MASTER

A Progress Report to

THE U.S. DEPARTMENT OF ENERGY

by

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Magnetic Measurements of the Transuranium Elements

and

Charge State Characterization of Actinides in Monazite

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Magnetic Measurements of the Transuranium Elements

A micromagnetic susceptometer for the purpose of measuring extremely small sample quantities (on the microgram level) was designed, constructed, and calibrated in previous years. The 1979 progress report[1] gives details of its operation. This device has operated without significant downtime in this funding period and much progress has been made in the magnetic characterization of elements beyond Am in the periodic table. Our program has roughly doubled man's knowledge of magnetism in Cm, Bk, and Cf and we have made the only Es magnetic measurements to date. The incorporation of an automatic data collection system in this period has made our analysis much more accurate and has allowed quicker turnaround of compounds and metals for study.

The following sections give a summary of results obtained for the compounds and metals studied this year.

Curium

Our previous measurements[1] on Cm-248 metal did not exhibit a unique low temperature antiferromagnetic transition in small fields (< 1600 G) as has been observed by others[2] in high fields (> 10,000 G). These studies[1] had shown a field and history dependent transition in the temperature range 55-80 K. Once the transition was observed to be of antiferromagnetic character at 55 K. During other measurements the susceptibility was constant below 80 K. In this funding period we pursued this anomaly by looking (1) at a larger sample (> 1 mg) and (2) at a freshly prepared sample of mass 130 μg to determine if the effects were due to a small number of crystallites with an anisotropy which we are unable to overcome in our largest fields. Both of the new samples had an indication of a maximum susceptibility in the range 60-65 K indicating an antiferromagnetic transition but the smaller sample had a transition at lower temperature to a large permanent moment per atom ($\sim .2\ \mu_B$). The large sample had the behavior expected for a classical, polycrystalline sample; i.e., an antiferromagnetic transition in the range 63-65 K with the susceptibility at 4.2 K being $\sim$ 2/3 of the maximum. This is illustrated in Fig. 1. Both samples gave the expected paramagnetic behavior at high temperatures as determined from a Curie-Weiss fit. The average moment value of 7.8 μ_B is very close to the theoretical value of 7.94 μ_B for the 3+ ion based on Hund's Rule and L-S coupling.

One of the preliminary samples[1] had shown a high temperature maximum in susceptiblity at about 200 K. This sample was nominally of the dhcp crystal structure but had one x-ray line attributable to the fcc form.

This lead us to undertake to prepare a pure fcc sample for measurement. Since this is the high temperature structure it was prepared by quenching a sample from the melt. The sample exhibited a transition at 205 K to a ferrimagnetic state. The average saturation moment, determined by cooling in a field of 16 kG, was 0.4 μ_B. By fitting the high temperature susceptibility to a two-site ferrimagnetic susceptiblity of the form,

$$X = \frac{(C_1 + C_2)T - 2\lambda C_1 C_2}{T^2 - T_N^2} \qquad \text{with} \quad C_i = \frac{N\mu_i^2}{6k} ,$$

a moment of 6.5 μ_B at one site and 5.7 μ at the other was determined. (The difference was constrained to be 0.8 μ_B.) Also we obtained λ = 231 ± 49 and T_N = 205 ± .6 K. Attempts to convert this same sample to the pure dhcp form were unsuccessful.

Einsteinium

During this contract period we have made the first quantitative magnetic measurements on compounds of ^{253}Es as well as the first qualitative measurements on ^{253}Es metal. This is an extremely difficult measurement due to the short half-life of 20 days, due to ingrowth of Bk daughter as an impurity, due to the small masses available (∿ 3 μg), and due to the high specific activity. One Es_2O_3 sample of mass 4.08 μg was determined to exhibit Curie-Weiss behavior with μ_{eff} = 10.1 μ_B and a θ_p of 44.9 K. An EsF_3 sample of mass 3.25 μg also exhibited Curie-Weiss behavior with μ_{eff} = 11.1 μ_B and θ = 40 K. Both values are close to the free ion; 3+ value of 10.6 μ_B expected theoretically, considering the error of determining mass by gamma-counting the samples. Figure 2 is a plot of the inverse susceptibility versus temperature for EsF_3. An attempt was

made to vapor deposit Es metal on a Platinum disk. This sample had no indication of magnetic transitions in the range 4.2 K - 350 K, but, since the sample signal is comparable to that from the Platinum disk, work is still underway to obtain quantitative values for the susceptibility.

Californium

A sample of CfO_2 was prepared by heating Cf_2O_3 at $\sim$ 300°C in an atomic oxygen atmosphere. Since CfO_2 decomposes upon heating to Cf_2O_3 (the more stable form) the two processes compete. Simultaneous measurements of the magnetic susceptibilities of a 26.0 μg sample of CfO_2, thus prepared, and a 34.7 μg sample of Cf_2O_3 were made. In this way it was desired to determine the actual composition assuming the Cf ions had the theoretical moment values of 9.62 μ_B and 10.6 μ_B in CfO_2 and Cf_2O_3 respectively. This is useful since the actual composition was heretofore determined from x-ray derived lattice spacings which must be corrected for lattice damage due to α decay. Unfortunately, we were only able to measure in the temperature range from 4.2 K to 90 K due to experimental problems. The plots of inverse susceptibility versus temperature showed some slight curvature and the values of 11.49 μ_B and 12.77 μ_B for CfO_2 and Cf_2O_3 were obtained from Curie-Weiss fits. These values are felt to be unreliable over such a small span. An alternate explanation for these high values is a large temperature independent contribution to the susceptibility arising from a low lying excited electronic state or ferromagnetic impurities in the samples. At present we are in the process of repeating these measurements.

Berkelium

Measurements were made on a 44.3 μg sample of BkF_4 at a time when 2% Cf had grown in. Its susceptibility was Curie-Weiss like with $\mu_{eff} = 7.80\ \mu_B$ and $\theta = 8$ K. This is to be compared with the theoretical free ion value of 7.94 μ_B for an f^7 electronic configuration. This experimental value indicates a well defined 4+ state for Bk in the compound and serves as a good ionic standard.

Simultaneous measurements were made on a "large" 338.7 μg sample of Bk metal with an ingrowth of 2% Cf. A Curie-Weiss fit to the high temperature data (50 K - 300 K) gives values of $\mu_{eff} = 9.67\ \mu_B$ and $\theta = 183$ K in very good agreement with the 3+, theoretical value of 9.72 μ_B. The low temperature behavior is characterized by a susceptibility maximum at 22 K in a 189 G field but with a large moment "turning-on" at 33 K. The maximum occurs at 25 K in a field of 800 G. Thus the low temperature data may be complicated by domain structure or a second crystal phase as in Curium metal.

This sample of metal was also cooled to a temperature of 2.3 K by pumping on the liquid Helium bath. This is a new feature added to the susceptometer during this funding period and is designed for a future search of superconductivity in actinide compounds. Bk metal is not superconducting down to this temperature.

Americium

Simultaneous measurement of the susceptibilities of large samples of AmF_3 and AmF_4 (> 1 mg) was undertaken to serve as ionic standards for Americium. Subsequently it was determined from spectrophotometric

analysis that the majority of the AmF_4 sample was AmF_3. The AmF_3 sample (1.113 mg) behaves similarly to Am metal with both a large, temperature-independent contribution and a small Curie-Weiss contribution to its susceptibility. The temperature-independent part of the molar susceptibility was determined to be: $X_m = 710.6 \times 10^{-6}$ emu/mole in comparison to 780×10^{-6} emu/mole for the metal. This term is attributable to low lying excited state for Am as is the case for Sm and Eu in the lanthanide series. The paramagnetic term is generally attributed to impurities, with the Curie-Weiss fit giving only 0.63 μ_B/Am. Kanellakopulos[3] has suggested that this term is due to a small portion of the sample in the Am^{2+} state which has a high moment of 6.2 μ_B. The two parts are separated by plotting χT versus T with the slope of the resulting straight line being the temperature independent part and the y-axis intercept the paramagnetic Curie constant. The quality of this fit is illustrated in Fig. 3.

Summary of Measurements

Sample	Mass (μg)	μ_{eff} (μ_B)	θ (K)	Type of Magnetic Transition	T_N or T_C (K)
^{248}Cm (dhcp)	130	7.56	180.4	AF?	60
^{248}Cm (dhcp)	1136.8	7.82	38.7	AF	64 ± 1
^{248}Cm (fcc)	152	6.33 5.93	--	Ferrimagnetic	205 ± .6
$^{253}Es_2O_3$	4.08	10.1	44.9	None above 4.2 K	--
$^{249}CfO_2$	26.0	11.49	20.9	None above 4.2 K	--
$^{249}Cf_2O_3$	34.7	12.77	40.0	None above 4.2 K	--
$^{249}BkF_4$	44.3	7.80	8	None above 4.2 K	--
^{249}Bk	338.7	9.67	183	AF	25 K @ 800 G
AmF_3	1113.0	.63	1.8	Temp. independent paramagnetism $\chi_m = 710 \times 10^{-6}$ (emu/mole)	
$^{253}EsF_3$	3.25	11.1	40	None above 4.2 K	--

Charge State Characterization of Radioactive Waste in Synthetic Monazite

The lanthanide orthophosphates are being investigated as an alternate means of primary containment for high level actinide wastes. Researchers at the Oak Ridge National Laboratory are involved in preparation of actinide doped compounds for all of the lanthanide transition series (La through Lu) for a study of leaching characteristics and E.S.R. classification. We have been aiding this study by identifying the charge state of ^{237}Np or ^{57}Fe either in the as-prepared compounds or following radioactive decay of ^{241}Am via the Mössbauer Effect. We feel that the final charge state will be an influential variable in the immobilization characteristics of the waste products stored in this synthetic monazite form.

The rationale for using these two Mössbauer isotopes involves the projected dissolution technique for spent fuel rods from a reactor. The fuel rods contain a significant fraction of radioactive iron from the stainless steel cladding and a small amount of Americium (and other transuranium elements) due to neutron absorption. Presumably partial assemblies of these spent rods will be dissolved in concentrated nitric acid, along with oxides of the lanthanide elements. Upon addition of ammonium phosphate and urea, to aid control of particle size, the precipitates will be formed as a mixture of low concentration actinides or iron in the rare earth orthophosphates. This step may be followed by a calcination process to remove waters of hydration at $\sim 800°C$ if it is an aid in providing better immobalization characteristics. Our studies therefore are made both prior to and following the heat and quench process.

The Mössbauer spectra are influenced by (a) local chemical effects, (b) local electric field gradients, and (c) local magnetic fields at the ^{237}Np or ^{57}Fe nuclei. In order to remove one complication (c) from the spectral distributions we have chosen to study only the $LaPO_4$ and $LuPO_4$ compounds since they exhibit no bulk magnetic properties. Both the isomer shift due to chemical bonding, and the quadrupole hyperfine interaction due to crystal field gradients are influenced by the charge state in these two nuclei. Figures 4 and 5 show the regions (represented by solid bars) of Doppler velocity which have been identified by previous researchers. There are seen to exist reasonably clear limits of the shift or splitting for these two Mössbauer elements in the many compounds which have been studied. In this figure several values of shift and splitting for the phosphates and oxides have been noted for later comparison with our unknown synthetic monazite compounds.

Iron Mössbauer Results

As a reference for the other spectra, Fig. 6 shows the Mössbauer spectrum for our ^{57}Co in rhodium standard source with an armco iron absorber. Two velocity scales (-10 mm/sec to +10 mm/sec and -4 mm/sec to +4 mm/sec) are shown for this pure magnetically split spectrum. Note the linewidth of each line is approximately equal to the natural linewidth of ^{57}Fe ($\sim$ 0.3 mm/sec).

Figure 7 shows our spectra for $FePO_4$ prepared by our precipitation technique. In the high velocity spectrum it is seen that no evidence exists for any iron metal (i.e., no absorption lines exist at the velocity of the peaks seen in Fig. 6). In the low velocity spectrum, it may be seen that a pure doublet (due to a single electric field gradient

site) spectrum is observed. The isomer shift (∿ -0.2 mm/sec) and the hyperfine splitting (∿ 0.7 mm/sec) are in good agreement with Fig. 4.

Figure 8 shows our spectra for 6 atomic percent ^{57}Fe precipitated with $LuPO_4$ both prior to and following a quench from 800°C. Again the results are consistent with either $FePO_4$ or $FePO_4 \cdot 4H_2O$ but we see broader unsymmetrical spectral lines indicating more than one kind of site. Statistics are poorer here due to strong absorption of the 14 keV Mössbauer γ-ray by the Lu atoms. It is seen in this figure that narrower lines are exhibited following the quench (suggesting a higher population of one of the kinds of sites) but that they are still larger than the natural line width seen in $FePO_4$ as in Fig. 7. No lines corresponding to the 2+ state $Fe_3(PO_4)_2 \cdot 8H_2O$ are produced by the preparation process (see Fig. 4).

Since $ScPO_4$ has the same tetragonal structure of $LuPO_4$ we have also placed 6 atomic percent ^{57}Fe in a $ScPO_4$ sample prepared by this technique. The resulting Mössbauer spectrum is seen in Fig. 9. Here several sets of spectra are seen. A small background distortion due to an iron magnetic spectrum at high velocities may be caused by iron metal particles at the 1% or lower level. The quadrupole doublet characteristic of $FePO_4$ is seen near zero velocity. An additional "mystery doublet" at ∿ -2.5 mm/sec could not be caused by any known isomer shift. Perhaps these lines are part of another pair buried beneath the $FePO_4$ spectrum at zero velocity (caused by $Fe_3(PO_4)_2$?). Further data to improve statistical resolution should answer this question.

Neptunium Mössbauer Results

The most interesting charge state determinations involve the question of the final configuration of a recoiling actinide atom following an energetic α-decay. The violent emission of the $\sim$ 5 MeV α is calculated to displace the nucleus approximately 200 lattice spacings from its initial site. Since the actinides which are of concern from an environmental viewpoint have long half lives (433 years for ^{241}Am), the ingrowth of the daughters occur slowly. The very dilute daughter component will have an unknown final chemical state which is not easily studied by other techniques in normal laboratory time frames. Fortunately only the recoillessly emitted γ-rays from the ^{237}Np nuclei are measured in a Mössbauer study. Thus within several excited state half-lives (of 68 nsec) a "flash" picture is made of the "final" state of the ^{237}Np daughter.

Figure 10 provides a summary of our actinide results to date. In part (a) we show the spectrum obtained with a metal ^{241}Am source and an NpO_2 absorber. Presumably the NpO_2 has Np atoms in a stable 4+ configuration. The isomer shift of +8 mm/sec is consistent with source Np nuclei in a higher charge state (between 4+ and 5+). The non-integer nature of these Np atoms in an Americium metal host is not unusual. Note that no other absorption lines are seen in the spectrum and the linewidth of 2 mm/sec (while much larger than the natural linewidth) is as good as any previously observed.

The same Am metal source used in 10a was then used with another absorber of 1% Np doped into $LaPO_4$ crystals. Though denoted as $NpPO_4$, the final Np configuration is not known and the charge state of the Np

is certainly not 3+. The fact that the isomer shift (relative to the Am metal source) is nearly zero (in fact +3 mm/sec) means that the Np atoms exist in a higher charge state (perhaps $Np^{+4.3}$). This spectrum has been shifted to the right so that the charge bands at the top apply. It is not reasonable to suggest that the ionicity of the Np is greater than that of NpF_4 (shown at the top) as the fluorine compounds always exhibit the highest isomer shift in a given charge band. Rather it is suggested that the Np exists in a very covalent 5+ configuration. Unfortunately the absorption spectrum of a similar small sample suggests the Np are in the 4+ state in disagreement with the Mössbauer conclusions above.

In Fig. 10c we show the results for a source of ^{241}Am doped into $LaPO_4$ crystals with the NpO_2 absorber. The charge bands at the top again apply. Two possible explanations for this complex spectrum exist. One is that the spectrum results from a local hyperfine interaction of coupled electric field gradient and magnetic field. A higher velocity spectrum shows no indication of other lines and we have found no single Hamiltonian consistent with this distribution. A second explanation is that the "flash" pictures made by many such decays result in several possible "final" configurations--each with a separate charge state. Three of the peaks are in the correct position to be the mixed 3+, 4+, and 5+ states. Even the quadrupole broadening of Fig. 5 is consistent with this picture. Of course these "flash" pictures are made within a few hundred nanoseconds after the Np nucleus comes to rest. That a distribution of charge states within this time frame would have environmental consequences is unknown. It is entirely possible that after several seconds some equilibrium well defined charge state is produced which is stable with respect to leaching.

Service Research

Inasmuch as we have the only operating Mossbauer program at ORNL and one of only two susceptometers we feel an obligation to provide service to others when it will not interfere with the main thrust of our funded program. Two such programs have been aided in 1980. In both cases we have provided critical information for the studies.

One study involved the reprocessing program. It also applies to the waste effort. In disposing of the low-level radioactive noble gases released upon dissolution of spent fuel elements, it is accepted practice to blow them up a smokestack. Unfortunately small iron-containing particles often accompany the noble gases up the stack and they provide an unacceptable background. Toward a solution to this problem, some of the particles were collected and found to be attracted by a horseshoe magnet. A temporarily obvious solution was then to place a magnetic separator in the effluent line. Upon addition of such a separator to a pilot plant it was found to be a very inefficient removal device. We cooperated with the group by studying the magnetic properties of the iron particles at temperatures they might experience in the effluent gas (up to 400°C). We found a clear transition from the ferromagnetic to the paramagnetic state at 250°C for the particles. The results suggest that the gases must be cooled prior to magnetic separation for an efficient operation.

Another study involves the synthetic fuel pilot plant at Wilsonville, Alabama. Operation has shown severe degradation of the iron plates in a cracking tower and has led to partial failure of the plates. We have examined some of the "oils" collected at various stages in this tower with

our Mössbauer spectrometer in an attempt to identify the insitu chemical state of the iron. Perhaps this will aid the understanding of the mechanism of degradation and suggest a prevention. Initial studies gave insufficient ^{57}Fe in the frozen "oils" for a reasonable statistical identification. Upon our suggestion some pure ^{57}Fe was subjected to the environment in the tower and also dissolved. These frozen "oils" have provided good spectra and we are in the process of interpreting them.

References

1. P. G. Huray, "A Progress Report to the U.S. Department of Energy--Magnetic Measurements of the Transuranium Elements," 1979.
2. B. Kanellakopulos, A. Blaise, J. M. Fournier, and W. Müller, Solid State Communications 17, 713-15 (1975).
3. B. Kanellakopulos, C. Aderhold, E. Dornberger, Radiochimica Acta 25, 89-92 (1978).

Original Proposal
Expenditure Statement

1-1-80 to 12-31-80

Category on Audit Trail	Date	Amount
1. Professional Salaries:	12-07-80	$ 43,658.62
(Includes - Principal Investigator,	1-08-80	- 16,747.29
Postdoctoral Res. Assoc.		26,911.33
Grad. Res. Asst.	12-80*	+ 1,545.05
BUDGET $ 30,175.00		$ 28,456.38
2. Clerical Salaries:	12-07-80	$ 3,352.21
	1-08-80	- 1,000.00
		2,352.21
	12-80*	+ 311.11
BUDGET $ 0.00		$ 2,633.32
3. Biweekly Salaries:	12-07-80	$ 0.00
	1-08-80	0.00
		0.00
	12-80*	0.00
BUDGET $ 955.00		$ 0.00
4. Fringe Benefits:	12-07-80	$ 5,246.90
		- 1,559.03
		3,687.87
	12-80*	+ 217.59
BUDGET $ 3,870.00		$ 3,905.46

TOTALS: Budget - $ 35,000 *Expended and Estimated - $ 34,995.16

APPROVED
REVISED
BUDGET

DOE DE-AS05-79ER10348

	1/1/80 - 1/1/81
SALARIES AND WAGES	
1. Principal Investigator	
20% Academic Year	$ 4,800.00
3 mos. summer	8,000.00
2. Postdoctoral Research Associate 100% effort	13,000.00
3. Graduate Research Assistant 100% effort	4,375.00
4. Undergraduate Research Assistant 100% effort for 3 months	955.00
Total Salaries and Wages	$31,130.00
TRAVEL	0
PUBLICATIONS	0
FRINGE BENEFITS - 15% x $25,800	3,870.00
INDIRECT COSTS - 43% x $31,130	13,385.90
Total Project Costs	$48,385.90
COST SHARING - The University of Tennessee will cost share by the reduction of indirect costs	$13,385.90
Total Requested from Agency	$35,000.00

Paul G. Murray
Principal Investigator

Head, Department of Physics

L. B. CEBIK
ASSISTANT DEAN FOR RESEARCH

Supplemental Funds
Expenditure Statement

1-1-80 to 12-31-80

Category on Audit Trail	Date	Amount
1. Travel:	12-07-80	$ 5,084.43
	1-08-80	- 1,473.73
		3,610.70
	12-80*	+ 1,050.00
BUDGET $ 2,000.00		$ 4,660.70
2. Printing and Duplications:	12-07-80	$ 50.75
	1-08-80	- 0.00
		50.75
	12-80*	0.00
BUDGET $ 1,000.00		$ 50.75
3. Operating Supplies:	12-07-80	$ 3,557.08
	1-08-80	- 0.00
		3,557.08
	12-80*	+ 1,000.00
BUDGET (see 5)		$ 4,557.08
4. Scientific Equipment:	12-07-80	$ 7,901.45
	1-08-80	- 0.00
		7,901.45
	12-80*	+ 730.00
BUDGET (see 5)		$ 8,631.45
5. Blanket P.O. to ORNL:	12-07-80	$ 0.00
	1-08-80	- 0.00
		0.00
	12-80*†	+ 12,000.00
BUDGET ($ 27,000 for 3, 4, and 5)		$ 12,000.00

TOTALS: Budget - $ 30,000.00 *Expended and Estimated - $ 29,899.98

†Contract legalities between purchasing agents, bookkeepers, and administrators have delayed payments until December 1980.

One check was mailed on December 1, 1980 for	- $ 4,893.78
for July, August, and September services. A bill for	- 1,389.91
has been received for October service. November and December bills will arrive in 1981. An estimate of	- 5,716.29
has been made since craft and liquid helium usage was heavy during these months.	$12,000.00

Supplementary
Budget
Request

to DOE DE-AS05-79ER10348

Travel	$ 2,000.00
Publications	$ 1,000.00
Crafts and Materials	$27,000.00
TOTAL SUPPLEMENTARY REQUEST OF AGENCY	$30,000.00

Paul G. Huray
Principal Investigator

William M. Bugg, Head
Department of Physics

Institutional Administrator
CARL O. THOMAS
DEAN FOR RESEARCH

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*SEE REVERSE SIDE FOR OBJECT CODE DESCRIPTION.

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GRANT AND CONTRACT BUDGET AND EXPENDITURE REPORT

REPORTING PERIOD 11/01/80 TO 11/30/80

PRINCIPAL INVEST AND ADDRESS: DR PAUL HURAY	ACCOUNT NAME: DOE DE-AS05-79ER10348	DEPARTMENT: PHYSICS	ACCOUNT NO: R01-1060-70
BUDGET ENTITY: KNOXVILLE		COLLEGE/MAJOR DIV.: COLLEGE OF LIBERAL ARTS	STATUS: FINAL — PAGE NO: 1
REPORTING ORG. AFFIBILITES: 121-01-10-060-000-02		FUNCTION: RESEARCH	RUN SEQUENCE: 777 — RUN DATE: 12/07/80

TOTAL FUNDS	DIRECT EXPENSE	INDIRECT EXPENSE	I/C CAL	COST SHARING	C/S CAL	I/C	C/S	CA	FILATED BALANCE	GRANT NUMBER	GRANT PERIOD	I/C
124,940.00	87,200.00	7,740.00	38.30	13,386.00	.00				B01996789	060063	01-01-80 TO 12-31-80	01

DATE	INTRANSIT NUMBER	PURCHASE ORDER NUMBER	TRANSACTION TYPE AND REFERENCE NUMBER	DESCRIPTION	BUDGET	INTRANSIT	UNPAID PURCHASE ORDERS OR ENCUMBRANCE	OBJECT CODE*	EXPENDITURES	FREE BALANCE
	BEGINNING BALANCE			- PROFESSIONAL SALARIES	48,175				42,013.57	6,161.43
11300			PV 35	MONTHLY				121	1,545.05	
11300			PV 35	MONTHLY				131	100.00	
	ENDING BALANCE			- PROFESSIONAL SALARIES	48,175				43,658.62	4,516.38
	BEGINNING BALANCE			- CLERICAL & SUPPORTING SALARIED					3,041.10	3,041.10-
11300			PV 35	MONTHLY				161	311.11	
	ENDING BALANCE			- CLERICAL & SUPPORTING SALARIED					3,352.21	3,352.21-
	BEGINNING BALANCE			- BIWEEKLY WAGES	955					955.00
	ENDING BALANCE			- BIWEEKLY WAGES	955					955.00
	BEGINNING BALANCE			- OPERATING & MISCELLANEOUS	26,070				12,307.25	13,762.75
11300			PV 35	STAFF BENEFITS				212	76.48	
11300			PV 35	STAFF BENEFITS				214	66.41	
11300			PV 35	STAFF BENEFITS				215	1.71	
11300			PV 35	STAFF BENEFITS				217	60.16	
11300			PV 35	STAFF BENEFITS				221	12.83	
11100		00035326	PO	CAMPBELL TOOL CO			526.15	39100		
11030			DV 651435	TECHNI-TOOL, INC.				39100	16.42	
11100			DV 655852	PAUL G. HURAY				31200	730.63	
11260			DV 664478	PERFORMANCE BUSINESS FORM				39100	216.87	
05270			TV 5837	TRANSPORTATION SERVICE				31300	450.40	
	ENDING BALANCE			- OPERATING & MISCELLANEOUS	26,070		526.15		13,939.16	11,604.69
	BEGINNING BALANCE			- EQUIPMENT & CAPITAL OUTLAY	12,000				7,901.45	4,098.55
11130		00035368	PO	TRANS ERA CORP			565.00	61200		
	ENDING BALANCE			- EQUIPMENT & CAPITAL OUTLAY	12,000		565.00		7,901.45	3,533.55
	TOTAL				87,200		1,091.15		68,851.44	17,257.41

	DETAIL OF ENCUMBERED REGULAR PURCHASE ORDERS	ORIG. AMT.	INTRANSIT	PAID-TO-DATE	BALANCE	
11100	00035326 CAMPBELL TOOL CO	526.15			526.15	391
11130	00035368 TRANS ERA CORP	565.00			565.00	612
	TOTAL OUTSTANDING REGULAR PURCHASE ORDERS				1,091.15	

	DETAIL OF UNENCUMBERED BLANKET PURCHASE ORDERS	ORIG. AMT.	INTRANSIT	PAID-TO-DATE	BALANCE	OBJ CO	PAID-TO-DATE THIS ACCOUNT
		**********	ENTIRE	PURCHASE ORDER	**********		
11110	00035336 ORNL	12,000.00			12,000.00	391	
	TOTAL OUTSTANDING BLANKET PURCHASE ORDERS				12,000.00		

BUDGET ANALYSIS

	MONTH EXPEND	YEAR-TO-DATE	PERIOD BUD	PERIOD INTRAN	PERIOD ENCUMB	OB CO	PERIOD-TO-DATE	FREE BALANCE
ACADEMIC SALARIES	1,545.05	6,802.25				121	21,148.81	
ACADEMIC EXTRA SERVICE	.00	5,333.34				122	15,997.33	
*TOT ACADEMIC SALARIES	1,545.05	12,135.59	33,800			12	37,146.14	3,346.14-
GTA, GA, GRA SALARIES	100.00	1,200.00				131	6,512.48	
*TOT GTA,GA,GRA SALARIES	100.00	1,200.00	14,375			13	6,512.48	7,862.52

Dec 80

UPON RECEIPT, ITEMS APPEARING ON THIS REPORT SHOULD BE VERIFIED FOR ACCURACY. IN REPORTING OR REQUESTING INFORMATION, PLEASE REFER TO ACCOUNT NUMBER AND TRANSACTION REFERENCE NUMBER

*SEE REVERSE SIDE FOR OBJECT CODE DESCRIPTION.

THE UNIVERSITY OF TENNESSEE

OFFICE OF THE TREASURER

GRANT AND CONTRACT BUDGET AND EXPENDITURE REPORT

REPORTING PERIOD 11/01/80 TO 11/30/80

PRINCIPAL INVEST. AND ADDRESS: DR PAUL HURAY	ACCOUNT NAME: DOE DE-AS05-79ER10348 BUDGET ENTITY: KNOXVILLE REPORTING ORG ATTRIBUTES (FUND BE COLL DEPT SUB FUNC): 121-01-10-060-000-02	DEPARTMENT: PHYSICS COLLEGE/MAJOR DIV.: COLLEGE OF LIBERAL ARTS FUNCTION: RESEARCH	ACCOUNT NO.: R01-1060-70 STATUS: FINAL PAGE NO.: 2 RUN SEQUENCE: 778 RUN DATE: 12/07/80

TOTAL FUNDS	DIRECT EXPENSE	INDIRECT EXPENSE	I/C CAL	COST SHARING	C/S CAL	I/C	C/S	CAL	RELATED BALANCE	GRANT NUMBER	GRANT PERIOD	I/C
124,940.00	87,200.00	7,740.00	38.30	13,386.00	.00				B01996789	060063	01-01-80 TO 12-31-80	01

DATE	INTRANSIT NUMBER	PURCHASE ORDER NUMBER	TRANSACTION TYPE AND REFERENCE NUMBER	DESCRIPTION	BUDGET	INTRANSIT	UNPAID PURCHASE ORDERS OR ENCUMBRANCE	OBJECT CODE*	EXPENDITURES	FREE BALANCE
				BUDGET ANALYSIS						
				MONTH EXPEND YEAR-TO-DATE	PERIOD BUD	PERIOD INTRAN	PERIOD ENCUMB	OB C	PERIOD-TO-DATE	FREE BALANCE
				SALARIES 311.11 1,913.88				161	2,913.88	
				OVERTIME .00 438.33				162	438.33	
				*TOT CLERICAL & SUPPORTIN 311.11 2,352.21				16	3,352.21	3,352.21-
				*TOT STUDENT EMPLOYEES	955			18		955.00
				RETIREMENT CONTRIB-TIAA/B .00				211	638.88	
				RETIREMENT CONTRIB-STATE 76.48 382.40				212	1,262.13	
				SOCIAL SECURITY CONTRIBUT 66.41 728.87				214	2,163.11	
				UNEMPLOYMENT COMPENSATION 1.71 10.66				215	73.06	
				RETIREMENT CONTRIB-TIAA/A 60.16 981.42				217	981.42	
				*TOT STAFF BENEFITS - REQ 204.76 2,103.35	5,070			21	5,118.60	48.60-
				GROUP INSURANCE 12.83 64.15				221	128.30	
				*TOT STAFF BENEFITS - OPT 12.83 64.15				22	128.30	128.30-
				OUT OF STATE 730.63 730.63				312	2,817.00	
				MTR VEH OPER-TRAVEL IN ST 450.40 864.20				313	2,267.43	
				*TOT TRAVEL 1,181.03 1,594.83	5,000			31	5,084.43	84.43-
				PRINTING .00				331	50.75	
				*TOT PRINTING, DUPLICATIN	1,000			33	50.75	949.25
				*TOT MAINTENANCE AND REPA	7,500			36		7,500.00
				OPERATING SUPPLIES 233.29 2,652.37			526.15	391	3,557.08	
				*TOT SUPPLIES 233.29 2,652.37	7,500		526.15	39	3,557.08	3,416.77
				EDUC & SCIENTIFIC EQUIPME .00 617.06			565.00	612	7,901.45	
				*TOT EQUIPMENT 617.06	12,000		565.00	61	7,901.45	3,533.55
				TOTAL 3,588.07 22,719.56	87,200		1,091.15		68,851.44	17,257.41

UPON RECEIPT, ITEMS APPEARING ON THIS REPORT SHOULD BE VERIFIED FOR ACCURACY. IN REPORTING OR REQUESTING INFORMATION, PLEASE REFER TO ACCOUNT NUMBER AND TRANSACTION REFERENCE NUMBER

*SEE REVERSE SIDE FOR OBJECT CODE DESCRIPTION.

THE UNIVERSITY OF TENNESSEE

OFFICE OF THE TREASURER

GRANT AND CONTRACT BUDGET AND EXPENDITURE REPORT

REPORTING PERIOD 12/01/79 TO 12/31/79

PRINCIPAL INVEST. AND ADDRESS: DR PAUL HURAY	ACCOUNT NAME: DOE DE-AS05-79ER10348	DEPARTMENT: PHYSICS	ACCOUNT NO.: R01-1060-70
BUDGET ENTITY: KNOXVILLE		COLLEGE/MAJOR DIV.: COLLEGE OF LIBERAL ARTS	STATUS: FINAL / PAGE NO.: 1
REPORTING ORG ATTRIBUTES: 121-01-10-060-000-02 (FUND, BS, COV, DIST, SUB, FUNC)		FUNCTION: RESEARCH	RUN SEQUENCE: 682 / RUN DATE: 01/08/80

TOTAL FUNDS	DIRECT EXPENSE	INDIRECT EXPENSE	I/C CAL	COST SHARING	C/S CAL	I/C	C/S	CAL	RELATED BALANCE	GRANT NUMBER	GRANT PERIOD	I/C
29,940.00	22,200.00	7,740.00	43.00	.00	.00				801996789	060063	01-01-79 TO 12-31-79	01

DATE	INTRANSIT NUMBER	PURCHASE ORDER NUMBER	TRANSACTION TYPE AND REFERENCE NUMBER	DESCRIPTION	BUDGET	INTRANSIT	UNPAID PURCHASE ORDERS OR ENCUMBRANCE	OBJECT CODE*	EXPENDITURES	FREE BALANCE
				BEGINNING BALANCE - PROFESSIONAL SALARIES	18,000				15,601.46	2,398.54
12319			PV 38	MONTHLY				121	833.33	
12319			PV 38	MONTHLY				131	312.50	
				ENDING BALANCE - PROFESSIONAL SALARIES	18,000				16,747.29	1,252.71
				BEGINNING BALANCE - CLERICAL & SUPPORTING SALARIED					1,000.00	1,000.00-
				ENDING BALANCE - CLERICAL & SUPPORTING SALARIED					1,000.00	1,000.00-
				BEGINNING BALANCE - OPERATING & MISCELLANEOUS	4,200				2,313.76	1,886.24
12319			PV 38	STAFF BENEFITS				212	63.75	
12319			PV 38	STAFF BENEFITS				214	51.08	
12319			PV 38	STAFF BENEFITS				215	4.17	
12059			DV 465364	WORLD TRAVEL SERVICE				31200	452.00	
12279			TV 9704	TRANSPORTATION SERVICE				31300	148.00	
				ENDING BALANCE - OPERATING & MISCELLANEOUS	4,200				3,032.76	1,167.24
				TOTAL	22,200				20,780.05	1,419.95

BUDGET ANALYSIS

	MONTH EXPEND	YEAR-TO-DATE	PERIOD BUD	PERIOD INTRAN	PERIOD ENCUMB	OB CO	PERIOD-TO-DATE	FREE BALANCE
ACADEMIC SALARIES	833.33	4,999.98				121	4,999.98	
ACADEMIC EXTRA SERVICE	.00	5,598.22				122	7,997.33	
*TOT ACADEMIC SALARIES	833.33	10,598.20	8,000			12	12,997.31	4,997.31-
GTA, GA, GRA SALARIES	312.50	2,083.33				131	3,749.98	
*TOT GTA,GA,GRA SALARIES	312.50	2,083.33	10,000			13	3,749.98	6,250.02
SALARIES	.00	1,000.00				161	1,000.00	
*TOT CLERICAL & SUPPORTIN		1,000.00				16	1,000.00	1,000.00-
RETIREMENT CONTRIB-TIAA/C	.00	283.90				211	403.85	
RETIREMENT CONTRIB-STATE	63.75	382.50				212	382.50	
SOCIAL SECURITY CONTRIBUT	51.08	600.60				214	747.66	
UNEMPLOYMENT COMPENSATION	4.17	25.02				215	25.02	
*TOT STAFF BENEFITS - REG	119.00	1,292.02	1,200			21	1,559.03	359.03-
OUT OF STATE	452.00	452.00				312	452.00	
MTR VEH OPER-TRAVEL IN ST	148.00	848.97				313	1,021.73	
*TOT TRAVEL	600.00	1,300.97	2,000			31	1,473.73	526.27
*TOT PRINTING, DUPLICATIN			1,000			33		1,000.00
TOTAL	1,864.83	16,274.52	22,200				20,780.05	1,419.95

JAN 80

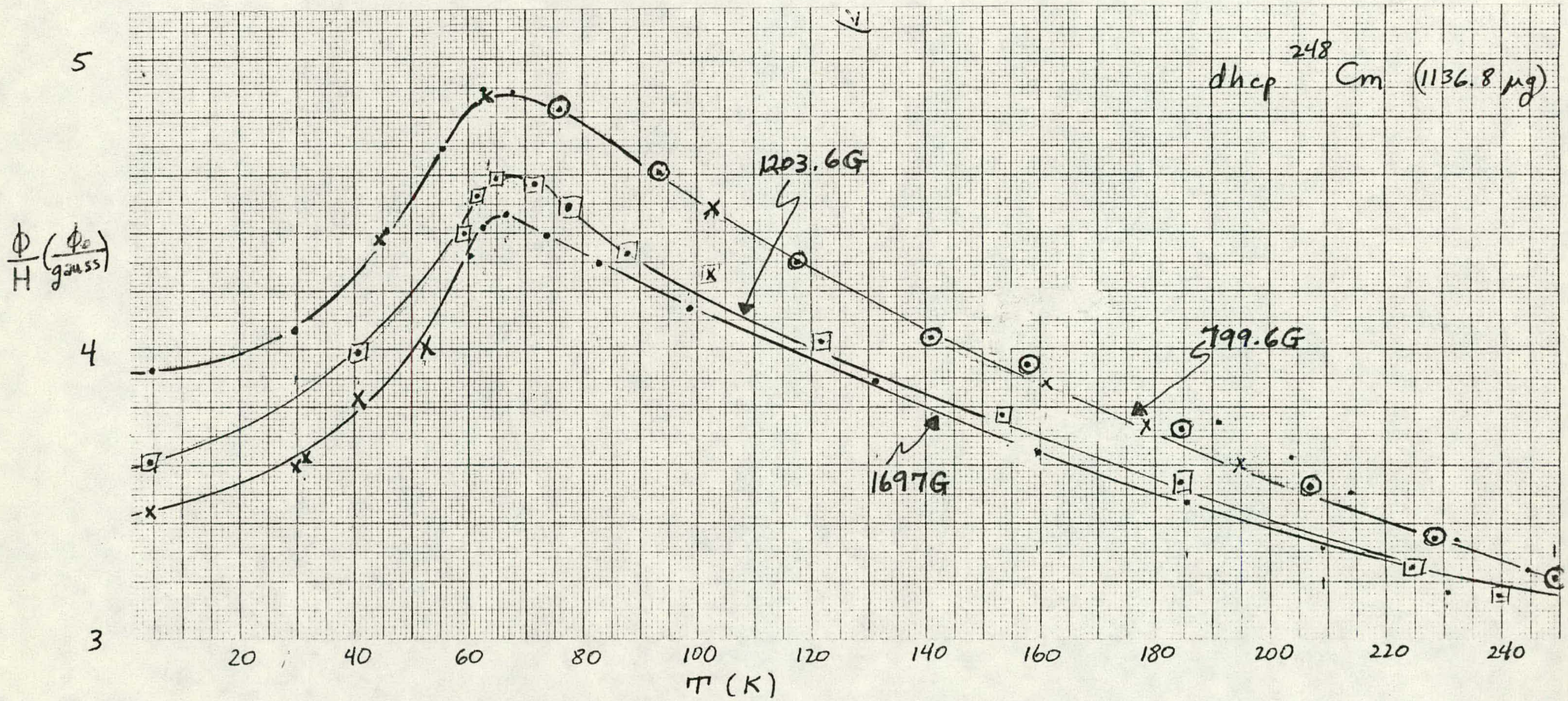
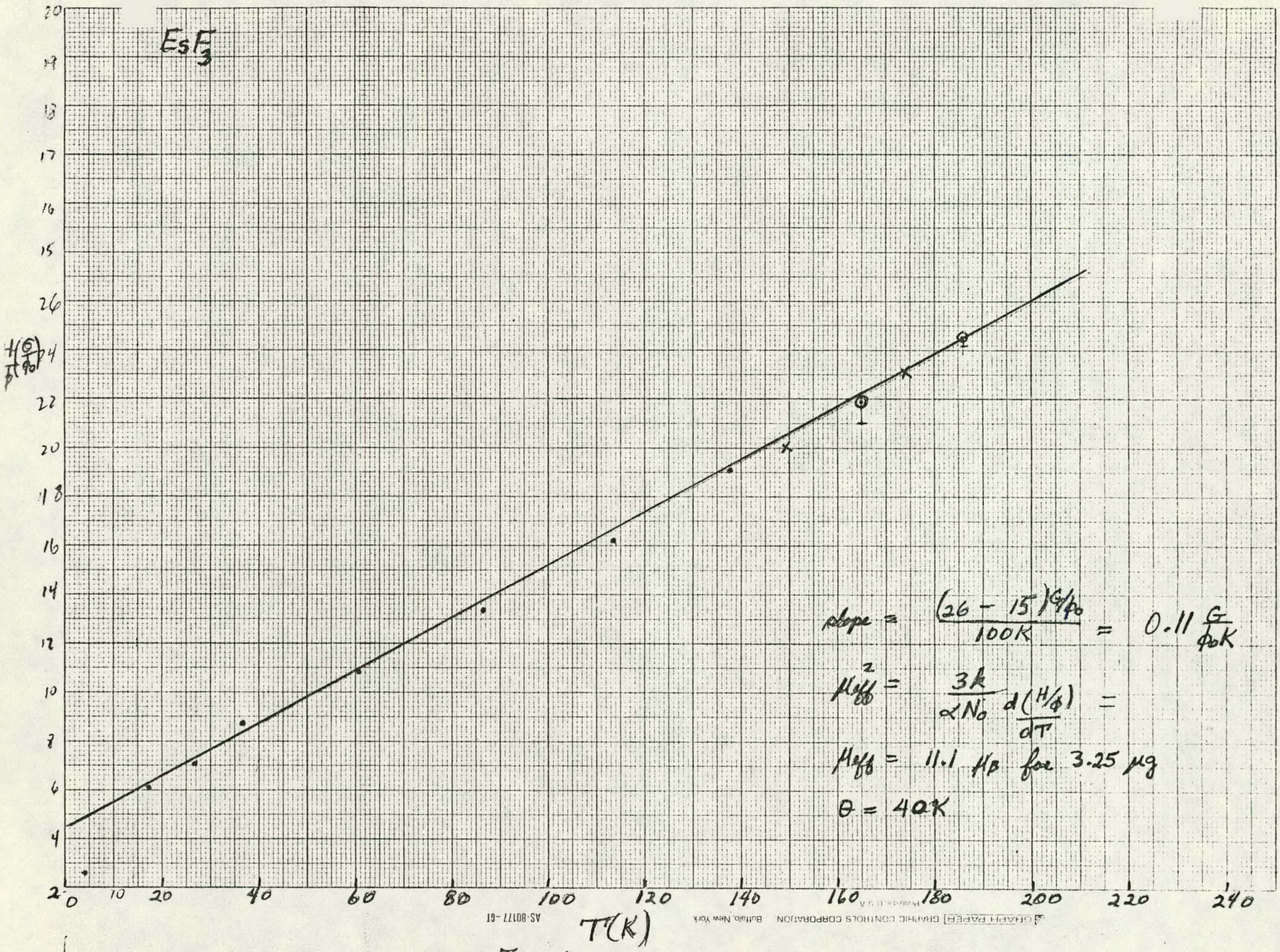

dhcp ^{248}Cm (1136.8 μg)
1203.6G
799.6G
1697G
$\frac{\phi}{H}\left(\frac{\phi_0}{gauss}\right)$
5
4
3
20
40
60
80
100
120
140
160
180
200
220
240
T (K)

Fig. 1

11/19/80



EsF_3
$\frac{H}{\phi}\left(\frac{G}{\phi_0}\right)$
T(K)
slope = $\frac{(26-15)G/\phi_0}{100K}$ = $0.11\frac{G}{\phi_0 K}$
$\mu_{eff}^2 = \frac{3k}{\alpha N_0}\frac{d(H/\phi)}{dT}$ =
μ_{eff} = 11.1 μ_B for 3.25 μg
θ = 40K

Fig 2

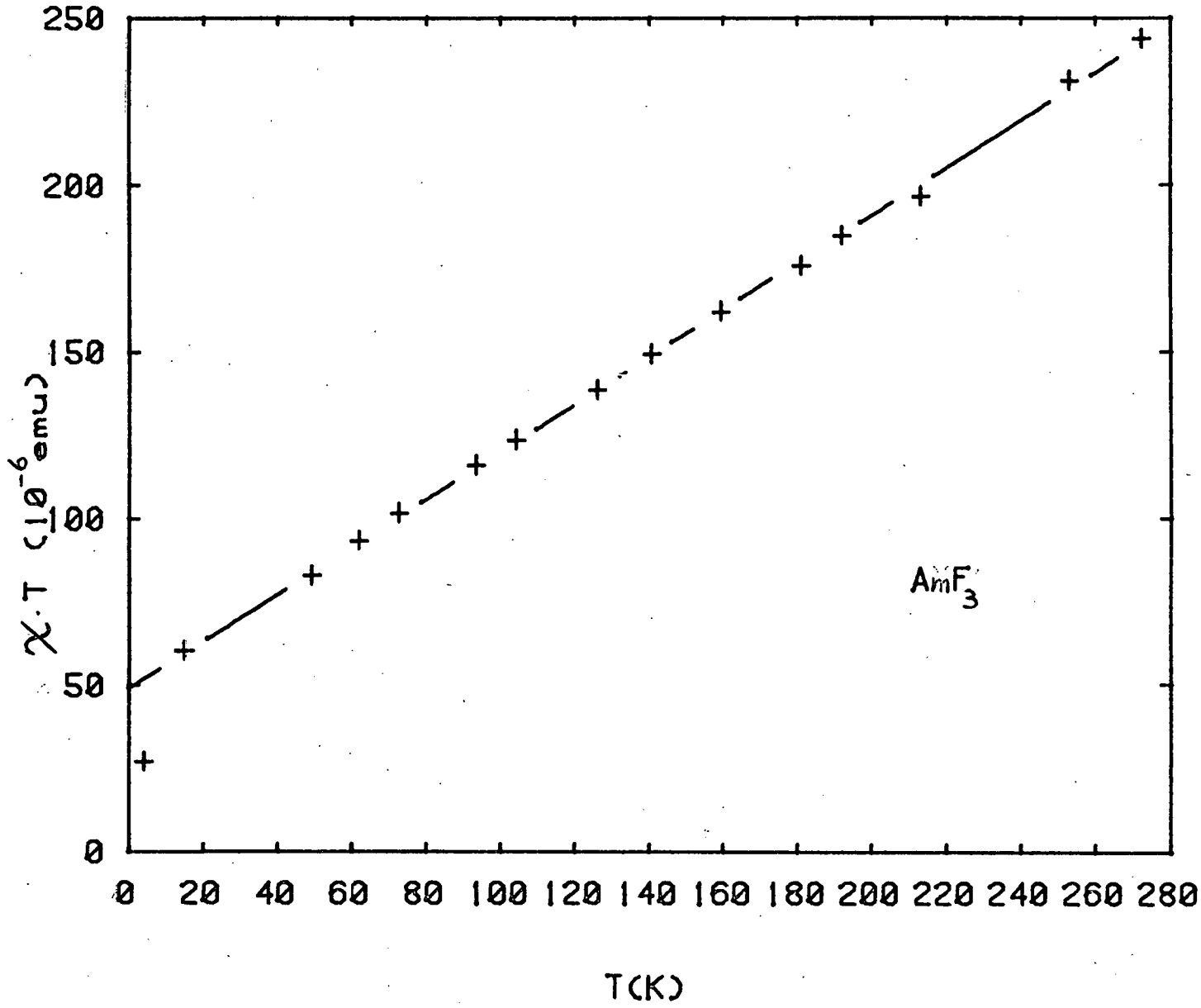
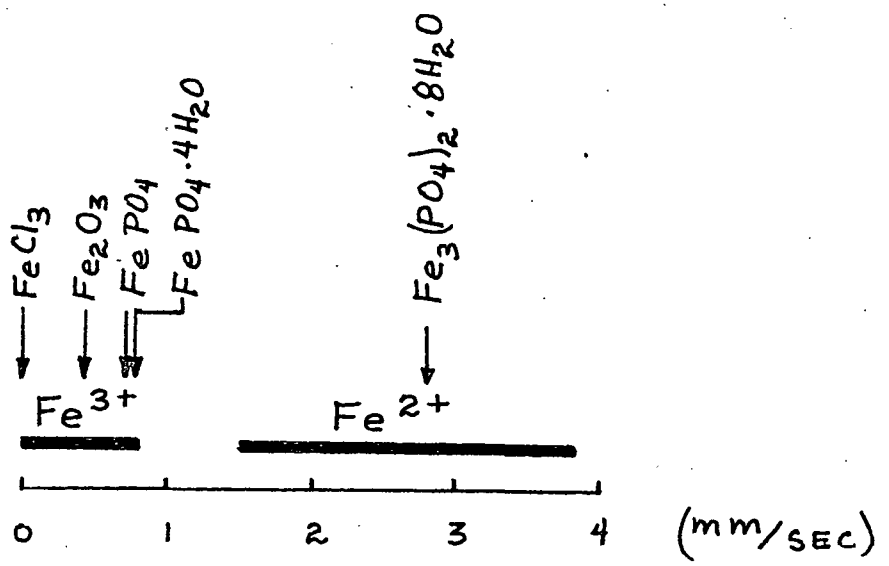
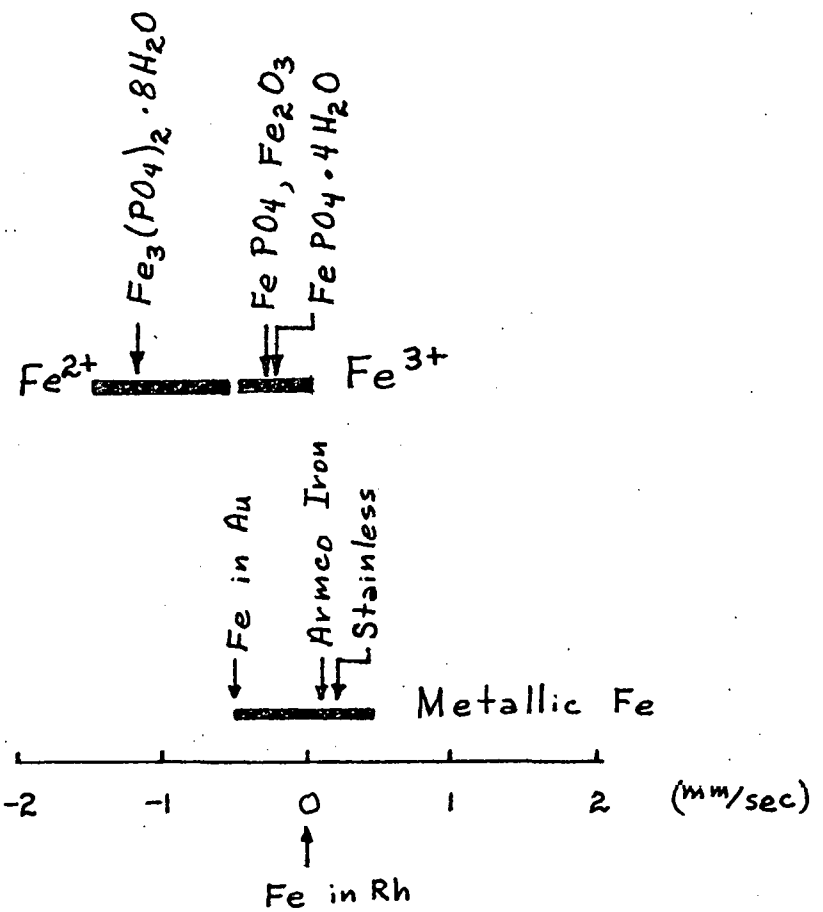

250
200
150
100
50
0
0 20 40 60 80 100 120 140 160 180 200 220 240 260 280
T(K)
χ·T (10⁻⁶ emu)
AmF3

Fig. 3



^{57}Fe Quadrupole Splitting



^{57}Fe Isomer Shifts

Fig. 4

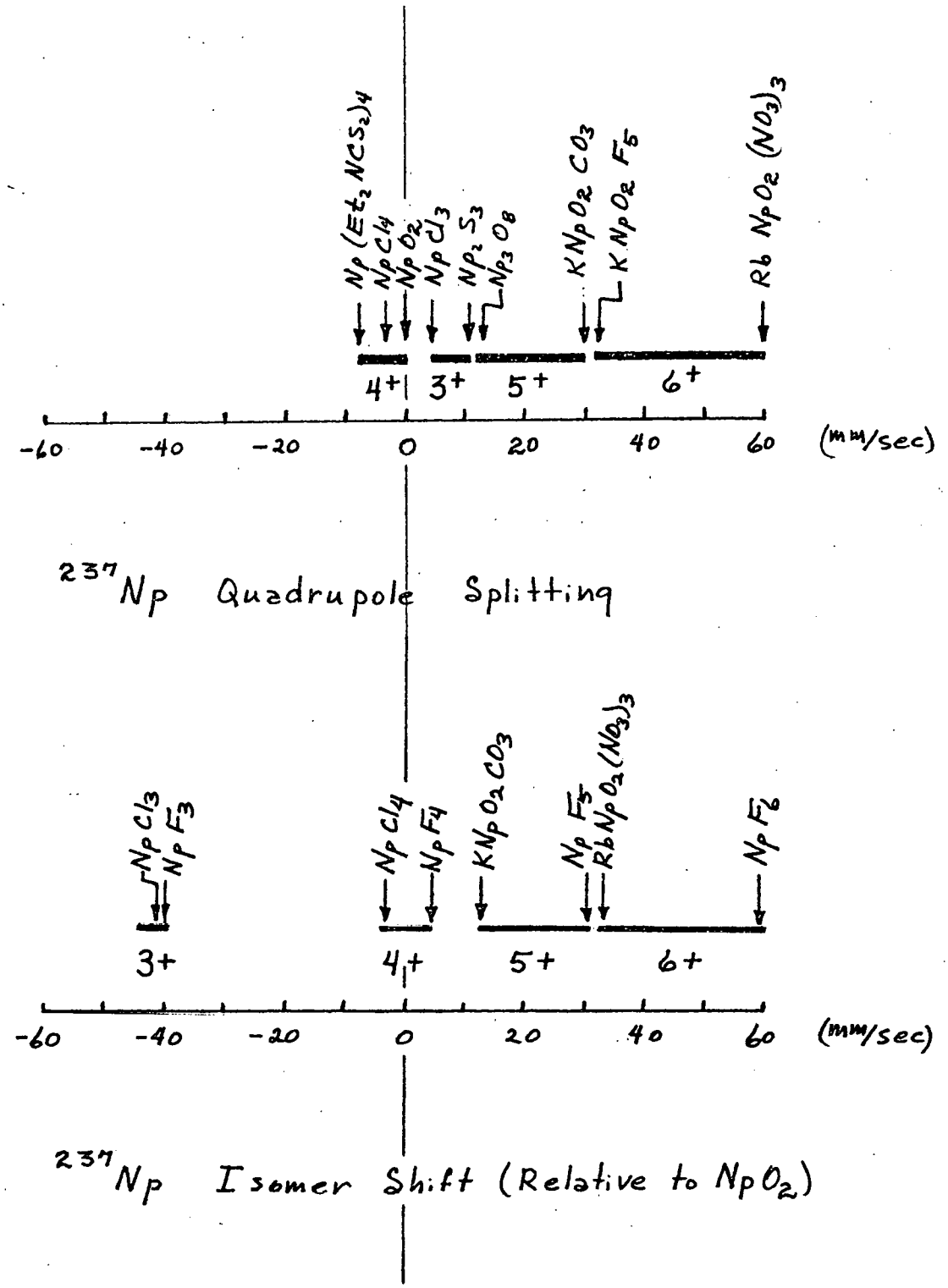
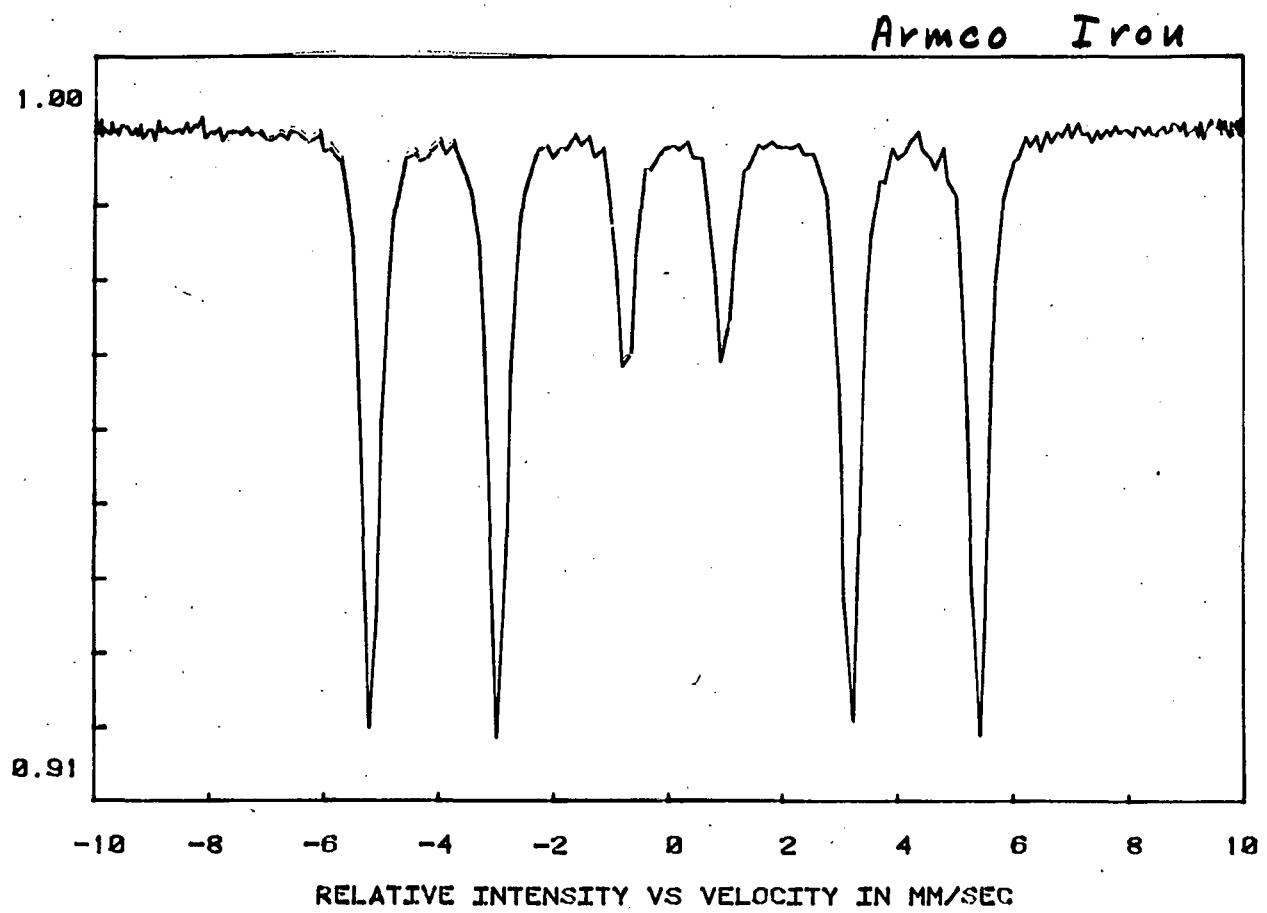

Np (Et2 NCS2)4
Np Cl4
Np O2
Np Cl3
Np2 S3
Np3 O8
K Np O2 CO3
K Np O2 F5
Rb Np O2 (NO3)3
4+
3+
5+
6+
-60
-40
-20
0
20
40
60
(mm/sec)
237Np Quadrupole Splitting
Np Cl3
Np F3
Np Cl4
Np F4
K Np O2 CO3
Np F5
Rb Np O2 (NO3)3
Np F6
3+
4+
5+
6+
-60
-40
-20
0
20
40
60
(mm/sec)
237Np Isomer Shift (Relative to Np O2)

Fig. 5


Armco Iron
1.00
0.91
-10
-8
-6
-4
-2
0
2
4
6
8
10
RELATIVE INTENSITY VS VELOCITY IN MM/SEC

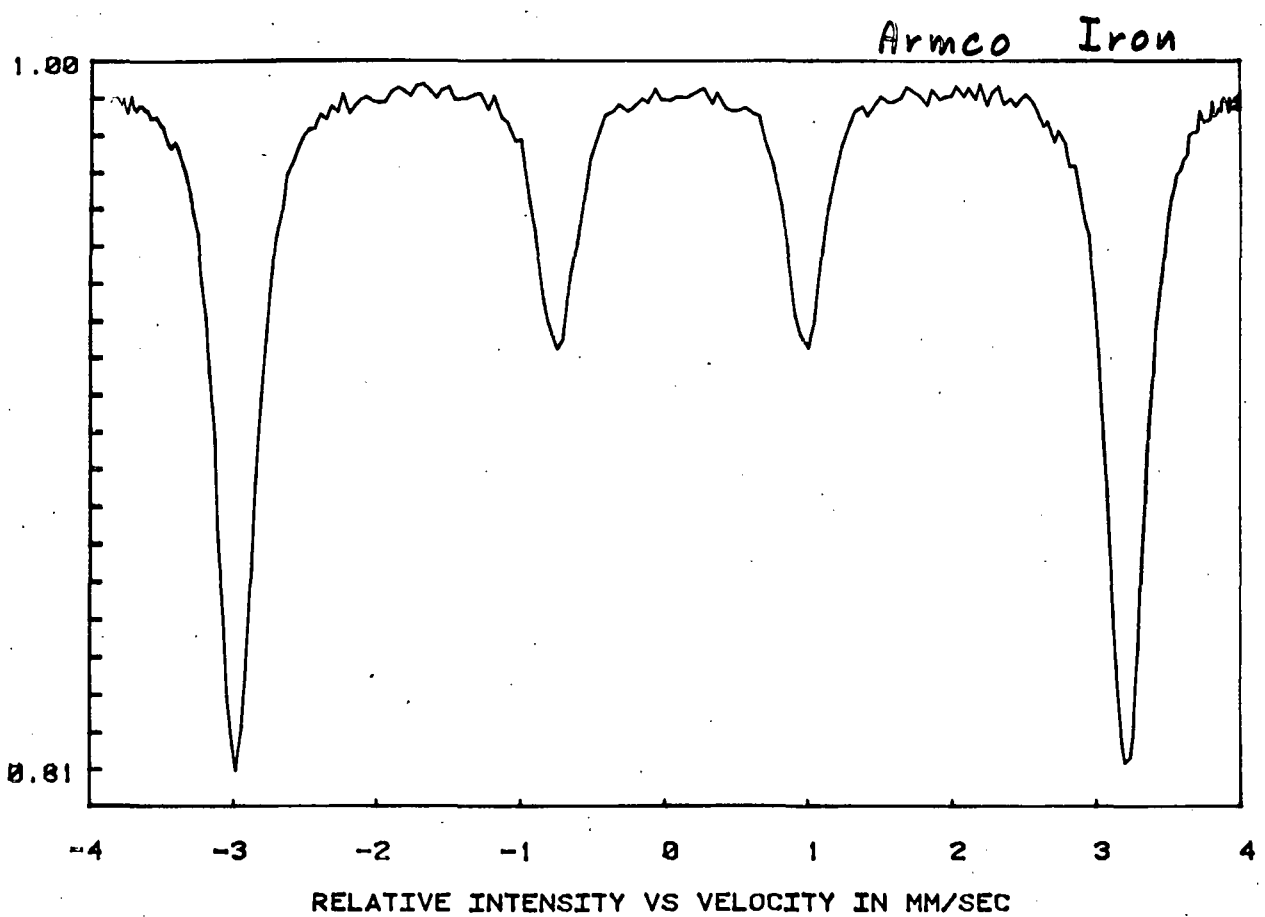
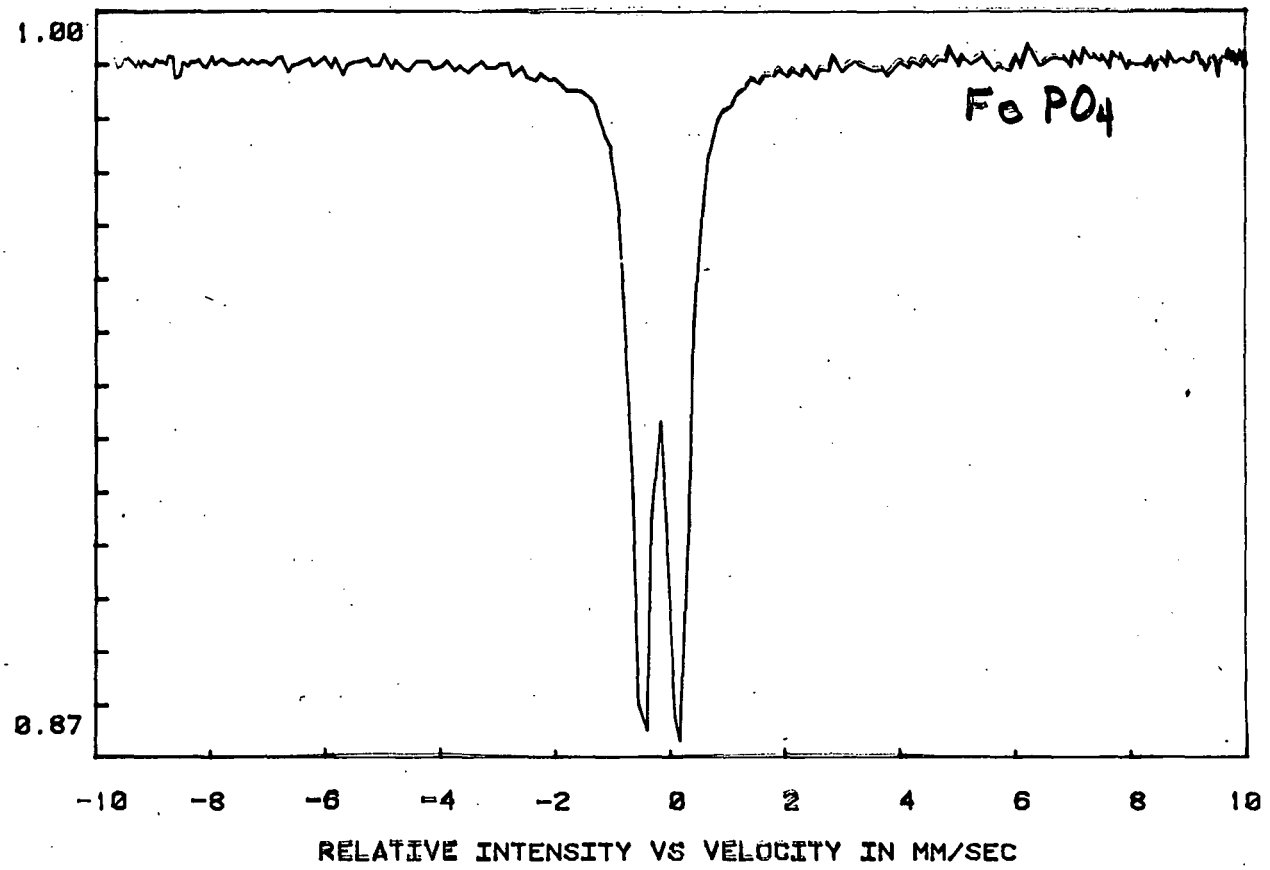

Armco Iron
1.00
0.81
-4
-3
-2
-1
0
1
2
3
4
RELATIVE INTENSITY VS VELOCITY IN MM/SEC

Fig 6.


1.00
0.87
Fe PO4
-10
-8
-6
-4
-2
0
2
4
6
8
10
RELATIVE INTENSITY VS VELOCITY IN MM/SEC

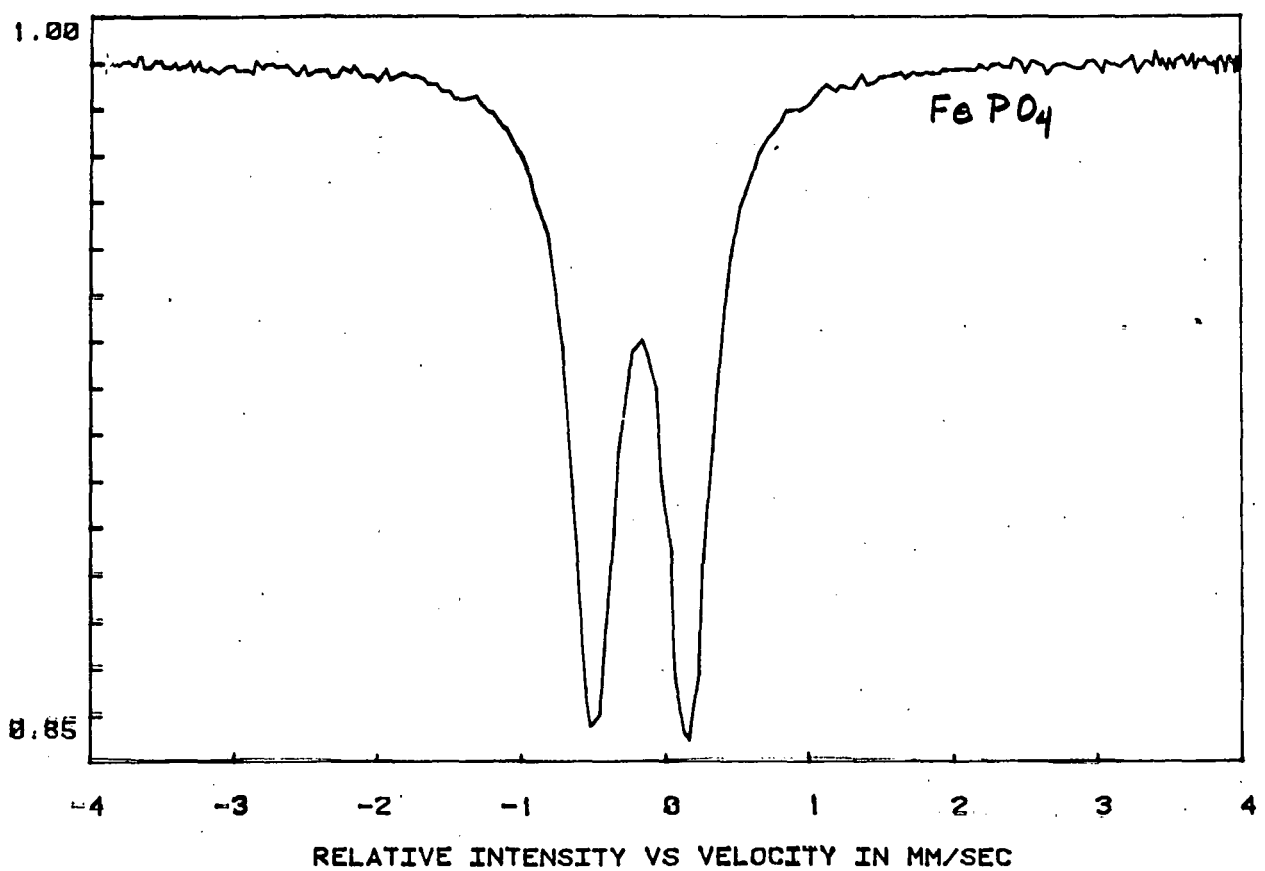
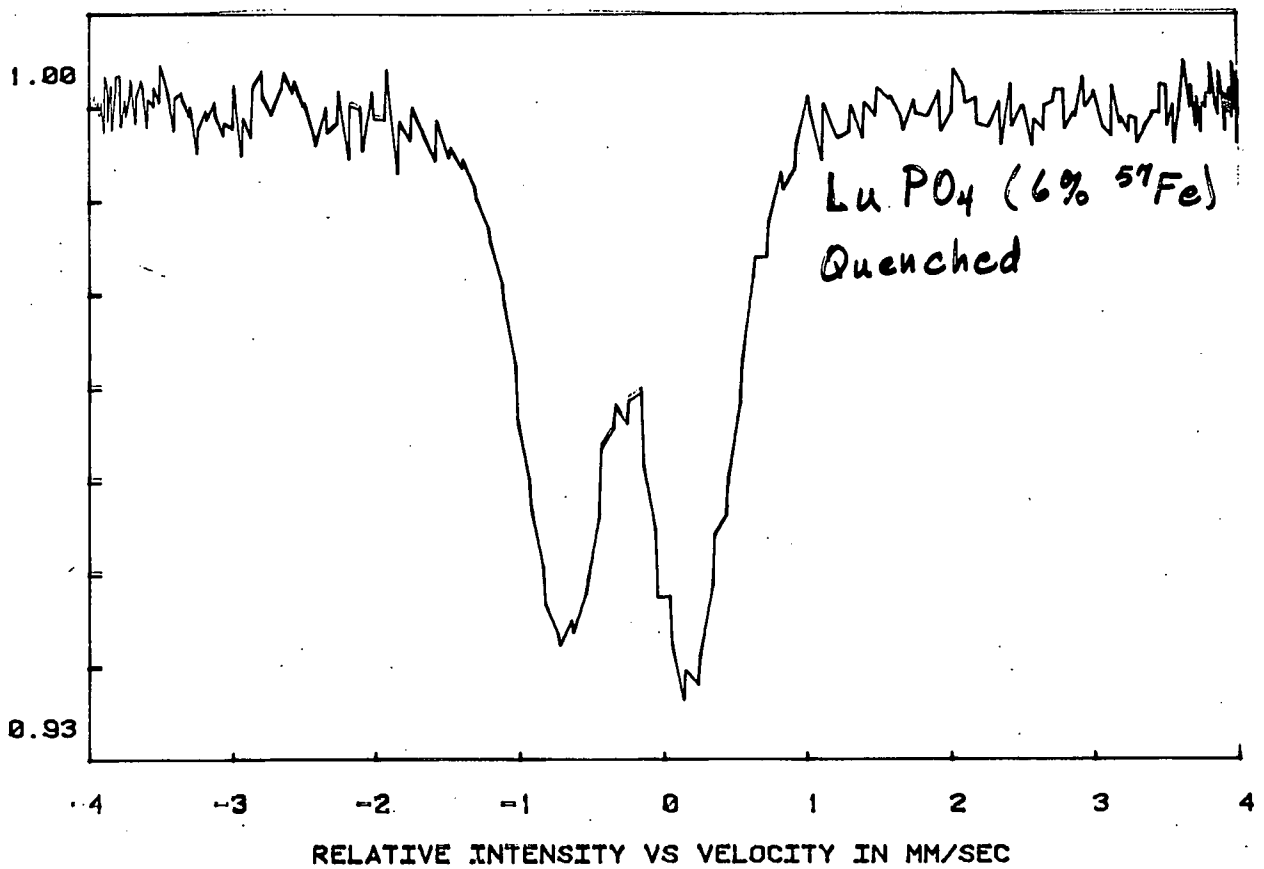

1.00
0.85
Fe PO4
-4
-3
-2
-1
0
1
2
3
4
RELATIVE INTENSITY VS VELOCITY IN MM/SEC

Fig 7


1.00
0.93
-4
-3
-2
-1
0
1
2
3
4
RELATIVE INTENSITY VS VELOCITY IN MM/SEC
Lu PO4 (6% 57Fe)
Quenched

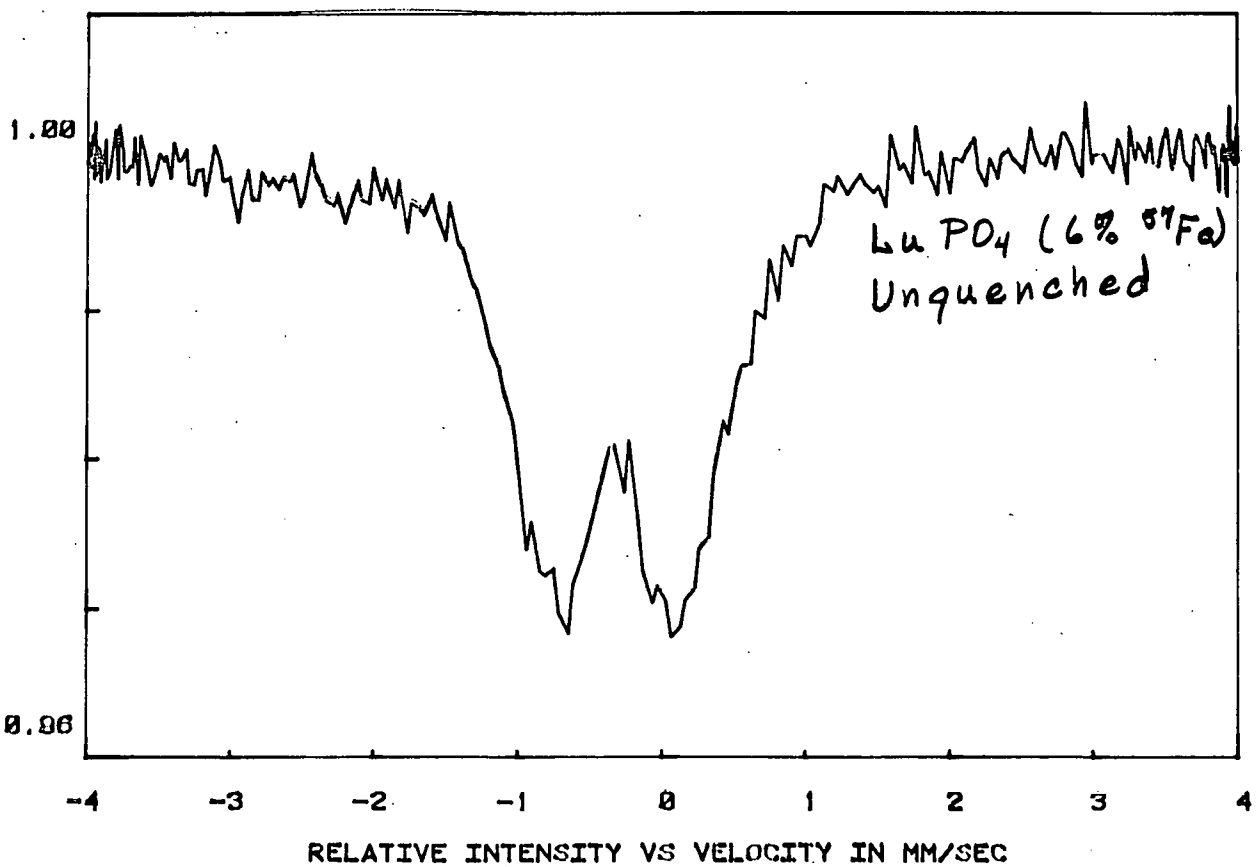

1.00
0.96
-4
-3
-2
-1
0
1
2
3
4
RELATIVE INTENSITY VS VELOCITY IN MM/SEC
Lu PO4 (6% 57Fe)
Unquenched

Fig. 8

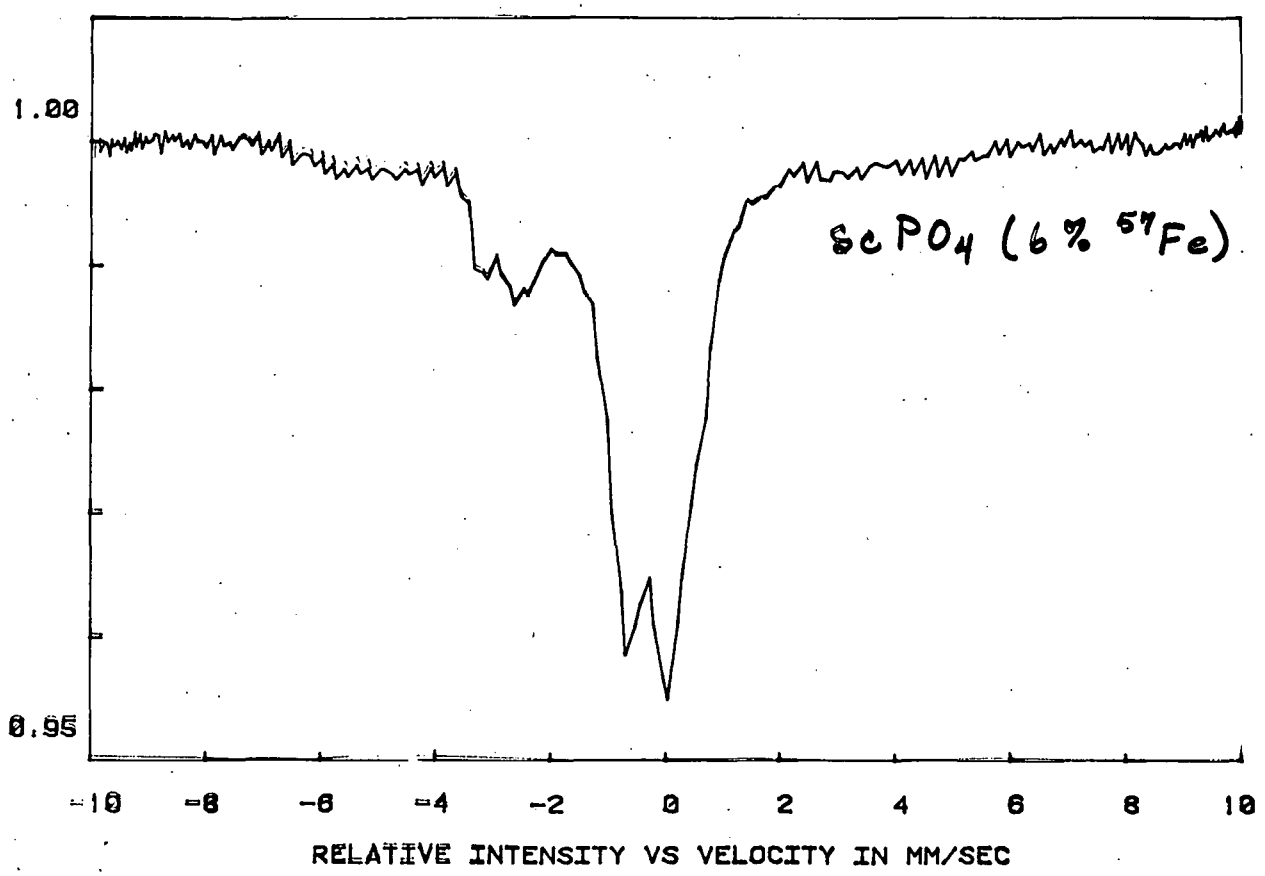

1.00
0.95
ScPO4 (6% 57Fe)
-10
-8
-6
-4
-2
0
2
4
6
8
10
RELATIVE INTENSITY VS VELOCITY IN MM/SEC

Fig. 9

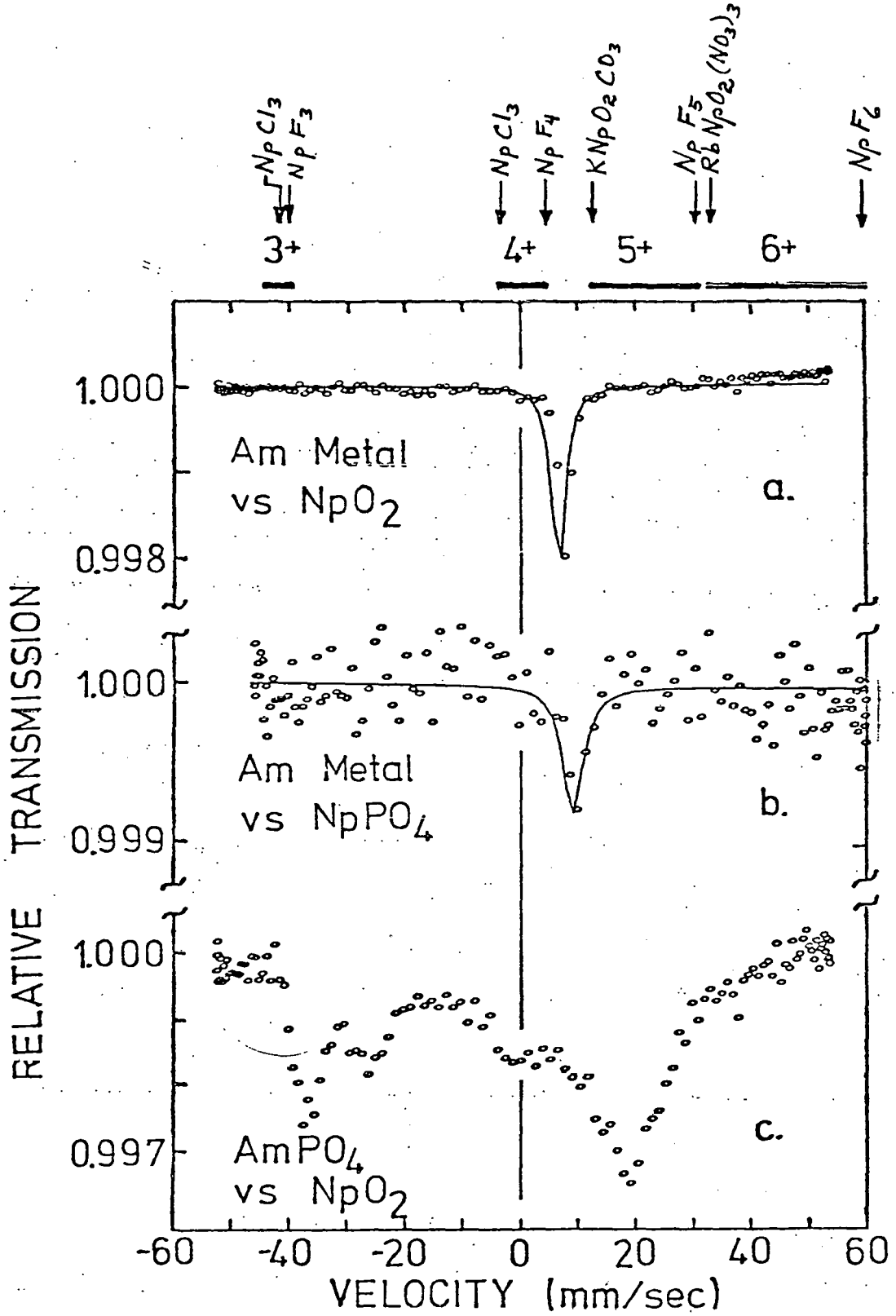

NpCl3
NpF3
NpCl3
NpF4
KNpO2CO3
NpF5
RbNpO2(NO3)3
NpF6
3+
4+
5+
6+
1.000
0.998
Am Metal
vs NpO2
a.
1.000
0.999
Am Metal
vs NpPO4
b.
1.000
0.997
AmPO4
vs NpO2
c.
RELATIVE TRANSMISSION
-60
-40
-20
0
20
40
60
VELOCITY (mm/sec)

Fig 10