Procedures to analyse gamma-ray spectra obtained from the ORTEC or nuclear data ND-680 system by ORTEC's analysis software packages incorporated into a separate IBM-PC computer

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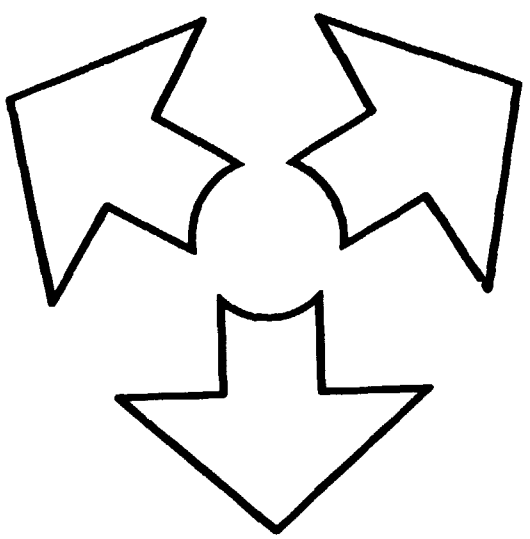
Zhang Xiu Zhen



Risø National Laboratory, DK-4000 Roskilde, Denmark
January 1990

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Abstract. A detailed description is presented for processing γ-spectra produced by means of Ortec or Nuclear Data spectrometry systems on an off-line IBM-PC. The ORTEC analysis software packages were transferred to and implemented on the PC A/T, and the different spectra were recorded on discs and subsequently brought into the format required by the program for the calculation of photo peak areas.

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Contents

Section 1

Introduction

The net area (net counts) of the detected photo peaks in a γ-spectrum is an essential quantity in gamma-ray spectrometry. The numerical value of the net peak area for a detected photo peak, however, depends on the data evaluation strategy adopted by the computer program analyzing the obtained γ-ray spectrum. For a photo peak disturbed by strong background or/and by neighbouring strong photo peaks, or in multiplet with other peaks, the value of the net peak area will vary significantly when determined by different programs. There is no way to affirm which program yields the most reliable results for the net peak area values for all γ-spectra obtained in practice. An approach to solve this problem is to analyze a γ-spectrum by different programs; this provides at least some information about the reliability of the net peak area calculation by comparison of the results.

In the Isotope laboratory there are three programs available for γ-spectrum analysis: ORTEC's analysis software packages integrated in the ORTEC γ-ray spectrometer system; Nuclear Data program PEAK in the ND-680 system and a home-developed program PEAKB in a IBM-PC computer. It is of course desirable to make it possible applying all three programs to analyze γ-spectra obtained from the existing γ-spectrometer systems.

This work reports two procedures for applying the ORTEC analysis software packages stored in a separate IBM-PC computer to process

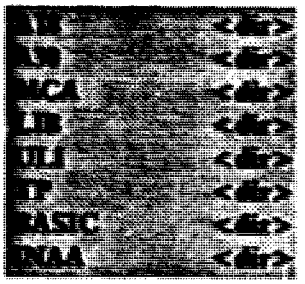
1. the γ-spectra obtained from ORTEC instruments but recorded on a disc as the transfer medium,
2. the γ-spectra obtained from the Nuclear Data ND-680 system but recorded on a disc as the transfer medium.

Section 2

Preparing to use the IBM-PC

2.1. Make sure the ORTEC's software packages have been incorporated into the separate computer.

C:\> DIR



2.2. Make the subdirectory INAAND for analyzing the γ-ray spectra obtained from the Nuclear Data ND-680 system

C:\> MD INAAND

C:\INAAND>

Section 3

Analysis of the γ-ray spectra from an ORTEC instrument by the ORTEC software packages stored in the separate IBM-PC

3.1. As a demonstration, an ORTEC γ-ray spectrum, 89080402.spc, obtained from the ORTEC instrument and recorded on a disc was processed using the IBM 100/150 MCA emulation software.

3.1.1. Copy the ORTEC γ-spectrum data file on the PC's hard disc.

Insert data disc into driver A:, then

---

* Grey colour : prompt by computer system
** Black colour : enter by user

3.1.2. Convert .spc file to .CHN file

3.1.3. Call MCA emulations software

The main menu of the system response will be shown on the computer screen window.

3.1.4. Load input file into MCA (current buffer of the PC)

Type ALT 9 (9-Recall)

The user will be prompted the filename:

Spectral graphics and textual information will be displayed as shown in Fig. 1 of the MCA manual.

3.1.5. Set Region-Of-Interest and perform calibration

· Type key ALT 6 (6-calculation)

Calculation menu is shown on the screen as Fig. 6
· press F2 Softkey, select ROI (Refer to page 30, MCA manual)
· Type key ALT 1 (1-calibration)

The system prompts as followed:

· Type ALT/2 Select second peak

Type ALT/1

Enter next peak channel and energy in keV

3.1.6. Print out results of calculations

Type 

Hardcopy output can be obtained that shows statistical data related to regions-of-interest in the selected MCB segment. Hardcopy output of the analysis of 89080402.spc is shown in Appendix 1

3.2. Spectrum data analysis using ORTEC Applications Manager Software Module, MCA 100/150 GELIGAM Software Module and Master Library.

3.2.1. Create a library of nuclides with gamma-ray energies, half-lives and branching ratios.

The existing library INAALIB.LIB, INAALONG.LIB in subdirectory INAA can be used. Otherwise it is necessary to build a library (Refer to ORTEC manual, GELIGAM Example of Operations (A30-B1), page 2, ULI part).

3.2.2. Build Sample file, Detector file, Analysis parameter file and Calibration file.

These files were already combined in the ORTEC γ-spectrum data file, 89080402.spc. They are 001001.SMP, 001001.DET, 001001.PRM, 001001.CLB. So it is not necessary to create these files when dealing with the γ-spectrum obtained from the ORTEC instrument. Otherwise these files should be created (Refer to ORTEC manual, Applications Manager (A18-B1) Example of Operations, and GELIGAM Example of Operations (A30-B1).)

3.2.3. Create intermediate disc file (.UFO)

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

VERSION NUMBER MENU

0 GERPAR VALUE
1 GAMMA-1
2 GAMMA-2
3 GAMMA-3
4 NAA-1
5 RESERVED
6 NAA-3
7 LLD

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

3.2.4. Read the .UFO file and perform the analysis. Results of the analysis are transferred to the .UFO file.

[redacted]

[redacted]

3.2.5. Generate a report file. The analysis results are formated according to the type of analysis performed.

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

3.2.6. Print the output of the analysis results

[redacted]

The output file is given in Appendix 2
(Analysis results of the γ-ray spectrum data, 89080402.spc)

Section 4

Analysis of the γ-ray spectrum from Nuclear Data ND-680 System by the ORTEC software packages available in the separate IBM-PC

As a demonstration, a ND γ-ray spectrum, 179037.SOO, obtained from the ND-680 system and recorded on a disc, was analyzed.

4.1. Enter input file and change the format of the input-file

[redacted]

4.1.1. [redacted]

[redacted]

4.1.2. Load [redacted] program
Execute [redacted], then NDOUT1.DAT is created.

4.1.3. Load [redacted] program
Execute [redacted], then NDOUT2.DAT is created.

```
[illegible]> [illegible]

[illegible]> [illegible]
```

4.1.4. Execute program ASCBIN-BAS

```
[illegible]> [illegible]

                    ASCBIN

            A SOFTWARE PRODUCT FROM

                 CAAC DENMARK

                     [illegible]

      ASCBIN CONVERTS AN ORTEC SPECTRUM FILE

          TO AN ASC FILE OR VICE VERSA
```

The system prompts with as shown above and ask user to select »options«

```
OPTIONS:

1) ORTEC FILE TO ASC FILE (CHN TO DAT)

2) ASC FILE TO ORTEC FILE (DAT TO CHN)

3) HELP

4) EXIT

WHICH OPTION? [illegible]

HAVE YOUR SPECTRA BEEN CREATED BY ASCBIN OPTION 1 (Y/N): [illegible]

NUMBER OF CHANNELS PER SPECTRUM (MAX 8192) [illegible]

NUMBER OF CHANNELS PER RECORD [illegible]

NUMBER OF SPECTRA TO BE CONVERTED (MAX 10) [illegible]

SPECTRUM NO. 1 INPUT FILENAME [illegible]

OUTPUT FILENAME [illegible]

ARE THE FILENAMES CORRECT (Y/N) [illegible]
```

Now the .CHN file was created, but the format of this file is different from that required. So the program ASCBIN will be excuted again but with the first option selection:

· C:\INAAND> ASCBIN

WHICH OPTION? 1

HAVE YOUR SPECTRA BEEN CREATED BY ASCBIN OPTION 1 (Y/N): Y

NUMBER OF CHANNELS PER SPECTRUM (MAX 8192) 8192

NUMBER OF SPECTRA TO BE CONVERTED (MAX 10) 1

SPECTRUM NO. 1 INPUT FILENAME 179037

OUTPUT FILENAME 179037.DAT

ARE THE FILENAMES CORRECT (Y/N) Y

In order to be analyzed by the ORTEC software packages, the program ASCBIN will be excecuted once more with the second option selected to convert the new formed .DAT file to .CHN file:

· C:\INAAND> ASCBIN

WHICH OPTION? 2

HAVE YOUR SPECTRA BEEN CREATED BY ASCBIN OPTION 1 (Y/N): Y

NUMBER OF CHANNELS PER SPECTRUM (MAX 8192) 8192

NUMBER OF SPECTRA TO BE CONVERTED (MAX 10) 1

SPECTRUM NO. 1 INPUT FILENAME 179037

OUTPUT FILENAME 179037.CHN

ARE THE FILENAMES CORRECT (Y/N) Y

Finally, the required .CHN file, i.e. 179037.CHN, was obtained.
The printout of the 179037.CHN was presented in Appendix 3.

4.2. Data analysis using the IBM 100/150 MCA Emulation Software.

Following the procedures presented in 3.1.3 to 3.1.6. The analysis results, given in Appendix 4, were obtained.

4.3. Analysis of the γ-ray spectra from Nuclear Data ND-680 system using ORTEC Software Application Manager Software Module, MCA 100/150 GELIGAM Software Module and MCA 100/150 Master Library.

4.3.1. Create a sample description file

```
C:\INAAND> \A18\Sample

Enter MCA number (  0): 1

Enter segment number (  1): 1

Enter sample description (2 x 64 characters)

 1> (NONE): AN UNKNOWN SAMPLE FROM DR. K. HEYDORN

 2> (NONE):

Any changes (NO)?
```

Now, the sample description file 001001.SMP was created in \INAAND subdirectory.

4.3.2. Create a Detector description file

```
C:\INAAND> \A18\Detector

Enter MCA number (  0): 1

Enter segment number (  1): 1

Enter detector number (  0): 0

Enter detector description (2 x 60 char.)

 1> Detector: GAMMA-X/S 72

 2> DATA FROM ND

Any changes (NO)?
```

Detector description file 001001.DET was created in \INAAND subdirectory.

4.3.3. Create a GERPAR file

GERPAR program can be used to create or modify an analysis parameter file

```
C:\INAAND> \A18\GERPAR
```

```
Enter MCA number (    1): 1

Enter segment number (    1): 1

Modify this file (N): Y

          VERSION NUMBER MENU
              0  GERPAR VALUE
              1  GAMMA - 1
              2  GAMMA - 2
              3  GAMMA - 3
              4  NAA-1
              5  RESERVED
              6  NAA - 3
              7  LLD

Enter version number (    0): 2

--- INTERACTIVE PARAMETER SECTION ---

Enter mnemonic (END): ALL

Units (  MICROCURIES  ):

Factor numerator (   1.000    ):

Factor denominator (   1.000    ):

First library filename (        .LIB): INAALIB.LIB

Sensitivity (  20.00    ):

Sorption correction (NO   )?

Decay correction (NO   )?

Turn MDA off (NO   )?

Intermediate printout (NO      )? Y

Peaked background correction (NO   )?

Recovery correction (NO   )?

Activity, Percent, or Total uncertainty (P):

1, 2, or 3 sigma (    2):

True coincidence correction (NO   ):

Random summing (NO   )?

Enter starting channel (50): 300
```

```
Enter ending channel (8000): 8100
Geometry correction (NO  )?
Five point low (NO  )?
Decay correct during acquisition (NO  )?
Enter mnemonic to change (END):
```

4.3.4. Create a preliminary .spc file

```
C:\INAAND> Convert

                    SPECTRUM CONVERSION ROUTINE
                    COPYRIGHT 1985 EG&G ORTEC
                    VERSION 2.08

Enter input filename (END): 179037.CHN
FILE NOT FOUND 00100L.SOR
FILE NOT FOUND 00100L.GEO
FILE NOT FOUND 00163L.QAF
FILE NOT FOUND 00100L.ROI
FILE NOT FOUND 00100L.SEQ
CONVERSION MADE
```

4.3.5. Create a new calibration file

```
C:\INAAND> \A30\CLB

                    CALIBRATION PROGRAM
                    COPYRIGHT 1984 EG&G ORTEC

Turn on the tracing (NO  )?
Enter calibration output filename (END): 001001.CLB
```

File already exists; do you want to replace it (NO)? Y

Enter calibration descripdon

1> This is another calibration

2>

Any changes (NO)?

Do you want to do a new energy-shape calibration? Y

Enter the spectrum filename (NONE): 179037.spc

179037.spc

ACQUIRED ON 01-JAN-86 AT 12:00:00

AN UNKNOWN SAMPLE FROM DR. K. HEYDORN

Is this the right file (NO)? Y

Start channel (50): 300

Stop channel (7950):

Five point low (NO):

CHANNEL NUMBER AND ENERGY (keV) PAIRS

Enter channel number (299): 787.9

Enter corresponding energy (keV) (1.000): 312.7

Enter channel number (299): 1256.0

Enter corresponding energy (keV) (1.000): 502.7

Enter channel number (299): 2518.0

Enter corresponding energy (keV) (1.000): 1013.7

Enter channel number (299):

Any changes (NO)?

Do you want to do a new efficiency calibration (NO):

Enter old calibration filename with efficiency calibration

(NONE): \INAA\001001.CLB

```
00100.CLB
CREATED ON 17-APR-89 AT 09:31:2
DESCRIPTION (NONE)
* * * END OF CALIBRATION * * *
```

6. Create an expected .spc file.

```
C:\INAAND> \A18\Conver
```

```
SPECTRUM CONVERSION ROUTINE
COPYRIGHT 1985 EG&G ORTEC
VERSION 2.08
```

```
Enter input file name (END): 179037.CHN
FILE NOT FOUND 00100.SOR
FILE NOT FOUND 00100.GEO
FILE NOT FOUND 00100.QAF
FILE NOT FOUND 00100.ROI
FILE NOT FOUND SEQNUM.SEQ
CONVERSION MADE
```

Now the required 179037.spc file was created; this can be analyzed by the ORTEC software, in the same way as the γ-ray spectrum data obtained directly from the ORTEC instrument.

7. Executing program AN1

```
C:\INAAND> \A30\AN1
```

```
ANALYSIS PROGRAM PART 1
COPYRIGHT 1986 EG&G ORTEC
VERSION 2.06
```

[redacted]

[redacted]

[redacted]

PERSON NUMBER MENU

0 GERPAR VALUE
1 GAMMA-1
2 GAMMA-2
3 GAMMA-3
4 NAA-1
5 RESERVED
6 NAA-2
7 LLD

[redacted]

--INTERACTIVE PARAMETER SECTION--

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted]

[redacted] 001001 CLB

8. Executing program AN2

[redacted] A30 AN2

[redacted]

[redacted]

[redacted]

[redacted] 179037 UFO

[redacted]

9. Executing program RPT

[redacted] A30 RPT

[redacted]

[redacted]

[redacted]

[redacted] 179037 RPT

[redacted]

[redacted]

10. **Print out the analysis results.**

[redacted] PRINT 179037 RPT

The output is given in Appendix.

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1. K. Heydorn, »Encyclopedia of Medical Devices and Instrumentation«, Volume 3, Neutron Activation Analysis. John Wiley & Sons, 1988.

2. IBM-PC DOS 3.20 manual

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5. ORTEC manual
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   - ADCAM™ Multichannel Analyzer 100/150 Operator's Manual
   - Software File Structure Manual for the IBM-PC
   - Software Loading Instructions for IBM-PC
   - A18-B1 Applications Manager
   - Application Manager (A18-B2) Examples of Operation
   -
   - Basic Gamma-Ray Spectroscopy
   - A30-B1 GELIGAM Germanium Analysis Software
   - Geligam (A30-B1) Examples of Operation
   - Model A53 Master Library for Master Library Members.

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Title and author(s)

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