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Peak Map User's Manual

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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.

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ACRONYMS & DEFINITIONS

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 a 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 GENIETM 2000 software package

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

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1. 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.

1.1. 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 Appendix A is an overview of the parameters used in the matching algorithm and Appendix C provides instructions on the installation of the software.

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2. USAGE

This chapter describes the usage and 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+letter)
- 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 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 or pressing F5 to toggle between the two modes. The window will toggle between Figure 2-1 and Figure 2-2, display a subset of the columns in the remaining grids, and hiding peak input information.

Irespective of the mode, the window contains three grid views, one on the left for the peaks in matching mode or written nuclides in library mode and two on the top and bottom of the right side of the window. The upper right grid displays the found nuclides from either a matching line or searched nuclide. The bottom right grid shows all the characteristic lines from the selected nuclide and any daughters in equilibrium with the nuclide. This grid can be filtered by expanding the the Line Filters which can include/exclude Daughter Lines, x-Rays, Gamma-Rays, provide a minimum yield and a window the line energies. The strip at the bottom of the screen presents information about loaded spectra/peak files, and the nuclide library file that is being written.

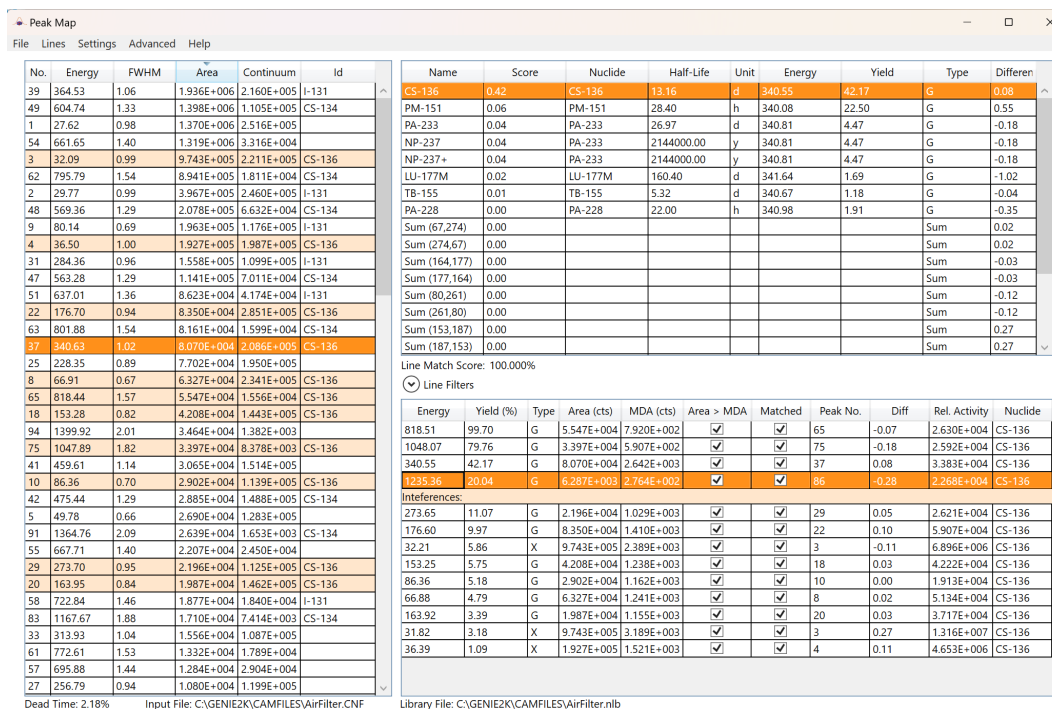


Figure 2-1. Peak Map window in matching mode performing peak matches.

2.1. Matching Mode

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.

Matching Mode as shown in Figure 2-1 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 2.1.2); but the input data fits into three categories: peak information, time information, and efficiency calibration Information. Peak Information includes the location of the peak (*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 4.9), Natural (Equation 4.10), and Empirical (Equation 4.11). The calibration curve is computed (Equation 4.15) on-the-fly and will be recalculated when any of the calibration settings are changed.

2.1.1. *Tips for Matching*

2.1.2. *Peak Inputs*

2.2. Library Mode

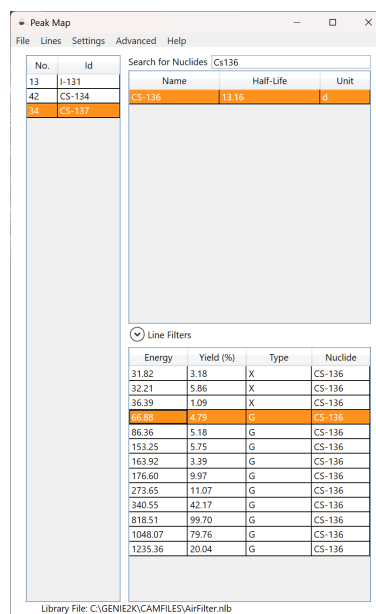


Figure 2-2. Peak Map window in library Mode

3. MENU NAVIGATION

3.1. File Menu

3.2. Lines Menu

3.3. Settings Menu

3.4. Advanced

3.5. Help Menu

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4. 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.

4.1. 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.

4.2. 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.

4.2.1. 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 4.1 $k = T_{1/2}, D, y, SP$ respectively.

$$S_N = 1.0 \cdot \prod_{k=0}^3 s_k, i : \{T_{1/2}, D, Y, SP\} \quad (4.1)$$

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

$$S_{T_{1/2}} = \exp \left[C_{1/2} \cdot \left(\frac{\Delta T}{T_{1/2}} \right) \right] \quad (4.2)$$

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 4.2 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.

$$S_D = \exp \left[C_D \cdot \frac{(\delta_E \cdot \Delta E)^2 \cdot y}{100} \right] \quad (4.3)$$

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 4.4). The score is simply multiplied by the fractional yield of the reference line (y_r), linearly reducing the score. The half-life penalty (Equation 4.2) mirrors the decay equation, a small penalty for few half-lives and a very large penalty for many half-lives. The deviation penalty (Equation 4.3) is also an exponential to severely penalize lines that approach the search tolerance (δ_E).

$$S_y = \frac{y_r}{100} \quad (4.4)$$

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 4.5 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.

$$S_{SP} = \begin{cases} P, & \text{there are less than 3 peaks} \\ P, & \text{there is no peak that matches the energy sum of the 2 largest peaks} \\ 1, & \text{otherwise} \end{cases} \quad (4.5)$$

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.

4.2.2. 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 4.6 is all the lines that should be detected with (di) 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 4.6 to exceed 100% if lines that should not have been detected were. It might indicate and interference.

$$S_L = C_L \cdot \frac{\sum_i^N y_i \sqrt{\epsilon_i}}{\sum_i^N \delta_i \cdot y_i \sqrt{\epsilon_i}} \cdot 100 \quad (4.6)$$

4.2.3. Comparative Calculations

The comparative calculations are required for the Line Scoring to be accurately calculated. The calculation of MDA Equation 4.7 and relative activity Equation 4.8 are required for the determination of δ_i in Equation 4.6. 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.

$$MDA = 2.71 + 2\sqrt{\mu_i} \quad (4.7)$$

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.

$$A_i = \frac{A_r \cdot \epsilon_i \cdot y_i}{\epsilon_r \cdot y_r} \quad (4.8)$$

4.2.3.1. Efficiency

An efficiency calibration is essential of the determination of the relative activity (Equation 4.8). 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 4.9, Natural in Equation 4.10 and Empirical Equation 4.11.

$$\log(\epsilon) = \sum_{i=-1}^M b_i \cdot \frac{1}{E} \quad (4.9)$$

$$\ln(\epsilon) = \sum_{i=0}^M b_i \cdot [\ln(E)]^i \quad (4.10)$$

$$\ln(\epsilon) = \sum_{i=0}^M b_i \cdot \left[\frac{0.5 \cdot (E_0 + E_H)}{E} \right]^i \quad (4.11)$$

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.

$$w_j = \left(\frac{\epsilon}{\sigma_\epsilon} \right)^2 \quad (4.12)$$

Given N Efficiency Points and a order of M the Equations 4.9, 4.10 and, 4.11 can be rewritten in matrix form.

$$\mathbf{A} \vec{b} \vec{w} = \vec{\epsilon} \vec{w} \quad (4.13)$$

For simplicity and clarity, the weights will be rolled into the \mathbf{A} and $\vec{\epsilon}$. Since the efficiencies $\left(\vec{\epsilon} \right)$ are measured values there is no solution to Equation 4.13 we must find a estimated solution $\left(\vec{b}^* \right)$ that minimizes the Equation 4.14.

$$\| \vec{\epsilon} - \mathbf{A} \vec{b}^* \| \quad (4.14)$$

This is achieved using the least squares method, where both sides of Equation 4.13 are multiplied by transpose of \mathbf{A}^T and the result is inverted to give $\vec{\epsilon}$. The solution is given in Equation 4.15.

$$\vec{b}^* = \mathbf{A}^T \vec{\epsilon} \cdot \left(\mathbf{A}^T \mathbf{A} \right)^{-1} \quad (4.15)$$

4.3. 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.

4.3.1. 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.

4.3.2. 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 4.16.

$$\bar{E} = \frac{\sum_i^N E_i \cdot y_i}{\sum_i^N y_i} \quad (4.16)$$

The uncertainty in the energy of the combined peak ($\sigma_{\bar{E}}$) is the weighted average standard deviation in the line energies. Equation 4.3.2 is used to determine the uncertainty in the combined line energy.

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

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 4.3.2 is used for the addition.

$$\bar{y} = \sum_i^N y_i$$

Uncertainty in the combined yield ($\sigma_{\bar{y}}$) in equation 4.3.2 is just propagation of errors of the yield uncertainty as determined in the Uncertainty section.

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

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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. centroid to line energy 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 when summing is not likely.

Unmatched Line Constant

Notation: C_L **Default:** 1.0 The constant to adjust the severity of an unmatched in 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 in keV where there may be an 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: $\{1.0e-4, 1.4e-17, -8.7e-19\}$. 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: $\left\{ \begin{array}{ccc} 20.0 & 0.999999999999 & 0.000000000005 \\ 1510 & 0.999999999999 & 0.000000000005 \\ 3000 & 0.999999999999 & 0.000000000005 \end{array} \right\}$

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 4.2

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.

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APPENDIX C. Software Installation

You must have administrative privileges to install the software. The software is installed by double clicking on setup.msi and running the installer. The software can be uninstalled either through the Programs and Features in the control panel or by running the setup.exe again.



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