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BGSUB and BGFIX: FORTRAN Programs to Correct Ge(Li) Gamma-Ray Spectra for Photopeaks from Radionuclides in Background

N. H. Cutshall
I. L. Larsen

ENVIRONMENTAL SCIENCES DIVISION
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OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
operated by
UNION CARBIDE CORPORATION
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ABSTRACT

CUTSHALL, N. H., and I. L. LARSEN. 1980. BGSUB and BGFIX: FORTRAN programs to correct Ge(Li) gamma-ray spectra for photopeaks from radionuclides in background. ORNL/TM-7051. Oak Ridge National Laboratory, Oak Ridge, Tennessee. 30 pp.

Two FORTRAN programs which provide correction and error analysis for background photopeak contributions to low-level gamma-ray spectra are discussed. A peak-by-peak background subtraction approach is used instead of channel-by-channel correction. The accuracy of corrected results near background levels is substantially improved over uncorrected values.

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INTRODUCTION

Background count rates interfere with the measurement of minute quantities of radionuclides. Therefore, data reduction procedures used with high sensitivity analytical systems involve a correction for background counts based on a measurement of count rates in the absence of a sample. Gamma-ray spectra from NaI(Tl) detectors are typically adjusted by subtracting a background spectrum from a sample spectrum. Commercially available spectrum analysis algorithms for data from high-resolution Ge(Li) detectors employ a different tactic. The area under a baseline drawn below a photopeak is estimated and subtracted from a gross numerical integral across the photopeak (Fig. 1a) (Baedecker 1971). This subtraction corrects for Compton continuum interferences from high-energy gamma emissions within the sample and for photons scattered from the surroundings into the detector. It does not, however, correct for photopeaks from radionuclides in the background (Fig. 1b). Therefore, analyses of such radionuclides at levels near background using available computer algorithms yield erroneous results which must be corrected. Even where great care in selection of shielding materials is taken, most backgrounds contain photopeaks from naturally occurring ^{40}K, ^{214}Pb, ^{214}Bi, ^{228}Ac, ^{212}Pb, ^{208}Tl, and often from fallout ^{137}Cs and ^{60}Co. We have devised and implemented a new correction scheme for background photopeaks that functions with commercially produced data reduction programs. The original version was written in the CLASS (TM)

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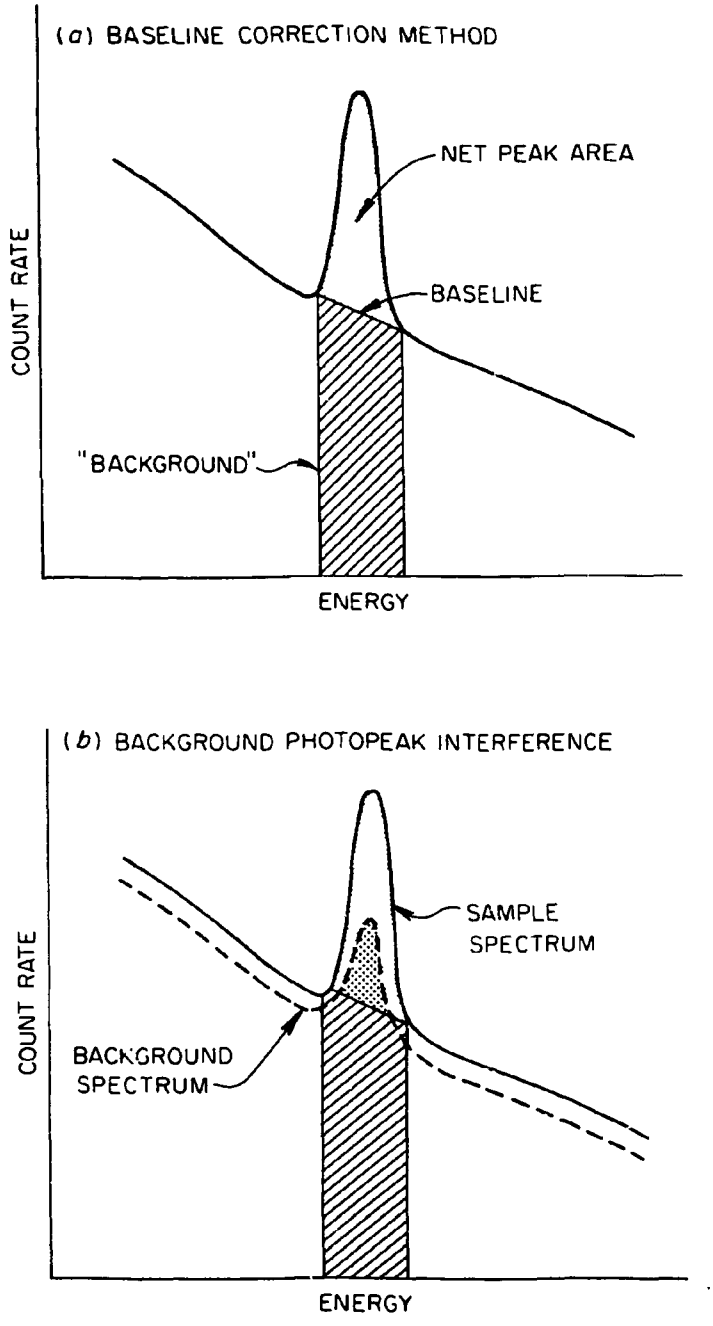

Fig. 1. Idealized gamma-ray photopeaks: (a) conventional baseline correction procedure, (b) interference from a background photopeak.

language to operate in a Canberra Quanta System at Oregon State University (Cutshall 1975). The version reported here is written in MIDAS/FORTRAN IV (TM) and is used in a Nuclear Data Model 6620 system. While the computer language and file format for the two versions are different, the strategy employed and the flow diagram (Fig. 2) in each version are the same.

Rather than the channel-by-channel background subtraction method used for NaI(Tl) spectra, our routine uses a peak-by-peak method. Channel-by-channel subtraction of spectra near background often results in over-correction of some channels (i.e., "negative" net counts) and also yields irregularities where instrumental drift occurs or energy calibration is performed between sample and background analyses. Such features may interfere with some peak-searching routines. Furthermore, channel-by-channel subtraction requires manipulation of two large spectral data arrays or files. On the other hand, in peak-by-peak subtraction only the smaller files of peak data need to be manipulated and therefore less memory is required. By inserting a background correction step between peak measurement and quantitative radionuclide computation, the quantitative routines operate on data which are corrected for background photopeaks (Fig. 3).

Two programs are used: the first modifies a background peak data file and the second performs the corrections on sample peak files.

BGFIX -- Background Peak File

Routine BGFIX converts a peak data file generated by Nuclear Data's program APS.PEAK (NDC 1976) into a background file. Since the

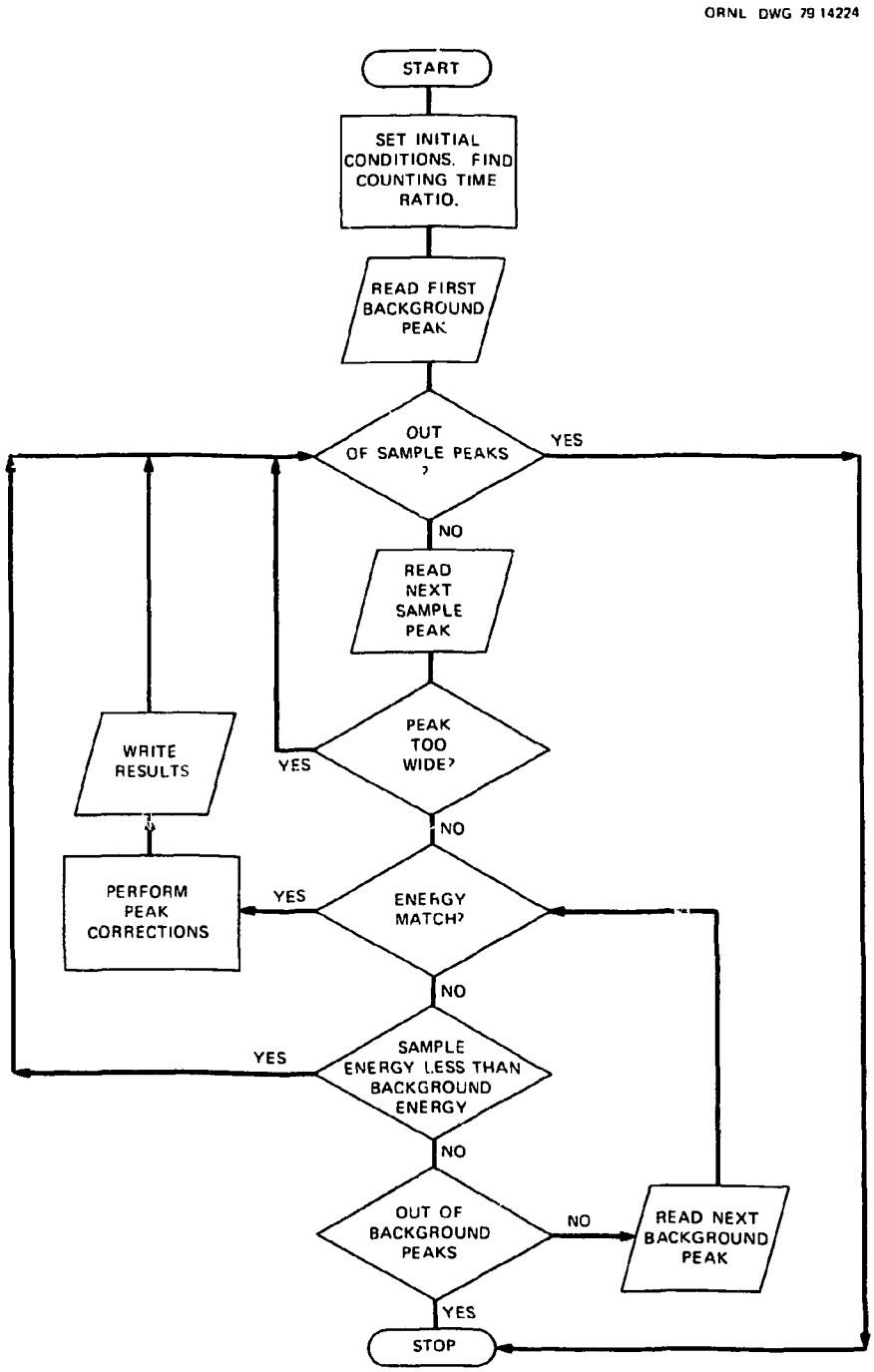

Fig. 2. Flowchart for BGSUB.

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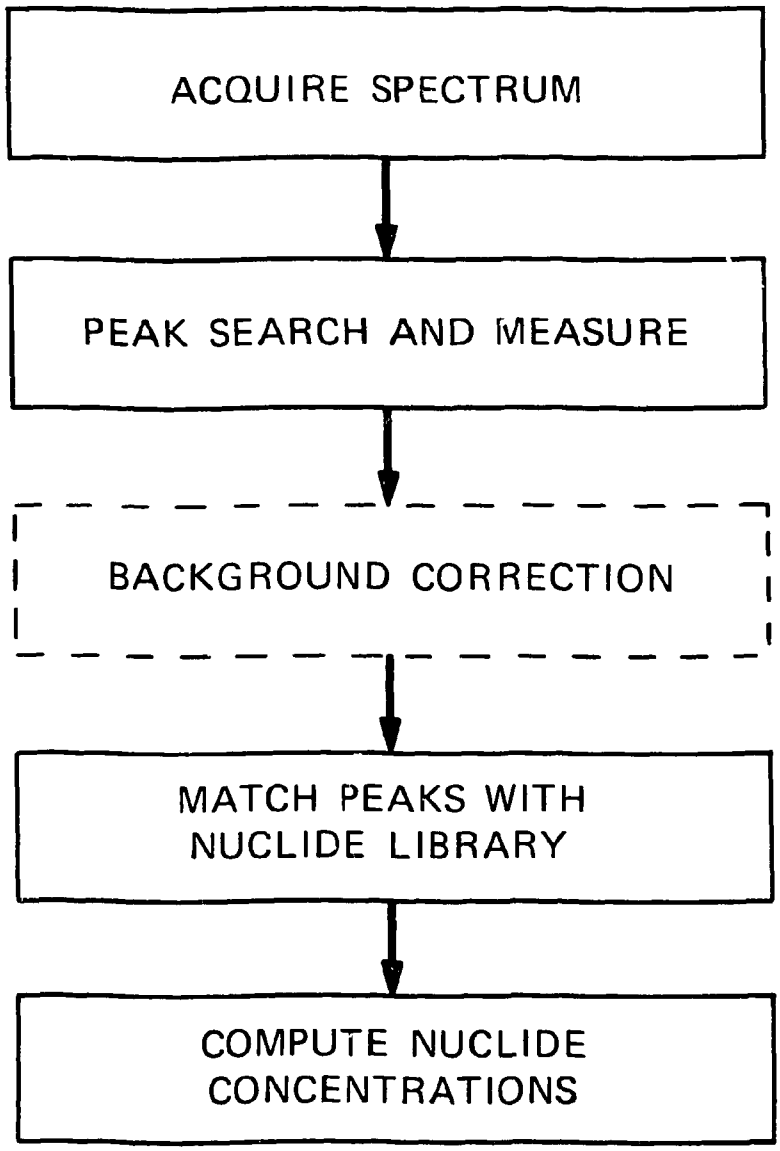

Fig. 3. Sequence of data reduction steps in sample analysis by gamma-ray spectrometry showing insertion of background correction step.

peak file does not normally contain the duration of the count, this value must be written into the file. BGFIX reads the elapsed live time (spectral format) from the data file header in logical unit-12 (LU12), converts the number to floating point format and writes the result into the peak data file in LU1. The number is written into words 2 and 3 of record 1. Record 1 is 27 words long and normally contains only the value for the number of peaks in the file in the first word.

To use BGFIX a background spectrum is first acquired and subjected to peak search (APS.PEAK). Then BGFIX is run. The modified WORK.PKFIL is REPlaced into a file called WORK.BGFIL. (WORK.BGFIL is originally created by COPYing a background WORK.PKFIL.) Finally, logical unit-10 is defined as WORK.BGFIL.

BGSUB -- Peak Area Correction

BGSUB is the program that performs background corrections on sample peak files. An energy comparison for peaks in background and sample peak files is made. If the difference between the sample peak energy and the background peak energy is less than ± 1 FWHM (Full Width Half Maximum), it is arbitrarily assumed that correction is appropriate. The sample peak area value is replaced by the difference between the sample peak area and the background peak area after allowance for the relative counting time of the sample and background.

$$\text{CORRECTED AREA} = \text{SAMPLE AREA} - \text{BACKGROUND AREA} * \text{TR},$$

$$\text{where TR} = \frac{\text{SAMPLE ELAPSED LIVE TIME}}{\text{BACKGROUND ELAPSED LIVE TIME}} .$$

The percent error term is also modified (assuming independent error) to reflect propagation of uncertainty.

$$\text{CORRECTED \% ERROR} = \frac{\sqrt{\left(\text{SAMPLE AREA} * \text{SAMPLE ERROR}\right)^2 + \left(\text{BACKGROUND AREA} * \text{BACKGROUND \% ERROR} * \text{TR}\right)^2}}{\text{CORRECTED AREA}}$$

BGSUB prints a table showing the energy, FWHM, the old area, and the new area for each peak corrected (Table 1).

If the FWHM of the sample peak exceeds 3.0 kev then no correction is made and the program goes to the next sample peak. Without this provision spurious broad peaks sometimes reported when the sensitivity parameter is set too small may appear to match the background peak energy. When BGSUB is used with detectors having poor resolution it may be necessary to change the 3.0 kev criterion to a larger value. Alternatively, the peak energy matching criterion could be changed from FWHM to an absolute value such as 2.0 kev. The first version of BGSUB used the energy matching criterion from the nuclide identification subroutine to decide whether or not corrections were needed.

BGSUB is run following the sample peak file generation (APS.PEAK) and prior to the nuclide identification/quantification program (APS.NID) (Fig. 3 and Appendix III). For samples containing radioactivity only slightly higher than background levels, the computed concentrations are significantly altered by BGSUB (Table 2).

Furthermore, for the ^{232}Th series, the two nuclides ^{228}Ac and ^{212}Pb appear to be in equilibrium in the uncorrected data, but perhaps not at equilibrium in the corrected data (Table 2). (The hypothesis that $^{212}Pb = {}^{228}Ac$ is rejected by an asymptotic t-test

Table 1. Typical BGSUB output table showing corrections for background photopeaks

BACKGROUND CORRECTIONS MADE
BACKGROUND COUNTING TIME= 226812. SECONDS

PK	FWHM	ENERGY	OLD AREA	OLD % ERROR	NEW AREA	NEW % ERROR
2	1.19	76.88	46.	65.53	29.	102.05
3	1.57	92.70	64.	29.75	46.	41.61
4	1.40	238.41	244.	11.95	198.	14.76
5	0.79	241.87	12.	153.18	10.	170.56
6	1.65	295.03	90.	19.02	84.	20.34
8	1.31	351.57	174.	10.43	168.	10.84
10	2.20	582.89	117.	12.70	103.	14.57
12	1.54	609.00	151.	9.05	144.	9.53
13	1.98	661.52	56.	19.03	51.	20.86
14	2.54	911.76	98.	11.20	96.	11.48
17	2.37	1460.54	191.	7.65	174.	8.42

Table 2. Computed radionuclide concentrations before and after background correction. Sample was 6.7 g of fish ash, counted for 1000 min on a Ge(Li) detector. Error term is 1 standard deviation.

	Before BGSUB pCi/g ± s.d.	After BGSUB pCi/g ± s.d.
^{137}Cs	0.80 ± 0.09	0.34 ± 0.09
^{40}K	49.3 ± 1.7	40.4 ± 1.7
^{214}Pb	1.26 ± 0.15	0.80 ± 0.15
^{214}Bi	1.40 ± 0.18	0.95 ± 0.18
^{228}Ac	1.31 ± 0.23	0.87 ± 0.24
^{212}Pb	1.18 ± 0.11	0.45 ± 0.11
Annihilation	1.67 ± 0.09	0.06 ± 0.09

(∞ d.f.) at the α = 0.2 level but not at α = 0.1. While the difference is not highly significant, it implies that the sample in question should be re-examined).

To precisely evaluate the impact of background correction, a series of low-level "samples" were prepared from standardized reference materials and reagent potassium chloride. These were analyzed and the results reduced (using commercial programs) both with and without background peak correction. Results (Table 3) also demonstrate that failure to correct for background peaks yields errors that are frequently significant compared to estimates of counting error. Corrected results, on the other hand, more nearly correspond to the amounts theoretically present.

Conclusions

Commercial software packages for reduction of spectra from Ge(Li) detectors do not adequately account for interference from background photopeaks in very low-level gamma-ray spectrometry. Results can be accurately and efficiently corrected for background interferences using peak-by-peak subtraction of areas. FORTRAN programs BGFIX and BGSUB conveniently perform such corrections for Nuclear Data programs in the ND6620 system.

Table 3. Results reported by commercial computer programs for standard "samples" before and after background correction

Nuclide	γ-energy (kev)	Amount taken pCi	Amounts reported (pCi ± 1 s.d.) Before BGSUB	After BGSUB
^{214}Bi	609	4	8 ± 1	3 ± 1
		7	11 ± 1	6 ± 1
		10	14 ± 1	9 ± 1
		15	18 ± 1	14 ± 1
^{40}K	1462	64	146 ± 12	70 ± 13
		92	172 ± 11	96 ± 11
		93	184 ± 11	107 ± 12
		109	207 ± 10	131 ± 11
		186	259 ± 12	180 ± 13
^{228}Ac	911	8	14 ± 3	10 ± 3
		12	20 ± 3	16 ± 3
^{208}Tl	583	8	15 ± 2	9 ± 2
		12	20 ± 2	14 ± 2

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Baedecker, Philip A. 1971. Digital methods of photopeak integration in activation analysis. Anal. Chem. 43(3):405-410.

Cutshall, Norman H. 1975. Ecological studies of radioactivity in the Columbia River estuary and adjacent Pacific Ocean. Progress Report to USERDA. (RLO-2227-T12-54). Reference 75-2, School of Oceanography, Oregon State University, Corvallis, Oregon.

Nuclear Data Corporation (NDC). 1976. ND6620 Operating Instructions. Nuclear Data Corporation, Schaumburg, Illinois.

APPENDIX I

LISTINGS OF BGFIX AND BGSUB

PROGRAM BGFIX LISTING

```
C       PROGRAM TO READ COUNTING TIME FROM A SPECTRUM
C       IN LU-12 (DISKFILE) AND WRITE IT INTO A PEAKFILE
C       IN LU-1.   N. H.  CUTSHALL ORNL  16 AUG 1979.
        DEFINE FILE 1 (200,27,U,NPK)
        DEFINE FILE 12 (0,2,U,NREC)
        READ(12'13)ISEC1,ISEC2
        CALL CHOP(ISEC1,ISEC1)
        CALL SFLOAT(ISEC1,TB)
        READ (1'1)IBGPKS
        WRITE(1'1)IBGPKS,TB
        CALL EXIT
        END
```

APPENDIX I: (Continued)

PROGRAM BGFIX LISTING

```
C       PROGRAM TO CORRECT FOR PEAKS FROM BACKGROUND.
C       WORKS BETWEEN APS.PEAK AND APS.SPLIN.
C       REQUIRES A BACKGROUND PEAKFILE IN LU=10.
C       BACKGROUND PEAKFILE GENERATED BY PROGRAM
C       NAMED BGFIX.   N.H. CUTSHALL ORNL 16 AUG 1979
        DEFINE FILE 1 (200,27,U,IP)
        DEFINE FILE 10 (200,27,U,IB)
        DEFINE FILE 12 (0,2,U,NREC)
        IP=1
        IB=1

C       DETERMINE THE COUNTING TIME RATIO
        READ(10'IB)IBMAX,TB
        READ(12'13)ISEC1,ISEC2
        CALL CHOP(ISEC1,ISEC1)
        CALL SFLOAT(ISEC1,TS)
        TR=TS/TB

C       PREPARE FOR THE PRINTOUT
        WRITE(6,20)
        WRITE(6,21)
        WRITE(6,24)TB
        WRITE(6,20)
        WRITE(6,22)
        WRITE(6,23)

20      FORMAT('************************************************************')
21      FORMAT('              BACKGROUND CORRECTIONS MADE ')
22      FORMAT(10X,'                OLD      OLD %     NEW     NEW %')
23      FORMAT('  PK     FWHM  ENERGY    AREA     ERROR    AREA     ERROR')
24      FORMAT('          BACKGROUND COUNTING TIME= ',F8.0,'SECONDS')
25      FORMAT(I4,2F8.2,F8.0,F8.2,F8.0,F8.2)

C       LOOK FOR ENERGY MATCH FOR PEAKS IN SAMPLE AND BACKGROUND
        READ(10'IB)K1,K2,K3,Y1,K4,K5,Y2,BFW,BAR,BEN,Y3,BER
        READ(1'IP)IPMAX
50      IF(IP.GT.IPMAX+1)GO TO 400
        READ(1'IP)J1,J2,J3,X1,J4,J5,X2,SFW,SAR,SEN,X3,SER
        IF(SFW.GT.3.0) GO TO 50
60      IF (ABS(SEN-BEN).LT.SFW) GO TO 300
        IF (SEN.LT.BEN)GO TO 50
        IF (IB.GT.IBMAX+1) GO TO 400
        READ(10'IB)K1,K2,K3,X1,X2,K4,K5,BFW,BAR,BEN,X3,BER
        GO TO 60

C       THIS SECTION DOES PEAK CORRECTIONS AND PRINTOUT
300     SARN=SAR-TR*BAR
        SERN=ABS(SQRT((SER*SAR)**2)+((TR*BER*BAR)**2))/SARN)
        IP=IP-1
        WRITE(6,25)J1,SFW,SEN,SAR,SER,SARN,SERN
        IF (SARN.LT.0.1) SARN=0.000000001
        WRITE(1'IP)J1,J2,J3,X1,J4,J5,X2,SFW,SARN,SEN,X3,SERN
        GO TO 50

C       THIS SECTION TERMINATES OUTPUT
400     WRITE(6,20)
        CALL EXIT
        END
```

APPENDIX II

INSTRUCTIONS FOR IMPLEMENTATION OF BGSUB

1. The FORTRAN programs for BGFIX and BGSUB should be compiled, linked, and copied into the "APS" file following instructions in the Nuclear Data Manual (NDC 1976).
2. A background count of sufficient duration (i.e. $\geq$ sample counting time) should be acquired and a peak search completed.

   ```
   DEF 1, WORK.PKFIL
   R PEAK.
   ```

3. Use BGFIX to modify the peak data file

   ```
   DEF 1, WORK.PKFIL )
   DEF 12, DATA MAIN )
   R BGFIX ) .
   ```

   Then COPY (or REPlace) the modified file into the background file:

   ```
   COPY     WORK.PKFIL     WORK.BGFIL ) .
   ```

4. To use the program, define logical unit 10 as the background peak file:

   ```
   DEF 10, WORK.BGFIL ) .
   ```

5. When a sample spectrum is to be reduced, use the command:

   ```
   R BGSUB ) .
   ```

   following the peak search.

APPENDIX III

TYPICAL JOBSTREAM USING BGFIX

```
DEF 1,WORK.PKFIL
DEF 2,NUCL.LIB2
DEF 3,WORK.SUMFIL
DEF 4,WORK.UNFIL
DEF 5,TTY
DEF 6,LP
DEF 7,TTY
DEF 8,DATA.MAIN
DEF 9
DEF 10,WORK.BGFILM
DEF 11,EFF.MARSED
DEF 12,DATA.MAIN
R WRITE
1
R HEAD
R PEAK
R BGSUB
R SPLIN
R NID
R REPORT
ENDJOB,,T
```