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ENSDF Analysis and Utility Codes

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Theory and Evaluation
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ENSDF Analysis and Utility Codes

Their Descriptions and Uses

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Summary

The ENSDF analysis and checking codes are briefly described, along with their uses with various types of ENSDF datasets. For more information on the programs see “Read Me” entries and other documentation associated with each code (<http://www.nndc.bnl.gov/nndc/ensdfpgm/H>). The current status and platform availability may be obtained at http://www.nndc.bnl.gov/nndcscr/ensdf_pgm/code_status.html.

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How to Use the Programs

FMTCHK

FMTCHK should be run every time the ENSDF formatted file has been manually changed before executing any of the other programs. All fatal errors (indicated by “<F>”) should be corrected. If possible, all errors (indicated by “<E>”) should be corrected. Warning messages (indicated by “<W>”) should be checked to see if there are problems that may need correction. For small input files, use of the default options is recommended. For larger files, the user may wish to make several iterations, starting with fatal errors only. This program should also be run on the final version before submittal to the NNDC.

Notes:

1. It is sometimes difficult to judge whether a message should be flagged as an error or warning. If you disagree with an error message, please indicate this along with your reasons on submittal or before. In some instances, error messages are given because of the possible effects on other programs. Two examples are:
 - a. It is considered an error when a mixing ratio is given and there is no associated mixed multipolarity. This is a problem since programs such as RULER or HSICC will be unable to perform the proper calculations. Note that the converse (*i.e.*, a mixed multipolarity given with no mixing ratios) may be addressed by assuming a 50%/50% admixture of the two multipolarities.
 - b. It is considered an error when an “FL=” is not given and there are no final levels with a certain limit or there are more than one level which may be considered the final level based on $E_{\text{level}} - E_{\gamma}$. This is a problem, particularly for complex level schemes such as in the adopted dataset, for level scheme programs such as ENSDAT or Isotope Explorer and programs such as GTOL, which do a least-squares adjustment of the level energies, or programs such as PANDORA.

ENSDAT and TREND

ENSDAT produces level schemes, bands, and tables in a format similar to that of the *Nuclear Data Sheets* and may be used to visual expect the results. TREND provides a simpler ASCII presentation of the tabular data that does not require a PostScript printer or viewer. One should also be able to copy the list of keynumbers generated by ENSDAT into the clipboard and paste this into the keynumber form of the NNDC Web NSR to obtain the NSR entries corresponding to these keynumbers.

Adopted Levels, Gammas Datasets

As well as ENSDAT, FMTCHK, and TREND, applicable programs for these datasets are ADDGAM, GTOL, HSICC, PANDORA, and RULER. ADDGAM and PANDORA are useful in constructing the dataset. In addition, PANDORA may be used iteratively to aid in physics decisions, checking assignments, and updating source datasets based on changes in the adopted data. GTOL is useful only in obtaining the least-squares adjustment of the level energies; for complex datasets, the matrix to be inverted may be singular (see Additional notes under GTOL for methods of handling this problem). RULER may be used in the comparison mode to provide additional information in obtaining γ -multipolarity assignments. HSICC and RULER should also be run to provide the internal conversion coefficients and $BE\lambda$ Ws and $BM\lambda$ Ws, respectively; note that HSICC should be executed before RULER. HSICC should also be run to provide the internal conversion coefficients; note that there is no need to delete the “S G” records generated by HSICC; the publication program automatically suppresses these when the evaluation is prepared for submission to Academic Press. Figure 1 shows the approximate order in which the programs are run. Note that this is an iterative process and, as changes are made, various programs will need to be rerun (in particular, FMTCHK).

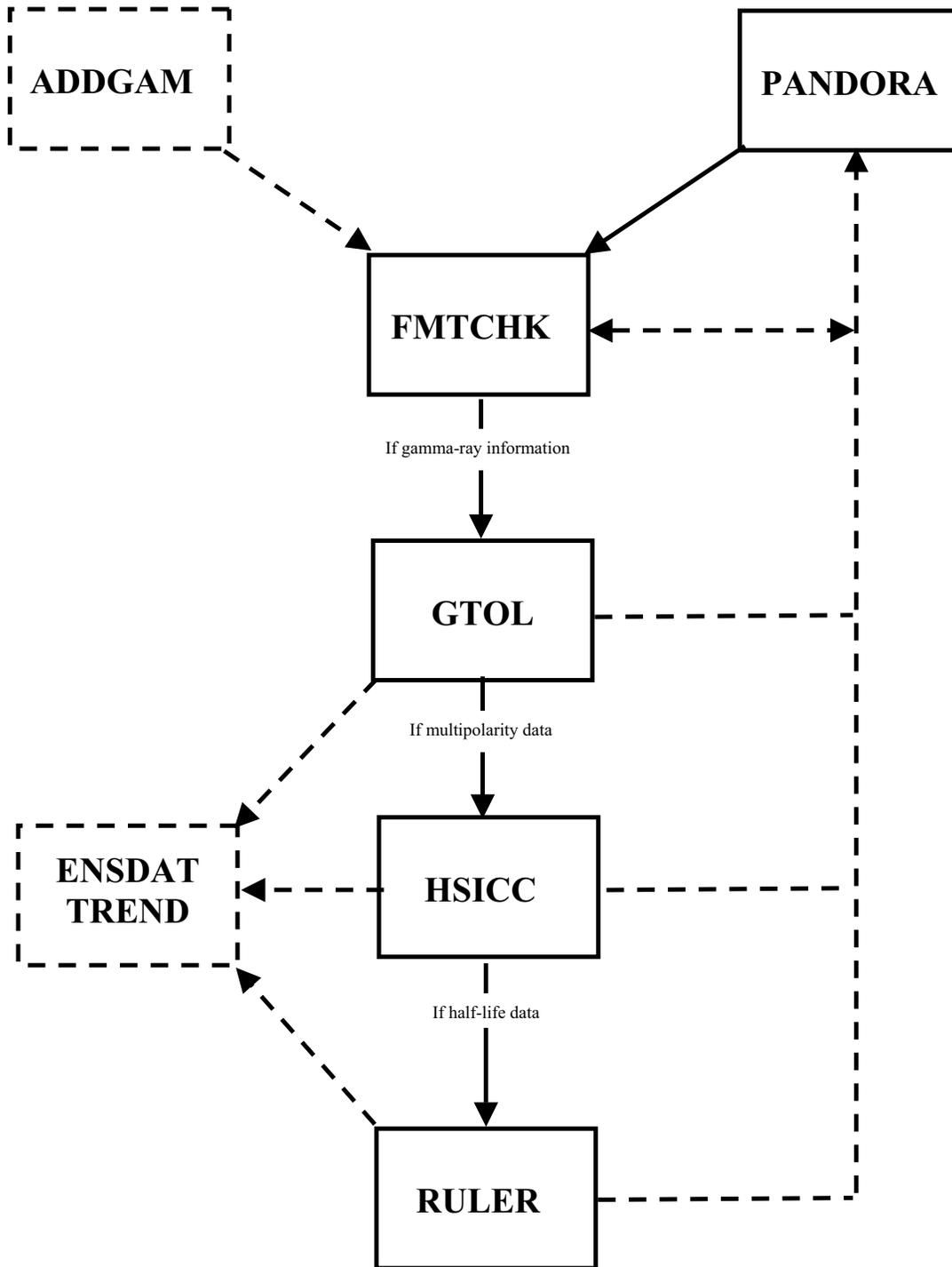


Figure 1: Flowchart of programs for Adopted Levels, Gammas datasets

Decay Datasets

Along with ENSDAT, FMTCHK, and TREND, applicable programs for these datasets are ALPHAD (for α decay), GABS, GTOL, HSICC, LOGFT (for β^\pm/ϵ decay), RadList, and RULER. Figure 2 shows the approximate order in which the programs are run. Note that this is an iterative process and, as changes are made, various programs will need to be rerun (in particular, FMTCHK).

1. ALPHAD should be used to obtain the hindrance factors and, for even-even ground-state nuclei, r_0 . For other nuclei, an r_0 must be supplied.
2. GABS may be used to combine the data from up to three sources to obtain I_γ -normalization (NR), the branching ratios (BR), and absolute I_γ s. HSICC should run on the input data or the internal conversion coefficients from the adopted dataset should be used.
3. GTOL may be used to provide a least-squares adjustment of the level energies. It should be used to check the uncertainties and placement of the γ s. If there are a large number of γ s and few whose energies deviate from the calculated energies, the experimental uncertainties may be overestimated; on the other hand, if there are a large number of deviations, the uncertainties may be underestimated. Also, for any deviation of over $\approx 3\sigma$, the placement of the transition should be carefully checked. GTOL should also be used to obtain the intensities of particles feeding the levels; this should be done before ALPHAD and LOGFT are employed and may be useful in deriving I_γ -normalization (NR).
4. HSICC may be used to check experimentally measured internal conversion coefficients against theory. If the adopted internal conversion coefficients are not used, HSICC should be executed to produce this information for the data set. This should be done before GABS, GTOL, or RadList are used.
5. LOGFT is required to obtain the $\log ft$ s, I_{β^+} and I_ϵ , and partial electron-capture fractions. This should be done before using RadList. If one is not using measured intensities, GTOL should be used to obtain I_{β^-} and $I_{\epsilon+\beta^+}$.
6. RadList should be used to check the calculated energy deposited with that predicted by the Q -value and branching ratios. If X-ray intensities are measured, these should be compared to those calculated by the program. If discrepancies cannot be resolved, these should be noted in the dataset. ALPHAD, HSICC, and LOGFT should have been used before doing these checks.
7. If $T_{1/2}$ s have been measured, RULER may be used to check or further limit multipolarities based on other methods (*e.g.*, from experimental conversion coefficients).

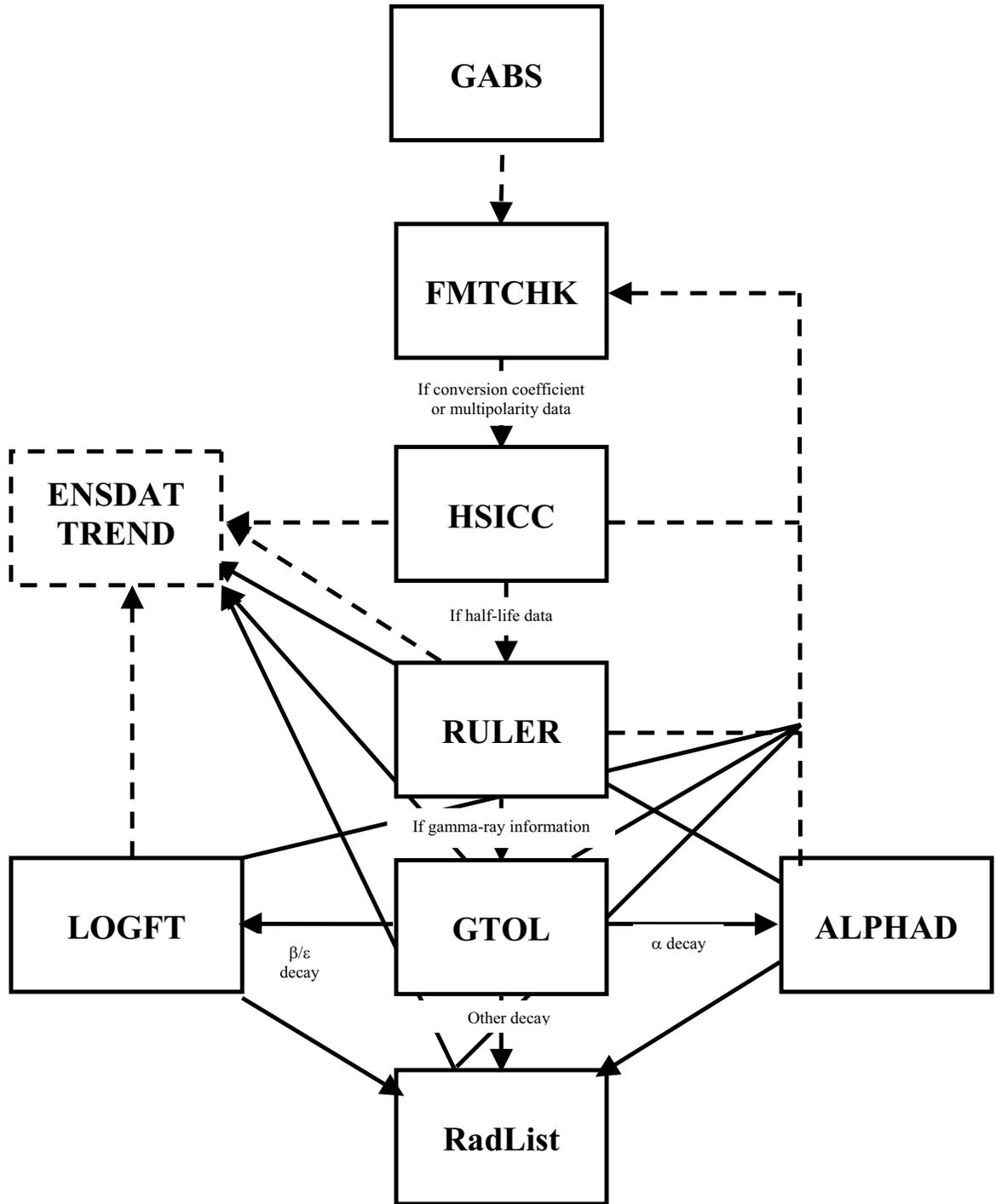


Figure 2: Flowchart of programs for decay datasets

Reaction Datasets

Along with ENSDAT, FMTCHK, and TREND, applicable programs for these datasets are GTOL, HSICC, and RULER. For (thermal n, γ) datasets, RadList may also prove of use. Figure 3 shows the approximate order in which the programs are run. Note that this is an iterative process and, as changes are made, various programs will need to be rerun (in particular, FMTCHK).

1. GTOL's primary use is to do a least-squares adjustment of the level energies and to check the uncertainties and placement of the γ s as described above. Note that it is now common for authors to omit the $\Delta\gamma$ s; if the evaluator cannot obtain a good estimate of these, it may be better to use the author's level energy values. It is also useful for checking for intensity imbalance problems if relative intensities are given.
2. HSICC may be used to check experimentally measured internal conversion coefficients against theory. While it is generally not required to include the conversion and partial conversion coefficients for reaction datasets, it is very useful to do this for (thermal n, γ) datasets.
3. If half-lives ($T_{1/2}$) have been measured, RULER may be used to check or further limit multiplicities based on other methods (*e.g.*, from experimental conversion coefficients).
4. RadList may be used to check the energy balance of (thermal n, γ) datasets by tricking it into believing the dataset is an IT decay dataset. This is done by changing the DSID on the ID record, adding an appropriate Parent record (level energy equal to the neutron separation energy) and a BR of 1.0 on the Normalization record.

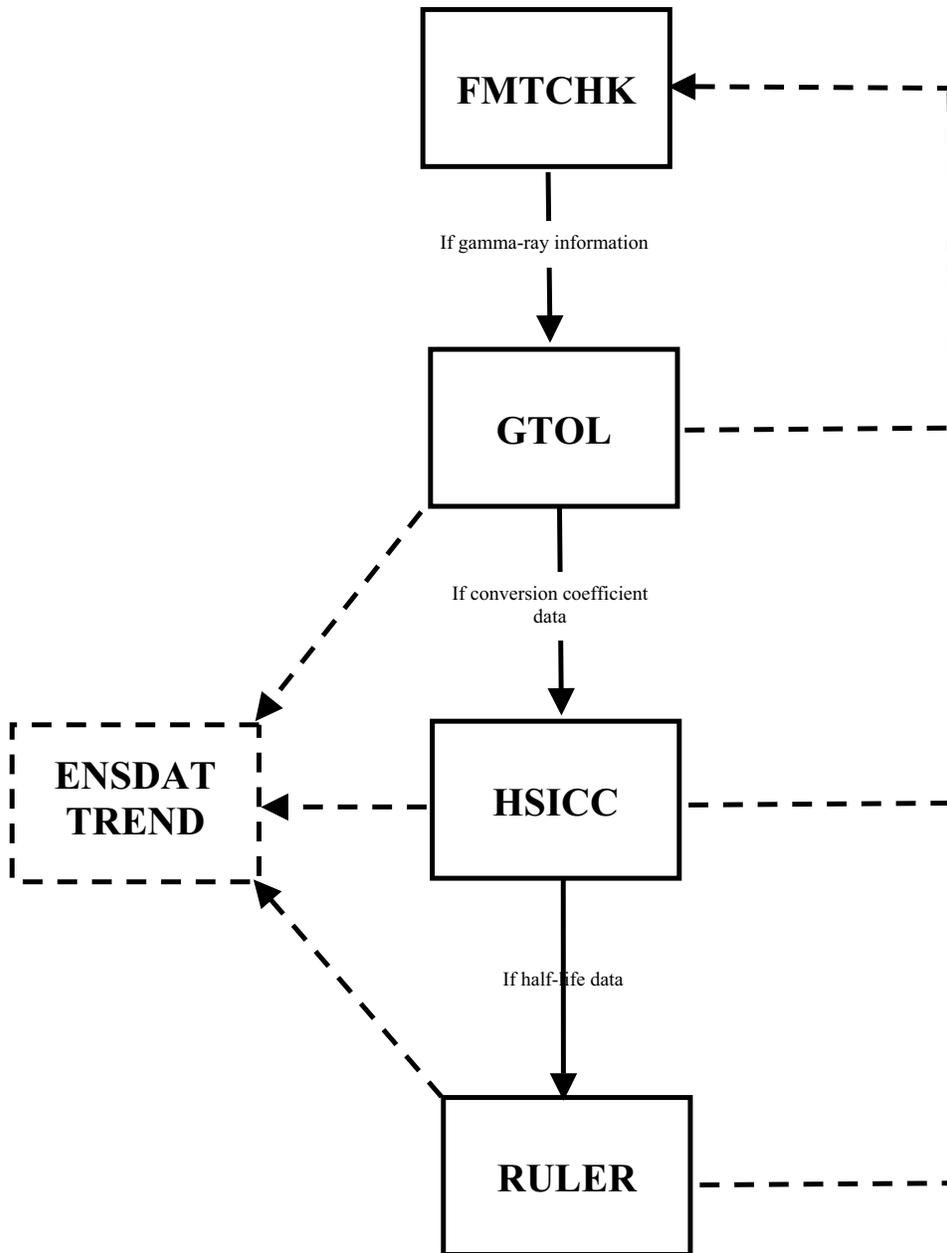


Figure 3: Flowchart of programs for reaction datasets

ADDGAM

Version 1.4 [Feb. 7, 2001]

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This program adds γ s to the Adopted Levels when all γ s come from one data set. If γ s come from more than one data set but are non-overlapping, the program may be run successively with different γ data sets as input.

Input files (ENSDF format):

- 1) Data set containing the adopted levels. Sample input file: ADDGAML.DAT
- 2) Data set containing the gammas to be added. Sample input file: ADDGAMG.DAT

Output file: Merged set containing the information in (1) and the γ s from (2). Sample output file: ADDGAM.NEW

Terminal dialog: The user will be asked to provide the file names for the data set containing the adopted levels, the file for the gammas to be added, and the file for the new data set.

Compilation and loading instructions: This program requires subroutines from the NSDFLIB package.

Additional documentation: None

ALPHAD

Version 1.6 [Feb. 7, 2001]

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(Original Authors: H.V. Michels, Y. Sanborn, R.C. Ward)

This program calculates the α hindrance factors and theoretical $T_{1/2}$ and, for even-even ground state to ground state transitions, r_0 using Preston's spin-independent equations (M.A. Preston. Phys. Rev. 71, 865 (1947)).

The program reads an ENSDF-formatted file and produces a report of the hindrance factors, theoretical $T_{1/2}$ s, and r_0 s calculated by the program. This report will also summarize any problems encountered or assumptions made. There is also an option to produce a new file using containing the HF's calculated. r_0 s may be specified on an ALPHA comment record by "HF" in columns 10 and 11 and a dollar sign ("\$\$") in column 12 or blanks in columns 12 through 19. The first value and uncertainty in columns 20 through 80 preceded by an R ("R") and an equal sign ("=") or approximate sign ("AP") will be taken as r_0 .

Sample input file: ALPHAD.DAT

Sample output files:

1. ALPHAD.RPT - Report of calculations
2. ALPHAD.NEW - New ENSDF file containing the hindrance factors (HF's) calculated by the program.

Terminal dialog:

1. **Input data file (Default: ALPHAD.DAT):**
2. **Output report to file (Y/N):**
The default is "Y". If NO is answered, the report will be displayed on the terminal. If YES is answered, the following query will appear:
Output report file (Default: ALPHAD.RPT):
3. **Echo input (Y/N):**
The default is "Y". In this case the input file will be copied to the report file.
4. **Rewrite input with hinderance factor (Y/N):**
The default is "Y". If YES is answered, the following query will appear:
Output data set file (Default: ALPHAD.NEW):

If the report output is to a file, the terminal output will note the progress in the calculations and report warning messages.

Compilation and loading instructions: This program requires subroutines from the NSDFLIB package.

Additional notes:

1. Calculation of Δr_0 : Five values are calculated: $r_0(T_{1/2}(\alpha), E_\alpha)$, $r_0(T_{1/2}(\alpha) + \Delta T_{1/2}(\alpha), E_\alpha)$, $r_0(T_{1/2}(\alpha) - \Delta T_{1/2}(\alpha), E_\alpha)$, $r_0(T_{1/2}(\alpha), E_\alpha + \Delta E_\alpha)$, and $r_0(T_{1/2}(\alpha), E_\alpha - \Delta E_\alpha)$. $\Delta r_0 = \sqrt{((|r_0(T_{1/2}(\alpha) + \Delta T_{1/2}(\alpha), E_\alpha) - r_0(T_{1/2}(\alpha) - \Delta T_{1/2}(\alpha), E_\alpha)|)/2)**2 + ((|r_0(T_{1/2}(\alpha), E_\alpha + \Delta E_\alpha) - r_0(T_{1/2}(\alpha), E_\alpha - \Delta E_\alpha)|)/2)**2)}$. r_0 and Δr_0 as calculated are output in the report file and so are $r_0(T_{1/2}(\alpha) + \Delta T_{1/2}(\alpha), E)$, $r_0(T_{1/2}(\alpha) - \Delta T_{1/2}(\alpha), E)$, $r_0(T_{1/2}(\alpha), E + \Delta E)$, and $r_0(T_{1/2}(\alpha), E - \Delta E)$.
2. If either the value or the uncertainty for E_{parent} , Q_α , or E_{level} is non-numeric and E_α and ΔE_α are numeric, E_α and ΔE_α are used in the calculations. NOTE: For systematic uncertainties in Q_α from the Audi-Wapstra Mass Tables, the input data should be modified to use the estimated uncertainty and the new output edited to change DQP back to "SY".
3. If there is more than one non-numeric uncertainty involved, the order of precedence is limits (*e.g.*, GT or LT) and then "AP", "CA", and "SY" for the new output.

Additional documentation: None.

Acknowledgements: I thank Y. Akevali and M.J. Martin for many useful discussions on the physics involved, for their many suggestions on improving the output, and for testing various versions of this code.

COMTRANS (COMment TRANSlation)

Version 7.0 [August 8, 2003]

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The program COMTRANS is a nuclear structure evaluator tool for translating comments in the Evaluated Nuclear Structures Data File (ENSDF) from the all upper case form to the upper/lower case form. In addition, translations of code words found in the NSD dictionary are made into a rich text type of format (*e.g.*, |a replaces ALPHA and {+56}Fe replaces 56FE). These comments no longer need to be used with the NSD dictionary. However, evaluators should note that adding a code word to such a translated comment means they must change the lower case comment flag (c or t) in column 7 to an upper case comment flag (C or T) or rerun the file using COMTRANS. Otherwise, ENSDAT (and the publication code), which do not translate lower case comment (c or t) cards), will output the code word unchanged. Finally, the input file is converted into an Y2K compliant form if it is not in that form. All keynumbers are changed from the old six-character keynumber (85AU01) into the new eight-character Keynumber (1985AU01). The keynumbers fields of the ID and Q cards are also changed to comply with the Y2K formats.

The program asks for an input file name, an output file name and options. The ENSDF translation dictionary file must be in the same directory from which the program is executed. The input and output files may include a disk and directory path.

Program files:

1. comtrans_sl.exe
2. ensdf_dic.exe - dictionary creation program.

Text files:

1. ensdf_dic.dat - sequential text file of the dictionaries used to create ra_ensdf_dic.dat.

Input files:

1. An ENSDF formatted file. Sample input file: comtrans.tst
2. ra_ensdf_dic.dat - (direct access binary file) contains the ENSDF translation dictionaries used by ENSDAT and COMTRANS; must be in the execution directory.

Sample output file: comtrans.out (Y2K compliant)

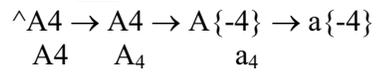
Terminal dialog: The program will request the following information:

1. Input
2. Output

Compilation and loading instructions: Only the executable is supplied.

Additional notes:

1). Should **not** be run on ENSDF or XUNDL files submitted to the NNDC.



2). Useful to run before using Isotope Explorer 2 or ENSDAT.

- a. Isotope Explorer 2 assumes that the comments have been translated into a “rich text” format and does not carry out a dictionary lookup.
- b. ENSDAT may be faster since it will not have to do a dictionary lookup for the comments.

Limitations:

1. No triple correlations.
2. Spins up to 20 are allowed, except when unobserved transitions are involved. For unobserved transitions the maximum spin is 10. These limitations are valid if the computer can handle double precision reals of up to 10^{76} .
3. Effects of internal conversion on the deorientation coefficients for mixed transitions are neglected. See Anicin *et al.*, Nucl. Instrum.Meth. 103, 395 (1972) for this usually very small effect.

NOTE: Except for the changes made in input and output units and to conform to ANSI-77 standard, this code is as provided by the author.

Input file: All records have the following format:

COL. 1-2 Symbol that determines type of card.

COL. 3-72 Free format reals or integers. Separator: any character different from '0-9', '.' and '!'. Everything following a '\$' is ignored. This can be used for comments on the data cards. Only DATA and GO cards are necessary. Uncert. = 0 for δ means that δ is kept fixed. new data with same name as existing data replace the latter.

Options (parameters in () are optional):

CL	Clear data
DU	Dump common blocks (for debugging)
OU A	A = 0 short output (default) A > 0 FULL OUTPUT
ST ST1,(ST2)	Step size (in degrees) for $\tan^{-1}(\delta_1)$ and $\tan^{-1}(\delta_2)$, respectively
EN	End of run
GO RJ1,RJ2,(RJ3)	Read spins and go. RJ's are reals or integers (e.g., 5/2- = -2.5, 2+ = 2, 0- = -0) Maximum 6 spins.
HE ANY TEXT	Header
LI A,B,C,D	Limits $\tan^{-1}(\delta_1)$ to A to B and $\tan^{-1}(\delta_2)$ to c to d
UN (DU(1), DU(2), DU(3))	Unobserved transitions, δ s. Defaults = 0.0
Correlation and DELTA data	
A2 A2,DA2	$A_2, \Delta A_2$
A4 A4,DA4	$A_4, \Delta A_4$
D NTR (,DELTA,DDELTA)	Transition number, $\delta, \Delta\delta$. Defaults: none, 0, 0
Conversion coefficient data (maximum 5 items)	

** NTR, EXP, DEXP, L1, H1(L2,H2)	where ** is any unique combination of symbols (e.g., CC, AK) NTR The number of the transition (1 or 2) EXP Experimental value DEXP Uncertainty L1 Theoretical value for the lower multipole (SHELL1) H1 Theoretical value for the higher multipole (SHELL1) For ratios SHELL1/SHELL2: L2 Theoretical value for the lower multipole (SHELL1) H2 Theoretical value for the higher multipole (SHELL2)
-------------------------------------	---

Sample input data set: DELTA.DAT

Output file (Short output marked with an asterisk (*)):

For each spin combination (each GO card):

* Option and data cards read

* Header

* Data

Header

χ^2 and best theoretical values of data (step in δ_1)

* Best δ_1

Header

* Plot of χ^2 versus $\tan^{-1}(\delta_1)$

Header

χ^2 and best theoretical values of data (step in δ_2)

* Best δ_2

* Plot of χ^2 versus $\tan^{-1}(\delta_2)$

* 'END OF ANALYSIS FOR THIS SPIN COMBINATION'

Optionally a dump of common block variables can be obtained.

Sample output: DELTA.RPT

Terminal dialog: The user will be requested to supply the input file name and the output file name.

Compilation and loading instructions: No special instructions

Additional documentation: DELTA - A computer program to analyze gamma-gamma correlations from unaligned states. L.P. Ekstrom. Nuclear Physics LUNFD6/(NFFR-3048) 1-27,(Lund University. 1983).

ENSDAT (Evaluated Nuclear Structure Drawings and Tables)

Version 9.7 [Sep. 11, 2000]

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The program ENSDAT (Evaluated Nuclear Structure Drawings And Tables) is similar to the production program for the Nuclear Data Sheets but more limited in its application. Only ENSDF data files can be used as input and a PostScript file, list of keynumbers in NSR, and a report file are output. As the default, all possible tables, band drawings, and gamma drawings are done for each dataset encountered in the input file. However, it is possible to choose one or more of these groups of output (see below). In addition, it is possible to modify the default tables and drawings by adding commands to the input file using control cards. (see the file `enscmds.txt`.) A final page is output to the PostScript file, which gives a listing of all the keynumbers, encountered in the input file.

Program files:

1. `ensdat.exe`
2. `ensdf_dic.exe` - dictionary creation program.

Text files:

1. `enscmds.txt` - instructions for using commands in the input file.
2. `ensdf_dic.dat` - sequential text file of the dictionaries used to create `ra_ensdf_dic.dat`.

Input files:

1. An ENSDF formatted file. Sample input file: `adopted.186`.
2. `ra_ensdf_dic.dat` - contains - translation dictionaries. `ensdf_dic.exe` must be run to create the ISAM files used by ENSDAT and COMTRANS.

Outputs:

1. PostScript file of tables and drawings in a form similar to the Nuclear Data Sheets.
2. Report file summarizing work done and any errors noted.
3. File listing the keynumbers (NSR) found in the input file.

Sample output files: `ad_186.log` and `ad_186.ps`.

Terminal dialog: The program will request the following information:

1. Input - input file specification
2. Output - output file name
3. Options - one or more of the following options can be entered, separated by a blank:

TABLE Level, gamma, and radiation information will be output in tabular format.
BAND Band drawings will be output. Radplot type drawings are also output.
DRAW Gamma drawings will be output.

NOAUTO No drawings or tables will be generated except those that are specified by the user on control cards, added to the input file. If none of these options are used, all tables, band drawings (if any), and gamma drawings (if any) will be output to the PostScript file.

4. View output - Yes or No (optional - see installation instructions for details)

Command Line dialog: ENSDAT *input output [option]*

Compilation and loading instructions: Only the executable is supplied.

Additional documentation: Following the output file name, several options are available to the user. The output file name must be followed by a blank and then, if desired, one or more of the following options:

TABLE	Level, gamma, and radiation information will be output in tabular format.
BAND	Band drawings will be output.
DRAW	Gamma drawings will be output.
NOAUTO	No drawings or tables will be generated except those, which are specified by the user on control cards added to the input file.

As before, if none of these options are used, all tables, band drawings (if any), and gamma drawings (if any) will be output to the PostScript file.

FMTCHK

Version 9.0g [August 4, 2003]

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(Original author: Bruce J. Barton)

This program analyzes the format of an ENSDF formatted file to verify that it conforms to "Evaluated Nuclear Structure Data File. A Manual for Preparation of Data Sets" by J.K. Tuli, Brookhaven National Laboratory Report BNL-NCS-63155-01/02 (2001) and subsequent memos.

Input file (ENSDF format): Sample input file is DATA.TST

Output file: A report file indicating possible errors or warnings is generated. Sample output file: FMTCHK.RPT. Brief explanations of the fatal error (prefix <F>), error (prefix <E>), warning (prefix <W>), and informational (prefix <I>) messages are given in READFMTC.ME or READFMTC.HTML.

Terminal dialog: The user will be asked to supply the input and output file names, if errors only should be reported or the complete file reported (default: errors only), if continuation records should be checked (default: check continuation records), if only fatal errors should be reported (default: no), if warning messages should be suppressed (default: no suppression). This query will be suppressed if only fatal errors are to be reported), and if the checking of the XREF *versus* DSID should be suppressed.

As the data sets in the input file are processed, this will be indicated on the terminal. After each data set is processed, the total number of fatal error, error, and warning messages will be reported. If both adopted data sets and "source" data sets are in the file, the X records and IDENTIFICATION records will be compared and any discrepancies listed.

Compilation and loading instructions: This program requires subroutines from the NSDFLIB package.

Additional documentation: None.

Additional notes:

1. For level energies of the form X, Y, Z, *etc.* or E + X, E + Y, E + Z, *etc.*, an arbitrary energy is assigned to the first occurrence of the character based on the energy of the previous level energy. This is reported as an informational message in the report file and is used to see if the levels are in the proper energy order.

GABS

Version 9.2 [Feb. 7, 2001]

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GABS calculates absolute gamma-ray intensities and a decay-scheme normalizing factor (NR) for converting relative intensities to absolute values per 100 decays of the parent nucleus. The program calculates the decay mode branching ratios (BR) for radionuclides that decay through several decay modes. It also calculates the uncertainties in all these quantities.

Input file: GABSPC reads up to three data sets (ENSDF format). See the documentation for modifications to the standard ENSDF format for use by this program. Sample input: GABS.IN.

Output files:

1. Report file summarizing the results of the calculations (default: GABSPC.RPT).
2. New ENSDF formatted file containing the results of the calculations (may not already exist). Sample output: GABS.OUT

Terminal dialog: The program will ask for an input file name, a report file name, if a new file should be created ("Y"; default is no, case insensitive), and, optionally, the name of the output file.

Compilation and loading instructions: This program requires subroutines from the NSDFLIB package.

Additional documentation: PROGRAM GABSPC (Version 9, May 2000). Edgardo Browne, Lawrence Berkeley National Laboratory. Adapted for IBM PC by Coral M. Baglin (September 1991).

GTOL

Version 6.4a [July 11, 2001]

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(Original authors: W.B. Ewbank, Nuclear Data Project, Oak Ridge National Laboratory; B.J. Barton, National Nuclear Data Center, Brookhaven National Laboratory; and L.P. Ekstrom and P. Andersson, Department of Nuclear Physics, Lund University)

In this program, gamma-ray energies are used to derive a set of least-squares adjusted level energies. The net feeding at each level is calculated from the input γ intensities and conversion coefficients. Unplaced or questionable γ s, or γ s whose final level is ambiguous or unknown are ignored.

The program parses the DSID of each data set and, if there is no indication of possible gamma records within the data set, skips it. In addition, the program will not calculate the intensity balancing for adopted data sets.

Input file: An ENSDF formatted file with the following optional information:

An option record with 'OPTION' in col. 1-6 may precede any data set and contain any of the following options in free format:

Option	Meaning
NOREC	No recoil correction, <i>i.e.</i> , recoil correction has already been applied to E_γ
RECOIL	Perform recoil correction (DEFAULT)
MARKED	Process only data sets preceded by a card with '*GTOL' in col. 1-5
ALL	Process all data sets (DEFAULT)
DEG=	For the current data set, override default assumption of 1 keV where no uncertainty on the gamma energy is given. Following the equal sign may be either a number or a number followed by a percent sign. A number alone indicates the uncertainty on E_γ in keV while a number followed by a percent sign indicates the fractional percent uncertainty to be assigned.
DRI=	For the current data set, assume a default uncertainty for the relative I_γ when none given. A number alone indicates the uncertainty on I_γ in the current relative units while a number followed by a percent sign indicates the fractional percent uncertainty to be assigned.
DTI=	For the current data set, assume a default uncertainty for when none given. A number alone indicates the uncertainty on $I_{\gamma+ce}$ in the current relative units while a number followed by a percent sign indicates the fractional percent uncertainty to be assigned.

Note that an option card resets the defaults.

A level energy can be held fixed by adding the letter 'F' somewhere in the energy field (columns 10 - 21). If the output option to create a new file containing the adjusted level energies is chosen, 'F' will be removed and a level documentation record will be added (LEVEL ENERGY HELD FIXED IN LEAST-SQUARES ADJUSTMENT).

If DRI= or DTI= are specified on an OPTION record, the assumed uncertainty may be overridden for an individual intensity, by adding an "E" separated from the intensity in either the RI or TI fields.

If DEG=, DRI=, or DTI= are specified on an OPTION record and a new file is created, FOOTNOTE COMMENTS will be generated and inserted as necessary.

Sample input file: DATA.TST

Output files:

1. Report file. The report file will contain a summary of the data input and actions taken by the program (*e.g.*, unplaced or questionable γ s ignored) and the following optional outputs for each data set:
 - a. Comparison of input gamma energies to those calculated based on the adjusted level energies.
 - b. Comparison of calculated net feedings to each level with values input on B, E, or A records

Note: if the calculated net feeding overlaps zero within three standard deviations, the program will calculate estimated upper limits (90% confidence level) using two methods suggested by Louis Lyons in *Statistics for Nuclear and Particle Physicists* (Cambridge University Press) and report these estimates if they differ by more than 0.01. The two methods are:

- i. $(\text{Integral of } gdB \text{ from } 0 \text{ to } B1) / (\text{Integral of } gdB \text{ from } 0 \text{ to infinity}) = 0.9$ where g is the normal (Gaussian) distribution.

- ii. $B_I < B_M + 1.28\sigma$.
- c. If a new file is generated a comparison of the old and new records will also be generated.

Sample output file: GTOL.RPT

- 2. New file containing the adjusted level energies (optional). Sample output file: None

Terminal dialog: The program will request the input and report (default: GTOL.RPT) file names and ask if you wish a new file created (default: no new file) and for the new file name, to suppress the gamma-energy comparison (default: no suppression), and to suppress the intensity comparison (default: no suppression). The progress of the program will be noted on the terminal as well as possible problems.

Compilation and loading instructions: This program requires subroutines from the NSDFLIB package.

Additional documentation:

B.J. Barton and J.K. Tuli. Physics analysis programs for nuclear structure evaluation. Brookhaven National Laboratory Informal Report BNL-NCS-23375/R (1977).

L.P. Ekstrom and P. Andersson. FORTRAN 77 versions of string handling subprograms and the programs GTOL and MEDLIST. Nuclear Physics Report LUNFD/(NFFR-3049)/1-27, (Lund University, Sweden. 1983).

Additional notes:

1. If the level energies are of the form X, Y, Z, *etc.* or E + X, E + Y, *etc.*, the least-squares fit is done separately for each group of states and merged back into the final results. Similar to FMTCHK, an arbitrary energy is assigned to the level based on the energy of the previous energy. This is used to sort the levels in the energy comparison but is not used when creating the new output file.
2. FMTCHK should be rerun if a new file is created since the order of the level energies may have changed as a result of the least-squares adjustment. This may occur when there are two closely lying levels or if there is a series of levels with unknown energies (*e.g.*, E + X) interspersed with levels of known energy.
3. If the connecting information is too sparse, the matrix created may be singular and cannot be inverted (this generally occurs for adopted datasets and other datasets where there are levels with no de-exciting γ s). In such instances, check the report file for levels that do not de-excite and fix these levels.
4. As noted above, uncertainly placed γ s are ignored in the least-squares fit and the intensity balance calculations. This means possible additional iterations to obtain an estimate of the excitation energies and their possible contributions to the uncertainties of the intensity balances:
 - a. To obtain an estimate of the excitation energies of levels only connected by such transitions, modify the input by removing the “?” in column 80 of the relevant gamma records and adding “F” in the energy fields of any connected level records which also are fed or de-excited by other γ s. Factor the results of the new least-squares fit into the original file.

- b. To obtain an idea of the effect of uncertainly placed γ s on the intensities, modify the input file by removing all “?” in column 80 of the gamma records. By comparing the original intensity balance calculations with the new one, you will be able to estimate the effect of these transitions on the balance uncertainties.

HSICC Program Package

The HSICC program package consists of the programs HSICC (calculates internal conversion coefficients), HSMRG (merges new gamma records created by HSICC with the original input data), BLDSHST (builds a direct access file of the internal conversion coefficient table), and SEQHST (recreates a sequential file of the internal conversion table from the direct access file). These are described separately on the following pages.

Compilation and loading instructions: HSICC requires subroutines from the NSDFLIB package; the others do not.

HSICC Program Package — HSICC

Version 11.13f [Oct. 9, 2001]

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This program calculates internal conversion coefficients by spline (cubic) interpolation tabulated values from Hager and Seltzer for the K, L, and M shells and from Dragoun, Plajner, and Schmetzler for the N + O +... shells.

Input files:

1. ENSDF formatted file. Sample input file: DATA.TST. NOTE: The input data should not be modified before running the code HSMRG.
2. ICC index file (created by the program BLDHST).
3. Binary file of ICCs (created by the program BLDHST).

Output files:

1. Complete report of calculations. Sample output file: HSCALC.LST.
2. New G/2G records generated by the program. This is used as input to the program HSMRG. Sample output file: CARDS.NEW.
3. Comparison of new and old G/2G records. Sample output file: COMPAR.LST.

Terminal dialog: The program will ask for the following information:

1. Input files
 - a. Name of input ENSDF file (default: DATA.TST)
 - b. Name of ICC index file (default: ICCNDX.DAT)
 - c. Name of ICC binary table file (default: ICCTBL.DAT)
2. Output files
 - a. Name of file from complete report (default: HSCALC.LST)
 - b. Name of file containing new G/2G records (default: CARDS.NEW)
 - c. Name of comparison file (default: COMPAR.LST)

Additional documentation:

R.S. Hager and E.C. Seltzer. Internal Conversion Tables. Part 1: K-, L-, M-Shell Conversion Coefficients for $Z = 30$ to $Z = 103$. Nucl. Data A4, 1 (1968).

O. Dragoun, Z. Plajner, and F. Schmutzler. Contribution of Outer Atomic Shells to Total Internal Conversion Coefficients. Nucl. Data Tables A9, 119 (1971).

B.J. Barton and J.K. Tuli. Physics analysis programs for nuclear structure evaluation. Brookhaven National Laboratory Informal Report BNL-NCS-23375/R (1977).

Additional notes: If E_γ is near the threshold for internal conversion, new records are not created.

HSICC Program Package — HSMRG

Version 7.1a [Sept. 17, 2001]

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(Original author: Bruce J. Barton)

This program merges the new (corrected) G-records created by HSICC with the input dataset file to create an updated dataset file.

Input files:

1. Input data file (ENSDF format). This must be the same input file used by HSICC. Sample input file: DATA.TST
2. Correction file of G-records created by HSICC. Sample input file: CARDS.NEW

Output file: Updated file (ENSDF format). Sample output file: CARDS.MRG

Terminal dialog: The program will ask for the names of the input file used by HSICC (default: DATA.TST), the correction file created by HSICC (default: CARDS.NEW), and the merged data file (default: CARDS.MRG).

Additional documentation: none

HSICC Program Package — BLDHST

Version 3.6 [Feb. 9, 2001]

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(Original author: Bruce J. Barton)

This program builds the Hager-Seltzer direct access table plus index from a sequential file.

Input file: A sequential access symbolic file of 80 character records (Z, SHELL, EG, E1, E2, E3, E4, M1, M2, M3, M4) = (I3, A2, F7.2, 8E8.2). Data file included: ICCSEQ.DAT. For MS-DOS, four additional files, H1.DAT through H4.DAT, are included covering Z = 3 - 34, Z = 35 - 59, Z = 60 - 82, and Z = 83 - 103, respectively.

Output files:

1. Direct access table consisting of a binary file of 11 word (44 bytes) records. 13004 records in the file if ICCSEQ.DAT is used as input.
2. An index consisting of a direct access binary file of one word (4 bytes) records. The Zth record is the integer record number pointer to the direct access table.

Terminal dialog: The program will first ask for the sequential input file name (default: ICCSEQ.DAT) and then the output table and index file names (defaults: ICCTBL.DAT and ICCNDX.DAT).

Additional documentation: none

HSICC Program Package — SEQHST

Version 3.4 [Feb. 9, 2001]

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(Original author: Bruce J. Barton)

This program converts the Hager-Seltzer direct access table to a sequential text file format.

Input file: The direct access table is a binary file of 11 word records. 13004 records in the file.

Output file: The text file is a sequential access symbolic file of 80 character records (Z, SHELL, EG, E1, E2, E3, E4, M1, M2, M3, M4) = (I3, A2, F7.2, 8E8.2). Data file included: ICCSEQ.DAT.

Terminal dialog: The program will first ask for the binary table file name (default: ICCTBL.DAT) and then the sequential output file name (default: ICCSEQ.DAT).

Additional documentation: none

LOGFT

Version 7.2a [Mar. 20, 2001]

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(Original authors: N.B. Gove and M.J. Martin, Nuclear Data Project, Oak Ridge National Laboratory, and B.J. Barton, National Nuclear Data Center, Brookhaven National Laboratory)

This program calculates $\log ft$ for beta decay. It also calculates the partial capture fractions for electron capture, the electron capture to positron ratio for positron decay, and the average beta energies. It will do special calculations for first and second forbidden unique; all other categories are treated as allowed.

Input files:

1. ENSDF formatted file. Sample input included: DATA.TST
2. Radial wave function data. Data file included: LOGFT.DAT

Output files:

1. Report file. Sample output included: LOGFT.RPT
2. New ENSDF formatted file with appropriate values for B and E cards updated. Sample output included: LOGFT.NEW

Terminal dialog: The program will ask for the names of the input data file (default: DATA.TST), the report file (default: LOGFT.RPT), the file containing the wave function data (default: LOGFT.DAT), and the file to be created (default: LOGFT.NEW).

Compilation and loading instructions: This program requires subroutines from the NSDFLIB package.

Additional documentation: N.B. Gove and M.J. Martin. Log-f tables for beta decay. Nuclear Data Tables A10, 206 (1971).

Additional notes:

1. New records will not be created if there are non-numeric parent or level energies, Q-values, or associated uncertainties.
2. If Lyon's method 1 has been used to estimate the intensity, LOGFT should also be run using the original values.

NSDFLIB

Version 1.5d [June 28, 1999]

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This subroutine package consists of three subroutine packages F77STR (Fortran 77 String Processing Library), NSDCNV (Fortran 77 Conversion Routines), and NSDMTH (Fortran 77 Mathematical Routines). All elements of the package have been written to conform to the ANSI standard for Fortran 77, and are therefore machine independent. The version number and date given in this "read me" is for F77STR.

Input file: none

Output file: none

Terminal dialog: none

Compilation and loading instructions: This subroutine package is required by most of the ENSDF analysis and utility codes and should be compiled and linked as necessary with them.

Additional documentation: Internal National Nuclear Data Center memo
NSDFLIB.MEM

PANDORA

Version 6.6a [Mar. 28, 2001]

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This program provides the following physics checks for an ENSDF file.

1. Decay data sets have a P-card
2. An L-CARD with $T_{1/2} > 0.1$ S should have MS FLAG.
3. Check consistency of spin/parity of levels with multipolarity connecting transitions.
4. For a transfer reaction with even-even target $J = L+1/2$.
5. For $3.6 < \log ft < 5.9$, $J^{i-1} \leq J^f \leq J^{i+1}$, no parity change. For 1U in cols. 78-79 and $\log ft \geq 8.5$ $J^f = J^{i \pm 2}$, parity change.
6. For alpha decay, if the mass is odd and $HF < 4$, $J^f = J^i$, no parity change.
If J^f or $J^i = 0$, parity change = $(-1)^{(J^f - J^i)}$
7. Levels out of order.

Input files: ENSDF formatted file. Sample input file: PANDIN.DAT.

Output files:

1. FILE.ERR. Errors and warnings about the input data. Sample output file: FILE.ERR.
2. FILE.GAM. Report of the γ s in the input file arranged by A, Z, E_γ , and DSID. Sample output file: FILE.GAM.
3. FILE.GLE. Report of the γ s in the input file arranged by A, Z, $E_{(\text{parent level})}$, E_γ , and DSID. I_γ given are branching ratios ($I_{(\text{strongest } \gamma)} = 100$). Sample output file: FILE.GLE.
4. FILE.LEV. Report of the levels in the input file arranged by A, Z, E_{level} , and DSID. Sample output file: FILE.LEV.
5. FILE.RAD. Report of β/ϵ in input file arranged by A, Z, $E_{\beta/\epsilon}$, and DSID. Sample output file: FILE.RAD.
6. FILE.REP. Reports ignored records, levels that have no match in adopted levels, frequency of XREF symbols, new XREF symbols, *etc.* Sample output file: FILE.REP.
7. FILE.XRF. Reports the cross-reference records. The cross-reference symbols are also given in FILE.LEV. Sample output file: FILE.XRF.
8. New ENSDF formatted file with XREFs added or modified. Sample output file: PANDOR.OUT.

Generation of the files reporting on the gammas, levels, and radiations and the new ENSDF formatted file is optional. There is no option to specify file names for the FILE.* outputs.

Terminal dialog: The program will ask for the input file name and then if the user wishes the level, gammas, and radiation reports (default: 0 for no) and a new file generated (default: 0 for

no). If new output is specified, the user will be queried for the output file name. As generation of the various output files is completed, this will be noted on the terminal.

Compilation and loading instructions: This program requires subroutines from the NSDFLIB package.

Additional documentation: Internal document (PANDOR.PSC).

RadList

Version 5.5 [October 5, 1988]

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This program is designed to calculate the nuclear and atomic radiations associated with the radioactive decay of nuclei. It uses as its primary input nuclear decay data in the ENSDF format. Listings or computer files containing the energies, intensities, and dose rates for various nuclear radiations are produced. These outputs also contain the energies, intensities, and dose rates of the associated atomic radiations. Optionally the continua spectra for β^\pm decay and for internal bremsstrahlung associated with β^\pm and electron-capture decay may be calculated.

Input files:

1. ENSDF formatted file. The following optional records as defined in cols. 1-9 of the record are allowed:
 - a. MERGE/ENDMERGE Specifies that the radiations from the data sets contained between them will be merged on output (ignored if the data-base option is selected)
 - b. PAGE Causes the radiation listing output to begin on a new page for the following data set.
 - c. PARAMETER Various parameters affecting the calculations or output of the program may be given in cols. 10 - 80 of this record which immediately precedes a data set and only affects that data set. The parameters are:
 - i. ALLGAM Overrides the minimum intensity cutoff for radiations and outputs all gammas. No value should be given for this parameter.
 - ii. MAXEC Specifies the number of electron-capture branches to be listed in the radiation listing (default = 0).
 - iii. MAT Specifies a material number for ENDF-6 output (default is based on the Z and A of the parent).
 - iv. RIMIN Specifies the minimum intensity cutoff (in percent) for radiations (default = 0.001% except for the data-base option [$10^{-12}\%$]).
 - v. WEIGHT Specifies an arbitrary weighting fraction. Not allowed with database and ENDF-6 options.

Sample input file: RADLST.INP. See the report for an explanation of what is tested within this sample input.

2. Atomic electron binding energies, fluorescence and Auger-electron yields: One of the following two data files must be present:
 - a. Direct access binary file (ATOMIC.DAT). The program will generate this file if it does not exist and the following file is available.
 - b. Sequential file (default name: MEDNEW.DAT). Data file provided with distribution.
3. Atomic mass data: If neither of the two following files is present, the program will calculate atomic masses based on the Garvey-Kelson formalism.
 - a. Direct access binary file (WAPSTB.DAT). The program will generate this file if it does not exist and the following file is available.
 - b. Sequential file (default name: RADMAS.DAT). Data file provided with distribution.

Output files: With the exception of the report file, these files are options.

1. Report file: The input data are listed in cols 2-81 and messages reporting possible problems or assumptions made are given in cols 82-133. Possible severe errors are noted on a line following the record in question.
After all relevant radiation data have been analyzed, there will be a summary of the energy deposited by the radiations and recoiling nuclei and a comparison between the sum of these deposited energies and the energy expected from the branching ratios and Q values.
2. Radiations listing: Fortran-formatted file containing the nuclear and atomic radiations obtained by the program. See the report for additional details.
3. Database file: Presents the data generated by the program in a fixed computer-readable format. See the report for additional details.
4. ENDF-6 format file: MT = 1, MF = 451 (comments) and MT = 8, MF = 457 (decay data) sections are generated.

Either the ENSDF-6 file or the database file may be generated but not both.

Terminal dialog:

1. The program will ask which output files should be generated (defaults: radiation listing; no ENDF-like file or database file).
2. Unless the database option is chosen, the user will be asked if the continua should be calculated (default: no).
3. The names of the input and report files will be requested (defaults: RADLST.INP and RADLST.RPT).
4. If the binary data files are not present, the user will be asked for the names of the sequential files.
5. The user will be asked the names of the various output files to be generated (defaults: ENSDF.RPT, NUDAT.OUT, and ENDF.RAW).
6. The source of the atomic data and the mass data will be noted.
7. As each data set or group of data sets are processed, a summary of the results will be displayed on the terminal.

Sample terminal dialogs and outputs: Following are descriptions of the sample files included in the distribution. NOTE: This supersedes Appendix B of the report. The various outputs in these files are separated by “%%%%%%” followed by the type of output and in some cases only show those outputs where there are major differences.

1. RADLST1.OUT: Normal options
2. RADLST2.OUT: ENDF option

3. RADLST3.OUT: Database file option
4. RADLST4.OUT: Continua with bremsstrahlung chosen
5. RADLST5.OUT: ENDF with continua with bremsstrahlung chosen

Compilation and loading instructions: This program requires subroutines from the NSDFLIB package.

Additional documentation: T.W. Burrows. The program RADLST. Brookhaven National Laboratory Report BNL-NCS-52142 (1988).

RULER

Version 1.31a [July 15, 2002]

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This program either calculates the reduced electromagnetic transition strengths and compares these to the Recommended Upper Limits (RUL) or calculates BELW and BMLW for inclusion in ENSDF data sets. Primarily designed to work on ADOPTED LEVELS, GAMMAS datasets but will process any dataset whose DSID indicates the presence of gammas.

Input file: ENSDF formatted file. Sample input file: RULER.IN

Output files:

1. The report file will list the datasets and note any problems or assumptions by the program. Comparison mode: will show the calculations and compare the results to the RULs noting possible violations; calculation mode: will show the calculations and compare the old and new values for BELWs and BMLWs. Sample output files: RULER1.RPT (comparison) and RULER2.RPT (calculation).
2. Optionally a new file will be created containing the calculated BE λ Ws and BM λ Ws. Sample output file: RULER.OUT.

Terminal dialog: The program will request the input and report file specifications, the mode of operation (answer is case sensitive), and, optionally, the new file specifications.

Compilation and loading instructions: This program requires subroutines from the NSDFLIB package.

Additional documentation: Distribution memo (RULER.PSC)

TREND

Version 8.3 [Feb. 7, 2001]

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(Other author: Bruce J. Barton)

This program generates ENSDF data tables report and allows the user to view and control the output file on the screen.

Input file: An ENSDF formatted file. Sample input file: DATA.TST.

Outputs: Tabular representations of the ENSDF data similar in organization to the Nuclear Data Sheets are generated either as a report file or as a file capable of being viewed interactively on an ANSI (VT100 equivalent) or VT52 terminal.

Sample output file: TREND.RPT (132 columns; 66 lines per page)

Terminal dialog: The program will request the following information:

1. Input file name
2. Output file name
3. If the output file exists, does the user wish to view it?
4. 80 or 132 column display (no defaults)
5. Lines per page (defaults: 60 if 80 column display; 66 if 132 column display). The user should specify 24 for screen display.

If the user has specified "TT:" or "TTY:" (case insensitive) as the output file name, answered yes to viewing an existing file, or 24 lines per page, the tables will be displayed on the screen with a prompt line at the bottom. The user may scroll up and down through the tables.

Compilation and loading instructions: This program requires subroutines from the NSDFLIB package.

Additional documentation: None