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PABS: A Computer Program to Normalize Emission Probabilities and Calculate Realistic Uncertainties

D. S. Caron*, E. Browne#, and E. B. Norman*

* *Nuclear Engineering Department, University of
California, Berkeley, California 94720*

#Nuclear Science Division

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D. S. Caron^{*}, E. Browne[#], and E. B. Norman^{*}

^{*} Nuclear Engineering Department, University of California, Berkeley, California 94720

[#] Lawrence Berkeley National Laboratory, University of California, Berkeley, California 94720

1 Abstract

The program PABS normalizes relative particle emission probabilities to an absolute scale and calculates the relevant uncertainties on this scale. The program is written in Java using the JDK 1.6 library. For additional information about system requirements, the code itself, and compiling from source, see the README file distributed with this program. The mathematical procedures used are given below.

2 Introduction

Absolute radiation emission probabilities are commonly used in nuclear structure, often for testing nuclear wave functions. These quantities are also of special importance for calculating average radiation energies per disintegration, in particular for the contribution of particle emission to reactor decay heat. Experimental absolute particle emission probabilities are evaluated and stored in the Evaluated Nuclear Structure Data File (ENSDF)[1]

Relative particle emission probabilities are usually deduced from areas of spectral peaks and reported on an arbitrary relative scale. Absolute particle emission probabilities may be deduced from relative probabilities, and are expressed on an absolute scale per nuclear disintegration, or in percent (per 100 disintegrations). These relative and absolute scales are linearly related through a single normalization factor. However, the relation between the statistical uncertainties in these two scales, which is given here, is not so straightforward.

3 Mathematical Procedure

The absolute emission probability (p_i) of a particle group (i) is given by

$$p_i[\%] = \frac{I_i}{\sum_k I_k} \times 100 \quad (1)$$

where I_i is the experimental relative spectral intensity of the i -th particle group. Its uncertainty $dp_i[\%]$ is given in ref. [2] as:

$$\frac{dp_i[\%]}{p_i[\%]} = \left[\left(\frac{dI_i}{I_i} \right)^2 \left(1 - \frac{2I_i}{\sum_k I_k} \right) + \frac{\sum_k dI_k^2}{\left(\sum_k I_k \right)^2} \right]^{1/2} \quad (2)$$

Where dI_i is the statistical uncertainty in I_i . Notice that this normalization ($\sum p_i[\%]=100$) has introduced a correlation between these quantities. PABS calculates the effect of this correlation on the uncertainties $dp_i[\%]$ using equations (1) and (2).

4 Program input

Data may be entered into PABS manually using the table at the main window of the program, passed in the form of a properly formatted input data set, or a combination thereof. A data set comprises information on the various particle groups emitted by a decaying nucleus. Each group is defined by three pieces of information:

1. A unique alpha-numeric identifier (ID)
2. A group intensity (I), in an arbitrary relative unit
3. An uncertainty associated with the relative intensity (dI)

The identifier is processed as a string and may contain up to 10 alpha-numeric characters. The intensity and its uncertainty are processed as double precision floating point numbers and may therefore be entered as either decimal numbers or in computerized scientific notation.

4.1 Manual data entry

Manual input may be entered directly into the table at the main program window of PABS. A field at the top of the window is provided for the title card. The table column headings specify the order and units of data input. Only the first three columns, which correspond to the identifier, the intensity, and its uncertainty, are accessible to the user; the last two are reserved for program output.

Data for each particle-group must be entered on a single row. Additional rows may be inserted below the currently selected one (or appended to the end of the table if no row has been selected) using the *Insert Row* function. A selected row may be removed from the table using the *Remove Row* function. Alternatively, if the first three columns of a particle-group are cleared of input data (the last two columns need not be empty), the data for that particle group will be removed from the calculation. Advanced editing options (such as *copy*, *cut*, *paste*, or other forms of re-ordering the input data) are not provided by PABS and it is therefore recommended that a text editor be used for such operations. Rows which are left entirely blank, regardless of their position in the table, have no effect on the calculation.

4.2 Input data set entry

Input data sets may be created externally using an ASCII text editor or may be generated from data entered into the main program window by calling the *Save Input* function of PABS. The latter option automatically formats the input data set according to program standards, whereas the former needs to conform to the following rules:

1. Line one of the input data set is reserved for the title card, which is replicated and printed in the output file.

2. Data for each particle group definition must be complete and entered in the order of ID, I, dI on a single line, with fields separated by commas, and in the relative units previously stipulated in this section.
3. Leading and trailing blanks is allowed between the three entries and the commas separating them or the carriage return, which terminates the data entry for each particle group.
4. Blank lines are permitted anywhere in the input data set and have no effect upon how data have been imported.
5. Full-line comments are allowed anywhere in the input data set and are denoted by a leading '%' character. The program does not read these comments, and thus are not printed in the output file.
6. File names for input data sets should conform to the operating system requirements of the host computer. Any file extension, or none at all, may be used.

The Import function of PABS reads into the program the information contained in an input data set.

5 Program output

The results of program calculations are displayed in the main window of PABS by calling the *Calculate* function. These may be printed to an output file by calling the *Save Output* function, which first performs the calculation (if it has not yet occurred), and then prompts the user for an output file name. The output file format is the same as that of an input file, with the additional entries of normalized particle emission probabilities (p_i) and their associated normalized uncertainties (dp_i). If no title card is present for the calculation, the default title card, which contains the date and time of the calculation, is printed in its place.

The program attempts to display each output value in decimal format; however, it will print individual particle emission probabilities and their respective uncertainties in computerized scientific notation as required by the precision of the uncertainties (See Section 5.1)

5.1 Significant figures and precision

PABS calculates and reports the uncertainty in the normalized particle emission probability with a maximum of two significant figures for values ≤ 25 , and with just one for > 25 . This normalized particle emission probability is then rounded and displayed with a precision determined by its uncertainty.

6 Example calculations

An example calculation is shown in this section describing proper input file format and demonstrating program results. Input data sets and output files for several cases are distributed with the program.

6.1 ^{240}Pu alpha decay

The physical data for the alpha decay of ^{240}Pu are provided in [3] and given below in an input data set:

Pu-240 alpha decay

% IDs are alpha energies rounded to the nearest keV

% ID, I[rel.], dI[rel.]

5168-keV, 73.51, 0.36

5124-keV, 26.39, 0.21

5022-keV, 0.071, 0.001

As a result of calling the *Import* function of the program and subsequently the *Calculate* function, the main window of PABS would appear as shown in Figure 1.

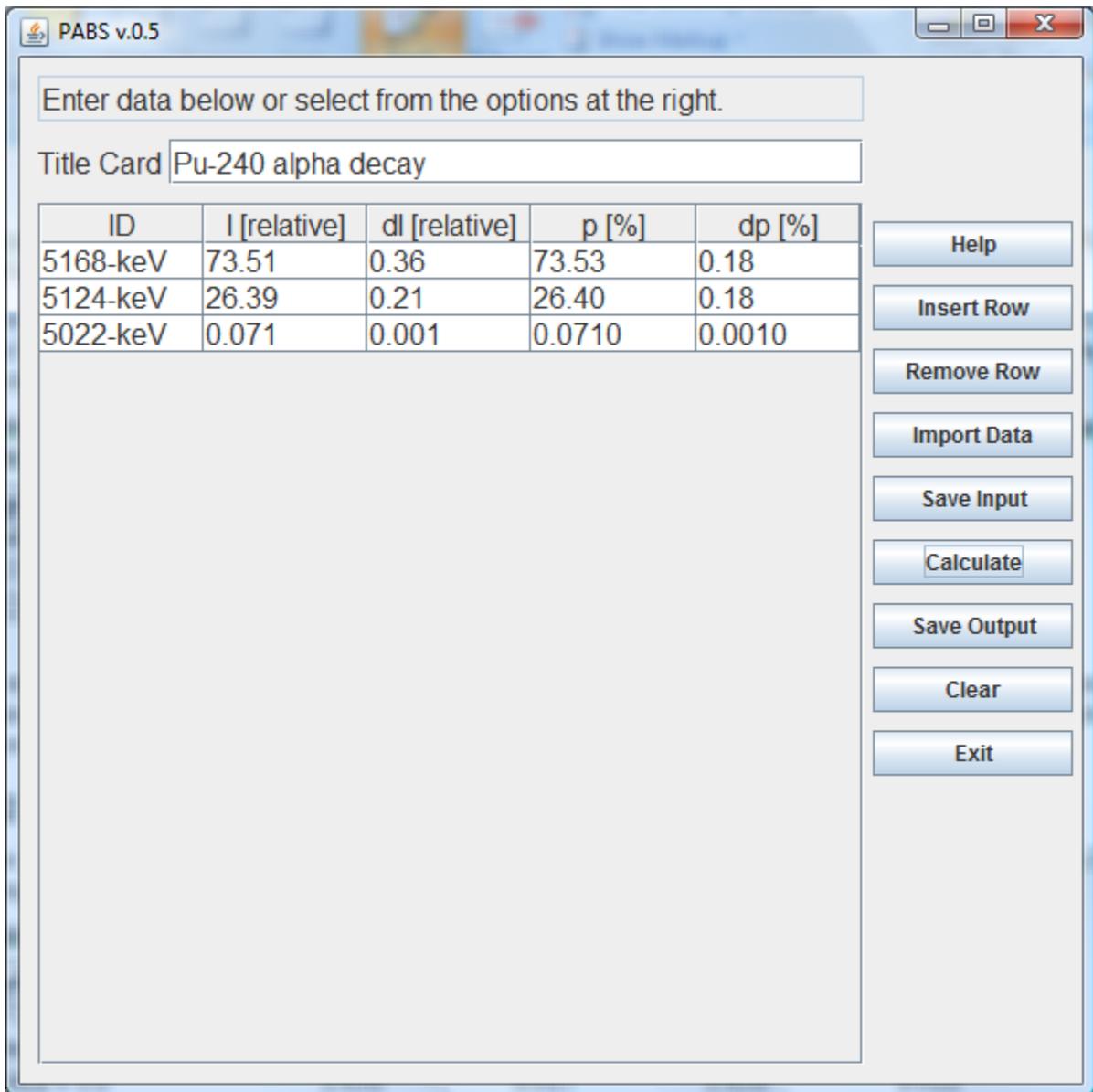


Figure 1. PABS main window as it appears following the ^{240}Pu calculation.

Choosing the *Save Output* function would generate the following output file:

```
Pu-240 alpha decay
% ID,I[rel.],dI[rel.],p[%],dp[%]
5168-keV,73.51,0.36,73.53,0.18
5124-keV,26.39,0.21,26.40,0.18
5022-keV,0.071,0.001,0.0710,0.0010
```

Notice that the calculated emission probabilities are essentially the same as the input values because the latter have been given on the same scale (per 100 emitted particles). However, their calculated uncertainties are significantly different due to the constraint imposed by the normalization procedure (i.e., the sum of the absolute emission probabilities should be 100 %, without any statistical uncertainty).

Now, consider a variation on this example. The same input data as that which appeared previously can be specified on an arbitrary relative scale as is shown in Table 1, along with the corresponding normalized emission probabilities and uncertainties.

Table 1. Normalization of ^{240}Pu alpha decay data with input values given on an arbitrary relative scale.

Alpha energy [keV]	I [rel.]	dI [rel.]	p [%]	dp [%]
5168.17 ± 0.15	100.00	0.49	73.53	0.18
5123.62 ± 0.25	35.90	0.29	26.40	0.18
5021.5 ± 0.5	0.0966	0.0014	0.0710	0.0011

As expected, the calculated normalized particle emission probabilities and their associated uncertainties are identical to those shown in the previous case, with the exception of the least significant digit in the uncertainty of the third alpha particle group.

Write to E. Browne at ebrowne@lbl.gov for a copy of the PABS executable JAVA program, including sample data.

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References

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