PROGRAM SPECTRA

An extension of LINEAR to linearize all MF=5 spectra.

2012/05/28 - Added MF=15 neutron induced, photon spectra.
2021/01/26 - MF=6 Still NOT Implemented

First released in 2010 - Earlier below dates refer to LINEAR.

VERSION 74-1 (MAY 1974)
VERSION 75-1 (APRIL 1975)
VERSION 76-2 (OCTOBER 1976)
VERSION 77-1 (JANUARY 1977)
VERSION 78-1 (JULY 1978)
VERSION 79-1 (JULY 1979) CDC-7600 AND CRAY-1 VERSION.
VERSION 80-1 (MAY 1980) IBM, CDC AND CRAY VERSION.
VERSION 80-2 (DECEMBER 1980)
VERSION 81-1 (MARCH 1981)
VERSION 82-1 (JANUARY 1982) IMPROVED COMPUTER COMPATIBILITY.
VERSION 83-1 (JANUARY 1983) *MAJOR RE-DESIGN.
*PAGE SIZE INCREASED - 1002 TO 3006.
*ELIMINATED COMPUTER DEPENDENT CODING.
*NEW, MORE COMPATIBLE I/O UNIT NUMBER.
*ADDED OPTION TO KEEP ALL ORIGINAL ENERGY POINTS FROM EVALUATION.
*ADDED STANDARD ALLOWABLE ERROR OPTIONS.
(CURRENTLY 0.1 PER-CENT)
VERSION 83-2 (OCTOBER 1983) IMPROVED BASED ON USER COMMENTS.
VERSION 84-1 (APRIL 1984) IMPROVED BASED ON USER COMMENTS.
VERSION 84-2 (JUNE 1984) *UPDATED FOR ENDF/B-VI FORMATS.
*SPECIAL I/O ROUTINES TO GUARANTEE ACCURACY OF ENERGY.
*DOUBLE PRECISION TREATMENT OF ENERGY (REQUIRED FOR NARROW RESONANCES).
*FORTRAN-77/H VERSION
VERSION 85-1 (AUGUST 1985)
VERSION 86-1 (JANUARY 1986) *ENDF/B-VI FORMAT
VERSION 87-1 (JANUARY 1987) *DOUBLE PRECISION TREATMENT OF CROSS SECTION
VERSION 88-1 (JULY 1988) *OPTION...INTERNALLY DEFINE ALL I/O FILE NAMES (SEE, SUBROUTINE FILEIO FOR DETAILS).
*IMPROVED BASED ON USER COMMENTS.
VERSION 89-1 (JANUARY 1989) *PSYCHOANALYZED BY PROGRAM FREUD TO INSURE PROGRAM WILL NOT DO ANYTHING CRAZY.
*UPDATED TO USE NEW PROGRAM CONVERT KEYWORDS.
*ADDED LIVERMORE CIVIC COMPILER CONVENTIONS.
VERSION 90-1 (JUNE 1990) *EXTENDED TO LINEARIZE PHOTON INTERACTION DATA, MF=23 AND 27
*ADDED FORTRAN SAVE OPTION
*UPDATED BASED ON USER COMMENTS.
*NEW MORE CONSISTENT ENERGY OUTPUT ROUTINE.
*WARNING...INPUT PARAMETER FORMAT HAS BEEN CHANGED...SEE DESCRIPTION BELOW.
VERSION 91-1 (JULY 1991) *ADDED INTERPOLATION LAW 6 - ONLY USED FOR CHARGED PARTICLE CROSS SECTIONS FOR COULOMB PENETRABILITIES.
VERSION 92-1 (JANUARY 1992) *ADDED NU-BAR (TOTAL, DELAYED, PROMPT) POLYNOMIAL OR TABULATED ALL CONVERTED TO LINEARLY INTERPOLABLE
*INCREASED PAGE SIZE FROM 3006 TO 5010
*ALL ENERGIES INTERNALLY ROUNDED PRIOR TO CALCULATIONS.
*COMPLETELY CONSISTENT I/O AND RUNDINGS
Routines - TO MINIMIZE COMPUTER
VERSION 92-2 (JULY 1992) *CORRECTED CONVERSION OF NU-BAR FROM POLYNOMIAL TO TABULATED - COPY SPECTRA SPONTANEOUS NU-BAR (BY DEFINITION THE SPONTANEOUS NU-BAR IS NOT AN ENERGY DEPENDENT QUANTITY).

VERSION 93-1 (MARCH 1993) *UPDATED FOR USE WITH LAHEY COMPILER ON IBM-PCS. INCREASED PAGE SIZE FROM 5010 TO 30000 POINTS SPECTRA

VERSION 94-1 (JANUARY 1994) *VARIABLE ENDF/B DATA FILENAMES TO ALLOW ACCESS TO FILE STRUCTURES (WARNING - INPUT PARAMETER FORMAT HAS BEEN CHANGED) CLOSE ALL FILES BEFORE TERMINATING (SEE, SUBROUTINE ENDIT) SPECTRA

VERSION 96-1 (JANUARY 1996) *COMPLETE RE-WRITE SPECTRA *IMPROVED COMPUTER INDEPENDENCE SPECTRA *ALL DOUBLE PRECISION SPECTRA *ON SCREEN OUTPUT SPECTRA *UNIFORM TREATMENT OF ENDF/B I/O SPECTRA *IMPROVED OUTPUT PRECISION SPECTRA *DEFINED SCRATCH FILE NAMES SPECTRA *ALWAYS INCLUDE THERMAL VALUE SPECTRA INCREASED PAGE SIZE FROM 30000 TO 60000 POINTS SPECTRA

VERSION 99-1 (MARCH 1999) *CORRECTED CHARACTER TO FLOATING POINT READ FOR MORE DIGITS SPECTRA UPDATED TEST FOR ENDF/B FORMAT VERS. BASED ON RECENT FORMAT CHANGES SPECTRA *GENERAL IMPROVEMENTS BASED ON USER FEEDBACK SPECTRA


VERS. 2000-1 (FEBRUARY 2000) *ADDED MF = 9 AND 10 LINEARIZATION SPECTRA *GENERAL IMPROVEMENTS BASED ON USER FEEDBACK SPECTRA

VERS. 2002-1 (MAY 2002) *OPTIONAL INPUT PARAMETERS SPECTRA
VERS. 2004-1 (JAN. 2004) *GENERAL UPDATE BASED ON USER FEEDBACK SPECTRA
VERS. 2005-1 (JAN. 2005) *ALWAYS KEEP ORIGINAL TABULATED NU-BAR POINTS SPECTRA
VERS. 2006-1 (FEB. 2006) *CORRECTED INT=6 NEAR Threshold SPECTRA NO SUBDIVIDE BELOW MINIMUM XMIN SPECTRA
VERS. 2007-1 (JAN. 2007) *CHECKED AGAINST ALL ENDF/B-VII. SPECTRA INCREASED PAGE SIZE FROM 60,000 TO 600,000 POINTS SPECTRA

VERS. 2010-1 (JUNE 2010) *ADDED MF = 5 - MF = 6 STILL PLANNED SPECTRA 72 CHARACTER FILE NAMES SPECTRA ONLY PROCESS MF=5 - SKIP ALL OTHERS TO PREVENT CONFLICT WITH LINEAR THINNING SPECTRA
VERS. 2012-1 (Aug. 2012) *Added MF=15, neutron induced photon spectra SPECTRA *Added CODENAME SPECTRA *32 and 64 bit Compatible SPECTRA *Added ERROR stop SPECTRA
VERS. 2015-1 (Jan. 2015) *Extended OUT9 SPECTRA *Replaced ALL 3 way IF Statements SPECTRA *Corrected MF=15 Data - it was adding SEND between sub-sections SPECTRA
VERS. 2017-1 (May 2017) *Increased page size to 3,000,000 SPECTRA *Updated based on user feedback SPECTRA *Changed DGAMMA to REDGAMMA to avoid conflict with possible RESERVED NAME SPECTRA *All floating input parameters changed to character input + IN9 conversion SPECTRA
VERS. 2018-1 (Jan. 2018) *Additional Interpolation Law Tests SPECTRA *Check Maximum Tabulated Energy to insure it is the same for all MTs SPECTRA
VERS. 2019-1 (June 2019)
if not, print WARNING messages.

*Corrected END Histogram linearized - SPECTRA
Previously deleted last point - ERROR SPECTRA
to assume this has Y=0 - now keep SPECTRA
point, but insure Y = 0. SPECTRA

VERS. 2020-1 (Mar. 2020) *Added Target Isomer State SPECTRA
VERS. 2021-1 (Jan. 2021) *Updated for FORTRAN 2018 SPECTRA
VERS. 2023-1 (Feb. 2023) *Decreased page size from 3,000,000 to 120,000 SPECTRA

OWNED, MAINTAINED AND DISTRIBUTED BY
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THE NUCLEAR DATA SECTION
INTERNATIONAL ATOMIC ENERGY AGENCY
A-1400, VIENNA, AUSTRIA
EUROPE

ORIGINAL WRITTEN BY
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AUTHORS MESSAGE
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THE REPORT DESCRIBED ABOVE IS THE LATEST PUBLISHED DOCUMENTATION FOR THIS PROGRAM. HOWEVER, THE COMMENTS BELOW SHOULD BE CONSIDERED THE LATEST DOCUMENTATION INCLUDING ALL RECENT IMPROVEMENTS. PLEASE READ ALL OF THESE COMMENTS BEFORE IMPLEMENTATION.

AT THE PRESENT TIME WE ARE ATTEMPTING TO DEVELOP A SET OF INDEPENDENT PROGRAMS THAT CAN EASILY BE IMPLEMENTED ON ANY ONE OF A WIDE VARIETY OF COMPUTERS. IN ORDER TO ASSIST IN THIS PROJECT, IT WOULD BE APPRECIATED IF YOU WOULD NOTIFY THE AUTHOR OF ANY COMPILER DIAGNOSTICS, OPERATING PROBLEMS OR SUGGESTIONS ON HOW TO IMPROVE THIS PROGRAM. HOPEFULLY, IN THIS WAY FUTURE VERSIONS OF THIS PROGRAM WILL BE COMPLETELY COMPATIBLE FOR USE ON YOUR COMPUTER.

PURPOSE
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THIS PROGRAM IS DESIGNED TO CONVERT ENDF/B FILE 3, 23 AND 27 DATA TO LINEAR-LINEAR INTERPOLABLE FORM. ANY SECTION THAT IS ALREADY LINEAR-LINEAR INTERPOLABLE WILL BE THINNED. IN THE FOLLOWING DISCUSSION FOR SIMPLICITY THE ENDF/B TERMINOLOGY---ENDF/B TAPE---WILL BE USED. IN FACT THE ACTUAL MEDIUM MAY BE TAPE, CARDS, DISK OR ANY OTHER MEDIUM.

ENDF/B FORMAT
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THIS PROGRAM ONLY USES THE ENDF/B BCD OR CARD IMAGE FORMAT (AS OPPOSED TO THE BINARY FORMAT) AND CAN HANDLE DATA IN ANY VERSION OF THE ENDF/B FORMAT (I.E., ENDF/B-I, II, III, IV, V OR VI FORMAT). IT IS ASSUMED THAT THE DATA IS CORRECTLY CODED IN THE ENDF/B FORMAT AND NO ERROR CHECKING IS PERFORMED. IN PARTICULAR IT IS ASSUMED THAT THE MAT, MF AND MT ON EACH LINE IS CORRECT. SEQUENCE NUMBERS (COLUMNS 76-80) ARE IGNORED ON INPUT, BUT WILL BE CORRECTLY OUTPUT ON ALL LINES. THE FORMAT OF SECTION MF=1, MT=451 AND ALL SECTIONS OF MF=3 MUST BE CORRECT. THE PROGRAM COPIES ALL OTHER SECTION OF DATA AS HOLLERITH AND AS SUCH IS INSENSITIVE TO
THE CORRECTNESS OR INCORRECTNESS OF ALL OTHER SECTIONS.

OUTPUT FORMAT
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IN THIS VERSION OF LINEAR ALL ENERGIES WILL BE OUTPUT IN F (INSTEAD OF E) FORMAT IN ORDER TO ALLOW ENERGIES TO BE WRITTEN WITH UP TO 9 DIGITS OF ACCURACY. IN PREVIOUS VERSIONS THIS WAS AN OUTPUT OPTION. HOWEVER USE OF THIS OPTION TO COMPARE THE RESULTS OF ENERGIES (THE NORMAL ENDF/B CONVENTION OF 6 DIGITS TO THE 9 DIGIT OUTPUT FROM THIS PROGRAM DEMONSTRATED THAT FAILURE TO USE THE 9 DIGIT OUTPUT CAN LEAD TO LARGE ERRORS IN THE DATA DUE TO TRUNCATION OF ENERGIES TO 6 DIGITS DURING OUTPUT.

ENTIRE EVALUATIONS ARE OUTPUT, NOT JUST THE LINEARIZED DATA CROSS SECTIONS, E.G. ANGULAR AND ENERGY DISTRIBUTIONS ARE ALSO INCLUDED.

DOCUMENTATION
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THE FACT THAT THIS PROGRAM HAS OPERATED ON THE DATA IS DOCUMENTED BY THE ADDITION OF 3 COMMENT LINES AT THE END OF EACH HOLLERITH SECTION IN THE FORM ************* PROGRAM SPECTRUM (2023-1) ************* FOR ALL DATA GREATER THAN 1.00000-10 IN ABSOLUTE VALUE DATA LINEARIZED TO WITHIN AN ACCURACY OF 0.1 PER-CENT THE ORDER OF SIMILAR COMMENTS (FROM RECENT, SIGMA1 AND GROUPIE) REPRESENTS A COMPLETE HISTORY OF ALL OPERATIONS PERFORMED ON THE DATA BY THESE PROGRAMS.

THESE COMMENT LINES ARE ONLY ADDED TO EXISTING HOLLERITH SECTIONS, I.E., THIS PROGRAM WILL NOT CREATE A HOLLERITH SECTION. THE FORMAT OF THE HOLLERITH SECTION IN ENDF/B-V DIFFERS FROM THE THAT OF EARLIER VERSIONS OF ENDF/B. BY READING AN EXISTING MF=1, MT=451 IT IS POSSIBLE FOR THIS PROGRAM TO DETERMINE WHICH VERSION OF THE ENDf/B FORMAT THE DATA IS IN. WITHOUT HAVING A SECTION OF MF=1, MT=451 PRESENT IT IS IMPOSSIBLE FOR THIS PROGRAM TO DETERMINE WHICH VERSION OF THE ENDF/B FORMAT THE DATA IS IN, AND AS SUCH IT IS IMPOSSIBLE FOR THE PROGRAM TO DETERMINE WHAT FORMAT SHOULD BE USED TO CREATE A HOLLERITH SECTION.

REACTION INDEX
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THIS PROGRAM DOES NOT USE THE REACTION INDEX WHICH IS GIVEN IN SECTION MF=1, MT=451 OF EACH EVALUATION. THIS CONVENTION HAS BEEN ADOPTED BECAUSE MOST USERS DO NOT REQUIRE A CORRECT REACTION INDEX FOR THEIR APPLICATIONS AND IT WAS CONSIDERED WORTHWHILE TO INCLUDE THE OVERHEAD OF CONSTRUCTING A CORRECT REACTION INDEX IN THIS PROGRAM. HOWEVER, IF YOU REQUIRE A REACTION INDEX FOR YOUR APPLICATIONS, AFTER RUNNING THIS PROGRAM YOU MAY USE PROGRAM DICTIN TO CREATE A CORRECT REACTION INDEX.

SECTION SIZE
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SINCE THIS PROGRAM USES A LOGICAL PAGING SYSTEM THERE IS NO LIMIT TO THE NUMBER OF POINTS IN ANY SECTION, E.G., THE TOTAL CROSS SECTION MAY BE REPRESENTED BY 200,000 DATA POINTS. FOR ANY LINEARIZED SECTION THAT CONTAINS 60000 OR FEWER POINTS THE ENTIRE OPERATION WILL BE PERFORMED IN CORE AND THE LINEARIZED DATA WILL BE OUTPUT DIRECTLY TO THE ENDF/B FORMAT. FOR ANY SECTION THAT CONTAINS MORE POINTS THE DATA WILL BE LINEARIZED A PAGE AT A TIME (1 PAGE = 60000 POINTS) AND OUTPUT TO SCRATCH. AFTER THE ENTIRE SECTION HAS BEEN LINEARIZED THE DATA WILL BE READ BACK FROM SCRATCH AND OUTPUT TO THE ENDF/B FORMAT.
SELECTION OF DATA

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THE PROGRAM SELECTS DATA TO BE LINEARIZED BASED EITHER ON EITHER MAT (ENDF/B MAT NO.) OR ZA AS WELL AS MF AND MT NUMBERS. THIS PROGRAM ALLOWS UP TO 100 MAT/MF/MT OR ZA/MF/MT RANGES TO BE SPECIFIED BY INPUT PARAMETERS. THE PROGRAM WILL ASSUME THAT THE ENDF/B TAPE IS IN MAT ORDER, REGARDLESS OF THE CRITERIA USED TO RETRIEVE MATERIALS. IF RETRIEVAL IS BY MAT RANGE THE PROGRAM WILL TERMINATE WHEN A MAT IS FOUND THAT IS ABOVE ALL REQUESTED MAT RANGES. IF RETRIEVAL IS BY ZA RANGE THE PROGRAM WILL SEARCH THE ENTIRE ENDF/B TAPE.

PROGRAM OPERATION

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EACH SECTION OF DATA IS CONSIDERED SEPARATELY. EACH SECTION OF ENDF/B DATA TO LINEARIZE IS REPRESENTED BY A TABLE OF ENERGY VS. CROSS SECTION AND ANY ONE OF FIVE ALLOWABLE INTERPOLATION LAWS BETWEEN ANY TWO TABULATED POINTS. THIS PROGRAM WILL REPLACE EACH SECTION OF DATA CROSS SECTIONS BY A NEW TABLE OF ENERGY VS. CROSS SECTION IN WHICH THE INTERPOLATION LAW IS ALWAYS LINEAR IN ENERGY AND CROSS SECTION BETWEEN ANY TWO TABULATED POINTS.

DATA IS READ AND LINEARIZED A PAGE AT A TIME (ONE PAGE CONTAINS 60000 DATA POINTS). IF THE FINAL LINEARIZED SECTION CONTAINS TWO PAGES OR LESS, DATA POINTS IT WILL BE ENTIRELY CORE RESIDENT AFTER IT HAS BEEN LINEARIZED AND WILL BE WRITTEN DIRECTLY FROM CORE TO THE OUTPUT TAPE. IF THE LINEARIZED SECTION IS LARGER THAN TWO PAGES, AFTER EACH PAGE IS LINEARIZED IT WILL BE WRITTEN TO SCRATCH. AFTER THE ENTIRE SECTION HAS BEEN LINEARIZED IT WILL BE READ BACK FROM SCRATCH, TWO PAGES AT A TIME, AND WRITTEN TO THE OUTPUT TAPE.

KEEP EVALUATED DATA POINTS

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SOMETIMES IT IS CONVENIENT TO KEEP ALL ENERGY POINTS WHICH WERE PRESENT IN THE ORIGINAL EVALUATION AND TO MERELY SUPPLEMENT THESE POINTS WITH ADDITIONAL ENERGY POINTS IN ORDER TO LINEARIZE THE CROSS SECTIONS. FOR EXAMPLE, IT IS OFTEN CONVENIENT TO KEEP THE THERMAL VALUE (AT 0.0253 EV) OR THE VALUE AT 14.1 MEV. THE CURRENT VERSION OF THIS PROGRAM WILL ALLOW THE USER TO KEEP ALL ORIGINAL EVALUATED DATA POINTS BY SPECIFYING 1 IN COLUMNS 34-44 OF THE FIRST INPUT LINE. THIS WILL TURN OFF THE BACKWARD THINNING (SEE UCRL-50400, VOL. 17, PART A FOR EXPLANATION) AND RESULT IN ALL ORIGINAL ENERGY POINTS BEING KEPT. CAUTION SHOULD BE EXERCISED IN USING THIS OPTION SINCE IT CAN RESULT IN A CONSIDERABLE INCREASE IN THE NUMBER OF DATA POINTS OUTPUT BY THIS CODE.

FOR ALL USERS WHO ARE NOT INTERESTED IN THIS OPTIONS NO CHANGES ARE REQUIRED IN THE INPUT TO THIS PROGRAM, I. E. IF COLUMNS 34-44 ARE BLANK (AS FOR ALL PREVIOUS VERSIONS OF THIS CODE) THE PROGRAM WILL OPERATE EXACTLY AS IT DID BEFORE.

ALLOWABLE ERROR

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ALLOWABLE ERROR MUST ALWAYS BE SPECIFIED IN THE INPUT TO THIS PROGRAM AS A FRACTION, NOT A PER-CENT. FOR EXAMPLE, INPUT THE ALLOWABLE FRACTIONAL ERROR 0.001 IN ORDER TO OBTAIN DATA THAT IS ACCURATE TO WITHIN 0.1 PER-CENT.

THE CONVERSION OF THE DATA FROM THE GENERAL INTERPOLATION FORM TO LINEARLY INTERPOLABLE FORM CANNOT BE PERFORMED EXACTLY. HOWEVER, ITS CAN BE PERFORMED TO VIRTUALLY ANY REQUIRED ACCURACY AND MOST IMPORTANTLY CAN BE PERFORMED TO A TOLERANCE THAT IS SMALL COMPARED TO THE UNCERTAINTY IN THE CROSS SECTIONS THEMSELVES. AS SUCH THE CONVERSION OF CROSS SECTIONS TO LINEARLY INTERPOLABLE FORM CAN BE PERFORMED WITH ESSENTIALLY NO LOSE OF INFORMATION.

THE ALLOWABLE ERROR MAY BE ENERGY INDEPENDENT (CONSTANT) OR ENERGY DEPENDENT. THE ALLOWABLE ERROR IS DESCRIBED BY A TABULATED
FUNCTION OF UP TO 20 (ENERGY, ERROR) PAIRS AND LINEAR INTERPOLATIONSPECTRA BETWEEN TABULATED POINTS. IF ONLY ONE TABULATED POINT IS GIVEN THESE SPECTRA ERROR WILL BE CONSIDERED CONSTANT OVER THE ENTIRE ENERGY RANGE. SPECTRA WITH THIS ENERGY DEPENDENT ERROR ONE MAY OPTIMIZE THE OUTPUT FOR SPECTRA ANY GIVEN APPLICATION BY USING A SMALL ERROR IN THE ENERGY RANGE OF INTEREST AND A LESS STRINGENT ERROR IN OTHER ENERGY RANGES. SPECTRA

DEFAULT ALLOWABLE ERROR

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IN ORDER TO INSURE CONVERGENCE OF THE LINEARIZING ALGORITHM THE SPECTRA ALLOWABLE ERROR MUST BE POSITIVE. IF THE USER INPUTS AN ERROR THAT IS NOT POSITIVE IT WILL AUTOMATICALLY BE SET TO THE DEFAULT SPECTRA VALUE (CURRENTLY 0.001, CORRESPONDING TO 0.1 PER-CENT) AND SPECTRA INDICATED AS SUCH IN THE OUTPUT LISTING. SPECTRA

COULOMB PENETRABILITY (INTERPOLATION LAW = 6)

INTRODUCED FOR ENDF/B-VI. THIS IS DEFINED AS,

\[ \text{SIG}(E) = C_1 \times \exp\left(-\frac{C_2}{\sqrt{E - T}}\right) \]

THIS PROGRAM ONLY CONSIDERS EXOTHERMIC REACTIONS - T = 0

\[ \text{SIG}(E) = C_1 \times \exp\left(-\frac{C_2}{\sqrt{E}}\right) \]

WARNING...THIS INTERPOLATION LAW SHOULD ONLY BE USED FOR REACTIONS WHICH HAVE A POSITIVE Q-VALUE (EXOTHERMIC REACTIONS), SINCE HERE WE ONLY CONSIDER T = 0.0 IN THE FORMALISM. IN ALL OTHER CASES A WARNING MESSAGE WILL BE PRINTED.

INPUT FILES

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UNIT DESCRIPTION

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2 INPUT LINES (BCD - 80 CHARACTERS/RECORD)

10 ORIGINAL ENDF/B DATA (BCD - 80 CHARACTERS/RECORD)

OUTPUT FILES

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UNIT DESCRIPTION

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3 OUTPUT REPORT (BCD - 120 CHARACTERS/RECORD)

11 FINAL ENDF/B DATA (BCD - 80 CHARACTERS/RECORD)

SCRATCH FILES

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UNIT DESCRIPTION

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12 SCRATCH FILE (BINARY - 180000 WORDS/RECORD)

OPTIONAL STANDARD FILE NAMES (SEE SUBROUTINE FILEIO)

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UNIT FILE NAME

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2 SPECTRA.INP

3 SPECTRA.LST

10 ENDFB.IN

11 ENDFB.OUT

12 (SCRATCH)

INPUT PARAMETERS

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FOR VERSIONS EARLIER THAN 90-1 THIS PROGRAM ONLY ALLOWED THE USER TO SPECIFY BY INPUT PARAMETERS WHICH MATERIALS (MAT) TO PROCESS. FOR EACH REQUESTED MATERIAL NEUTRON INTERACTION CROSS SECTIONS (MF=3) WOULD BE LINEARIZED AND THE REMAINDER OF THE MATERIAL WOULD BE COPIED.

FOR VERSIONS 90-1 AND LATER THIS PROGRAM WILL ALLOW THE USER TO SPECIFY BY INPUT PARAMETERS EXACTLY WHAT SECTIONS OF DATA
TO PROCESS. FOR EACH SECTION OF DATA, SPECIFIED BY MAT, MF, MT SPECTRA RANGES, SECTIONS OF MF=3, 23 AND 27 WILL BE LINEARIZED AND ALL SPECTRA OTHER REQUESTED SECTIONS WILL BE COPIED. ALL SECTIONS WHICH ARE NOT EXPLICITLY REQUESTED WILL BE SKIPPED AND WILL NOT APPEAR ON SPECTRA ENDF/B FILE OUTPUT BY THIS PROGRAM.

WITH THIS NEW PROCEDURE YOU CAN MINIMIZE THE SIZE OF THE ENDF/B SPECTRA FILE OUTPUT BY THIS PROGRAM, E.G., IF YOU ONLY WANT NEUTRON SPECTRA CROSS SECTIONS FOR SUBSEQUENT PROCESSING YOU NEED ONLY REQUEST SPECTRA ONLY MF=3 DATA.

HOWEVER, YOU MUST UNDERSTAND THAT ONLY THOSE SECTIONS WHICH YOU EXPLICITLY REQUEST WILL APPEAR ON THE ENDF/B FILE OUTPUT BY SPECTRA THIS PROGRAM. FOR EXAMPLE, IF YOU WISH TO DOCUMENT EXACTLY SPECTRA HOW YOU LINEARIZED THE DATA BY INCLUDING COMMENTS IN MF=1, MT=451 SPECTRA THEN YOU MUST EXPLICITLY REQUEST THAT MF=1, MT=451 BE PROCESSED SPECTRA FOR EACH MATERIAL THAT YOU REQUEST. SIMILAR IF YOU WANT THE ENTIRE EVALUATION YOU MUST REQUEST ALL MF AND MT TO BE OUTPUT.

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<thead>
<tr>
<th>LINE</th>
<th>COLS</th>
<th>DESCRIPTION</th>
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<tbody>
<tr>
<td>1</td>
<td>1-11</td>
<td>SELECTION CRITERIA (0=MAT, 1=ZA)</td>
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<tr>
<td>12</td>
<td>22</td>
<td>MONITOR MODE SELECTOR</td>
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<td></td>
<td>= 0 - NORMAL OPERATION</td>
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<td>= 1 - MONITOR PROGRESS OF LINEARIZING OF THE DATA.</td>
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<td>EACH TIME A PAGE OF DATA POINTS IS WRITTEN TO</td>
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<td></td>
<td>THE SCRATCH FILE PRINT OUT THE TOTAL NUMBER OF</td>
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<td>POINTS ON SCRATCH AND THE LOWER AND UPPER</td>
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<td>ENERGY LIMITS OF THE PAGE (THIS OPTION MAY BE</td>
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<td>USED IN ORDER TO MONITOR THE EXECUTION SPEED</td>
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<td></td>
<td>OF LONG RUNNING JOBS).</td>
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<td>23-33</td>
<td></td>
<td>MINIMUM CROSS SECTION OF INTEREST (Barns).</td>
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<td>(IF 0.0 OR LESS IS INPUT THE PROGRAM WILL</td>
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<td>USE 1.0E-10). ENERGY INTERVALS WILL NOT BE</td>
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<td>SUB-DIVIDED IF THE ABSOLUTE VALUE OF THE CROSS</td>
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<td>SECTION WITHIN THE INTERVAL IS LESS THAN THIS VALUE.</td>
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<td>AN EXCEPTION TO THIS RULE IS NEAR THRESHOLDS ENERGY</td>
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<td>INTERVALS WILL BE SUB-DIVIDED UNTIL CONVERGENCE</td>
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<td>REGARDLESS OF THE MAGNITUDE OF THE CROSS SECTION.</td>
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<td>34-44</td>
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<td>KEEP ORIGINAL EVALUATED DATA POINTS.</td>
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<td>= 0 - NO.</td>
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<td>= 1 - YES - ADDITIONAL POINTS MAY BE ADDED IN ORDER</td>
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<td>TO LINEARIZE DATA, BUT ALL ORIGINAL</td>
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<td>DATA POINTS WILL BE INCLUDED IN THE</td>
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<td>RESULTS.</td>
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<td>2</td>
<td>1-72</td>
<td>ENDF/B INPUT DATA FILENAME</td>
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<td>(STANDARD OPTION = ENDFB.IN)</td>
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<td>3</td>
<td>1-72</td>
<td>ENDF/B OUTPUT DATA FILENAME</td>
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<td></td>
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<td>(STANDARD OPTION = ENDFB.OUT)</td>
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<tr>
<td>4-N</td>
<td>1-6</td>
<td>LOWER MAT OR ZA LIMIT</td>
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<td></td>
<td>7-8</td>
<td>LOWER MF LIMIT</td>
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<td>9-11</td>
<td>LOWER MT LIMIT</td>
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<td></td>
<td>12-17</td>
<td>UPPER MAT OR ZA LIMIT</td>
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<td>18-19</td>
<td>UPPER MF LIMIT</td>
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<td>20-22</td>
<td>UPPER MT LIMIT</td>
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<td>UP TO 100 RANGES MAY BE SPECIFIED, ONLY ONE RANGE</td>
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<td>PER LINE. THE LIST OF RANGES IS TERMINATED BY A</td>
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<td>BLANK LINE. IF THE UPPER MAT LIMIT OF ANY REQUEST</td>
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<td>IS LESS THAN THE LOW LIMIT IT WILL BE SET EQUAL TO</td>
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<td>THE LOWER LIMIT. IF THE UPPER LIMIT IS STILL ZERO</td>
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<td>IT WILL BE SET EQUAL TO 999999. IF THE UPPER MF OR</td>
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<td>MT LIMIT IS ZERO IT WILL BE SET TO 99 OR 999</td>
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<td>RESPECTIVELY.</td>
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<tr>
<td>5-VARY</td>
<td>1-11</td>
<td>ENERGY FOR ERROR LAW</td>
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<tr>
<td>12-22</td>
<td>ALLOWABLE FRACTIONAL ERROR FOR ERROR LAW.</td>
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<td>THE ACCEPTABLE LINEARIZING ERROR MAY BE SPECIFIED TO</td>
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<td>BE EITHER ENERGY INDEPENDENT (DEFINED BY A SINGLE</td>
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<tr>
<td></td>
<td></td>
<td>ERROR), OR ENERGY DEPENDENT (DEFINED BY UP TO 20</td>
</tr>
<tr>
<td></td>
<td></td>
<td>ENERGY, ERROR PAIRS). FOR THE ENERGY DEPENDENT CASE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>LINEAR INTERPOLATION WILL BE USED TO DEFINE THE ERRORSPECTRA</td>
</tr>
<tr>
<td></td>
<td></td>
<td>AT ENERGIES BETWEEN THOSE AT WHICH IT IS TABULATED.</td>
</tr>
</tbody>
</table>
In all cases the error law is terminated by a blank line. If only one energy, error pair is given the law will be considered to be energy independent. If more than one pair is given it will be considered energy dependent (note, energy independent form will run faster than the equivalent energy dependent form). For an energy dependent error law all energies must be ascending energy order. For convergence of the linearizing algorithm all errors must be positive. If an allowable error is not positive it will be set equal to the standard option (currently 0.001, corresponding to 0.1 per-cent). If the first error line is blank it will terminate the error law and the error will be treated as energy independent, equal to the standard option (currently 0.1 per-cent). (See example input 4).

Example input no. 1
-------------------
Retrieve data by ZA in order to find all uranium isotopes and thorium 232. Retrieve all neutron interaction cross sections (MF=3). All energy intervals in which the cross section is at least 1 micro-barn (1.0E-06 barns) will be subdivided. Backward thinning will be performed. From 0 to 100 ev linearize to within 0.1 per-cent accuracy. From 100 ev to 1 kev vary accuracy between 0.1 and 1.0 per-cent. Above 1 kev use 1 per-cent accuracy.

Explicitly specify the standard filenames.

In this case the following 11 input lines are required

<table>
<thead>
<tr>
<th>Energy</th>
<th>Lower</th>
<th>Upper</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00000+</td>
<td>0</td>
<td>1.00000-</td>
<td>0</td>
</tr>
<tr>
<td>0.00000+</td>
<td>2</td>
<td>1.00000-</td>
<td>0</td>
</tr>
<tr>
<td>0.00000+</td>
<td>3</td>
<td>1.00000-</td>
<td>0</td>
</tr>
<tr>
<td>0.00000+</td>
<td>9</td>
<td>1.00000-</td>
<td>0</td>
</tr>
</tbody>
</table>

Example input no. 2
-------------------
Same as the above case, except linearize all data to within the standard accuracy (currently 0.1 per-cent). In order to use the standard accuracy you need not specify any error law at all. In this case include the hollerith section, MF=1, MT=451, for each material.

Leave the definition of the filenames blank - the program will then use standard filenames.

In this case the following 9 input lines are required

<table>
<thead>
<tr>
<th>Energy</th>
<th>Lower</th>
<th>Upper</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00000+</td>
<td>0</td>
<td>1.00000-</td>
<td>0</td>
</tr>
<tr>
<td>(use default filename = ENDFB.IN)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(use default filename = ENDFB.OUT)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Example input no. 3
-------------------
Linearize all materials on an ENDF/B tape to within an accuracy of 0.5 per-cent (0.005 as a fraction). In this case you need not
SPECIFY THE MAT, MF, MT RANGES.

READ THE ENDF/B DATA FROM \ENDFB6\ZA092238 AND WRITE THE ENDF/B DATA TO \ENDFB6\LINEAR\ZA092238.

IN THIS CASE THE FOLLOWING 6 INPUT LINES ARE REQUIRED

\ENDFB6\ZA092238
\ENDFB6\LINEAR\ZA092238
(RETRIEVE ALL DATA, END REQUEST LIST)
5.00000-03
(END OF ERROR LAW)

NOTE THAT IN THIS CASE IF THE INPUT HAD SPECIFIED AN EQUIVALENT ENERGY DEPENDENT ERROR LAW BY GIVING A NUMBER OF ENERGY POINTS AT EACH OF WHICH THE ERROR IS 0.5 PER-CENT THE PROGRAM WOULD TAKE LONGER TO RUN (I.E., ONLY USE AN ENERGY DEPENDENT ERROR LAW WHEN IT IS NECESSARY).

EXAMPLE INPUT NO. 4

IN ORDER TO LINEARIZE ALL MATERIALS ON AN ENDF/B TAPE TO THE STANDARD OPTION OF 0.1 PER-CENT IT IS ADEQUATE TO INPUT A SET OF COMPLETELY BLANK LINES WHICH WILL AUTOMATICALLY INVOKE ALL OF THE STANDARD OPTIONS.

LEAVE THE DEFINITION OF THE FILENAMES BLANK - THE PROGRAM WILL THEN USE STANDARD FILENAMES.

IN THIS CASE THE FOLLOWING THREE INPUT LINES ARE REQUIRED

\ENDFB6\ZA092238
\ENDFB6\LINEAR\ZA092238
(RETRIEVE ALL DATA, END REQUEST LIST)
(USE DEFAULT FILENAME = ENDFB.IN)
(USE DEFAULT FILENAME = ENDFB.OUT)
(0.1 PER-CENT ERROR, END OF ERROR LAW)

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