

SANDIA REPORT

SAND2020-2523 O

Unlimited Release

Printed 2,2020

Peak Map User's Manual

Gamma Matching and Nuclide Library Generation

Version 1.2

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia National Laboratories is a multission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Approved for public release; further dissemination unlimited.



Sandia National Laboratories

Issued by Sandia National Laboratories, operated for the United States Department of Energy by National Technology and Engineering Solutions of Sandia, LLC.

NOTICE: This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof, or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof, or any of their contractors.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865) 576-8401
Facsimile: (865) 576-5728
E-Mail: reports@adonis.osti.gov
Online ordering: <http://www.osti.gov/bridge>

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Rd
Springfield, VA 22161

Telephone: (800) 553-6847
Facsimile: (703) 605-6900
E-Mail: orders@ntis.fedworld.gov
Online ordering: <http://www.ntis.gov/help/ordermethods.asp?loc=7-4-0#online>



SAND2020-2523 O
Unlimited Release
Printed 2,2020

Peak Map User's Manual

Gamma Matching and Nuclide Library Generation

Version 1.2

Elliott J. Leonard

Abstract

Peak Map is a software tool that allows users to generate nuclide library files for gamma spectroscopy from a nuclear data reference. This document lays out the necessary information for the usage of the Peak Map software tool. It includes directions for the correct usage of the software and information on the algorithms used in the software.

Acknowledgment

Thanks to Michael Enghauser (mwengha@sandia.gov) and Sean Forunier (sdfourn@sandia.gov) for technical direction and help with testing.

Contents

Nomenclature	9
About this Manual	10
Modes	13
Matching Mode	13
Tips for Matching	15
Peak Inputs	16
Library Mode	17
File Menu	18
Lines Menu	18
Settings Menu	19
Advanced	19
Help Menu	19
Matching	20
Scoring	20
Nuclide Scoring	20
Line Scoring	21
Comparative calculations	22
Efficiency	22
Library	23
Uncertainty	23
Combining Lines	24

Appendix

A	Settings description	25
A.1	Matching	25
A.2	Library	26
A.3	Spectral	26
B	Decay Chains	28
C	Software Installation	29

List of Figures

1	Empty Peak Map Window	11
2	Matched Result of 661.7 keV	14
3	Peak Map window in library Mode	17
C.1	Installation wizard screens	30

List of Tables

1	Peak Input Options.....	17
---	-------------------------	----

Nomenclature

SNL Sandia National Laboratories

DOE United States Department of Energy

NNSA National Nuclear Security Administration

ICRP-107 International Commission on Radiological Protection publication 107 *Nuclear Decay Data for Dosimetric Calculations*

keV Kilolectronvolts, unit of energy 1000 times the energy needed to move an electron across one volt

MDA Minimum Detectable Activity, the point at which a false positive peak identification is set to fixed percentage, typically 5%

ROI Region of Interest, an span of channels on a gamma spectra representing an important region

CAM Configuration Access Method, a proprietary file type of storing spectral information used in the Mirion Canberra GENIE™ 2000 software package

CSV Comma Separated Variable file, a text based file for tabular data were columns are delimited with a comma and rows with new Lines

Introduction

Peak Map is a software tool that assists the user with matching unknown peaks from gamma spectroscopy measurements with corresponding decay signatures and generating nuclide libraries to be used in gamma spectroscopy analysis. The system uses nuclear data for the International Commission on Radiological Protection publication 107: *Nuclear Decay Data for Dosimetric Calculations* (ICRP-107) as a nuclear data reference however, the system is designed in such a way other data references can be used in future releases. Peak matching is done by matching the energy of a peak to find nuclides with corresponding gamma line signatures and then provides a score. The score based on the difference in energy of the peak and line, the photon yield of the, and the half-life of the nuclide in relation to the time between the reference date and the measurement date. To further increase the confidence of the selection, the other signature lines of the parent, and of the daughters in equilibrium, are provided with a line match score that is determined by whether the lines that should be detected have matching peaks in the list. The signature lines and the matching nuclide information can then be written to a nuclide library file.

About this Manual

This manual is a complete description of the tool and guidance document for users of the system. It is broken into chapters, the first chapter [Introduction](#), is an overview of the tool and this document. Chapter [Usage](#) describes how to use the tool to accomplish the goals of the user and Chapter [Technical](#) describes the algorithms and equations used within the software. [Appendix A](#) is an overview of the parameters used in the matching algorithm and [Appendix C](#) provides instructions on the installation of the software.

Usage

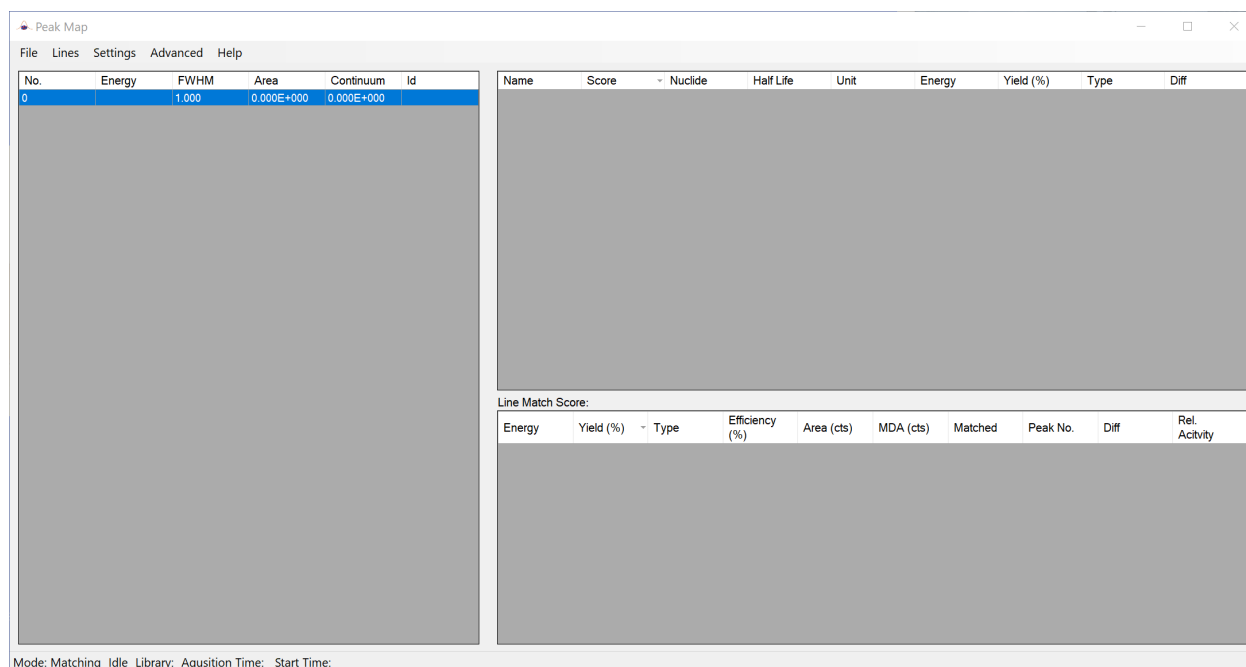


Figure 1: Peak Map window immediately after the tool is launched.

This chapter describes the usage and the the complete functionality of the tool. It is broken into the menus available to the user. The terminology is as follows:

- Left Click - Use the mouse left button
- Right Click - Use the right mouse button
- Navigate - Move through the menus as directed, using the mouse or keyboard (ALT+_iletter_i)
- Select - Click on a row
- Selected - Highlighted row
- Multi-Select - Select multiple rows by using the left click while holding the Control key (CTRL) or the Shift Key (SHIFT)
- Drag and Drop - Left click and hold on a file, move the mouse over the Peak Map tool, and release the mouse button

The window, [Figure 1](#), consists of three grid views, one on the left for the peaks (if applicable) and two on the top and bottom of the left side of the window. The upper grid displays the nuclide and the line that is was used for the match. The bottom grid shows all the characteristic lines from the selected nuclide and any daughters in equilibrium with the nuclide. Between the two grids is the line match score or the score determined by the number of detectable lines that are associated with peaks. The strip at the bottom of the screen presents information about loaded peaks files, and the nuclide library file that is being written.

The columns in the peaks grid are as follows:

- **No.** - An identification number for the peak.
- **Energy** - The energy of the peak centroid in kiloelectronvolts (keV).
- **FWHM** - The Full width at half maximum of peak in keV.
- **Area** - The number of counts in the peak.
- **Continuum** - The number of counts in the continuum under the peak.
- **Id** - The nuclides, separated by a comma, matched to the peak.

The columns in the nuclides grid are as follows:

- **Name** - The nuclide to be associated with matched lines or decay chain (see [Appendix B](#) for a discussion on the decay chains).
- **Score** - The score associated with the match of the nuclide to the selected peak.
- **Nuclide** - The actual nuclide that emits the characteristic line.
- **Half-Life** - The half-life of the nuclide listed in the **Name** column.
- **Unit** - The unit of half-life.
- **Energy** - The characteristic energy of the line matched with the peak in keV.
- **Yield** - The photon yield, in percent, of the matched line from the nuclide in the **Name** column. This includes nuclide branching ratios if applicable.
- **Type** - Emission type: **X** for x-rays, **G** for gamma rays.
- **Diff** - The Difference between the peak centroid energy and the characteristic energy of the matched line in keV.

The column in the lines grid are as follows:

- **Energy** - The energy of the characteristic line in keV.

- **Yield** - The photon yield, in percent, of the characteristic line in the **Name** column. This include nuclide branching ratios if applicable.
- **Type** - Emission type, **X** for x-rays **G** for gamma rays.
- **Efficiency** - The detection efficiency, in percent, at the energy of the characteristic line. This will be zero if there is no efficiency information.
- **Area** - The expected area of a peak, based on the selected peak, for this line.
- **MDA**- The minimum area (95th confidence interval) a peak would need to have to be detected.
- **Matched** - Checked if a peak was found that matches to the line.
- **Peak No.** - The identification number of the matched peak, blank if **Matched** is unchecked.
- **Diff** - The difference between the matched peak centroid and the line energy in keV. Blank if the **Matched** is unchecked.
- **Rel. Activity** - The expected activity, based on the selected peak, of this line relative to the other lines. Blank if the **Matched** is unchecked.
- **Name** - Library Mode only. The name of the nuclide emitting the line.

Modes

The tool has two modes, [Matching Mode](#) and [Library Mode](#). The former is for matching a list of peaks to signature lines and nuclides then writing a nuclide library file. The latter, is for entering nuclides and writing them and the signature lines to a nuclide library file. Library mode is useful for quickly creating nuclide libraries of known nuclides. The tool always opens in the matching mode by default, but can be switched to the library mode by navigating to **Settings** → **Mode** or and selecting the desired mode pressing F5 for matching mode and F6 for library mode. The window will toggle between [Figure 1](#) and [Figure 3](#), display a subset of the columns in the remaining grids, and hiding peak input information.

Matching Mode

Matching Mode allows for increasing complexity and more sophistication in the matching and scoring algorithms depending on the availability of information. The minimum amount of information required is a single peak centroid energy. The tool will accept various peak input formats (details in [Peak Inputs](#)); but the input data fits into three categories: peak information, time information, and efficiency calibration Information. Peak Information includes the location of the peak

Name	Score	Nuclide	Half Life	Unit	Energy	Yield (%)	Type	Diff
BA-137M	0.891	BA-137M	2.552	m	661.657	89.739	G	0.043
CS-137	0.891	BA-137M	30.167	y	661.657	84.713	G	0.043
MN-50M	0.239	MN-50M	1.750	m	661.500	25.000	G	0.200
PD-98	0.158	PD-98	17.700	m	662.200	19.720	G	-0.500
Y-84M	0.057	Y-84M	39.500	m	660.500	15.677	G	1.200
LA-132M	0.044	LA-132M	24.300	m	663.070	11.606	G	-1.370
LA-132	0.042	LA-132	4.800	h	663.070	9.044	G	-1.370
RE-181	0.030	RE-181	19.900	h	661.800	2.960	G	-0.100
BI-204	0.025	BI-204	11.220	h	661.580	2.541	G	0.120
TL-200	0.022	TL-200	26.100	h	661.350	2.276	G	0.350
NB-88M	0.019	NB-88M	7.780	m	661.600	1.911	G	0.100
HO-154M	0.018	HO-154M	3.100	m	661.500	1.784	G	0.200
RH-95	0.015	RH-95	5.020	m	661.000	1.539	G	0.700
AT-204	0.013	AT-204	9.200	m	662.720	1.382	G	-1.020
BI-202	0.013	BI-202	1.720	h	662.550	1.310	G	-0.850
CS-121	0.011	CS-121	155.000	s	661.100	1.166	G	0.600
HG-191M	0.011	HG-191M	50.800	m	662.000	1.140	G	-0.300
HO-170	0.011	HO-170	2.760	m	662.900	1.188	G	-1.200
LI-126	0.010	LI-126	81.600	m	662.100	1.051	G	-0.400

Line Match Score: 94.571%

Energy	Yield (%)	Type	Efficiency (%)	Area (cts)	MDA (cts)	Matched	Peak No.	Diff	Rel. Activity
31.819	2.160	X	9.927E-001	2.608E+001	2.710E+000	<input type="checkbox"/>			0.000E+000
32.206	3.977	X	9.926E-001	4.803E+001	2.710E+000	<input type="checkbox"/>			0.000E+000
36.317	0.380	X	9.917E-001	2.000E+000	2.710E+000	<input checked="" type="checkbox"/>	2	0.983	5.306E+000
36.392	0.736	X	9.917E-001	2.000E+000	2.710E+000	<input checked="" type="checkbox"/>	2	0.908	2.739E+000
37.261	0.156	X	9.915E-001	2.000E+000	2.710E+000	<input checked="" type="checkbox"/>	2	0.039	1.290E+001
661.657	89.739	G	8.587E-001	1.253E+003	0.000E+000	<input checked="" type="checkbox"/>	1	0.043	1.626E+001

Figure 2: The matched result of 661.7 keV and 37.3 keV peak centroids. The parent, Cs-137, and daughter, Ba-137m, are both displayed in the **Name** column. They have different yields (89.739% vs 84.713%) because of Cs-137 only decays into Ba-137m 94.4% of the time.

(*centroid/energy*), and the size (*area*) and the underlying continuum (*Continuum*). These parameters can be entered into the peaks grid manually one by one. Time information includes the length of the count (*Acquisition time*), the time elapsed from the time the acquisition began (*Start Time*), and the time the sample was collected (*Sample Time*). The time parameters are used in **Nuclide Scoring** to help filter out short lived nuclides that may be impossible to detect given the span of time between *sample time* and *start time* and the half-life of the nuclide. These parameters are entered through the **Settings Menu** or loaded through a compatible input file. Efficiency calibration information allows for the **Line Scoring** and comparative peak calculations to occur (*area*, *MDA*, and *relative activity*) as well as the efficiency at the line energy. The calibration curve model, order of polynomial and efficiency measurements (*Energy*, *Efficiency*, *Efficiency Uncertainty*) can be entered through **Settings Menu** or loaded through a compatible input file. There are three available models: Linear (**Equation 9**), Natural (**Equation 10**), and Empirical (**Equation 11**). The calibration curve is computed (**Equation 15**) on-the-fly and will be recalculated when any of the calibration settings are changed.

Matching is performed by loading or entering a **peak input file** and selecting a peak in the peaks grid or entering an energy in the peaks grid and pressing **Enter**. This will then find all the nuclides, including decay chains (**Appendix B**), in the library with a line that has an energy within the tolerance (default of the FWHM, if available or 1 keV otherwise). The nuclides are then scored (**Nuclide Scoring**) based on the deviation of the peak centroid and the line energy (**Equation 3**), the half-life score (**Equation 2**), and the yield of matched line (**Equation 4**). This matched line is referred to as the *reference line*. If the nuclide has a parent with a longer or comparable half-life, the parent will appear in the nuclides grid with the name of the parent in the **Name** column and the matched nuclide in the **Nuclide** column. The **Half-Life** column will show the half-life of the nuclide displayed in the **Name** column. Yields of daughters take into account parent decay

branching ratios. [Figure 2](#) shows an example of a match of the 661.7 keV peak from Ba-137m. The peak can be attributed to the much longer lived Cs-137, a common practice.

Sum and escape peaks, single and double, are included in the search. Sum peaks will be heavily penalized if two conditions are not met:

1. There at least three peaks and,
2. The two largest peaks sum to a energy that is close to another peak centroid.

The list of matched nuclides is sorted by the largest scores to the smallest with nuclides failing the score cutoff completely removed from the nuclides grid. Selecting any nuclide in the nuclide grid will display the lines in the line grid associated with that nuclide and, unless otherwise specified, the daughters in equilibrium. The display of daughter lines can be toggled on and off through the right click anywhere in the tool.

The Line Match score ([Equation 6](#)) is displayed between the nuclide and peak grids. It represents the the number of peaks above MDA, peaks that should be detected, that are found in the peaks grid. The column **Matched** shows the peaks matched with a line from the selected nuclide, the peaks matched with lines will also be highlighted in the peaks grid. The **Diff** and **Rel. Activity** columns display the deviation of a matched peak centroid to the energy line and the activity of the line given the efficiency and yield based on the reference line.

Tips for Matching

- The first nuclide is not always the best match because the line match score is not part of the nuclide score. It is therefore best to select several nuclides before deciding.
- Start at high energy peaks and work toward low energy. Many low energy peaks (less than 80 keV) are x-rays from the nuclides that also have more distinct gamma emissions in the higher energies.
- Start with the largest peaks, the matched nuclides will likely have other lines reducing the effort needed.
- Avoid jumping around to different peaks, finish with one peak before moving on.
- If the efficiency calibration is a good representation, the relative activity across the energy lines should be uniform for a correctly identified nuclide.
- If a line peak has a relative activity that is different from the others, it might be an interference with another nuclide.
- Look for peak areas that should be above the MDA and determine why they were not found.

- Enter as much information about the spectrum as possible, information unlocks the more sophisticated matching tools.
- Ignore the comparative analysis if there are no peak areas or efficiency calibration.

The nuclide and lines can be written to a nuclide library for use in vendor supplied gamma spectroscopy software. To generate or append a library, a library must be loaded. This can be done from, the [File Menu](#) menu. Selecting **New...** will generate a new library file or overwrite the library if a file with the same name exists. **Open...** will append the nuclides and lines to the selected file. Both options will open a window where to browse for a file or a save location. Three file types are available: .nlb, .cnf, .tlb. The .nlb and .cnf files are CAM file types to be used in the GENIE™ 2000 software package. The third (tlb) is a text based library that can be opened with any text editor. Once the file is ready to be written, the file name will appear in the status strip and the write options in [Lines Menu](#) will become active. To write the lines, determine how they should be written and select the appropriate option from the [Lines Menu](#). The options are as follows:

- **Selected** - Write the lines that have been selected in the Lines Grid
- **Matched** - Write only the lines that have matching peaks, delineated by a check mark in the **Matched** column. Available in Matching Mode only.
- **Yield...** - Write the lines above a minimum yield percentage in the window that opens after this option is selected.
- **All** - Write every line in the Lines Grid.

Every line, independent of the option chosen, will be written to the selected nuclide. Lines from daughters in equilibrium can be associated with their parent or a decay chain ([Appendix B](#)) by selecting the desired nuclide in the nuclide grid. **Note:** Attributing daughter lines with parents will write the lines to the parent nuclide, (with the parent half-life) and the line yield will be adjusted for branching ratios.

The key line for the nuclide is determined by finding the line with the largest abundance that does not have any lines from other nuclides that are within the interference band. The symmetrical band can be adjusted with the **Key Line Interference** parameter described in [Appendix A](#) section: [Key Line Interference](#).

Peak Inputs

There are several ways to import peak and spectral information. [Table 1](#) shows the available inputs and the data that is automatically (A) and manually (M) loaded. A Mirion Canberra GENIE™ 2000 Configuration Access Method (CAM) file can be loaded. This will load all the peak information, time information and calibration information, if available in the file. The peaks must have already been located and areas determined before the file is loaded. Continuum information is read

Table 1: Peak input options and the class of data that is automatically loaded (A) or manually loaded (M)

Input Type	Peak Info.	Time Info.	Efficiency Cal.
CAM	A	A	A
CSV	A	M	M
User	M	M	M

directly from the spectrum so the MDA calculations are complete. Another way to load data into the tool is to import a PeakEasy ROI Data Comma Separated Value (CSV) file. This will have all the peak information, but efficiency calibration and time information will need to be loaded manually. The PeakEasy file type uses linear interpolation between peaks to determine the continuum, which is a degradation of accuracy in the MDA from the CAM file but serves as a good approximation. The final method of entering data is completely manual; every piece of information must be entered manually and there is no way of determining the continuum so only the MDA calculations for found peaks will be accurate, if peak area was entered. An array of peak energies can be pasted into the peaks grid with typical Windows paste operations. The other input file types can be dragged and dropped into the window or open through the [File Menu](#) → **Input....** CAM files can take a few seconds to load, but once the file is loaded the peaks will appear in the peaks grid, and the input file name will be displayed in the status strip at the bottom of the window.

Library Mode

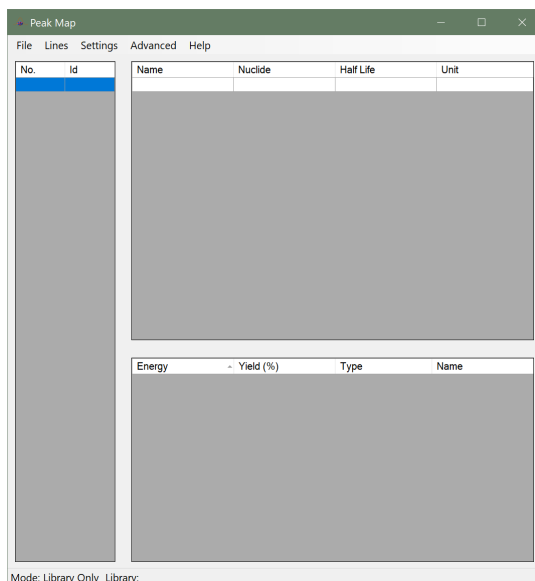


Figure 3: Peak Map window in library Mode

Library Mode ([Figure 3](#)) allows for the searching of nuclide names and the displaying and library generation of the resultant nuclides and lines. Selecting library mode from the [Settings Menu](#) or

pressing F6 opens the nuclides grid **Name** column to editing. Typing a nuclide (e.g. Cs137, or CS-137, 137cs) in any row will search for that nuclide and its daughters in equilibrium. An incomplete entry can also be entered, for example, only the chemical symbol or and isomer number. The former will find all isotopes of the chemical entered chemical symbol, and the former all the isomers of the entered number and the associated daughters. If the entered value is part of a decay chain ([Appendix B](#)) the entire chain will be retrieved and displayed. Clicking on the nuclide in the grid will display all the associated lines with that nuclide, and daughters if applicable. The lines from the daughters can be toggled on or off from the [Lines Menu](#) or right clicking and clicking **show daughter lines**. The lines can be written to the library in the same as in the [matching mode](#) and the nuclides added will show up in the left most pane. Nuclides and all their lines can be removed by selecting the nuclides to remove and right clicking and selecting **Clear Selected**. **Clear Current Row** will delete just the row that was right-clicked on, and **clear Matches** will clear the whole table.

Menu Navigation

File Menu

- **Open Input...** - Open a window to browse to an input file, a list of the inputs can be found in [Peak Inputs](#)
- **Close Input** - Clear the peaks and other spectral information and return the program to the state when it was opened.
- **New...** - Create a new nuclear data library to write the nuclides and lines, see [Library Mode](#) for details.
- **Open...** - Open an existing nuclear data library to write the nuclides and lines, see [Library Mode](#) for details.
- **Save Library** - Close the open nuclear data library.
- **Exit** - Exit the tool.

Lines Menu

- **Show Daughter Lines** - Toggle showing the lines from the daughter nuclide. If this is unchecked on the lines from the nuclide in the **Name** column will be displayed.
- **Selected** - Write the lines that have been selected in the Lines Grid
- **Matched** - Write only the lines that have matching peaks, delineated by a check mark in the **Matched** column. Available in Matching Mode only.

- **Yield...** - Write the lines above a minimum yield percentage in the window that opens after this option is selected.
- **All** - Write every line in the Lines Grid.
- **Write** - Write to the library via the checked means of writing (Selected, Matched, Yield, All)

Settings Menu

- **Matching...** - Adjust the parameters used in the matching algorithm. See [Matching](#) for a description of the algorithms and [Section A.1](#) for the parameters.
- **Spectral...** - Enter or change the remaining information about the spectrum. See [Section A.1](#) for a description of the of the spectral parameters.
- **Library...** - Adjust the parameters used in the library writing algorithm. See [Library](#) or the description of the algorithms and [Section A.1](#) for the specifics of the parameters
- **Matching** - Change the mode to Matching ([Matching Mode](#))
- **Library** - Change the mode to Library ([Library Mode](#))

Advanced

- **Rebuild Library Database...** - Generate a new SQLite database containing all the nuclide and line data from the library file with the settings in the app.config file. The software deploys with the database necessary. The only reason to do this is if the default settings and the built in decay chains are not adequate for the user's purposes.

Help Menu

- **About** - View the information about the tool

Technical

The following algorithms are used to perform all the calculations in the tool. They are provided for clarity, transparency and to allow advanced users to tweak the parameters to fit their specific needs. There are two main categories of algorithms, one for matching and one for nuclide library generation.

Matching

The matching algorithms are used in [Matching Mode](#) to assist the user in determining which nuclides are present in a set of peaks. The correctness of a matched is judged by two scores: the nuclide score and the line score. Both scores depend on the amount of information in the input file. See [Peak Inputs](#) for more information on the data from the various inputs.

Scoring

The score is a series of penalties ascribed to the selected nuclide (**Name** column) in the Nuclides Grid based on the number of elapsed half-lives, the deviation of the peak centroid from the matched line energy, and the yield of the matched line. The line score is a metric of the number of lines that should have been detected that have a matching peak.

Nuclide Scoring

The nuclide score begins at a value of 1.0 and is assigned a penalty for elapsed half-lives, deviation of peak centroid line energy and sum peak, and the yield of the matched line with the subscripts for S in [Equation 1](#) $k = T_{1/2}, D, Y, SP$ respectively.

$$S_N = 1.0 \cdot \prod_{i=0}^3 S_k, \quad i: \{T_{1/2}, D, Y, SP\} \quad (1)$$

The subscript $T_{1/2}$ represents the penalty for the number of half-lives ($T_{1/2}$) that have elapsed during the start of [Acquisition Time](#) and the [Sample Time](#) (ΔT) and is shown in [Equation 2](#). The

severity of the penalty can be adjusted using the [Half-Life Constant](#) ($C_{1/2}$).

$$S_{T_{1/2}} = \exp \left[C_{1/2} \cdot \left(\frac{\Delta T}{T_{1/2}} \right) \right] \quad (2)$$

The score is further reduced by measurement between the peak centroid and the line energy from the reference (ΔT). The line search tolerance (δ_E) which is set to the Peak FWHM, if available, and the line yield is also accounted for in this determination. The product of the ΔT and δ_E is squared to ensure it is always positive and the S_D acts as a penalty. Just as with the half-life penalty the severity can be adjusted with a constant [Line Deviation Constant](#) (C_D). For nuclides, the deviation penalty as expressed in [Equation 3](#) accounts for yield (y_r) of the reference line. For escape peaks and sum peaks, the yield is excluded as it is strongly dependent on the counting geometry and such calculations are unnecessary for these purposes.

$$S_D = \exp \left[C_D \cdot \frac{(\delta_E \cdot \Delta E)^2 \cdot y}{100} \right] \quad (3)$$

The lines that appear in a spectra are likely the most abundant lines from the nuclide. To account for this the score is further reduced by the yield penalty ([Equation 4](#)). The score is simply multiplied by the fractional yield of the reference line (y_r), linearly reducing the score. The half-life penalty ([Equation 2](#)) mirrors the decay equation, a small penalty for few half-lives and a very large penalty for many half-lives. The deviation penalty ([Equation 3](#)) is also an exponential to severely penalize lines that approach the search tolerance (δ_E).

$$S_y = \frac{y_r}{100} \quad (4)$$

Sum peaks require at least three peaks to be present in a spectrum for the possibility of sum peaks to arise. Furthermore, the chance of multiple sum peaks is greatly reduced if the two peaks with the largest area do not sum a peak in the peaks grid. The accounting for these facts is done with the sum peak score (S_{SP}) expressed in [Equation 5](#) which acts as cutoff essentially removing the possibility of sum peaks if there are not three peaks and the largest peaks do not sum to a peak in the spectrum.

$$S_{SP} = \begin{cases} P, & \text{there are less than 3 peaks} \\ P, & \text{there is no peak that matches the energy sum of the 2 largest peaks} \\ 1, & \text{otherwise} \end{cases} \quad (5)$$

The [Sum Peak Penalty](#) is an adjustable parameter and as with the other penalty constants which allows the user to finely tune the nuclide scores within a session of matching.

Line Scoring

Once a nuclide is selected in the nuclides grid the line score is generated and represented as a percent. This score is a measure of the lines that were found in the peaks grid against the lines

that should have been found. To determine which lines should have been found, an efficiency calibration is required, as well as a measurement of continuum where MDA can be determined. For the i^{th} line attributed to the nuclide, the Minimum detectable activity (MDA_i), efficiency at the line energy (ϵ_i), and the activity (a_i) relative to the reference line (denoted with subscript r) is calculated using the [Comparative calculations](#). The reference line is the line found that matches the highlighted peak in the peaks grid. The denominator in [Equation 6](#) is all the lines that should be detected with (δ_i) indicating if it should have been detected. The numerator is the number of lines found in the spectra. The severity of the penalty can be scaled with (C_L) and is described in [Appendix A](#) section: [Unmatched Line Constant](#). It is possible of the [Equation 6](#) to exceed 100% if lines that should not have been detected were. It might indicate and interference.

$$S_L = C_L \cdot \frac{\sum_{i=0}^N y_i \sqrt{\epsilon_i}}{\sum_{i=0}^N \delta_i \cdot y_i \sqrt{\epsilon_i}} \cdot 100, \quad \begin{cases} \delta_i = 1, a_i > MDA_i \\ \delta_i = 0, \text{ otherwise} \end{cases} \quad (6)$$

Comparative calculations

The comparative calculations are required for the [Line Scoring](#) to be accurately calculated. The calculation of MDA [Equation 7](#) and relative activity [Equation 8](#) are required for the determination of δ_i in [Equation 6](#). The MDA is calculated using the Currie method at the 95% confidence level, where μ_i is the continuum counts at the energy of the i^{th} line of the selected nuclide.

$$MDA = 2.71 + 2 \cdot \sqrt{\mu_i} \quad (7)$$

The relative activity is based off the activity of the reference line (A_r). It requires the efficiency and yield of both the reference line (ϵ_r and y_r , respectively), and the efficiency and yield of the i^{th} line.

$$A_i = \frac{A_r \cdot \epsilon_i \cdot y_i}{\epsilon_r \cdot y_r} \quad (8)$$

Efficiency

An efficiency calibration is essential of the determination of the relative activity ([Equation 8](#)). Following the convention in gamma spectroscopy the efficiency calibration is a curve regression fitted to several peak areas across the energy range as compared to a known standard. There are three available models: Linear found in [Equation 9](#), Natural in [Equation 10](#) and Empirical [Equation 11](#).

$$\log(\epsilon) = \sum_{i=-1}^M b_i \cdot \frac{1}{E}^i \quad (9)$$

$$\ln(\epsilon) = \sum_{i=0}^M b_i \cdot [\ln(E)]^i \quad (10)$$

$$\ln(\epsilon) = \sum_{i=0}^M b_i \cdot \left[\frac{0.5 \cdot (E_0 + E_H)}{E} \right]^i \quad (11)$$

The curve allows for an energy E and the fit of the curve is controlled by the fitting coefficients (b_i) can be entered in the Spectral Settings menu, described in [Appendix A](#) section: [Calibration Parameters](#).

The efficiency curves are calculated from the efficiency measurements loaded from the spectral file or entered manually in the [Efficiency Points](#). The coefficients(b_i) are determined by using weighted least squares methodology. It is also known that the efficiency measurement is associated with uncertainty, and logically, measurements of high uncertainty should contribute less to the solution. Thus, a weight, that is a function of the uncertainty is applied to both sides of the efficiency equation.

$$w_j = \left(\frac{\epsilon}{\sigma_\epsilon} \right)^2 \quad (12)$$

Given N [Efficiency Points](#) and a order of M the Equations [9](#), [10](#) and, [11](#) can be rewritten in in matrix form.

$$\mathbf{A}\vec{b}\vec{w} = \vec{\epsilon}\vec{w} \quad (13)$$

For simplicity and clarity, the weights will be rolled into the \mathbf{A} and $\vec{\epsilon}$. Since the efficiencies($\vec{\epsilon}$) are measured values there is no solution to [Equation 13](#) we must find a estimated solution (\vec{b}^*) that minimizes the [Equation 14](#).

$$\| \vec{\epsilon} - \mathbf{A}\vec{b}^* \| \quad (14)$$

This is achieved using the least squares method, where both sides of [Equation 13](#) are multiplied by transpose of \mathbf{A}^T and the result is inverted to give \vec{b}^* . The solution is given in [Equation 15](#).

$$\vec{b}^* = \mathbf{A}^T \vec{\epsilon} \cdot (\mathbf{A}^T \mathbf{A})^{-1} \quad (15)$$

Library

The generation of nuclear data libraries for use in gamma spectroscopy software requires the calculation of uncertainty because ICRP-107 does not list uncertainties. The tool will also combine lines that may be unreasonable in a spectrum. The limit on how close peaks must be to be combined are outlined in [Appendix A](#) section: [Resolution Limit](#). Line combination can be disabled in [Appendix A](#) section: [Line Combination](#) if it is not desired. Also the tool will ask the user to confirm the combination of lines each time it detects combination a situation.

Uncertainty

The uncertainty for any number is assigned as half the last digit of precision. ICRP-107 lists energies in MeV and yields in gammas per decay in scientific notation with six digits. Therefore, the uncertainty can be six orders of magnitude smaller than the listed value. The uncertainty is 0.5 of the last non-zero significant digit, the median between the precision of the listed value. This sample logic applies to half-life values, which are listed as floats in ICRP-107.

Combining Lines

No gamma spectroscopy technology has perfect charge collection, and by continuation the peaks are not infinitely thin. As a result, there is a possibility that lines from a single nuclide may need to be combined if they are smaller than the resolution of the system used to collect the spectrum. This is particularly prevalent within the x-ray region of the spectrum. The energy of the combined peak is simply the yield (y_i) weighted average of the line energies (E_i) over the number of peaks to combine (N) and is given in [Equation 16](#).

$$\bar{E} = \frac{\sum_i^N E_i \cdot y_i}{\sum_i^N y_i} \quad (16)$$

The uncertainty in the energy of the combined peak ($\sigma_{\bar{E}}$) is the weighted average standard deviation in the line energies. [Equation 17](#) is used to determine the uncertainty in the combined line energy.

$$\sigma_{\bar{E}} = \sqrt{\frac{\sum_i^N y_i \cdot (E_i - \bar{E})^2}{\frac{N-1}{N} \sum_i^N y_i}} \quad (17)$$

The yield of the newly combined peak is just simple addition of the yields. It is possible for this yield to exceed 100% if the nuclear decay structure has many high yield instantaneous decays. [Equation 18](#) is used for the addition.

$$\bar{y} = \sum_i^N y_i \quad (18)$$

Uncertainty in the combined yield ($\sigma_{\bar{y}}$) in [Equation 19](#) is just propagation of errors of the yield uncertainty as determined in the [Uncertainty](#) section.

$$\sigma_{\bar{y}} = \sqrt{\sum_i^N (\sigma_{y_i})^2} \quad (19)$$

Appendix A

Settings description

A.1 Matching

Algorithm Settings

Enable Half-Life Score

Default: True. Turn on or off the half life scoring. May be necessary if a very large amount of a short lived nuclide may be present.

Half-Life Constant

Notation: $C_{1/2}$ **Default:** -0.0051. The constant to adjust the severity of the half-life penalty.

Line Deviation Constant

Notation: C_D **Default:** -0.5. The constant to adjust the severity of the deviation of peak centroid to line energy penalty.

Sum Peak Penalty

Notation: P **Default:** 0.1. The penalty assigned to possible sum peaks for not sum peaks not being likely.

Unmatched Line Constant

Notation: C_L **Default:** 1.0. The constant to adjust the severity of the Line Match score.

Limit Settings

Parent/Daughter Half-Life Ratio

Default: 1.0. The ratio of the parent's half-life to the daughter's to serve as indication if the pair are in equilibrium and will be added as a pair or a single nuclide.

Score Limit

Default: 0.001. The cutoff for lowest score to be included in the nuclides grid.

Yield Limit

Default: 0.1. The smallest line yield to be included in the search or lines grid.

A.2 Library

Line Combination Settings

Line Combination

Default: True. Turn on or off the line combination during library generation.

Resolution Limit

Default: 0.5. The largest difference between line energies in keV to still be considered individually resolved.

Key Line Interference

Default: 3.0 The symmetrical band limit (keV) where there may be and interference and to not set as the key line for that nuclide

A.3 Spectral

Calibration

Calibration Model

Default: Linear. The type of curve fit to use to model the efficiency of the count.

Calibration Parameters

Default: $\{b_1 = -0.0001, b_2 = 1.4e - 17, b_3 = -8.7e - 19\}$ The fitting constants for the calibration model. The default is a constant calibration of 100% efficiency across the entire spectrum.

Order

Default: 5 or 2. The number of terms in the calibration equation. Changing this will recalculate the calibration parameters.

Efficiency Points

Default: $\{(E, 0.999999999999, 0.000000000005) \text{ where } E = (20, 1510, 3000) \text{ keV}\}$. The efficiency measurements used to determine the efficiency equation

Time

Acquisition Time

The date and time the count was started.

Count Time

The time the sample was counted in seconds.

Sample Time

The date and time the sample was collected or reference date or time. The difference between [Acquisition Time](#) and [Sample Time](#) is the ΔT in [Equation 2](#)

Appendix B

Decay Chains

A nuclear decay chain can occur when a nuclide decays into another radioactive nuclide but with much shorter half-life, which in turn decays into another radioactive nuclide, and so on. There are several naturally occurring decay chains with the very long lived naturally occurring actinides, Th-232 and U-238, U-235 and one anthropogenic, Np-237. Since every known isotope above Bi-208 is unstable, these actinides must go through a series of decays. The shortest of the four is the Np-237 with a 2.1 million year half-life, far outstripping every daughter until the stable isotopes. The other three follow the same pattern, albeit with much longer parent half-lives. It is therefore, possible to see all or some the emissions from the photon emitting daughter nuclides. It is important to note, that some of these chains contain Radon, which is a gas and will leave the sample. In all cases the prediction of the nuclide concentrations depends on the ability to retain the radon gas.

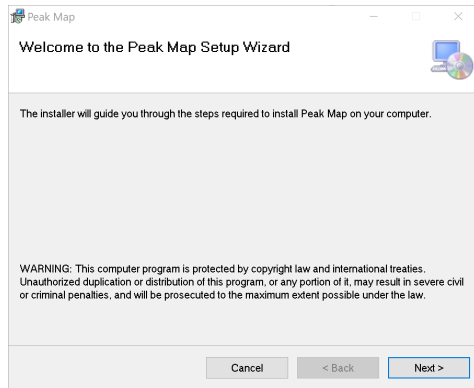
Much shorter decay chains consisting of a parent decaying into a radioactive daughter which then reaches stable occur frequently in many radioactive nuclides. These are functionally the same as the much longer decay chains. It is often the case that one might want to attribute the decay of the entire chain to that of the longer lived parent. The tool provides this flexibility through the **Name** and **Nuclide** columns in the nuclides grid. In this case the name being that of the parent and the nuclide being the actual emitting nuclide.

For many applications the emissions for the daughters of the large decay chains can simply be attributed to the chain itself as the determination of exact concentrations of each daughter can be problematic. As such, the tool is distributed with the Th-232, and U-238, U-235, and Np-237 decay chains defined in their entirety. If a peak is matched with a daughter line in a chain the parent of the chain or any of the four parents are searched for in [Library Mode](#) will appear in the **Name** column appended by a “+”. Selecting a decay chain will display all of the lines of all the daughters with the branching ratio adjusted yields.

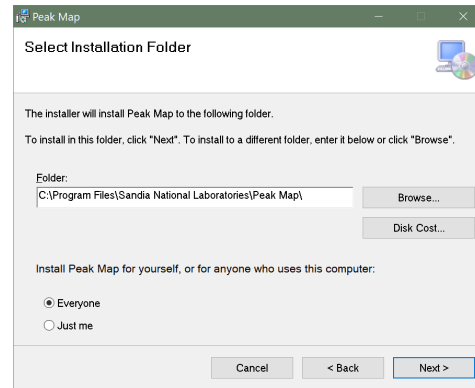
Appendix C

Software Installation

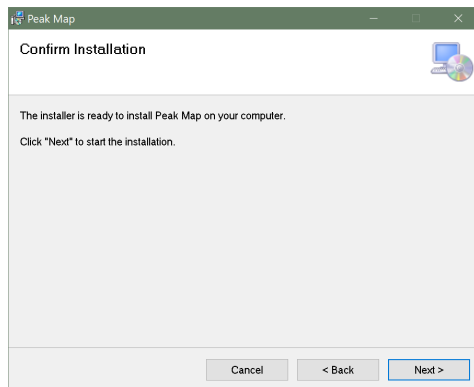
You must have administrative privileges to install the software. The software is installed by double clicking on either setup.exe or setup.msi and running the installer. The wizard launched by setup.exe will guide the user through the installation process as shown in [Figure C.1](#). Only the installation directory and selection of users are available to change, this is done on the Subfigure [C.1b](#). The software can be uninstalled either through the Programs and Features in the control panel or by running the setup.exe again.



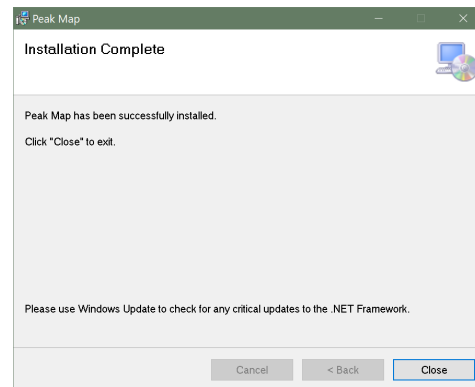
(a) Welcome screen



(b) Folder selection screen



(c) Confirmation screen



(d) Installation complete screen

Figure C.1: Installation wizard screens

Index

Algorithms, [20](#)

- Average Peak Energy, [24](#)
- Average Peak Energy Uncertainty, [24](#)
- Average Peak Yield, [24](#)
- Average Peak Yield Uncertainty, [24](#)
- Empirical Efficiency, [22](#)
- Energy Deviation Penalty, [21](#)
- Half-Life Penalty, [21](#)
- Library, [23](#)
- Line MDA, [22](#)
- Line Relative Activity, [22](#)
- Line Score, [21](#)
- Line Yield Penalty, [21](#)
- Linear Efficiency, [22](#)
- Matching, [20](#)
- Natural Efficiency, [22](#)
- Peak Combination, [24](#)
- Sum Peak Score, [21](#)
- Total Score, [20](#)
- Uncertainty, [23](#)

Efficiency Calibration, [14](#), [22](#)

- Empirical, [22](#)
- Generation, [23](#)
- Linear, [22](#)
- Natural, [22](#)

Library Mode, [17](#), [19](#)

Line

- Deviation, [13](#), [15](#)
- Energy, [12](#)
- Grid, [12](#)
- Key, [16](#)
- Match Score, [15](#)
- MDA, [13](#), [22](#)
- Reference, [14](#), [22](#)
- Relative Activity, [13](#), [15](#), [22](#)
- Score, [20](#)
- Type, [13](#)
- Yield, [13](#)

Matching Mode, [13](#), [19](#)

Nuclide

- Emission Type, [12](#)
- Grid, [12](#)
- Reference Line, [14](#)
- Score, [14](#)
- Yield, [12](#)

Peaks, [13](#)

- Area, [12](#)
- Average Energy, [24](#)
- Average Energy Uncertainty, [24](#)
- Average Yield, [24](#)
- Average Yield Uncertainty, [24](#)
- Centroid, [12](#)
- Combination, [24](#)
- Continuum, [12](#)
- Energy, [12](#)
- Escape, [15](#)
- FWHM, [12](#)
- Grid, [12](#)
- Sum, [15](#)

Score, [20](#)

- Cutoff, [15](#)
- Energy Deviation, [21](#)
- Half-Life, [21](#)
- Line, [20](#), [21](#)
- Line Match, [15](#)
- Nuclide, [14](#), [20](#)
- Sum Peak, [21](#)
- Yield, [21](#)

Time, [14](#)

- Acquisition, [14](#)
- Sample, [14](#)
- Start, [14](#)

