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PROGRESS REPORT

HIGH RESOLUTION POSITRON Q-VALUE MEASUREMENTS
AND NUCLEAR STRUCTURE STUDIES FAR FROM
THE STABILITY LINE

DOE/ER/10434--3

DE82 013242

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(February 28, 1982)

PROGRESS REPORT NO. DOE/ER/10434-13

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REPORT OF PROGRESS DURING THE PERIOD 1 MARCH 1981 AND 28 FEBURARY 1982.

Essentially all of the work on the electron capture and positron decay of ^{206}Fr and ^{208}Fr and the energy levels of ^{206}Rn and ^{208}Rn , was completed last year. This serves as an excellent example of the type of spectroscopy which one could do at UNISOR until very recently when several new techniques have improved our versatility. Presently UNISOR has the capability of determining ground state spins using a laser pumping technique developed by the UNISOR-UT collaboration. The USC-ORNL collaboration has just completed developing the techniques to perform accurate Q-value measurements of high energy positron decays using intrinsic Ge detectors. The most serious corrections are associated with the scattering and the interference caused by annihilation radiations which can be accurately calculated using a detailed Monte Carlo technique. A reprint of an article describing the application of the technique to known decays and giving extensive correction coefficients is reproduced in Appendix B. Since the publication of that paper, this technique has been subjected to more stringent tests and has been applied to a variety of positron end-point-energy measurements in decays of ^{82}Sr , ^{27}Si , ^{58}Cu , ^{77}Rb and ^{77}Kr . Preprints of papers describing this work appear as appendices.

The following experiments have been completed, analyzed and written for publication:

a) The Monte Carlo calculated corrections were checked by performing the following reactions $^{27}\text{Al}(p,n)^{27}\text{Si}$ and $^{\text{Nat}}\text{Ni}(p,n)^{58}\text{Cu}$ which both positron decay with known end point energies of 3787.0 ± 1.3 and 7540.6 ± 2.4 keV respectively. Using our Monte Carlo calculations we obtained corrected values, from our raw data, to compare to the above of 3793 ± 16 and 7537 ± 38 keV respectively. The accurate values above were obtained by

direct mass measurements which can not be done in cases of short lived isotopes. Previously, scintillation techniques were used in such cases with typical uncertainties of 6 to 10% as opposed to the 0.42% obtained using our technique. This then represents a major breakthrough in β^+ Q-value measurements.

b) The neutron deficient nuclide ^{77}Rb was produced in the reaction $^{60}\text{Ni}(^{20}\text{Ne}, p3n)^{77}\text{Rb}$ using $^{20}\text{Ne}^{+5}$ ions from ORIC. End point energies were obtained from the β^+ - γ coincidence experiments and in a singles experiment. Separate spectra were collected in coincidence with the 179, 245, 394 keV γ rays in ^{77}Kr as well as with the annihilation radiations. When the γ ray energies are added back we obtained 4249 ± 41 , 4245 ± 63 , 4253 ± 71 , and 4253 ± 124 keV respectively which can be averaged and added to $2m_0c^2 = 1.022$ MeV to yield a Q-Value of 5272 ± 26 keV.

c) In a parasite experiment, the end point energies of the positron spectra from the decay of ^{77}Kr were also measured. The accepted decay energy is 3005 ± 30 keV; however, our final result was 2760 ± 42 keV and the discrepancy at this time is not understood.

d) The neutron deficient nuclide ^{76}Rb was produced in the reaction $^{60}\text{Ni}(^{20}\text{Ne}, p4n)^{76}\text{Rb}$ again using the $^{20}\text{Ne}^{+5}$ beam from ORIC. The coincidence spectrum of γ - β^+ events was thought from previous studies to procede mainly to the first 2^+ excited state at 424 keV. The observed end-point energy was 4558 ± 30 keV, corresponding to a Q-value of 5.90 MeV, and is in sharp conflict with the predicted Q-value of 8.43 ± 0.25 MeV.¹³

e) The serious discrepancy in the Q-value of the decay of ^{76}Rb caused us to return to the reaction $^{60}\text{Ni}(^{20}\text{Ne}, p4n)^{76}\text{Rb}$ to perform a detailed γ - γ -t experiment to confirm the earlier decay scheme. We found that the difficulty was indeed with the decay scheme. When the experiment was

performed again it was found indeed that most of the β^+ strength was to the highly excited state at 2571 keV and that coincidence with the 424 keV γ ray was through complex γ ray cascades. The final result for the Q-value is then $4558 \pm 30 \text{ keV} + 2571 + 1.022 \text{ MeV} = 8063 \pm 32 \text{ keV}$ which is in much better agreement with the predicted value of $8430 \pm 250 \text{ keV}$ and in any case we feel that it is correct.

Another activity supported by this contract involved a positive response by the PI to a request to install a conversion electron detection system on line to the Argonne National Laboratory's Heavy Ion Linear Accelerator. This system was developed earlier by the PI (Nucl. Instr. Meth. 107, (1973) 453; 116 (1974) 521) and installed at UNISOR. It was later discovered that the isotope separator products don't suffer serious enough interference with internal conversion measurements to preclude the use of a more efficient bare Si(Li) detector. The mini-orange-filtered, Si(Li) detector is more than adequate to prevent interference of photons with low energy electrons.

The final effort we have to report concerns the in-depth study, of the nuclear spectroscopy required to settle some of the basic issues in the controversy over the spectrum of antineutrinos from a nuclear reactor. One of the goals of this study was to determine if research at UNISOR might shed light on this issue. The results of this study are most interesting in that since our theoretical work of 1980, there have been a significant number of experiments at on-line separator projects which have produced detailed spectroscopic data on decay schemes, β^- Q-values, and branching ratios. When we attempted to predict these results with the empirical techniques, described in Phys. Rev. C22, 594 (1980), we did so with good agreement particularly at the high energy end where our technique is claimed by some to fail. In addition we determined that if about nine new decay

schemes were determined, the important issue of the contribution of the shortest lived fission fragments to the high energy end of the spectrum would be essentially settled. Our study has clearly identified those isotopes. We have determined, however, that it is very probable that the new Hollifield facility may allow us to use multinucleon transfer reactions on the heavy projectiles to study neutron rich isotopes as well as we now study neutron deficient isotopes using heavy ion reactions. The ion source difficulties have been examined by the UNISOR staff and it seems that techniques used at GSI, will very probably work at UNISOR.

Preprints of four papers describing the details of this year's efforts are appendices to this report.

List of Appendices

- Appendix A Precision Mass Differences in Light Rubidium and Krypton Isotopes Utilizing Beta Endpoint Measurements
- Appendix B Paper Presented at the 4th International Conference on Nuclei far from Stability
- Appendix C Monte Carlo Calculations Predicting the Response of Intrinsic GE Detectors to Electrons and Positrons
- Appendix D Reactor Antineutrino Spectra and Nuclear Spectroscopy of Isotopes far from Beta Stability

APPENDIX A

PRECISION MASS DIFFERENCES IN LIGHT RUBIDIUM AND KRYPTON ISOTOPES UTILIZING BETA ENDPOINT MEASUREMENTS

PRECISION MASS DIFFERENCES IN LIGHT RUBIDIUM AND KRYPTON
ISOTOPES UTILIZING BETA ENDPOINT MEASUREMENTS

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Abstract

A technique for precise determination of beta endpoints with an intrinsic germanium detector has been developed and checked with the known positron spectra of ^{27}Si and ^{58}Cu . These isotopes were produced in the (pn) reactions on ^{27}Al and natural nickel targets. Decay energies of 5272 ± 26 , 8063 ± 44 and 2760 ± 42 keV have been obtained for mass-separated samples of ^{77}Rb , ^{76}Rb and ^{77}Kr . Mass surface systematics in this region have been examined and found to be consistent.

Many mass determinations have been made utilizing direct reaction measurements and discrete energy charged-particle spectroscopy. However, mass determinations on a vast majority of nuclides far from stability require accurate spectroscopic information combined with mass differences derived from direct beta endpoint measurements. The results of these measurements are fraught with inconsistencies due mainly to the continuous nature of beta spectra as well as to the complications which result in attempts to determine detector response functions. Intrinsic germanium spectrometers have energy resolutions of a few keV and can be energy calibrated by γ -ray photopeaks; hence, they are replacing plastic scintillator spectrometers [1,2]. Generalized electron response functions for intrinsic germanium detectors are difficult to determine. The problem has been approached in a number of ways, including shape function calculations of known β emitters [3] and empirical electron response function calculations determined from monoenergetic electron beams [4]. A β spectrometer utilizing a superconducting solenoid to channel the β particles has been reported earlier [5] and analysis of the detector distorted data has been accomplished through an iterative technique [6]. It has also been demonstrated that a small detector yields straight Fermi-Kurie plots over the higher energy portion of the spectrum without a magnetic filter [7]. This technique requires further correction in the case of positrons because of the interference of the annihilation radiation; however, this correction has been shown to be straight forward [8].

The technique used in this work utilizes a Monte Carlo approach [8,9] to predict the energy shift in the endpoint due to the presence of the annihilation radiation and has been described in detail in reference 8. Some of the relevant formulae used in our beta spectrum analyses are given

in reference 9. The detector analyzed in the calculations of reference 8 has dimensions 1.6 cm. diameter by 0.7 cm. thick, which were those of the detector used in the measurements described here. Calculated energy shifts (ΔE_0), due to annihilation interference, were found to vary smoothly over the energy range from 2.5 to 9.0 MeV and were easily fit to the quadratic polynomial [8]:

$$\Delta E_0 = 0.1572 + 0.0115 E_0 - 0.007 E_0^2, \quad (1)$$

where E_0 is the correct endpoint energy. Thus, a 4.0-MeV endpoint would be measured as 4.192 MeV. The special case where one 511 γ -ray escapes (e.g. 511 gated spectra) were fit to the cubic polynomial:

$$\Delta E_0 = 0.0488 + 0.0390 E - 0.00582 E^2 + 0.000301 E^3, \quad (2)$$

and in this case a 4.0-MeV endpoint would be measured as 4.131 MeV.

The most important consideration in the Fermi-Kurie analysis was avoiding the inclusion of data in a nonlinear region. Since a departure from linearity occurs 200-300 keV below the endpoint energy for a detector of these dimensions [9], a second β -ray branch within this range can create a serious problem. If no second component exists, then, in principle, data points can be added from below as long as the endpoint energy resulting from a fit to the Fermi-Kurie function remains constant. A reasonable criterion is χ^2 minimization in which the fitting range is chosen to minimize χ^2 below the "break point", which is the beginning of the high energy nonlinearity caused by annihilation radiations [8]. The fitting routines and the Monte Carlo calculations were tested by measuring the endpoint energies of the positron branches in the decay of ^{27}Si and ^{58}Cu produced in (p,n) reactions on ^{27}Al and $^{\text{NAT}}\text{Ni}$ targets respectively. Singles spectra yield endpoint energies of 3903 ± 8 keV for ^{27}Si and 7667 ± 49 and 7639 ± 42 keV for ^{58}Cu where the errors are strictly fitting errors. Application of

equation (1) gives corrections due to annihilation radiation interference of 191 and 204 keV respectively. Additional corrections due to energy losses in the beryllium entrance window of 107 ± 30 keV and 68 ± 19 keV have been included, yielding final endpoints for the ^{27}Si and ^{58}Cu positron spectra of 3779 ± 23 and 7537 ± 38 keV which are in excellent agreement with the accepted values of 3787.0 ± 1.3 and 7540.6 ± 2.4 keV respectively [10].

The general mass surface between the $f_{7/2}$ and $g_{9/2}$ shells has not been extensively explored. The mass systematics in this region should prove very interesting because of the large variety of shell model states and because of the proximity of the proton drip and $Z = N$ lines to the region. In order to utilize the best characteristics of the UNISOR on-line mass separator facility [11] and in some cases to exploit the relative stability of the daughter isotopes to minimize contamination, our investigation was begun in the light rubidium isotopes. In addition, there have been some direct mass measurements made in this region which greatly assist in the systematic understanding of our data [12].

The neutron-deficient nuclides ^{77}Rb and ^{76}Rb were produced in the reaction $^{60}\text{Ni}(^{20}\text{Ne}, \text{pxn})$ using $^{20}\text{Ne}^{+5}$ ions accelerated with the Oak Ridge Isochronous Cyclotron (ORIC) and subsequently mass separated using the on-line separator UNISOR [11]. Although ^{77}Kr is copiously produced in the $^{60}\text{Ni}(^{20}\text{Ne}, 2\text{pn})$ reaction, the surface ionization source used in these experiments preferentially ionizes the Rb isotopes. Thus, our ^{77}Kr results are derived from the daughter decay of ^{77}Rb . Fig. 1 shows a typical gamma-ray-gated, Fermi-Kurie plot for the decay of ^{77}Rb along with the accepted decay scheme [13]. Endpoint energies were obtained for the beta spectra gated by the 179-, 234-, 511- and 394-keV gamma rays as well as for the singles spectrum. After making the appropriate corrections for electron

scattering and annihilation radiation interference and adding in the gamma-ray energies, a weighted average of 4250 ± 26 keV was obtained which corresponds to $Q_{EC} = 5272 \pm 26$ keV. This result is in agreement with the value 5180 ± 390 keV given by Westgaard et al. [14] but disagrees with the value 4882 ± 150 keV given by Liptak et al. [15]. Both previous results were measured using scintillation spectrometers. The results are given in Table I.

The β^+ decay of ^{77}Kr ($J^\pi = 5/2^+$) has long been known to proceed in approximately equal proportions to states at 130 keV ($J^\pi = 5/2^+$) and 276 keV ($J^\pi = 3/2^+$) in ^{77}Br . The accepted beta decay energy for ^{77}Kr is 3005 ± 30 keV [10] based upon earlier beta spectrometer measurements [16]. Since the mass of ^{77}Br has been measured very precisely [17,18] by (p,n) threshold reactions on ^{77}Se , the present beta endpoint energies can be used to determine the mass of ^{77}Kr . Thus, by measuring the endpoint energies of beta spectra in coincidence with the 130- and 146-keV transitions in ^{77}Br , an independent check of the Q_{EC} for ^{77}Kr was achieved. The major complication in these measurements arises from the interference from the ^{77}Rb decay. Normal subtraction techniques still leave a small residual ^{77}Rb background. This subtraction was approximately accomplished by first fitting a straight line to the higher energy ^{77}Rb data, subtracting the calculated line in the Fermi-Kurie plot, and then converting to a ^{77}Kr plot. A subtraction range of 2000-3500 keV was used for ^{77}Rb which yielded an endpoint energy of 1528 ± 10 keV for the 146-keV gated spectrum, while subtraction ranges of 1800-3300 keV and 2200-3700 keV gave endpoints of 1528 and 1530 keV, respectively. No background subtraction criteria was found which yielded an endpoint ~ 200 keV higher. After making the appropriate corrections, the final value of 1737 ± 37 keV is obtained. The 130-keV gated spectrum behaved similarly and yielded an endpoint of 1752 ± 124 keV (the large error is due

to the small ~ 100 -keV data range used in the fits). The weighted average of 1738 ± 36 keV gave a final value of $Q_{EC} = 2760 \pm 42$ keV, significantly below the value quoted above. This 245 keV discrepancy can not easily be explained by an error in the energy calibration or in the response of the detector at ~ 1.5 MeV. The straight-line approximation for the ^{77}Rb background is not strictly valid, but this approximation tends to result in a higher measured value.

The decay of ^{76}Rb has been previously studied [14, 19], with most of the decay strength being observed to the 2^+ first excited state of ^{76}Kr . Since the separator ion source produces neither ^{76}Kr nor ^{76}Sr and since in any case ^{76}Kr is not a positron emitter, the measured β^+ spectrum was completely attributable to ^{76}Rb . Essentially no events were recorded above 5 MeV (8 MeV was the collection limit). The measured endpoint energy for the $2^+ \rightarrow 0^+$ transition gated-spectrum was 4558 ± 30 keV, with no major second components observed above 3.5 MeV. In fact, the final χ^2 minimization criterion was based on the quality of fit of this ^{76}Rb data. The final corrected value for Q_{EC} is 5.90 MeV assuming the decay proceeds via the 2^+ first excited state. Surprisingly, the predicted Q_{EC} is 8.43 ± 0.25 MeV [12] and this 2.53 MeV discrepancy cannot be easily explained. Other potential phenomena, nuclear deformation for example, would tend to increase the decay energy rather than reduce it. Recent laser measurements [20] have shown the spin of ^{76}Rb to be 1, but a 1^+ state should exhibit a significant decay branch to the 0^+ ground state of ^{76}Kr . Our sensitivity to weak higher energy transitions is $< 1\%$ and no such transition was observed, while the weak $0^+ \rightarrow 0^+$ isospin forbidden transition observed in ^{78}Rb by Rehfield [21] was confirmed in the present work. Most of the decay strength in ^{78}Rb proceeds via high-lying excited states [22], but the odd particles in ^{78}Rb

reside in $p_{3/2}$ and $g_{9/2}$ orbitals, differing greatly from ^{76}Rb where the odd particles reside in $p_{3/2}$ and $p_{1/2}$ orbitals. However, the decays appeared to us to be similar.

The first clue to resolving this mystery comes from earlier work [23] done at CERN, where a β^+ spectrum gated with a 2573 γ -ray ($I_{2573} = 70\%$ of $2^+ \rightarrow 0^+$) yielded an endpoint of 4.74 ± 0.40 MeV. Close examination of our data showed the intensity of this γ -ray to be 30^{+20}_{-10} of the $2^+ \rightarrow 0^+$ transition. Crude β^+ endpoint measurements as well as γ - γ coincidence data from this and an earlier experiment [24] were used to construct the partial decay scheme shown in Fig. 2. Most of the decay strength apparently proceeds via the 2571-keV level which decays either directly to the ground state or cascades down through the 424-keV 2^+ level. Since a 1^+ ground state for ^{76}Rb has been tentatively ruled out, a 1^- state would seem most likely. An allowed decay, indicated by a $\log ft$ of 5.1 for decay to the 2571 level, would suggest either a 1^- or 2^- J^π for the 2571 level. The strongly observed ground state transition would further suggest that this state is 1^- because the M2 transition rate dictated by a 2^- state would be very slow, allowing more favorable competing decays. The γ -ray energy of 2571 keV, added to our corrected decay energy, yields a final Q_{EC} of 8063 ± 44 keV (summarized in Table I), which is in much better agreement with the prediction of 8.43 ± 0.25 MeV [10]. It seems then that the difficulty was with the earlier decay scheme.

These newly measured β -decay energies follow the systematics taken from ref. 10 and shown in Fig. 3 relatively well. One of the original objectives of this work was to accurately measure the masses of the light krypton isotopes by combining precise mass difference measurements with the direct mass measurements [11]. These direct mass measurements have been questioned [25,26] and thus any new mass difference measurements must have

a credible base. A more recent evaluation [27] of the direct mass measurements has, however, improved our agreement substantially as demonstrated in Table II. The mass of ^{77}Br has been determined very precisely by (p,n) threshold measurements [17,18], giving the A=77 mass chain a solid base. Since ^{76}Kr is not a β emitter, it does not permit the use of ^{76}Br as a base. Recent results [28] utilizing the $^{78}\text{Kr}(p,t)^{76}\text{Kr}$ reaction have given a mass excess value for ^{76}Kr of -68968 ± 15 keV. We intend to extend these measurements to ^{75}Rb , ^{74}Rb and the light krypton isotopes.

We wish to thank E. H. Spejewski and R. L. Mlekodaj for experimental assistance, H. K. Carter and J. D. Cole for Computer analysis assistance and S. Raman and G. Leander for useful discussions. We further wish to thank the staff at ORIC which made this work possible. The Oak Ridge National Laboratory is operated for the U.S. Department of Energy by Union Carbide Corporation under Contract No. W-7405-eng-26. This work was supported in part by the Department of Energy under contracts DEAS 0979 ER10434 and DE-AC05-76OR00033.

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FIGURE CAPTIONS

- Fig. 1. Kurie plot of the 179-keV gated data from the decay of ^{77}Rb . Only one-third of the data points have been plotted. Decay scheme has been taken from ref. [13].
- Fig. 2. Proposed partial decay scheme for ^{76}Rb . The assigned spins and parities are from in-beam gamma work [24].
- Fig. 3. Beta decay energy systematics for light rubidium and krypton isotopes. Predictions are taken from ref. [10].

TABLE I. BETA ENDPOINTS RESULTS

Corrected	Annihilation			Gamma		
	Nuclide	Gate	Endpoint	Correction	Energy	Endpoint*
		(keV)	(keV)	(keV)	(keV)	(keV)
	⁷⁷ Rb	179	4089±26	196	245	4249±41
	⁷⁷ Rb	245	4085±54	192	245	4245±63
	⁷⁷ Rb	394	3886±63	190.6	450.8	4253±71
	⁷⁷ Rb	Singles	4272±28	193.5	66.5	4252±42
	⁷⁷ Rb	511	4212±120	131	66.5	4253±124
						5272±26
	⁷⁷ Kr	130	1690±120	173	130	1752±124
	⁷⁷ Kr	146	1528±20	172	276	1737±37
						2760±42
	⁷⁶ Rb	424	4558±30	195	2571	7041±44
						8063±44

*All values corrected for foil energy loss; 107±30 keV at 4.0 MeV and 105±30 keV at 1.0 MeV. Error of 30 keV is due to straggling and has been added in quadrature.

TABLE II. COMPARATIVE MASS EXCESS VALUE

Nuclide	^{78}Rb	^{77}Rb	^{76}Rb	^{77}Kr
Q_{EC} (keV)	7242(20) ^{a)}	5272(26) ^{b)}	8063(44) ^{b)}	2760(42) ^{b)}
Direct Mass Measurement				
Mass Excess (keV) ^{c)}	-67061(66)	-65100(105)	-60763(146)	
A	78	77	76	77
Mass Excess of Daughter (keV)	-74150(8)	-70481(43) ^{b)} (-70236(30)) ^{d)}	-68968(15) ^{e)}	-73241(3.8) ^{d)}
Derived Parent Mass	-66908(22)	-65209(50) ^{c)} (-64964(36)) ^{d)}	-60905(47)	-70481(43)
Difference from Direct Measurements (keV)	153	-109 (+136)	-142	

a) Ref. [21] b) This work c) Ref. [27] d) Ref. [12] e) Ref. [28]

ORNL-DWG 81-19100R

APPENDIX B

PAPER PRESENTED AT THE 4TH. INTERNATIONALS CONFERENCE
ON NUCLEI FAR FROM STABILITY

PRECISION MASS MEASUREMENTS UTILIZING BETA ENDPOINTS

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ABSTRACT

A technique for precise determination of beta endpoints with an intrinsic germanium detector has been developed. The energy calibration was derived from γ -ray photopeak measurements. This analysis procedure has been checked with a ^{27}Si source produced in a (p, n) reaction on an ^{27}Al target and subsequently applied to mass separated samples of ^{76}Rb , ^{77}Rb and ^{78}Rb . Results indicate errors < 50 keV are obtainable.

*) Oak Ridge National Laboratory is operated by Union Carbide Corporation for the U. S. Department of Energy under Contract No. W-7405-eng-26.

**) Supported by Department of Energy Contracts DEAS 0979ER10434 and DE-AC05-76OR00033.

I. INTRODUCTION

Many nuclear and particle physics experiments may be characterized by an attempt to measure the total energy and the energy distribution for a particle or composite group of particles. The total energy of a bound nuclear system is dominated by the mass of the agglomerated particles. Since the masses of the free neutron and proton are known with great precision, the most interesting potential energy part of a nuclear system is the binding energy. Many methods to determine the binding energy of an unknown nuclide have been devised including both direct and indirect measurements. The former tend to give smaller error bars (1-50 keV), while the latter techniques typically yield larger error bars (>50 keV). Because of small cross sections and a lack of suitable target nuclei for direct measurements, indirect methods are dictated. Where observation of radionuclide decay is required, mass separation¹ is often necessary to eliminate as much "background" from competing reaction products as possible. Discrete energy charged particle spectroscopy has long been used to determine both ground state and excited state masses, but this class of nuclei is limited to light neutron-deficient A series, to a small region above $Z = 50$ and to all the well-established alpha-particle emitters above neodymium. Although some mass determinations have been made by utilizing unique systematics, the vast majority of nuclides far from stability require direct beta endpoint measurements which are fraught with inconsistencies due to nondiscrete particle energies and to differing detector response functions.

Beta particle with plastic scintillators has long been a standard procedure^{2,3} with determined mass differences generally having errors > 100 keV. Thus, conversion to intrinsic germanium spectrometers has become an important step in attempts to attain endpoint measurements with errors < 20

keV. The energy calibration is generally much simpler (γ -ray photopeaks may be used), but the response function has been difficult to delineate. This latter problem has been solved in a number of ways, including shape function calculations on known β emitters⁴ and empirical electron response function calculations⁵ determined from a monoenergetic electron beam. A β spectrometer utilizing a superconducting solenoid to channel the β particles has been constructed⁶ and analysis of the detector distorted data has been accomplished through an iterative technique.⁷ This technique has been used to measure decay characteristics of ^{78}Rb .⁸

Since extra bombardment time for calibrations is not always available, an analysis of the raw electron or positron spectrum distorted by a germanium crystal has been attempted using the γ -ray energy calibration. The basic Monte Carlo approach^{9,10} has been successfully used in predicting gamma and negatron spectra as distorted by an intrinsic germanium detector. Further work has been necessary, however, to extend these calculations to positron spectra. Since this work is in the process of being published,¹¹ only a brief synopsis will be given here, in addition to results from the test case $^{27}\text{Si} (\text{GS}) \rightarrow ^{27}\text{Al} (\text{GS})$.

The general area between the $f_{7/2}$ and $g_{9/2}$ shells has been only loosely explored. The mass systematics should prove very interesting because of the large number of differing shell model states and because the proton dripline and $Z = N$ line should intersect in this region. In order to utilize the best characteristics of the UNISOR¹² on-line mass separator facility, the direct mass measurements of Ref. 13 and the relative stability of the krypton isotopes to minimize daughter contamination, measurements on the light rubidium isotopes were commenced. Results for ^{76}Rb , ^{77}Rb and ^{78}Rb will be presented.

II. TECHNIQUE

Although the techniques already mentioned^{4,7} have their advantages and seem to work well in interpreting β spectra measured with an intrinsic germanium detector, it was deemed advantageous to develop a technique whereby the energy calibration resultant from γ -ray photopeaks could be utilized. This process would eliminate the necessity for wasting bombardment time on calibrations and simplify the corrections to a standard Fermi-Kurie type calculation.

An attempt to completely calculate the response function of positrons in germanium has been started, but for present purposes a simplified version¹¹ has been developed to give positron endpoints. This Monte Carlo calculation simulates the effect of annihilation radiation on the shape of the observed Kurie plot. The code calculates the energy deposited in the detector from both the stopped positron and associated γ rays (511-keV annihilation pairs) and then proceeds to redistribute the peak intensity with a Gaussian smearing routine. All positrons were assumed to stop at the center of the detector. We have found that this assumption does not generally affect the calculated endpoint while it significantly reduces the computer time. The hypothetical detector used in these calculations had dimensions 1.6 cm by 0.7 cm, identical to that used in the measurements described herein. The code was run for theoretical endpoint energies ranging from 2.5 to 9.0 MeV. The calculated energy shift due to annihilation interference (ΔE_0) was found to vary smoothly over this energy range and could easily be fit by the quadratic polynomial:¹¹

$$\Delta E_0 = 0.1572 + 0.0115 E_0 - 0.0007 E_0^2, \quad (1)$$

where E_0 is the correct endpoint energy. Thus a 4.0-MeV endpoint would be measured as 4.192 MeV. Figure 1 shows a theoretical Kurie plot, an observed Kurie plot and the Monte Carlo simulation for the high energy portion of a

known positron emitter (^{82}Rb --see Ref. 11 for details). The slight disagreement on the high energy tail is unimportant for the purpose considered here, since least-squares fits are begun at the point where the Kurie function first becomes linear.

Avoiding the inclusion of data in the nonlinear region of the Kurie was an important consideration in our data analysis. Since this departure from linearity occurs 200 - 300 keV below the endpoint for a detector of these dimensions,¹¹ a second β -ray branch within this range could create a problem. Unless the statistics of a particular spectrum are very large, this break is not easy to detect. The analysis code thus searches for a consistent endpoint while removing data points in small increments from the high energy side. Removing a small number of data points from the low energy side often changes the endpoint and is probably due either to a second component or to not having properly found the original high energy break. To reduce the statistical error in a particular endpoint measurement, it is necessary to include as much data as possible in the fit. But a second component within the 200-keV break points is non-trivial to treat. A reasonable criterion for data inclusion near the break point has been χ^2 minimization; in principle, data can be added as long as the endpoint remains consistent and χ^2 is reduced. These procedures have been applied where possible to all of the spectra which will be presented.

III. EXPERIMENTAL

The choice of light rubidium isotopes was predicated upon the ease of extracting rubidium from the UNISOR integrated target ion source and the direct mass measurements¹³ which could be used as a basis, or in the case where the Krypton daughters are well characterized, provide a check for

those same direct mass measurements. It was thus decided to use ^{78}Rb as a check for our technique and commence actual measurements with ^{76}Rb and ^{77}Rb , produced in $^{60,62}\text{Ni}$ ($^{20}\text{Ne}, \text{pxn}$) reactions with ^{20}Ne ions accelerated in the Oak Ridge isochronous cyclotron. These reactions are not necessarily the best choice available, but the proximity of the target to the ion source made the choice of a nickel target imperative. Unfortunately, ^{78}Rb has proven to be anything but simple and has not served as the test originally envisioned. Some of the possible reasons will be mentioned later, but a fundamental necessity for such measurements is that the level structure of the daughter be strictly understood. The decay schemes relevant to this work as shown in Fig. 2 are reported in Ref. 14.

A stringent test of both the fitting routines and the Monte Carlo calculations was performed by measuring the ^{27}Si endpoint. Silicon-27 was produced in $^{27}\text{Al}(\text{p}, \text{n})$ reaction with ~ 11.4 MeV protons accelerated in the Oak Ridge EN tandem and then transported to a β - γ coincidence station by a helium-jet system for analysis. A continuous counting-collection cycle was utilized to measure both singles and 511-keV coincidence spectra of the ground state-to-ground state decay. The singles spectrum gave an endpoint of 3983 ± 11 keV and the coincidence spectrum yielded an endpoint of 3980 ± 30 where the errors are strictly statistical. Application of Eq. 1 results in a positron distortion correction of 191 keV which when subtracted yields 3792 and 3789 keV for the final endpoints for ^{27}Si , in excellent agreement with the accepted value of 3787.0 ± 1.3 keV.¹⁵ Final errors were calculated by adding the conservative estimate of ~ 10 keV in the correction factor in quadrature to the energy calibration error and the statistical error to give final endpoints of 3792 ± 16 keV and 3789 ± 32 keV for the singles and coincidence spectra, respectively. The slightly better agreement between

our results and previous work¹⁵ using the coincidence measurement is expected and such measurements should be utilized whenever possible.

Although the heavier neutron deficient nuclei are usually studied first, the order of discussion will be reversed for the sake of clarity. The decay of ^{76}Rb had been previously studied^{16,17} and the simple decay scheme shown in Fig. 2 is consistent with our observation. A Kurie plot of the singles spectra for ^{76}Rb is shown in Fig. 3. Since the ion source produces no ^{76}Kr or ^{76}Sr and since ^{76}Kr emits no β^+ particles, the measured spectrum was completely attributable to ^{76}Rb . Essentially no events were recorded above 5 MeV (8 MeV was the collection limit). The $2^+ \rightarrow 0^+$ and $4^+ \rightarrow 2^+$ transitions in ^{76}Kr are 424 and 612 keV, respectively. No evidence for the latter transition was observed, whereas most of the beta strength seemed to be channeled through the 2^+ , 424-keV level. Analysis of these data provides an excellent illustrative example of the ideal analysis procedure. Using a distortion break at ~ 4250 keV garnered from the singles spectrum, a series of fits was obtained by using a progressively larger data base. Fits were terminated when the endpoint obtained was no longer consistent. The final endpoint of 4584 ± 40 keV in Table 1 was chosen on the basis of the minimum χ^2 utilizing a 1000-keV range of data. Slightly differing ranges for fits could have been chosen, but would not have had a significant effect on the final value. This is clearly a best-case example and, as will be shown, other fits obtained are not quite as simple.

The spectrum of positrons in coincidence with annihilation radiation yield an endpoint of 4585 ± 52 keV. After correcting for annihilation radiation distortion, adding in the γ -ray energy and taking appropriate averages, a final Q_{EC} of 5835 ± 42 keV was obtained. The singles spectrum yielded a Q_{EC} of 5833 ± 16 keV. Results from all three analyses are sum-

marized in Table 2. It should also be noted that a lack of a ground state positron branch, in addition to the unobserved $4^+ \rightarrow 2^+$ transition suggest that the ground state spin and parity of ^{76}Rb is 2^+ , in accordance with Ref. 17.

Because the high cross section $^{60}\text{Ni}(^{20}\text{Ne}, 2\text{pxn})$ reactions are hindered when $x = 0$ or 1 , this permits a greater yield for the $^{60}\text{Ni}(^{20}\text{Ne}, \text{p}2\text{n})$ reaction as a percentage of the total reaction cross section. This larger yield is useful because the fragmented decay of ^{77}Rb (see Fig. 2) requires greater statistics. Furthermore, the five γ rays (66, 179, 245, 394, and 511 keV) should provide five independent measurements of the same value. Choice of data fitting region was much more difficult because of the level spacing, particularly for the 66-keV transition. Since the positron endpoint for ^{77}Kr is ~ 2 MeV, positrons from the ^{77}Kr daughter should not interfere. Thus, the only convergence criteria used were that the 66- and 511-keV gated spectra should yield the same endpoint and that the 179- and 245-keV gated spectra should also give the same endpoint. An attempt was made to obtain a consistent endpoint using only a 150- to 250-keV range below the distortion break in the Kurie plot for the 66- and 511-keV gated spectra and to minimize both χ^2 and the statistical error bar within the context of a very limited amount of data. Thus, a consistent endpoint utilizing the same analysis procedures as for ^{76}Rb was not possible. Instead, an endpoint sometimes had to be based on an average of all similar endpoints with consistent χ^2 values and statistical error bars because no particular subset of data could clearly be called best. For example, with the 245-keV gated data, reasonable fits for slightly differing energy ranges gave several endpoints with similar χ^2 values. The final value was taken to be a simple average with the largest statistical error, 4023 ± 28 keV. This

value is consistent with the 179-keV result of 4026 ± 18 keV. This averaging procedure was used only in the cases of the singles spectrum and the 66-, 245- and 394-keV gated spectra.

Figure 4 gives the Kurie plot for the high anergy 179-keV gated data. This plot shows the annihilation radiation distortion break, but only the singles spectrum makes it clear enough to choose a fitting region (as can be seen in the singles spectrum for ^{76}Rb in Fig. 3). Furthermore, most gated spectra do not have sufficient statistics to delineate this point. Therefore, careful analysis was required to discover where the fit should begin. This problem was particularly acute for the 66-keV gated data, where the final value of 4212 ± 28 could easily be calculated as 5-10 keV higher, but the 511-keV gated data could in no reasonable manner give such values and convergence was a necessary criterion. Table 3 summarizes our observations, including a final value for Q_{EC} of ^{77}Rb of 5102 ± 25 keV. The excellent agreement of the value derived from the singles spectrum only serves to indicate that in some cases good endpoints can be derived from such spectra. It should not be construed as a better measurement. The quoted error bars are based solely on statistics of the ~ 150 -keV fitting range from the positron distortion break. Obviously, singles spectra can only be used for special cases where no radioactivities (including the daughter) have endpoints above or in the same range as the nuclide of interest. It is also imperative to know the relevant decay scheme precisely for calculating proper endpoints; however an endpoint can also be used to locate a particular energy level in the daughter nucleus.

The plan to utilize ^{78}Rb as a preliminary check was quickly shattered once the data were obtained. Figure 5 compares the singles and 455-keV

gated positron spectra. It should be immediately evident that the endpoints of these two spectra differ by more than the 455 keV suggested by the decay scheme in Fig. 2. The 511-keV gated data also shows the very high energy trend, but because of the very small number of events, valid endpoints are not attainable. The final fitting range for the 455-keV gated data yields a corrected endpoint of 3150 ± 110 keV. This value was corroborated by fitting the equivalent range of 511-keV gated data, yielding 3160 ± 85 keV. Previously, the endpoint¹⁶ for ^{78}Rb has been obtained by gating on the 664-keV transition. Our final endpoint for this data of 2840 ± 70 keV is consistent with the decay scheme given in Fig. 2, but is not consistent with that given in Ref. 16 of 3410 ± 370 keV.

Although the singles spectrum high energy statistics are extremely poor (<10% or decay strength), a crude endpoint of 6060^{+300}_{-170} shows that perhaps previous decay scheme work¹⁸⁻²⁰ was incorrect. Recent work by Rehfield and Moore⁸ give an endpoint of 6221 ± 20 as being due to a 0^+ (GS) $\rightarrow 0^+$ (GS) isospin forbidden beta transition with a $\log ft$ value of 7.95. Since their measurement was begun after waiting 45 min to eliminate any 6 min ^{78m}Rb decays and because the sample was produced in the $^{78}\text{Kr}(p,n)$ reaction at 15 MeV, these beta particles must be from ^{78g}Rb . For reasons already elucidated, our sample was also pure ^{78}Rb , forcing the beta decays involving the 455- and 664-keV transitions to occur elsewhere in ^{78}Kr , transitions to occur elsewhere in ^{78}Kr , or necessitating a search for some very high energy γ transitions. Work on a more detailed decay scheme for ^{78}Rb is under way²¹ and it is hoped this will clarify these matters. Our present results thus tend to support the conclusions of Ref. 8.

IV. RESULTS AND CONCLUSIONS

Although our values for Q_{EC} for ^{77}Rb and ^{76}Rb should be considered preliminary, the base numbers should change little. The error bars should also be considered preliminary, with the statistical error dominating. Table 4 summarizes our results and also compares them with the direct mass measurements of Ref. 13. The decay energy for ^{77}Rb agrees well with one scintillator measurement¹⁶ (5180 ± 390 keV), but not with another²³ (4882 ± 150 keV). Furthermore, within quoted error bars, our value agrees with the direct mass measurements¹³, but the ~ 100 keV differences is of opposite sign from that in ^{78}Rb . These differences are noted because the direct mass measurements have been called into question.^{26,27}

The measured decay energy for ^{76}Rb is lower than most all predictions by ~ 2.5 MeV. Since the observed ^{76}Rb spectrum (unlike ^{78}Rb) indicated no significant high energy events, any large error in the reported spectroscopy would necessitate either a ground state-ground state transition with a branching ratio less than 1% or a different location for the 424-keV transition in ^{76}Kr . The error in the direct mass measurements does not account for this discrepancy. Unfortunately, the mass for ^{76}Kr has been measured only indirectly²² by observing the endpoint of delayed protons from the decay of ^{77}Sr . Clarification of all these bits of information will require two more important links--the mass of ^{76}Kr and better spectroscopic information in the decay of ^{76}Rb . The latter problem has been given a cursory inspection²⁸ with no real surprises. The first problem is currently under study here at Oak Ridge.

Another possibility which might explain the small Q_{EC} for ^{76}Rb is the correctness of the response of our detector to higher positron energies. Data have been obtained on the decay of ^{58}Cu ¹⁵ (Q_{β^+}) = 7540.6 ± 2.4 keV

and, although analysis is incomplete, the raw beta spectrum suggests the decay energy is within 100 keV of this number. Since a natural nickel target was used in the (p,n) reaction bombardments ($E_p = 11.4$ MeV), ^{60}Cu data were also obtained simultaneously. These spectra should provide a clue as to the validity of subtracting one component to obtain a second endpoint. If this technique is successful with ^{58}Cu and ^{60}Cu , then it will be applied to the ^{77}Kr contribution present as a low energy background in the ^{77}Rb spectra. An accurate decay energy for ^{77}Kr will provide a complete chain to ^{77}Br whose mass is known²⁹ to 3.8 keV from (p,n) threshold reactions.

Our measurements for ^{77}Rb and ^{76}Rb appear consistent with predictions¹¹ and thus questions arise about how these Q_{EC} values fit into the general nuclear mass surface systematics. It is clear, however, that much work remains.

We wish to thank E. H. Spejewski and R. L. Mlekodaj for experimental assistance and H. K. Carter and J. D. Cole for computer analysis assistance. We further wish to thank the staff at ORIC which made this work possible.

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TABLE 1.

 $^{76}\text{Rb } \beta^+$ Decay - 424-keV Gamma Gate Fits

Range from Distortion Break in Kurie Plot (keV)	Endpoint	Relative Chi-Square
600	4579	1.08
800	4583	1.03
1000	4584	1.00
1200	4584	1.13
1500	4500	1.12

TABLE 2.

 ^{76}Rb Endpoints Results

	Gamma Gate (keV)		<u>Singles</u>
	424	511	
Measured E_0 (keV)	4584±40	4585±42	4582±11
Annihilation Radiation Correction (keV)	-195	-195	-195
Gamma Energy (keV)	424	424	424
Q_{β^+} (keV)	4813	4814	4811
Weighted Mean (keV)	4813±30		
Q_{EC} (keV)	5835±42		5833±16

TABLE 3.

 ^{77}Rb Endpoint Results

	Gamma Gate (keV)				
	66	511	179	245	394
Measured E_0 (keV)	4212 $\pm$ 28	4208 $\pm$ 46	4026 $\pm$ 18	4023 $\pm$ 28	3812 $\pm$ 35
Annihilation Radiation Correction (keV)	-193.5	-193.5	-192.0	-192.0	-190.6
Gamma Energy (keV)	66.5	66.5	245	245	450.8
Q_{β^+} (keV)	4085 $\pm$ 30	4081 $\pm$ 48	4079 $\pm$ 21	4076 $\pm$ 30	4081 $\pm$ 37
Weight = $\sqrt{N}$	35	34	85	60	37
Weighted Mean (keV)	4080 $\pm$ 13				
Q_{EC} (keV)	5102 $\pm$ 25				
Singles Q_{EC} (keV)	5103 $\pm$ 15				

TABLE 4 Final Q_{EC} and Mass Excess Values

Nuclide	^{78}Rb	^{77}Rb	^{76}Rb
Q_{EC} (keV)	$7242 \pm 20^{\text{a)}}$	$5102 \pm 25^{\text{b)}}$	$5835 \pm 42^{\text{b)}}$
Direct Mass Measurement ^{c)} Mass Excess (keV)	-67076 ± 64	-65037 ± 105	-60668 ± 151
A	78	77	76
Mass Excess of Kr Isotopes (keV) ^{d)}	-74150 ± 8	-70236 ± 30	$-69100 \pm 200^{\text{e)}}$
Derived Rb Mass Excess ($M_{(\text{Kr})} + Q_{EC}(\text{Rb})$) (keV)	-66908 ± 22	-65134 ± 39	-63265 ± 205
Difference from Direct Measurements (keV)	168	-97	-2597

a) Ref. 8

b) This work

c) Ref. 13

d) Ref. 15

e) Based on Ref. 22

ORNL-DWG 81-9710

ORNL-DWG 81-9707

ORNL-DWG 81-9706

ORNL-DWG 81-10043

APPENDIX C

MONTE CARLO CALCULATIONS PREDICTING THE RESPONSE OF INTRINSIC GE DETECTORS TO ELECTRONS AND POSITRONS

A MONTE CARLO STUDY OF THE RESPONSE OF A GE DETECTOR
TO ELECTRONS AND POSITRONS*

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A Monte-Carlo code has been developed which predicts electron and positron response functions of a planar Ge detector. The operational flow-chart for the main program is given while the function of each required subroutine is discussed. The characteristics of the response functions were studied with respect to the bremsstrahlung, annihilation radiation and the total electron transit distance. It is found that electron spectra are primarily distorted near the full energy peak by bremsstrahlung while positron spectra are seriously distorted by both annihilation radiations and bremsstrahlung near the peak. The asymmetric full energy peak is found to result from low energy bremsstrahlung photons. The total transit distances calculated here are found to be in good agreement with those calculated with the Bethe-Bloch formula. The effects of bremsstrahlung, annihilation radiations and total stopping distance, calculated independently in the complete code, were used to construct an abbreviated version which reduced the computer time by a factor of 16. Sample computations are presented for a 16 mm diameter by 7 mm thick, planar detector. The calculated response functions reproduce experimental spectra accurately. The response functions were also used to analyze positron spectra and obtain their end point energies.

I. INTRODUCTION

Nuclear spectroscopy studies involve the experimental determination of the energies, spins and parities of nuclear levels as well as transition probabilities and decay energies. In beta decay (negatron or positron) an extremely fundamental quantity of interest is the Q-value which is determined from the beta end-point energy and knowledge of the decay scheme of the daughter nuclide. In studies of nuclides far from the line of beta stability, the half-lives are short and the well proven techniques of magnetic spectrometry can not usually be applied. In cases where the end-point energies are not much larger than 1 MeV, the Si(Li) detector is ideal because it has excellent energy resolution, collects the events corresponding to all energies at once and has a low atomic number, which minimizes the shape distortion effects of electron scattering. For the measurements involving beta spectra with end-point energies of between about 2 and 10 MeV it is difficult to Li-drift silicon to the required depletion depths, hence, single detectors appropriate for such energies are not available. In 1977 Aleklett [1] introduced a complex system in which the electrons enter the detector from the side, on a flat cut edge of a Si(Li) detector. Electrons which scattered out of the faces were detected in two other Si(Li) detectors which are used as anticoincidence detectors. This technique, though complex, was highly successful. In early attempts to use intrinsic Ge detectors for such studies, Moore, Hayakawa and Rehfield used a magnetic filter to eliminate the interference of γ rays [2]. It was later shown by Girard and Avignone [3] that even in cases involving complex decay schemes with many γ rays, accurate end-point energies can be determined from linear Fermi-Kurie plots if the diameter of the detector is chosen small enough to avoid β - γ summing, and the depth is chosen no thicker than necessary to stop the β -particles at the end-point energy. This technique has by now become a standard tool in on-line studies of β end-point energy

determinations [4-6]. Recently, Avignone et al. [7] have demonstrated that the major difficulty associated with using this technique for positron measurements was an effective shift in the Fermi-Kurie plot and a non linearity near the endpoint, both associated with the interference from annihilation radiations. The techniques used to calculate the corrections do to this effect were tested using positron spectra from the decays of ^{82}Sr , ^{27}Si and ^{58}Cu and the technique was applied to determine the Q-values of the positron decays of ^{76}Rb , ^{77}Rb and ^{77}Kr .

The present paper describes an extension of these Monte Carlo calculations to the determination of the β^- and β^+ response functions, including the effects of multiple electron scattering and bremsstrahlung, as well as annihilation radiation interference. In earlier work of this type, Rehfield and Moore [8] examined semiempirical response functions for β^- and β^+ particles. They approximated the effects of the backscatter and bremsstrahlung with a flat tail but later [9] improved their approximation to account for the backscattering with a flat tail and the bremsstrahlung with a triangular component. During this writing a far more complete study, both theoretical and experimental, appeared in print by Varley et al. [10]. In their earlier work, Decker et al. [4,5] experimentally studied the electron response of Ge using monenergetic electrons from 1.6 to 8 MeV, using a magnetic electron spectrometer. They divided the spectra into three components: a back-and side-escape tail, a bremsstrahlung escape tail, and the primary or full energy peak. In our earlier work, we only considered the interference of the annihilation radiations with positron spectra measured in Ge[7], while presently we report the extension of this work to include multiple electron scattering and bremsstrahlung escape as well.

In this paper we describe the details of two Monte-Carlo Codes; Code I is a detailed and complete code and Code II which uses parameterized functions calculated with Code I to calculate β^- and β^+ response functions within less computer

time. The detector size analyzed in these calculations was 16 mm in diameter and 7 mm thick. These dimensions were determined earlier to be optimum so that a practical balance between efficiency and freedom from γ ray interference was achieved [3]. The calculational techniques used here are similar to those used by Berger et al. [11] in their analyses of the response functions for Si(Li) detectors.

The response functions calculated with these codes are found to reproduce the experimental spectra very well. The final goal of this study is to allow the measurement of beta branching ratios as well as end-point-energy measurements, using planar, intrinsic Ge detectors. This technique was developed to support our Q-value measurements of positron emitters of neutron deficient nuclei, far from stability, which are performed with the UNISOR isotope separator on line to the ORIC cyclotron and HHIRF van de graaff accelerator at the Oak Ridge National Laboratory [12].

II. THEORETICAL CONSIDERATIONS

The theoretical bases for the various formulae used in our Monte-Carlo Codes are presented only very briefly below. The effects of electron and positron scattering are given equivalent treatment theoretically, while the treatment for the distortion due to annihilation radiations is treated in the usual way appropriate to gamma ray scattering and absorption.

2-1. Energy Losses

The passage of a beta particle (β^+ or β^-) through the detector is divided into many steps. We assume that the particle loses DE_i in a distance, called the stepping distance, W_i . The energy loss increment DE_i is mainly due to inelastic collisions with atomic electrons and to the emission of bremsstrahlung in the Coulomb field of nuclei. The total energy loss, called ETOT, is simply

given by,

$$ETOT \equiv \sum_i dE_i. \quad (1)$$

When the electron is stopped in the detector, ETOT is equal to the initial energy EI. At each step (i), there is an associated energy lost from the detector $DE_{(brem)}^i$, due to bremsstrahlung which escapes. The total energy which escapes from the detector due to this effect is called ESUM and is given by,

$$ESUM_{brems} = \sum DE_{brems}^i. \quad (2)$$

When a positron is stopped, it annihilates with an electron and produces annihilation photons. Since two-photon annihilation is strongly dominant, we assume that two photons of $h\nu = m_e c^2$ are produced, back-to-back. We call the total energy deposited in the detector by these two photons E_{annih} . The total energy losses, which are deposited in the detector are given by

$$E_{\beta^-} = ETOT - ESUM_{brems} \quad (3)$$

and

$$E_{\beta^+} = ETOT - ESUM_{brems} + E_{annih}. \quad (4)$$

2.2 Multiple Scattering

The direction of the momentum vector of beta particles in matter is mainly changed by multiple elastic scattering by nuclei. We assume in these calculations that at each stepping distance W_i , the particle's momentum vector is rotated through angles (θ, ϕ) which are selected using random variables with weightings in accordance with the Molière multiple scattering formula [13]. The angular distribution associated with Molière scattering is given by,

$$W(\theta)2\pi\theta d\theta = F(\theta^2)d\theta^2, \quad (5)$$

where θ is a parameter defined by $\theta \equiv \Theta/\chi_c \sqrt{B}$. Also, $\chi_c \equiv (\sqrt{1-\beta^2}/\beta^2)(44.8Z)(\sigma/A)^{1/2}$ and $\sigma \equiv \rho W_i$, where ρ is the density of the detector material and $\beta \equiv v/c$. The values of the function $F(\theta^2)$ are tabulated in reference [13]. The parameter B is a slowly varying parameter dependent on the number of collisions n and has

values of 3.36, 6.29 and 8.93 for $\log_{10} n = 1, 2$ and 3 respectively. Given the quantity $\log_{10} n$, the step distance W_i in cm is calculated by

$$W_i = \frac{A Z^{2/3} (1.13 + 3.76\gamma^2)}{\rho\gamma^2} \cdot 10^s, \quad (6)$$

when $s \equiv \log_{10} n - 8.215$ and $\gamma \equiv Z/137\beta$. For a given step distance, the angle θ is chosen using a random variable technique which will reproduce the Moliér angular distribution while ϕ is chosen randomly. We essentially replace a very large number of interactions with a finite number, one at each step distance W_i . For each value of the index i , the scattering angles θ and ϕ are chosen and the electron moves in the new direction, dictated by these angles, for a distance W_i with a reduced energy.

2.3 The Energy Loss Distribution

The distribution of energy losses DE_i , at each step, is given by the function $\phi(\lambda)$ derived by Landau [14] which is given as

$$\phi(\lambda) = \frac{1}{\sqrt{2\pi}} \exp \left\{ \frac{|\lambda| - 1}{2} - e^{|\lambda| - 1} \right\}, \quad (7)$$

where λ is a dimensionless parameter defined as,

$$\lambda \equiv (DE_i - DE_M)/aW_i. \quad (8)$$

In equation (8), DE_M is the most probable energy loss and $a \equiv 0.153(\rho Z/A)\beta^2$ MeV/cm. An expression for DE_M , which includes a correction D_{pol} , called the density effect due to the polarizability of the material, was derived by Sternheimer [15] as follows:

$$DE_M = aW_i \{ \ln[aW_i mc^2 \beta^2 / I^2 (1 - \beta^2)] - \beta^2 + K - D_{pol} \}. \quad (9)$$

In equation (8), I is the mean excitation energy and $K = 1.12$ as given in ref. (15). Subsequent to choosing a value for λ , in accordance with the distribution $\phi(\lambda)$, the energy loss for the i^{th} step is computed by use of equation (8).

2.4 Bremsstrahlung Cross Sections

The differential cross section $d\sigma(k, E_i)$, for the production of a bremsstrahlung photon of energy k , by a beta particle of initial energy E_i , can be calculated using formulae given by Koch and Motz [16]. For beta particle energies below 0.2 MeV, a nonrelativistic Born approximation, without screening corrections, is used which is written in the Heitler approximation as,

$$d\sigma_k = \frac{(Zr_o)^2}{137} \left(\frac{16}{3}\right) \frac{dk}{k} \frac{1}{p_o^2} \ln \left(\frac{p_o + p}{p_o - p}\right), \quad (10)$$

where p_o and p are the initial and final electron momenta respectively and where $r_o = e^2/mc^2 = 2.82 \times 10^{-13}$ cm. For beta particle energies above 0.2 MeV, a relativistic Born approximation without screening was used. This formula, given in ref. [16] is the Bethe-Heitler approximation which can be written as

$$d\sigma_k = \frac{4Z^2r_o^2 dk}{137 k} \left[1 + \left(\frac{E}{E_o}\right)^2 - \frac{2}{3} \frac{E}{E_o}\right] \left[\ln\left(\frac{2E_o E}{k}\right) - \frac{1}{2}\right]. \quad (11)$$

In equation (11), E_o and E are the initial and final electron energies, in units of $m_o c^2$, respectively. The total bremsstrahlung cross section $\sigma_t(E_i)$ is obtained by integrating $d\sigma(k, E_i)$ over k ,

$$\sigma_t(E_i) = \int_{E_{\min}}^{E_i} d\sigma, \quad (12)$$

where the minimum photon-energy $E_{\min} = E_i/100$ was arbitrarily adopted for these calculations. In order to simplify the Monte Carlo Code, a relative photon energy distribution $\sigma_R(EK)$ was calculated in terms of the relative energy $EK \equiv k/E_i$, using equations (10) and (11). An average distribution was used for beta energies on the interval $0.1 \leq E_i \leq 5$ MeV. The error introduced by using this average photon distribution is about 10%, while it leads to a significant simplification of the code.

2.5 The Photo-Electron, Angular Distribution

The energy losses due to escaping annihilation radiations and bremsstrahlung are accounted for in a code similar to that on which this work was originally based [17] and in our recent work [7]. In the present calculations we also account for energy lost due to photo-electrons which escape from the crystal. For this section of the code, we use the same techniques discussed above to determine when the electron escapes and how much energy it has deposited prior to escape. The only new factor is the angular distribution of the electrons. The direction of the photo-electron is chosen, relative to the direction of the absorbed photon, in accordance with an angular distribution $W(\theta)$. In cases in which the photon energies are below 100 keV, the nonrelativistic approximation of Sauter is used [18], which can be written as,

$$W(k\theta) 2\pi \sin\theta d\theta = \frac{C \sin^3\theta d\theta}{[1 - E\gamma/2mc^2 - \beta\cos\theta]}^4, \quad (13)$$

where c is a normalization constant. A relativistic formula given by Pratt et al. [19] is used in the present work when the photon energies are greater than 100 keV. This angular distribution is written as follows:

$$W(k\theta) 2\pi \sin\theta d\theta = \frac{C \sin^3\theta \{1 + \Gamma(1 - \beta\cos\theta)\} d\theta}{1 - \beta\cos\theta}, \quad (14)$$

where $\Gamma \equiv \frac{1 - 3\sqrt{1 - \beta^2} + 2(1 - \beta^2)}{2(1 - \beta^2)^{3/2}}$

In both equations (13) and (14), the photon energy k enters through the velocity v in β , in the usual way.

2.6 Selection of Parameters

There are several techniques employed in Monte-Carlo calculations, which are used to select a value of a given variable for a given trial, so that the known distribution of values of that variable is reproduced. These techniques can be shown to be equivalent to the use of a response-distribution function

$X(R)$, where R is random number ($0 \leq R \leq 1$). The function $X(R)$ is related to a given distribution $\phi(x)$ such that when a statistically significant set of random numbers $\{R\}$ is selected and related to a distribution $\phi(x)$ as follows:

$$R = \int_{x_0}^x \phi(x) dx / \int_{x_0}^{x(\max)} \phi(x) dx, \quad (15)$$

the distribution in X thus determined, would in fact be proportional to $\phi(x)$. The variable x could be θ in an angular distribution or λ in the Landau distribution for example. Each part of a Monte Carlo Code, involving a given distribution $\phi(x)$ and variable, x can be tested independently by performing the operations indicated by equation (15) and determining if in fact the distribution of selected values of x in fact reproduces $\phi(x)$.

III. OPERATION OF THE MONTE CARLO CODES

Schematic diagrams of the functional steps of the detailed Code I and the abbreviated Code II are shown in Fig. 1. The corresponding operational flow-chart is shown in Fig. 2. The distribution of beta particle trajectories is consistent with that for an isotropic source. The history of each beta particle is followed until it is stopped in the detector or escapes. Bremsstrahlung and annihilation photons as well as photo-electrons are followed until they either escape or are absorbed. Finally, the total energy for that event is computed. Below we discuss in detail the logic by which the code accomplishes this.

Let us assume that a beta particle with energy E_I arrives at the face of the detector from the source. Let us further assume that the entrance point is defined by the vector $\vec{P}_I$ which has a unit vector $\vec{S}_I$ in the direction of its momentum, on the surface of the detector. Further, let us assume that the beta particle suffers many collisions and that after n steps, the beta particle has energy E_n is located by vector $\vec{P}_n$ and has a direction unit vector $\vec{S}_n$. After the

step $n+1$, the total distance traveled is W_{n+1} while the scattering angles $(\theta, \phi)_{n+1}$ are calculated using subroutine ESCAT, which is based on the equations (5) and (6). In subroutine ESCAT, $\log_{10} n$ is chosen for the three different energy intervals corresponding to values 1, 2, and 3. In Table I we give corresponding values of W_i . The next direction vector $\vec{S}_{n+1}$ is then calculated from the scattering angles $(\theta_{n+1}, \phi_{n+1})$.

Subroutine LANDAU is used to calculate the energy loss DE_{n+1} of the $n+1$ step by use of equation (8), and by using the LANDAU distribution $\phi(\lambda)$ as discussed in Section 2-6. At this point, the most probable energy loss is calculated using equation (9). We note from Table I that DE_M is 5.68 keV at $E_m = 3$ keV and $\log_{10} n = 1$. The beta particle is considered to be stopped. Generally when the particle reaches a point at $n+1$, it has just lost energy DE_{n+1} and has a direction vector $\vec{S}_{n+1}$. The energy E_{n+1} is given by,

$$E_{n+1} = E_n - DE_{n+1}, \quad (16)$$

while the location vector $\vec{P}_{n+1}$ is given by

$$\vec{P}_{n+1} = \vec{P}_n + W_{n+1} (\vec{S}_n + \vec{S}_{n+1}). \quad (17)$$

In this way, the location and energy constantly evolve in finite steps until the electron either escapes or is absorbed.

Subroutine BREMS gives the bremsstrahlung escape-energy, DE_{brems} , as a function of the current beta energy E_n and the step distance W_{n+1} . When the beta energy E_n is larger than 3 MeV, the step distance is divided into ten intervals. In each interval, DE_{brems} is calculated with BREMS. The bremsstrahlung emission probability is obtained from W_{n+1} and the total bremsstrahlung cross section $\sigma_t(E_n)$, given by equations (11) and (13). The photon energy $k = EK \cdot E_n$ is then selected by use of the relative photon-energy distribution function $\sigma_R(EK)$, discussed in Section 2-4. The angular distributions are assumed to be isotropic, because low energy photons are primarily emitted. The energy loss DE_{brems} is then calculated using the photon response code used in our earlier work [17].

If after step $n+1$, $\vec{P}_{n+1}$ still locates a point inside of the detector, while also $E_{n+1} > 3$ keV, the code returns to statement 999 where another representative interval is taken. This is repeated until either $\vec{P}_i$ is outside of the detector, in which case the electron escapes, and $E_{\text{annih}} = 0$, or $\vec{P}_i$ is inside of the detector and $E_i < 3$ keV indicating a stopped particle. At this point, the energy deposited by the annihilation radiations is calculated using subroutine 1EN511 which is also fashioned after the γ ray code described in ref. [17], except that in subroutine 1EN511 the escape of both Compton- and photo-electrons are accounted for in a manner similar to that of the main code. It is found that approximately 10% of the 511 keV photo-peak is lost due to electron escape in the small detector analyzed in this work (16 mm diam. by 7 mm deep). The shape of the Compton tail is not noticeably changed by electron escape. The deposited energies are smeared according to a gaussian smearing routine SMEAR discussed in ref [17]. The smeared energies are converted into channel number and the distribution of events calculated this way represents the calculated spectrum.

An operational flowchart describing the abbreviated Code II is shown in Fig. 3. Code II is a simplified version of Code I, which depends on parameters and two data sets which were calculated using Code I. The parameters are the stopping rate, RSTOP, the average stopping depth or distance from the detector face, $\bar{Z}$ and the annihilation radiation absorption rate, R511, defined by

$$R511 = \frac{\text{Number of events } E_{\text{annih}} > 0.1 \text{ keV}}{\text{Number of stopped particles}} \quad (18)$$

These parameters were calculated as functions of the initial beta energy E_i . In Code II, we calculate the range, RANG, of electrons of energy E_i , which we calculate by the Bethe-Bloch formula which includes density and bremsstrahlung effects [19]. In this code when RSTOP is selected as a weighted random variable,

it is then determined whether a given beta particle stops or not. If a particle is determined to have only part of its energy deposited, then the total energy deposited is determined by the distribution calculated in detail by use of Code I, the results of which are shown in Fig. 4. The calculation assumes a source-to-detector distance of 8 mm which is a natural distance one would use with this size detector. The results do vary with this distance. In Code II, when the particle itself escapes from the detector, we neglect the bremsstrahlung and annihilation radiation effects, hence, $ESUM_{\text{brems}} = E_{\text{annih}} = 0$.

When the particle is stopped, the energy loss due to bremsstrahlung is taken into account. Photons are emitted when the beta particle traverses the range, RANG. This distance is divided into a number of steps JSTEP and a photon is emitted at each step. The parameter was fixed at 100, in Code II, by comparing spectra generated by both codes. The bremsstrahlung energy loss at each step distance is chosen to be the same in Code II. The depth at which a bremsstrahlung photon is emitted from the detector surface is given by

$$Z_i = (\bar{Z}/RANG) \sum_{j=1}^i W_j, \quad (19)$$

where $\bar{Z}$ is the average stopping depth. The X-Y coordinates of the stopped particle are chosen randomly for simplicity. The escape energy for bremsstrahlung is chosen using subroutine BREMS, which when summed over all steps yields the total bremsstrahlung escape energy $ESUM_{\text{brems}}$.

It is also assumed that the annihilation radiations are emitted from a depth $\bar{Z}$. The probability of absorption of a given energy by annihilation photons is given by the parameter R511 for $E_{\text{annih}} > 0.1$ keV, while the energy distribution of E_{annih} is given by subroutines DATA AND 511SHAPE. This routine is based on the normalized shape of the annihilation energy-losses and is independent of the depth $\bar{Z}$. This fact was proved using Code I. Using our results from Code I, we

assume that the 511 keV total energy rate is given by $R_{511} \times 0.011$. The energy losses $E_{\text{multistep}}$, E_{electron} and E_{positron} are obtained using equations in Section II above. These energies are converted into channel number with subroutine SMEAR to obtain the calculated spectra. Code II then, is a significantly simplified code which depends critically on results obtained using the detailed Monte-Carlo Code I. Its results were also directly checked with Code I.

IV. RESULTS AND DISCUSSION

The positron spectrum at $EI = 4.0$ MeV, calculated with the full Monte-Carlo version Code I, is shown in Fig. 5. The general features are in agreement with those shown in Fig. 6 of ref. [10]. Three main features are coded individually, namely, the electron escape tail, the bremsstrahlung escape, and the annihilation radiation contribution. The main source of distortions of the spectrum in the region of the full energy peak are due to bremsstrahlung and annihilation radiations of the stopped positrons. It should be noted that EI is the kinetic energy of the positron. With the approximation, made in this work, that the only difference between positrons and electrons is the distortion due to annihilations radiations, a positron spectrum is obtained by summing all three effects while an electron spectrum is obtained by eliminating annihilation radiation effects. As one test of our methods, we have calculated an electron spectrum at $EI = 4.0$ MeV and it was found to be in good agreement to the experimental spectrum given in reference [4].

The bremsstrahlung contribution consists of a low-energy part, for $ESUM_{\text{brems}}$ less than 20 keV, and a triangular part. Figure 6 shows the bremsstrahlung contribution to the spectrum for $EI = 1, 4$ and 6 meV, calculated with Code I. The triangular portion for $ESUM_{\text{brems}} > 20$ keV shows a strong dependence on EI . We also have noted that the relative intensity of the bremsstrahlung spectra are

not sensitive to the source-to-detector distance, if it is greater than about 8 mm. The low energy portion of the bremsstrahlung escape spectrum tends to degrade the peak energy resolution of both electron and positron spectra. Figure 7 shows both electron and positron spectra in the region of the full energy peaks. The pure "MULTISTEP" peak neglects photon effects. The low-energy tail was identified as a contribution due to the low energy portion of the bremsstrahlung contribution. The peak intensity difference between the multistep and electron spectra is due to the triangular portion of the bremsstrahlung contribution while the difference between the electron and positron peaks is due to the summing of positron and annihilation radiation energies.

The results of a detailed calculation of the total transit distance $W = \sum_i W_i$ for stopped beta particles is shown in Fig. 8. Up to $EI = 8$ MeV, W agrees well with the range, $RANG$, given by the Bethe-Bloch formula, including density, bremsstrahlung and polarization effects as given in ref. [19]. The stopping distance, $\bar{Z}$, from the entrance face of the detector also shows an almost straight-line dependence on EI .

The back, side, and forward escape rates were also calculated as functions of the initial particle energy EI , using Code I and are shown in Fig. 9. As expected, backscattering escape decreases with increasing EI , while side escape increases which clearly demonstrates the value of good collimation. Forward escape does not become important until the energy corresponds to a range which exceeds the thickness of the detector. The theoretical back-scattering curves are those given by Rehfield et al. [8]. The consistency of these results to the theoretical curves shows that this effect is not strongly dependent on the size of the detector.

The stopping rates RSTOP for SL, the source-to-detector distances of 8 and 100 mm are shown in Fig. 10. They are different but both gradually decrease with increasing initial energy. The difference between these two curves is as expected and again shows the merits of using a "good" geometry and the importance of having equivalent geometries for both the calculations and experiments being compared.

The annihilation radiation absorption rate R511, defined by equation (8), is also shown in Fig. 10. It was observed that the curve R511 was not sensitive to the source-to-detector distance SL, for $SL > 8$ mm. The curve R511 increases gradually from $EI = 1$ to $EI \cong 4$ MeV, when it essentially becomes constant with a value of about 0.35 up to 8 MeV. The shape of the contribution to the spectrum of annihilation radiations is itself found to be almost independent of initial particle energy EI.

The single escape peak rate $R(1\gamma)$ for annihilation radiations is defined as follows:

$$R(1\gamma) = \frac{N_p(1\gamma)}{N_t(E > 0.1)}, \quad (20)$$

where $N_p(1\gamma)$ is the total number of events under the one-annihilation-photon escape peak and, $N_t(E > 0.1)$ is the total number of annihilation photons which deposit more than 0.1 keV in the detector. The quantity $R(1\gamma)$ for a variety of source-to-detector distances, SL, are tabulated in Table II. Each value given is for a total of 10^5 beta events and was calculated using Code I. $R(1\gamma)$ has essentially a constant value of 0.011 for $EI = 4.0$ to 6.0 MeV and for $SL = 8$ m or infinity.

A quantity which we call the triangular bremsstrahlung rate RB_{tri} , defined in equation (21), is also shown as a function of EI in Fig. 10. We define,

$$RB_{tri} \equiv \frac{N(\Delta)}{N_{\beta}(\text{stop})} , \quad (21)$$

where $N(\Delta)$ is the total number of bremsstrahlung photons in the triangular part of the bremsstrahlung spectrum, for which $ESUM_{\text{brems}} > 20$ keV, and $N_{\beta}(\text{stop})$ is the total number of beta particles which stop in the detector. RB_{tri} is not sensitive to source distance SL , when $SL > 8$ mm, but continuously increases with EI almost linearly. The detector efficiency for an electron event to appear in the full energy peak is then $RSTOP(1-RB_{tri})$ while that for a positron it is $RSTOP(1-RB_{tri}-R511)$.

The central processing unit (CPU) time with an IBM 360, or equivalent computer is 17.4 seconds, on the average, per 100 electrons analyzed with Code I, at $EI = 4.0$ MeV. The average number of steps NS , each of distance W_i , has an approximately constant value ~ 200 for $EI = 2.2$ to 5.0 MeV. We have noted, however, that NS increases from a value of 94 at $EI = 0.2$ and decreases to a value of 125 over the interval $EI = 5.0$ to 8 MeV.

Code II was developed so as to exploit some of the constant or smoothly varying nature of these parameters and significantly shortens the computer time. The bremsstrahlung contribution is computed in Code II by allowing the bremsstrahlung photons to be emitted in a total number of steps, called $JSTEP$ (see Fig. 3). The bremsstrahlung rate RB_{tri} actually depends on how $JSTEP$ is chosen. This parameter was varied in Code II over a range from 10 to 1000. It was found that when $JSTEP = 100$, spectra calculated with Code II are very similar to those calculated with Code I. Figure 11 shows a positron spectrum for $EI = 4.0$ MeV, calculated with Code II and with $JSTEP = 100$. This calculation required 1.1 sec. per 100 sec., which is a factor of 16 less than the same calculation using Code I. This factor is somewhat dependent on EI . It has clearly been demonstrated, then, that an elaborate and detailed Monte Carlo Code can be used to

generate the behavior of certain parameters which can be used in a much simplified code with essentially equivalent results. The abbreviated code can then be used to do vary repetitious calculations, an example of which is the extraction of the best beta end-point energy from a raw spectrum, using an iterative technique [20].

In the present work, the multiple scattering distributions as well as the energy losses were assumed to be the same for electrons and positrons. We can however estimate the differences which would be reflected in the response functions by considering the theoretical backscattering coefficients shown in Fig. 9. The coefficient for positrons is several percent less than that for electrons for an incident energy E_i of between 0.1 and 10 MeV [11]. In addition, Berger et al. [21] have estimated the positron energy-loss to be approximately 3% less than that for electrons over the energy range from 0.5 to 10 MeV. We can then estimate that the escape tail of the positrons will be between 10 and 20% less than that of the electrons. The spectra are, however, strongly dominated by the full-energy peaks and the peaks are primarily distorted by bremsstrahlung and annihilation radiations from stopped particles. We conclude from this that the calculation of positron end point energies for continuous positron spectra, should not be significantly affected by neglecting the difference in the multiple scattering processes between electrons and positrons.

The use of the present calculations to extract end-point energies has been checked by measuring the well known positron spectrum in the decay of ^{27}Si , formed in the reaction $^{27}\text{Al} (p,n) ^{27}\text{Si}$. In the iterative technique, a series of allowed positron spectra were calculated and distorted by our response codes for many end-point energies. The end-points are varied until the Fermi-Kurie functions of the calculated, distorted-spectra overlap the measured one. Using this procedure we extracted an end-point energy of 3793 ± 16 keV for this decay.

This end-point energy has a well known value of 3787 ± 1.3 [22]. The error in a typical scintillation detector measurement would be more than an order of magnitude larger than our error, which clearly demonstrates the power of this technique.

We wish to express our appreciation to Dr. E. H. Spejewski and the UNISOR staff for their help during this work and also to Dr. K. S. Toth for his collaboration in the experimental measurements and for many valuable communications on this subject.

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* Supported by the U.S. Dept. of Energy under contracts DE-AS09-79ER10434 and DE-AC05-76OR00033.

**The Oak Ridge National Laboratory is operated by the Union Carbide Corporation for the U.S. Department of Energy under contract W-7405-eng-26.

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CAPTIONS FOR THE FIGURES

- Fig. 1. Schematic diagram of the processes calculated with Codes I and II.
- Fig. 2. Flow-chart of Code I.
- Fig. 3. Flow-chart of Code II. The parameters (RSTOP, $\bar{Z}$ and R511) and the data (TAIL and 511 SHAPE) were calculated using Code I.
- Fig. 4. The data called TAIL and parameter RSTOP in Code II are deduced from this multistep spectrum obtained by Code I at SL = 8 mm for 10^3 events at each initial beta energy EI. Intervals of 0.2 MeV have been used and each tail is divided into 20 channels. The primary peak is due to stopped beta particles in the detector.
- Fig. 5. Positron spectrum given by Code I at an initial energy EI = 4 MeV and SL = 8 mm for 10^4 events. The solid line shows the bremsstrahlung effects due to stopped particles in the detector. The dashed line shows the escape tail due to the multistep losses and the shaded area shows the annihilation radiation effects.
- Fig. 6. Bremsstrahlung spectra of $ESUM_{\text{brems}}$ due to particles stopped in the detector with EI = 1, 4 and 6 MeV. Each spectrum is taken for 10^5 events using Code I and a parallel beta beam.
- Fig. 7. Peak spectra showing the net positron and electron peaks and the pure multistep peak, calculated using Code I at EI = 4 MeV and SL = 8 mm for 10^5 events. The antisymmetric low-energy side of electron and positron peaks are due to low-energy bremsstrahlung from stopped particles. The high energy events, beyond positron peak, are due to the annihilation radiations.

- Fig. 8. The total transit distance $W = \sum_i W_i$ for stopped beta particles calculated with Code I. Also shown is the average stopping distance, $\bar{Z}$, from the detector surface. The beta range (RANG) was calculated with the Bethe-Bloch formula. These points were calculated with Code I.
- Fig. 9. Back, side and forward escape rates calculated with Code I at $SL = 8$ mm for 10^3 events at each energy. The solid and dashed lines are the backscattering coefficients of electrons and positrons respectively, given in reference [8].
- Fig. 10. The stopping rates RSTOP: (1) for a parallel beta beam and (2) at $SL = 8$ mm. (3) The annihilation absorption rate R511, and (4) the triangular bremsstrahlung rate RB_{tri} . These results were calculated using Code I.
- Fig. 11. A positron spectrum for initial particle energy $EI = 4$ MeV with $JSTEP = 100$, using Code II with 10^4 events.

TABLE I. Results of the subroutine ESCAT (E,W,THET,FI) and the most probable energy-loss DE_M .

$\log_{10} n$	Energy E(MeV)	$W(10^{-3})\text{cm}$	$DE_M(\text{keV})$
1	$E < 0.2$	< 0.115	$0.59 <$
2	$0.2 < E \leq 3.00$	$1.15 - 2.00$	$6.5 - 7.9$
3	$3.0 < E$	$20.0 - 20.3$	$100 - 110$

TABLE II. Escape peak rate $R(1\gamma)$ of a single 511 keV gamma-ray for the annihilation shape.

EI (MeV)	SL	$R(1\gamma)$
4.0	8mm	0.01050 ± 0.00069
4.0	Parallel	0.01082 ± 0.00065
1.0	Parallel	0.01124 ± 0.00073
6.0	Parallel	0.01166 ± 0.00069

CODE I

Ge DETECTOR

CODE II

CODE I

CODE II

ORNL-DWG 82-8289

APPENDIX D

REACTOR ANTINEUTRINO SPECTRA AND NUCLEAR SPECTROSCOPY OF ISOTOPES FAR FROM BETA STABILITY

REACTOR ANTINEUTRINO SPECTRA AND NUCLEAR SPECTROSCOPY
OF ISOTOPES FAR FROM BETA STABILITY*

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Recent decay scheme information, not included in our earlier calculations has been used to calculate the contribution of these isotopes to the fission spectrum of antineutrinos. This contribution has also been calculated using our earlier methods of extrapolating to nuclides further from beta stability and the agreement is good. Comparison of the total fission beta spectrum, calculated this way, to one of the recent measurements strongly implies that our extrapolation techniques, and probably all averaging techniques, fail suddenly for the last few important contributing isotopes far from stability. A list of the most important experimental nuclear spectroscopy, which would increase the accuracy of all such calculated spectra, is deduced from the present calculations. These experiments might be performed using heavy ion reactions as well as with thermal fission.

[Radioactivity: Fission ^{235}U ; antineutrino spectrum calculated in equilibrium. List of important nuclear spectroscopy experiments deduced.]

* Supported in part by the U.S. Department of Energy under contract DE-AS09-79ER10434.

I. INTRODUCTION

Reactor antineutrino experiments represented the first serious efforts to study the interactions of neutrinos with matter and they continue to play a central role in our understanding of neutrinos and their interactions. A recent review of the historical developments was given by Borovoi.¹ Presently, the central issue in this field involves the search for neutrino oscillations. An extensive list of references on this subject is given in reference 3 of the recent article by Avignone and Greenwood (AG).² Two events which have dominated this field recently are: (1) the evidence for possible neutrino oscillations observed in the experimental ratios of the cross sections for the reactions $d(\bar{\nu}_e, \bar{\nu}_e)Pn$ and $d(\bar{\nu}_e, e^+)nn$ by Reines, Sobel and Pasierb³ and (2), the conclusion by Lyubimov et al.⁴ that the shape of the 3H beta spectrum, near the end-point, implies a non zero electron antineutrino mass ($16\text{ev} \leq m_{\nu}c^2 \leq 46\text{ev}$). The effects of uncertainties in the final state interactions^{5,6} as well as the effects of neutrino spectrum shape on the cross sections of ref. (3) have been shown to be small.⁶ Further evidence supporting neutrino oscillations in reactor experiments was given by Silverman and Soni⁷ who analyzed three inverse beta decay experiments in a way which avoids uncertainties in calculated neutrino spectra and in absolute detector efficiencies. Other recent analyses of neutrino oscillations have been given by Barger, Whisnant and Phillips⁸ and by De Rújula et al.⁹ It was concluded in ref. (9) that sizeable oscillations between electron and tau neutrinos are compatible and perhaps indicated by existing data. On the other hand a recent report of the proton inverse beta decay experiment done at the Laue-Langevin reactor¹⁰ concludes that the data are consistent with no oscillations. These data were analyzed on the basis of two neutrino oscillations; however, and this

simplifying assumption may be overrestrictive. Three new experiments are underway at a variety of distances from two reactors which should produce new data by the Spring or Summer of 1982.¹¹ While none of the above analyses need depend on accurate knowledge of the fission spectrum of antineutrinos, more accurate and straightforward interpretation of the data would be possible if these spectra could be accurately calculated. In addition, this spectrum is of basic interest itself.

There have been a variety of attempts to calculate the fission spectrum of antineutrinos^{2,12-19} while there are mainly two methods of accounting for the decays to nuclides with unknown decay schemes. One is the use of beta strength functions $S_\beta = \sum_J \rho_J(E) B_J(E)$ where ρ is the calculated level density of the daughter nuclide and where B is the reduced transition probability. Klapdor²⁰ has recently pointed out, however that there is low energy structure in beta strength functions which can have drastic influence on the calculated neutrino spectra and further that calculations using this approach have not accounted for this structure.^{16,18,19} Other methods of accounting for unknown nuclear structure^{2,12-15} involves effectively obtaining B and ρ from the average properties of known nuclides. In particular (AG)² attributed to a nuclide with unknown structure, all of the energy levels of nuclides of the same atomic number Z , but which differ in neutron number N by an integral number of neutron pairs. The beta Q values were calculated using semiempirical mass formulae. The branching ratios are taken to be the renormalized collection of all of the experimental ratios in this same collection of nuclides. There are also a variety of pitfalls which one might encounter using these empirical techniques.

The obvious experimental test of these calculational techniques, which is independent of possible neutrino oscillations, is direct comparison to

the beta spectra from fissioning ^{235}U in secular equilibrium. There have been a variety of such measurements;²¹⁻²⁵ however, their results differ significantly.²⁴ The calculations of Davis et al.,¹⁶ for example, are in excellent agreement with the recent measurement of Schreckenbach et al.²⁴ while those of (AG)² are in good agreement with the measurements of Tsoulfanidis et al.²³ which differ significantly from those of ref. (24) particularly at higher beta energies. The delayed fission beta measurements of Dickens et al.²⁶ also were found to have a much softer spectrum than that of ref. (23) and motivated the much softer calculated fission antineutrino spectrum of Dickens.¹⁸ A more recent measurement by Borovoi et al.²⁵ are in much better agreement with the predictions of (AG)² and of Borovoi et al. (BDK).¹⁵ It seems as though there may also be inherent difficulties in the measurements which are not clearly understood. This leaves the calculations with no stringent reliable tests. One of the main motivations of the present work is to identify those isotopes which make the most important contribution to the fission antineutrino spectrum and which have yet unknown decay schemes.

II. ANTINEUTRINO SPECTRUM CALCULATIONS

In principle, one could calculate the antineutrino spectrum from the decays of fission fragments exactly, if one had exact knowledge of the primary fission yield $Y(ZA)$, the beta branching ratios $b_j(ZA)$, the excited state energies of daughter nuclides E_{zj} , and E_{oj} , the beta end point energies. In this case the spectrum is expressed as

$$N(E) = \sum_{Z,A,j} K(ZA)b_j(ZA)P_j(Z,A,E_{oj},E_\beta), \quad (1)$$

where $P_j(Z,A,E_{oj},E)$ is the normalized, allowed, Coulomb corrected anti-

neutrino spectrum with end-point energy E_{oj} , and $b_j(Z,A)$ is the beta branching ratio of the j th beta branch in the isotope (Z,A) . The weighting factor $K(AZ)$ is the sum over Z of the independent fission yields of all of the isotopes in the chain of mass A , up to and including Z .

All of the formulae and calculational techniques used here are given in detail in ref. (2). The first calculation we report here is that of the fission antineutrino spectrum due to a number of isotopes whose decay schemes were not known to us at the time of our earlier work (AG)². First the calculation was made using the beta branching ratios and energy levels given in the new references.²⁷⁻⁴³ This spectrum is labeled "New Knowns" in Figure 1. Next, the level schemes and beta branching ratios were deduced using the averaging techniques discussed in ref. (2) involving all other known isotopes, excluding this new set. The neutrino spectrum calculated with these parameters is labeled "Old Guesses" in Figure 1. One notes that between 6 and 10 MeV the agreement is good which indicates that the new nuclear spectroscopy data brought no surprises except that at low energies several strong beta branches caused wiggles in the spectrum. The collection of new known isotopes is typical of the remaining unknown isotopes in the number of steps from stability as well as general areas in the $N-Z$ plane. They come predominantly from the lower sides of the two fission mass peaks. If the proponents of the "softer" fission neutrino spectra are correct, then our averaging techniques fail but not smoothly. The densities of levels available to allowed beta decay of the remaining dozen unknown isotopes which dominate the fission antineutrino spectrum, must change drastically along with the pattern of beta strengths. If this is so, then other averaging techniques, based for example on the statistical model of the nucleus, very probably also fail to predict this sudden change in

properties. The softer spectra, if they are shown to be correct, are then somewhat fortuitous and we conclude that there can be no reliable theoretical antineutrino spectra from fission products until experimental nuclear spectroscopy is performed on the remaining important isotopes. We have determined from our calculations that there are nine isotopes whose decays could well dominate the antineutrino spectrum above 8 MeV, where the existing disagreements are the largest. The corresponding spectra calculated using the $(AG)^2$ technique are shown in Figure 2. Since most of these isotopes are near in proton number and are in a vicinity where sudden changes in p and B may well exist. For completeness we have used the newly known decay schemes in our averaging technique to simply update our spectrum. The main value of these calculations is to demonstrate the relative importance of known and unknown decay schemes at various neutrino energies as shown in Figure 3 and not to produce yet another calculated spectrum.

III. RESULTS AND CONCLUSIONS

In Table I we give values of the antineutrino spectra calculated here as well as those of refs. (2, 15, 16, 18). The column labeled "Present Known" is the spectrum of antineutrinos due to all of the isotopes with known beta branches and daughter energy levels. It is interesting to note that this portion of the spectrum accounts for all of the antineutrinos predicted by Dickens¹⁸ between 5 and 8 MeV. The new known spectrum accounts for 87, 84, 91 and $> 100\%$ of the antineutrinos predicted by DVMS¹⁶ at 5, 6, 7 and 8 MeV respectively. It should be emphasized that this spectrum (Present Known) does not rely on beta strength calculations or other averaging techniques nor on semiempirical mass formulae but only on measured nuclear

structure parameters and on fission yields. This implies that if the Dickens spectrum is correct or nearly so, none of the remaining isotopes with yet unknown decay schemes can have ground state beta branches while only a very weak average ground state beta branch would be consistent with the calculations of DVMS and measurements of Schreckenbach et al.²⁴ These observations raise serious questions, other than those pointed out by Klapdor,²⁰ concerning any techniques which smoothly average the known nuclear properties to extrapolate to nuclei with unknown decay schemes.

The majority of the new nuclear structure data used in the present calculations has come from nuclear spectroscopy performed with isotope separators on line to nuclear reactors.^{27,43} Projects such as TRISTAN, OSTIS, JOSEF, LOHENGRIN and OSIRIS for example have recently produced an explosion of new nuclear spectroscopic data. The isotopes listed in Fig. 2 are those which we predict dominate the high energy portion of the fission antineutrino spectrum, and may present special problems in some cases for the present separator ion sources. They may not all lend themselves to precisely the same techniques as those reported in refs. (27-43).⁴⁴ In addition some have small thermal fission yields which present further difficulties.

A new source of such data on neutron rich isotopes far from stability derives from multinucleon transfer reactions such as those observed in heavy ion reactions by Artukh et al.⁴⁶ and by Breuer et al.⁴⁶ This technique has recently been exploited at the GSI laboratory by Kirchner et al.⁴⁷ to produce the isotopes ^{179}Yb and $^{181,182}\text{Lu}$ in the reactions of 9MeV/nucleon, ^{136}Xe ions on tantalum and tungsten targets. This recent development enhances the probability that the list of isotopes shown in Figure 2, whose decays might dominate the high energy portion of the fission neutrino

spectrum, might be investigated with isotope separators on line to heavy ion accelerators as well as those on-line to nuclear reactors. One important motivation of this paper is to specifically identify and stimulate the needed nuclear spectroscopic measurements.

The authors are grateful to Professors Borovoi, Klimov and Kopeikin for communicating the results of their work, well in advance of their preprint, and to P. Vogel and J. K. Dickens for stimulating discussions on this subject. We also thank R. L. Mlekodaj and the UNISOR staff and E. F. Zganjar for advice concerning the multinucleon reactions and R. E. Chrien and his collaborators at TRISTAN for their informative hospitality on several occasions.

TABLE I. Comparison of the present calculations with several previous calculations.

Energy MeV	DVMS ^a	DICKENS ^b	AG ^c	Present Known	Present Unknown	Present Total	BDK ^d
1.0	2.38	2.22	2.12	2.12	1.98(-1)	2.32	- - - -
1.5	1.65	1.62	1.62	1.44	2.33(-1)	1.68	1.60
2.0	1.21	1.26	1.35	1.09	2.17(-1)	1.31	1.26
2.5	8.42(-1)	8.80(-1)	10.4(-1)	7.54(-1)	1.83(-1)	9.37(-1)	8.82(-1)
3.0	5.95(-1)	6.57(-1)	7.69(-1)	5.43(-1)	1.30(-1)	6.73(-1)	6.61(-1)
4.0	2.73(-1)	2.96(-1)	3.49(-1)	2.50(-1)	5.15(-2)	3.01(-1)	3.22(-1)
5.0	1.03(-1)	0.92(-1)	1.39(-1)	9.33(-2)	1.67(-2)	1.10(-1)	1.30(-1)
6.0	3.50(-2)	2.86(-2)	4.93(-2)	3.15(-2)	5.16(-3)	3.66(-2)	4.89(-2)
7.0	1.01(-2)	0.93(-2)	1.50(-2)	1.01(-2)	1.65(-3)	1.18(-2)	1.74(-2)
8.0	1.87(-3)	1.60(-3)	3.10(-3)	2.03(-3)	6.81(-4)	2.71(-3)	4.35(-3)
9.0	- - - -	- - - -	5.52(-4)	3.35(-4)	2.37(-4)	5.72(-4)	8.23(-4)
10.0	- - - -	- - - -	1.71(-4)	4.65(-5)	6.82(-5)	1.15(-4)	1.61(-4)

a Davis, Vogel, Mann and Schenter (ref. 16)

b Dickens (ref. 18)

c Avignone and Greenwood (ref. 2)

d Borovoi, Dobrynin and Kopeikin (ref. 15)

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ANTINEUTRINOS / FISSION / MeV

10^{-4}

10^{-5}

10^{-6}

TOTAL

- 1 ^{85}As
- 2 ^{86}As
- 3 ^{87}As
- 4 ^{88}As
- 5 ^{91}Br
- 6 ^{92}Br
- 7 ^{97}Rb
- 8 ^{102}Y
- 9 ^{132}In

ENERGY [MeV]

APPENDIX E

Monte Carlo Calculations Predicting the Response of Intrinsic Ge Detectors to Electrons and Positrons

This effort represents approximately 1.5 man years and 250 hours of
CPU time on an IBM 370 and equivalent computer.