160
0048          DO 80 K=1,J                                           SIMQ1170
0049          B(IB)=B(IB)-A(IA)*B(IC)                               SIMQ1180
0050          IA=IA-N                                               SIMQ1190
0051       80 IC=IC-1                                               SIMQ1200
0052          RETURN                                                SIMQ1210
0053          END                                                   SIMQ1220
```

APPENDIX D

COMPUTER PROGRAM FOR NUMERICAL SOLUTIONS OF THE QUADRUPOLE INTERACTION ENERGY SECULAR EQUATIONS

```
      C   COMPUTATION OF N Q R FREQUENCY FACTORS AND THEIR RELATIVE
      C   RATIOS AS A FUNCTION OF THE ASYMMETRY PARAMETER
      C
      C
0001        DIMENSION X(101),E(9,101),E97(101),E75(101),E53(101),E31(101),
           1R1(101),R2(101),R3(101),R4(101),R5(101),R6(101)
0002      1 READ(5,2)E1,N,J,K
0003        I=0
0004        A=0.0
0005        Y=0.01
0006        GO TO (4,5,6),N
0007      4 C1=E1
0008        X2=A*A
0009        C2=C1*C1
0010        C3=C2*C1
0011        E2=(2.*C3+20.*(1.-X2))/(3.*C2-7.*(3.+X2))
0012        D=ABS(E2-E1)
0013        IF(D-0.0001)8,8,9
0014      9 E1=E2
0015        GO TO 4
0016      8 I=I+1
0017        X(I)=A
0018        E(J,I)=E2
0019        E1=E2
0020        A=A+Y
0021        IF(A-1.)4,4,10
0022     10 IF(J-1)11,11,1
0023     11 WRITE(6,3)
0024        WRITE(6,30)
0025        DO 12 I=1,101
0026        E53(I)=E(5,I)-E(3,I)
0027        E31(I)=E(3,I)-E(1,I)
0028        R1(I)=E53(I)/E31(I)
0029     12 WRITE(6,13)X(I),E(5,I),E(3,I),E(1,I),E53(I),E31(I),R1(I)
0030        WRITE(6,60)
0031        GO TO 1
0032      5 C1=E1
0033        X2=A*A
0034        C2=C1*C1
0035        C3=C2*C1
0036        C4=C2*C2
0037        X3=1.+X2/3.
0038        X4=X3*X3
0039        DN=0.75*(C4-14.*X3*C2-35.*X4)
0040        DD=C3-21.*X3*C1-16.*(1.-X2)
0041        E2=DN/DD
0042        D=ABS(E2-E1)
0043        IF(D-0.0001)14,14,15
0044     15 E1=E2
0045        GO TO 5
0046     14 I=I+1
0047        X(I)=A
0048        E(J,I)=E2
0049        E1=E2
0050        A=A+Y
0051        IF(A-1.)5,5,16
```

```
0052          16 IF(J-1)17,17,1
0053          17 WRITE(6,18)
0054             WRITE(6,40)
0055             DO 19 I=1,101
0056             E75(I)=E(7,I)-E(5,I)
0057             E53(I)=E(5,I)-E(3,I)
0058             E31(I)=E(3,I)-E(1,I)
0059             R1(I)=E75(I)/E31(I)
0060             R2(I)=E53(I)/E31(I)
0061             R3(I)=E75(I)/E53(I)
0062          19 WRITE(6,20)X(I),E(7,I),E(5,I),E(3,I),E(1,I),E75(I),E53(I),
                1E31(I),R1(I),R2(I),R3(I)
0063             WRITE(6,60)
0064             GO TO 1
0065           6 C1=E1
0066             C2=C1*C1
0067             C3=C2*C1
0068             C4=C2*C2
0069             C5=C4*C1
0070             X2=A*A
0071             D1=3.+X2
0072             D2=1.-X2
0073             D3=D1*D1
0074             DN=4.*C5-22.*D1*C3-44.*D2*C2-48.*D1*D2
0075             DD=5.*C4-33.*D1*C2-88.*D2*C1+44.*D3/3.
0076             E2=DN/DD
0077             D=ABS(E2-E1)
0078             IF(D-0.0001)21,21,22
0079          22 E1=E2
0080             GO TO 6
0081          21 I=I+1
0082             X(I)=A
0083             E(J,I)=E2
0084             E1=E2
0085             A=A+Y
0086             IF(A-1.)6,6,23
0087          23 IF(J-1)24,24,1
0088          24 WRITE(6,25)
0089             WRITE(6,50)
0090             DO 26 I=1,101
0091             E97(I)=E(9,I)-E(7,I)
0092             E75(I)=E(7,I)-E(5,I)
0093             E53(I)=E(5,I)-E(3,I)
0094             E31(I)=E(3,I)-E(1,I)
0095             R1(I)=E97(I)/E31(I)
0096             R2(I)=E75(I)/E31(I)
0097             R3(I)=E53(I)/E31(I)
0098             R4(I)=E97(I)/E53(I)
0099             R5(I)=E75(I)/E53(I)
0100             R6(I)=E97(I)/E75(I)
0101          26 WRITE(6,27)X(I),E(9,I),E(7,I),E(5,I),E(3,I),E(1,I),E97(I),
                1E75(I),E53(I),E31(I),R1(I),R2(I),R3(I),R4(I),R5(I),R6(I)
0102             STOP
0103           2 FORMAT(F4.1,3I2)
0104           3 FORMAT(1H ,60X,7HI = 5/2//)
0105          13 FORMAT(10X,F5.2,6(10X,F8.5))
```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```
0106          18 FORMAT(1H ,60X,7HI = 7/2//)
0107          20 FORMAT(5X,F5.2,10(4X,F8.5))
0108          25 FORMAT(1H ,60X,7HI = 9/2//)
0109          27 FORMAT(F5.2,9(1X,F8.5),6(1X,F6.3))
0110          30 FORMAT(1H ,10X,4HASYM,13X,4HE5/2,14X,4HE3/2,14X,4HE1/2,13X,
                 15HE5-E3,13X,5HE3-E1,12X,7HE53/E31//)
0111          40 FORMAT (1H ,5X,4HASYM,7X,4HE7/2,8X,4HE5/2,8X,4HE3/2,8X,4HE1/2,
                 17X,5HE7-E5,7X,5HE5-E3,7X,5HE3-E1,6X,7HE75/E31,5X,7HE53/E31,5X,
                 27HE75/E53//)
0112          50 FORMAT(1H ,4HASYM,4X,4HE9/2,5X,4HE7/2,5X,4HE5/2,5X,4HE3/2,
                 15X,4HE1/2,4X,5HE9-E7,4X,5HE7-E5,4X,5HE5-E3,4X,5HE3-E1,
                 21X,7HE97/E31,7HE75/E31,7HE53/E31,7HE97/E53,7HE75/E53,
                 37HE97/E75//)
0113          60 FORMAT(1H1)
0114             END
```