

```

===== Groupie
PROGRAM GROUPIE Groupie
VERSION 76-1 (NOVEMBER 1976) Groupie
VERSION 79-1 (OCTOBER 1979) CDC-7600 AND CRAY-1 VERSION. Groupie
VERSION 80-1 (MAY 1980) IBM, CDC AND CRAY VERSION Groupie
VERSION 81-1 (JANUARY 1981) EXTENSION TO 3000 GROUPS Groupie
VERSION 81-2 (MARCH 1981) IMPROVED SPEED Groupie
VERSION 81-3 (AUGUST 1981) BUILT-IN 1/E WEIGHTING SPECTRUM Groupie
VERSION 82-1 (JANUARY 1982) IMPROVED COMPUTER COMPATIBILITY Groupie
VERSION 83-1 (JANUARY 1983) *MAJOR RE-DESIGN. Groupie
*ELIMINATED COMPUTER DEPENDENT CODING. Groupie
*NEW, MORE COMPATIBLE I/O UNIT NUMBERS. Groupie
*NEW MULTI-BAND LIBRARY BINARY FORMAT. Groupie
VERSION 83-2 (OCTOBER 1983) ADDED OPTION TO ALLOW SIGMA-0 TO BE Groupie
DEFINED EITHER AS MULTIPLES OF Groupie
UNSHIELDED TOTAL CROSS SECTION IN EACH Groupie
GROUP, OR POWERS OF 10 IN ALL GROUPS. Groupie
VERSION 84-1 (APRIL 1984) ADDED MORE BUILT IN MULTIGROUP ENERGY Groupie
STRUCTURES. Groupie
VERSION 85-1 (APRIL 1985) *UPDATED FOR ENDF/B-VI FORMATS. Groupie
*SPECIAL I/O ROUTINES TO GUARANTEE Groupie
ACCURACY OF ENERGY. Groupie
*DOUBLE PRECISION TREATMENT OF ENERGY Groupie
(REQUIRED FOR NARROW RESONANCES). Groupie
*MINIMUM TOTAL CROSS SECTION TREATMENT Groupie
VERSION 85-2 (AUGUST 1985) *FORTRAN-77/H VERSION Groupie
VERSION 86-1 (JANUARY 1986) *ENDF/B-VI FORMAT Groupie
VERSION 86-2 (JUNE 1986) *BUILT-IN MAXWELLIAN, 1/E AND FISSION Groupie
WEIGHTING SPECTRUM. Groupie
VERSION 88-1 (JULY 1988) *OPTION...INTERNALLY DEFINE ALL I/O Groupie
FILE NAMES (SEE, SUBROUTINES FILIO1 Groupie
FILIO2 FOR DETAILS). Groupie
*IMPROVED BASED ON USER COMMENTS. Groupie
VERSION 89-1 (JANUARY 1989) *PSYCHOANALYZED BY PROGRAM FREUD TO Groupie
INSURE PROGRAM WILL NOT DO ANYTHING Groupie
CRAZY. Groupie
*UPDATED TO USE NEW PROGRAM CONVERT Groupie
KEYWORDS. Groupie
*ADDED LIVERMORE CIVIC COMPILER Groupie
CONVENTIONS. Groupie
VERSION 91-1 (JUNE 1991) *INCREASED PAGE SIZE FROM 1002 TO 5010 Groupie
POINTS Groupie
*UPDATED BASED ON USER COMMENTS Groupie
*ADDED FORTRAN SAVE OPTION Groupie
*COMPLETELY CONSISTENT ROUTINE TO READ Groupie
FLOATING POINT NUMBERS. Groupie
VERSION 92-1 (JANUARY 1992) *ADDED RESONANCE INTEGRAL CALCULATION - Groupie
UNSHIELDED AND/OR SHIELDED - FOR Groupie
DETAILS SEE BELOW Groupie
*INCREASED NUMBER OF ENERGY POINTS Groupie
IN BUILT-IN SPECTRA - TO IMPROVE Groupie
ACCURACY. Groupie
*ALLOW SELECTION OF ZA/MF/MT OR Groupie
MAT/MF/MT RANGES - ALL DATA NOT Groupie
SELECTED IS SKIPPED ON INPUT AND Groupie
NOT WRITTEN AS OUTPUT. Groupie
*COMPLETELY CONSISTENT I/O ROUTINES - Groupie
TO MINIMIZE COMPUTER DEPENDENCE. Groupie
*NOTE, CHANGES IN INPUT PARAMETER Groupie
FORMAT - FOR ZA/MF/MT OR MAT/MF/MT Groupie
RANGES. Groupie
VERSION 92-2 (JUNE 1992) *MULTIBAND PARAMETERS OUTOUT AS Groupie
CHARACTER (RATHER THAN BINARY) FILE. Groupie
VERSION 93-1 (APRIL 1993) *INCREASED PAGE SIZE FROM 5010 TO Groupie
30000 POINTS Groupie
*ELIMINATED COMPUTER DEPENDENCE. Groupie
VERSION 94-1 (JANUARY 1994) *VARIABLE ENDF/B DATA FILENAMES Groupie
TO ALLOW ACCESS TO FILE STRUCTURES Groupie
(WARNING - INPUT PARAMETER FORMAT Groupie
HAS BEEN CHANGED) Groupie

```

	*CLOSE ALL FILES BEFORE TERMINATING	Groupie
	(SEE, SUBROUTINE ENDIT)	Groupie
VERSION 95-1 (JANUARY 1994)	*CORRECTED MAXWELLIAN WEIGHTING	Groupie
	*CHANGING WEIGHTING SPECTRUM FROM	Groupie
	0.1 TO 0.001 % UNCERTAINTY	Groupie
VERSION 96-1 (JANUARY 1996)	*COMPLETE RE-WRITE	Groupie
	*IMPROVED COMPUTER INDEPENDENCE	Groupie
	*ALL DOUBLE PRECISION	Groupie
	*ON SCREEN OUTPUT	Groupie
	*UNIFORM TREATMENT OF ENDF/B I/O	Groupie
	*IMPROVED OUTPUT PRECISION	Groupie
	*DEFINED SCRATCH FILE NAMES	Groupie
	*UP TO 1000 GROUP MULTI-BAND	Groupie
	CALCULATION (PREVIOUSLY 175)	Groupie
	*MAXIMUM NUMBER OF GROUPS REDUCED	Groupie
	FROM 3,000 TO 1,000	Groupie
	*UP TO 1000 MATERIALS	Groupie
	(PREVIOUSLY 100)	Groupie
	*CORRECTED USE OF MAXWELLIAN +	Groupie
	1/E + FISSION SPECTRUM	Groupie
	*ONLY 2 BAND VERSION DISTRIBUTED	Groupie
	(CONTACT AUTHOR FOR DETAILS)	Groupie
	*DEFINED SCRATCH FILE NAMES	Groupie
VERSION 99-1 (MARCH 1999)	*CORRECTED CHARACTER TO FLOATING	Groupie
	POINT READ FOR MORE DIGITS	Groupie
	*UPDATED TEST FOR ENDF/B FORMAT	Groupie
	VERSION BASED ON RECENT FORMAT CHANGE	Groupie
	*GENERAL IMPROVEMENTS BASED ON	Groupie
	USER FEEDBACK	Groupie
VERSION 99-2 (JUNE 1999)	*ASSUME ENDF/B-VI, NOT V, IF MISSING	Groupie
	MF=1, MT=451.	Groupie
VERS. 2000-1 (FEBRUARY 2000)	*ADDED MF=10, ACTIVATION CROSS SECTION	Groupie
	PROCESSING.	Groupie
	*GENERAL IMPROVEMENTS BASED ON	Groupie
	USER FEEDBACK	Groupie
VERS. 2002-1 (FEBRUARY 2002)	*ADDED TART 700 GROUP STRUCTURE	Groupie
	*ADDED VARIABLE SIGMA0 INPUT OPTION	Groupie
(MAY 2002)	*OPTIONAL INPUT PARAMETERS	Groupie
(NOV. 2002)	*ADDED SAND-II EXTENDED DOWN TO	Groupie
	1.0E-5 EV.	Groupie
(JUNE 2003)	*CORRECTED SAND-II 620 AND 640 GROUP	Groupie
	ENERGY BOUNDARIES DEFINITIONS.	Groupie
VERS. 2004-1 (SEPT. 2004)	*INCREASED PAGE SIZE FROM 30000 TO	Groupie
	120000 POINTS	Groupie
	*ADDED "OTHER" AS ADDITIONAL REACTION	Groupie
	TO IMPROVE MULTI-BAND FITTING	Groupie
	*ADDED ITERATION FOR "BEST" PARTIAL	Groupie
	PARAMETERS.	Groupie
	*DO NOT SKIP LOW TOTAL ENERGY RANGES	Groupie
	WHEN DEFINING AVERAGE CROSS SECTIONS -	Groupie
	THIS MAKES OUTPUT COMPATIBLE WITH	Groupie
	ANY STANDARD AVERAGING PROCEDURE	Groupie
OWNED, MAINTAINED AND DISTRIBUTED BY		Groupie
-----		Groupie
THE NUCLEAR DATA SECTION		Groupie
INTERNATIONAL ATOMIC ENERGY AGENCY		Groupie
P.O. BOX 100		Groupie
A-1400, VIENNA, AUSTRIA		Groupie
EUROPE		Groupie
ORIGINALLY WRITTEN BY		Groupie
-----		Groupie
DERMOTT E. CULLEN		Groupie
UNIVERSITY OF CALIFORNIA		Groupie
LAWRENCE LIVERMORE NATIONAL LABORATORY		Groupie
L-159		Groupie
P.O. BOX 808		Groupie
LIVERMORE, CA 94550		Groupie
U.S.A.		Groupie
TELEPHONE 925-423-7359		Groupie

AUTHORS MESSAGE

AT THE PRESENT TIME WE ARE ATTEMPTING TO DEVELOP A SET OF COMPUTER 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

- (1) UNSHIELDED GROUP AVERAGED CROSS SECTIONS
- (2) BONDARENKO SELF-SHIELDED GROUP AVERAGED CROSS SECTIONS
- (3) MULTI-BAND PARAMETERS

IN THE FOLLOWING 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

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 OR V 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 CARD IS CORRECT. SEQUENCE
NUMBERS (COLUMNS 76-80) ARE IGNORED ON INPUT, BUT WILL BE
CORRECTLY OUTPUT ON ALL CARDS. 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.

ALL FILE 3 CROSS SECTIONS THAT ARE USED BY THIS PROGRAM MUST BE LINEARLY INTERPOLABLE IN ENERGY AND CROSS SECTION (ENDF/B INTERPOLATION LAW 2). FILE 3 BACKGROUND CROSS SECTIONS MAY BE MADE LINEARLY INTERPOLABLE USING PROGRAM LINEAR (UCRL-50400, VOL. 17, PART A). THE RESONANCE CONTRIBUTION MAY BE ADDED TO THE BACKGROUND CROSS SECTIONS USING PROGRAM RECENT (UCRL-50400, VOL. 17, PART B). IF THIS PROGRAM FINDS THAT THE FILE 3 CROSS SECTIONS ARE NOT LINEARLY INTERPOLABLE THIS PROGRAM WILL TERMINATE EXECUTION.

CONTENTS OF OUTPUT

IF ENDF/B FORMATTED OUTPUT IS REQUESTED ENTIRE EVALUATIONS ARE OUTPUT, NOT JUST THE MULTI-GROUPED FILE 3 CROSS SECTIONS, E.G. ANGULAR AND ENERGY DISTRIBUTIONS ARE ALSO INCLUDED.

DOCUMENTATION

THE FACT THAT THIS PROGRAM HAS OPERATED ON THE DATA IS DOCUMENTED BY THE ADDITION OF THREE COMMENT CARDS AT THE END OF EACH HOLLERITH SECTION TO DESCRIBE THE GROUP STRUCTURE AND WEIGHTING SPECTRUM, E.G.

```

***** PROGRAM GROUPE (2004-1) *****
UNSHIELDED GROUP AVERAGES USING 69 GROUPS (WIMS)
MAXWELLIAN, 1/E AND FISSION WEIGHTING SPECTRUM

THE ORDER OF ALL SIMILAR COMMENTS (FROM LINEAR, RECENT AND SIGMAL)
REPRESENTS A COMPLETE HISTORY OF ALL OPERATIONS PERFORMED ON
THE DATA.

THESE COMMENT CARDS 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
-----
THIS PROGRAM DOES NOT USE THE REACTION INDEX WHICH IS GIVEN IN
SECTION MF=1, MT=451 OF EACH EVALUATION.

THIS PROGRAM DOES NOT UPDATE THE REACTION INDEX IN MF=1, MT=451.
THIS CONVENTION HAS BEEN ADOPTED BECAUSE MOST USERS DO NOT
REQUIRE A CORRECT REACTION INDEX FOR THEIR APPLICATIONS AND IT WAS
NOT 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
-----
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.

SELECTION OF DATA
-----
THE PROGRAM SELECTS MATERIALS TO BE PROCESSED BASED EITHER ON
MAT (ENDF/B MAT NO.) OR ZA. THE PROGRAM ALLOWS UP TO 100 MAT OR
ZA RANGES TO BE SPECIFIED. THE PROGRAM WILL ASSUME THAT THE
ENDF/B TAPE IS IN EITHER MAT OR ZA ORDER, WHICHEVER CRITERIA IS
USED TO SELECT MATERIALS, AND WILL TERMINATE WHEN A MAT OR ZA
IS FOUND THAT IS ABOVE THE RANGE OF ALL REQUESTS.

ENERGY ORDER AND UNITS
-----
ALL ENERGIES (FOR CROSS SECTIONS, WEIGHTING SPECTRUM OR GROUP
BOUNDARIES) MUST BE IN UNITS OF EV AND MUST BE IN ASCENDING
NUMERICAL ORDER.

ENERGY GRID
-----
ALTHOUGH ALL REACTIONS MUST TO LINEARLY INTERPOLABLE, THEY DO NOT
ALL HAVE TO USE THE SAME ENERGY GRID. EACH REACTION CAN BE GIVEN
BY AN INDEPENDENT ENERGY GRID. THIS PROGRAM WILL PROCEED FROM
THE LOWEST TO HIGHEST ENERGY SELECTING EACH ENERGY INTERVAL OVER
WHICH ALL DATA, FOR ANY GIVEN CALCULATION, ARE ALL LINEARLY
INTERPOLABLE.

GROUP STRUCTURE
-----
THIS PROGRAM IS DESIGNED TO USE AN ARBITRARY ENERGY GROUP
STRUCTURE WHERE THE ENERGIES ARE IN EV AND ARE IN INCREASING
ENERGY ORDER. THE MAXIMUM NUMBER OF GROUPS IS 1000.

THE USER MAY INPUT AN ARBITRARY GROUP STRUCTURE OR THE USER MAY
USE ONE OF THE SEVEN BUILT-IN GROUP STRUCTURES.
(0) 175 GROUP (TART STRUCTURE)

```

5

WEIGHTING FUNCTION THAT IS A PRODUCT OF THE ENERGY DEPENDENT
WEIGHTING SPECTRUM TIMES A BONDERENKO TYPE SELF-SHIELDING FACTOR.

$$WT(E) = S(E) / (TOTAL(E) + SIGMA0) ** N$$

WHERE...

```

S(E)      - ENERGY DEPENDENT WEIGHTING SPECTRUM (DEFINED BY
            TABULATED VALUES AND LINEAR INTERPOLATION BETWEEN
            TABULATED VALUES).

TOTAL(E)  - ENERGY DEPENDENT TOTAL CROSS SECTION FOR ONE MATERIAL
            (DEFINED BY TABULATED VALUES AND LINEAR INTERPOLATION
            BETWEEN TABULATED VALUES).

SIGMA0    - CROSS SECTION TO REPRESENT THE EFFECT OF ALL OTHER
            MATERIALS AND LEAKAGE (DEFINED WITHIN EACH GROUP TO BE
            A MULTIPLE OF THE UNSHIELDED TOTAL CROSS SECTION WITHIN
            THAT GROUP OR POWERS OF 10 - INPUT OPTION).

N         - A POSITIVE INTEGER (0, 1, 2 OR 3).

```

THE PROGRAM WILL USE ONE ENERGY DEPENDENT WEIGHTING SPECTRUM S(E) AND 25 DIFFERENT BENDERENKO TYPE SELF-SHIELDING FACTORS (25 SIGMA0 AND N COMBINATIONS) TO DEFINE 25 DIFFERENT AVERAGE CROSS SECTIONS, FOR EACH REACTION, WITHIN EACH GROUP.

THE 25 WEIGHTING FUNCTIONS USED ARE....

```

(1) - UNSHIELDED CROSS SECTIONS (N=0)
(2-22)- PARTIALLY SHIELDED CROSS SECTIONS (N=1 ,VARIOUS SIGMA0)
      THE VALUES OF SIGMA0 USED WILL BE EITHER,
      (A) THE VALUES OF SIGMA0 THAT ARE USED VARY FROM 1024
      TIMES THE UNSHIELDED TOTAL CROSS SECTIONS IN STEPS OF 1/2
      DOWN TO 1/1024 TIMES THE UNSHIELDED TOTAL CROSS SECTION
      (A RANGE OF OVER 1 MILLION, CENTERED ON THE UNSHIELDED
      TOTAL CROSS SECTION WITHIN EACH GROUP).
      (B) THE SAME CONSTANT VALUES OF SIGMA0 IN EACH GROUP. THE
      VALUES OF SIGMA0 USED INCLUDE 40000, 20000, 10000, 7000,
      4000, 2000, 1000, 700, 400, 200, 100, 70, 40, 20, 10, 7,
      4, 2, 1, 0.7, 0.4 (A RANGE OF 100,000 SPANNING MORE THAN
      THE RANGE OF SIGMA0 VALUES THAT MAY BE ENCOUNTERED IN
      ACTUAL APPLICATIONS)
(23) - TOTALLY SHIELDED FLUX WEIGHTED CROSS SECTION
      (N=1, SIGMA0=0)
(24) - TOTALLY SHIELDED CURRENT WEIGHTED CROSS SECTION
      (N=2, SIGMA0=0)
(25) - TOTALLY SHIELDED COSINE SQUARED WEIGHTED CROSS SECTION
      (N=3, SIGMA0=0)

```

FOR ALL OTHER REACTIONS (EXCEPT TOTAL, ELASTIC, CAPTURE AND FISSION) THE PROGRAM WILL USE THE ENERGY DEPENDENT WEIGHTING SPECTRUM $S(E)$ TO DEFINE THE UNSHIELDED (BONDERENKO $N=0$) AVERAGED CROSS SECTION WITHIN EACH GROUP.

CALCULATION OF RESONANCE INTEGRALS

IN A PURE ELASTIC ISOTROPICALLY SCATTERING MATERIAL WITH A
CONSTANT CROSS SECTION THE SPECTRUM WILL BE $1/E$ AND THERE WILL
BE NO SELF-SHIELDING.

IN THIS CASE IF THE CROSS SECTION VARIES WITH ENERGY THE SPECTRUM WILL STILL BE $1/E$ AND THE SELF-SHIELDING FACTOR WILL BE EXACTLY $1/\text{SIG-TOT}(E)$ - WHERE $\text{SIG-TOT}(E) = \text{SIG-EL}(E)$, SINCE THERE IS ONLY SCATTERING.

IF WE HAVE AN INFINITELY DILUTE AMOUNT OF A MATERIAL UNIFORMLY MIXED WITH A PURE ELASTIC ISOTROPICALLY SCATTERING MATERIAL WITH A CONSTANT CROSS SECTION THE STANDARD DEFINITION OF THE RESONANCE INTEGRAL CAN BE USED TO DEFINE REACTION RATES FOR EACH REACTION.

THE RESONANCE INTEGRAL IS DEFINED AS,

$$RI = (\text{INTEGRAL } E1 \text{ TO } E2) (\text{SIGMA}(E) * S(E) * WT(E) * DE)$$

[illegible]

$$\begin{aligned} S(E) &= 1/E \\ WT(E) &= 1 \quad - \text{NO SELF-SHIELDING} \end{aligned}$$
$$RI = \text{AVERAGE} * (\text{INTEGRAL } E1 \text{ TO } E2) (S(E)*WT(E)*DE)$$

FOR A $1/E$ SPECTRUM AND NO SELF-SHIELDING THIS REDUCES TO,

$$RI = \text{AVERAGE}^* \text{LOG}(E2/E1)$$

IN ANY OTHER SITUATION, INCLUDING ABSORPTION AND/OR ENERGY DEPENDENT CROSS SECTIONS, THE SPECTRUM WILL NOT BE $1/E$ - ABSORPTION WILL TEND TO DECREASE THE SPECTRUM PROGRESSIVELY MORE AT LOWER ENERGIES - ENERGY DEPENDENCE OF THE CROSS SECTION WILL LEAD TO SELF-SHIELDING.

HERE WE WILL NOT ATTEMPT TO PERFORM A DETAILED SPECTRUM
CALCULATION TO ACCOUNT FOR ABSORPTION.

HOWEVER, WE WILL EXTEND THE DEFINITION OF THE RESONANCE INTEGRAL TO ACCOUNT FOR SELF-SHIELDING EFFECTS BY ALLOWING FOR INCLUSION OF SELF-SHIELDING EFFECTS IN THE DEFINITION OF GROUP AVERAGES AND THEN DEFINING THE RESONANCE INTEGRAL AS,

$$RI = AVERAGE * LOG(E2/E1)$$

IN ORDER TO CALCULATE RESONANCE INTEGRALS YOU MUST FOLLOW THESE STEPS,

- 1) SELECT A 1/E SPECTRUM - ON FIRST LINE OF INPUT PARAMETERS.
- 2) SELECT THE ENERGY BOUNDARIES - NORMALLY ONLY 1 GROUP FROM 0.5 EV UP TO 20 MEV - HOWEVER, YOU ARE FREE TO SELECT ANY ENERGY RANGE THAT YOU WISH - YOU MAY EVEN SELECT MORE THAN 1 GROUP MERELY BY SPECIFYING MORE THAN 1 GROUP AS INPUT - THIS CAN BE USED TO DEFINE THE CONTRIBUTIONS TO THE RESONANCE INTEGRAL FROM INDIVIDUAL ENERGY RANGES.
- 3) SELECT THIS OPTION FOR THE UNSHIELDED AND/OR SHIELDED OUTPUT LISTING - ON THE SECOND LINE OF INPUT PARAMETERS.

WHEN THIS OPTION IS USED THE PROGRAM WILL CALCULATE GROUP AVERAGED CROSS SECTIONS - AS DEFINED ABOVE - PRIOR TO OUTPUT THE RESULTS WILL MERELY BE MULTIPLIED BY THE WIDTH OF THE GROUP ASSUMING YOU HAVE SELECTED A 1/E SPECTRUM - THERE IS NO CHECK ON THIS - THE PROGRAM MERELY MULTIPLIES THE GROUP AVERAGED CROSS SECTIONS BY,

LOG(E2/E1) - WHERE E2 AND E1 ARE THE GROUP ENERGY BOUNDARIES.

WARNING - IT IS UP TO YOU TO INSURE THAT YOU FOLLOW EXACTLY THE
STEPS OUTLINED ABOVE IF YOU WISH TO OBTAIN MEANINGFUL
RESULTS.

NOTE - OUTPUT IN THE ENDF/B FORMAT IS ALWAYS GROUP AVERAGED CROSS SECTIONS, REGARDLESS OF WHETHER YOU ASK FOR AVERAGED CROSS SECTIONS OR RESONANCE INTEGRALS - THIS IS BECAUSE DATA IN THE ENDF/B FORMAT IS EXPLICITLY DEFINED TO BE CROSS SECTIONS.

RESONANCE INTEGRAL OUTPUT CAN ONLY BE OBTAINED IN THE
LISTING FORMATS.

MINIMUM TOTAL CROSS SECTION TREATMENT

SINCE THE BONDARENKO SELF-SHIELDING DEPENDS ON 1/TOTAL CROSS SECTION, THE ALGORITHM WILL BECOME NUMERICALLY UNSTABLE IF THE TOTAL CROSS SECTION IS NEGATIVE (AS OCCURS IN MANY ENDF/B EVALUATIONS). IF THE TOTAL IS LESS THAN SOME MINIMUM ALLOWABLE VALUE (DEFINE BY OKMIN, PRESENTLY 1 MILLI-BARN) AN ERROR MESSAGE WILL BE PRINTED AND FOR THE SELF-SHIELDING CALCULATION ALL ENERGY

NOTE, FOR THE UNSHIELDED CALCULATIONS ALL CROSS SECTIONS WILL BE CONSIDERED WHETHER THEY ARE POSITIVE OR NEGATIVE. THEREFORE IF THE TOTAL CROSS SECTION IS NEGATIVE OR LESS THAN THE MINIMUM VALUE THERE MAY BE AN INCONSISTENCY BETWEEN THE UNSHIELDED AND THE SELF-SHIELDED CROSS SECTIONS. IF THE TOTAL CROSS SECTION IS NEGATIVE AND SELF-SHIELDED CROSS SECTIONS ARE CALCULATED THE PROGRAM WILL PRINT AN ERROR MESSAGE INDICATING THAT THE SELF-SHIELDED RESULTS ARE UNRELIABLE AND SHOULD NOT BE USED. THEREFORE IN THIS CASE THE PROGRAM WILL NOT ATTEMPT TO MODIFY THE UNSHIELDED RESULTS TO ELIMINATE THE EFFECT OF NEGATIVE CROSS SECTIONS, SINCE THE UNSHIELDED RESULTS ARE THE ONLY ONES WHICH TRULY REFLECT THE ACTUAL INPUT.

IN THE RESOLVED RESONANCE REGION (ACTUALLY EVERYWHERE BUT IN THE UNRESOLVED RESONANCE REGION) THE CROSS SECTIONS OUTPUT BY LINEAR-RECENT-SIGNAL1 WILL BE ACTUAL ENERGY DEPENDENT CROSS SECTIONS AND THE CALCULATIONS BY THIS PROGRAM WILL YIELD ACTUAL SHIELDED AND UNSHIELDED CROSS SECTIONS.

IN THE UNRESOLVED RESONANCE REGION PROGRAM RECENT USES THE UNRESOLVED RESONANCE PARAMETERS TO CALCULATE INFINITELY DILUTE AVERAGE CROSS SECTIONS. THIS PROGRAM WILL MERELY READ THIS INFINITELY DILUTE DATA AS IF IT WERE ENERGY DEPENDENT DATA AND GROUP AVERAGE IT. AS SUCH THIS PROGRAM WILL PRODUCE THE CORRECT UNSHIELDED CROSS SECTION IN THE UNRESOLVED RESONANCE REGION, BUT IT WILL NOT PRODUCE THE CORRECT SELF-SHIELDING EFFECTS.

ALL INTEGRALS ARE PERFORMED ANALYTICALLY. THEREFORE NO ERROR IS INTRODUCED DUE TO THE USE OF TRAPAZOIDAL OR OTHER INTEGRATION SCHEME. THE TOTAL ERROR THAT CAN BE ASSIGNED TO THE RESULTING AVERAGES IS JUST THAT DUE TO THE ERROR IN THE CROSS SECTIONS AND ENERGY DEPENDENT WEIGHTING SPECTRUM. GENERALLY SINCE THE THE ENERGY DEPENDENT WEIGHTING SPECTRUM APPEARS IN BOTH THE NUMERATOR AND THE DENOMINATOR THE AVERAGES RAPIDLY BECOME INSENSITIVE TO THE WEIGHTING SPECTRUM AS MORE GROUPS ARE USED. SINCE THE WEIGHTING SPECTRUM IS LOADED IN THE PAGING SYSTEM THE USER CAN DESCRIBE THE SPECTRUM TO ANY REQUIRED ACCURACY USING ANY NUMBER OF ENERGY VS. SPECTRUM PAIRS.

MULTI-BAND PARAMETERS ARE CALCULATED FOR THE TOTAL, ELASTIC, CAPTURE AND FISSION REACTIONS. WITH THE NUMBER OF GROUPS THAT ARE NORMALLY USED (SEE BUILT IN GROUP STRUCTURES) ALL OTHER REACTIONS RESULT IN A NEGLIGIBLE AMOUNT OF SELF-SHIELDING. AS SUCH THEIR EQUIVALENT BAND CROSS SECTION WILL MERELY BE THEIR UNSHIELDED VALUE WITHIN EACH BAND.

FOR ANY GIVEN EVALUATION, WITHIN ANY GIVEN GROUP THIS PROGRAM WILL GENERATE THE MINIMUM NUMBER OF BANDS REQUIRED WITHIN THAT GROUP. AS OUTPUT TO THE COMPUTER READABLE DISK FILE THE BAND PARAMETERS FOR EACH EVALUATION WILL BE FORMATTED TO HAVE THE SAME NUMBER OF BANDS IN ALL GROUPS (WITH ZERO WEIGHT FOR SOME BANDS WITHIN ANY GROUP). THE USER MAY DECIDE TO HAVE OUTPUT EITHER WITH THE MINIMUM NUMBER OF BANDS REQUIRED FOR EACH EVALUATION (E.G. 2 BANDS FOR HYDROGEN AND 4 BANDS FOR U-233) OR THE SAME NUMBER OF BANDS FOR ALL EVALUATIONS (E.G. 4 BANDS FOR BOTH HYDROGEN AND U-233).

8

INPUT CARDS				Groupie
-----				Groupie
CARD	COLS.	FORMAT	DESCRIPTION	Groupie
----	-----	-----	-----	Groupie
1	1-11	I11	SELECTION CRITERIA (0=MAT, 1=ZA)	Groupie
1	12-22	I11	NUMBER OF GROUPS.	Groupie
			=.GT.0 - ARBITRARY GROUP BOUNDARIES ARE READ	Groupie
			FROM INPUT FILE (N GROUPS REQUIRE	Groupie
			N+1 GROUP BOUNDARIES). CURRENT	Groupie
			PROGRAM MAXIMUM IS 1000 GROUPS.	Groupie
			BUILT-IN OPTIONS INCLUDE....	Groupie
			= 0 - TART 175 GROUPS	Groupie
			= -1 - ORNL 50 GROUPS	Groupie
			= -2 - ORNL 126 GROUPS	Groupie
			= -3 - ORNL 171 GROUPS	Groupie
			= -4 - SAND-II 620 (665) GROUPS TO 18 MEV	Groupie
			= -5 - SAND-II 640 (685) GROUPS TO 20 MEV	Groupie
			= -6 - WIMS 69 GROUPS	Groupie
			= -7 - GAM-I 68 GROUPS	Groupie
			= -8 - GAM-II 99 GROUPS	Groupie
			= -9 - MUFT 54 GROUPS	Groupie
			= -10 - ABBN 28 GROUPS	Groupie
			= -11 - TART 650 GROUPS	Groupie
			= -12 - TART 700 GROUPS	Groupie
			= -13 - SAND-II 665 GROUPS TO 18 MEV	Groupie
			= -14 - SAND-II 685 GROUPS TO 20 MEV	Groupie
1	23-33	I11	MULTI-BAND SELECTOR	Groupie
			= 0 - NO MULTI-BAND CALCULATIONS	Groupie
			= 1 - 2 BAND. CONSERVE AV(TOT), AV(1/TOT)	Groupie
			AND AV(1/TOT**2)	Groupie
			= 2 - 2 BAND. CONSERVE AV(TOT), AV(1/TOT)	Groupie
			AND AV(1/(TOT+SIGMA0)) WHERE	Groupie
			SIGMA0 = AV(TOT) IN EACH GROUP	Groupie
			= 3-5- MULTI-BAND FIT. CONSERVE AV(TOT) AND	Groupie
			MINIMIZE FRACTIONAL ERROR FOR ENTIRE	Groupie
			SELF-SHIELDING CURVE (SIGMA0 = 0 TO	Groupie
			INFINITY)	Groupie
			IF THE SELECTOR IS POSITIVE (1 TO 5) THE	Groupie
			MINIMUM NUMBER OF BANDS WILL BE OUTPUT FOR	Groupie
			EACH ISOTOPE INDEPENDENTLY. IF THE SELECTOR	Groupie
			IS NEGATIVE (-1 TO -5) THE SAME NUMBER OF	Groupie
			BANDS (ABS(SELECTOR)) WILL BE OUTPUT FOR	Groupie
			ALL ISOTOPES.	Groupie
1	34-44	I11	NUMBER OF POINTS USED TO DESCRIBE ENERGY	Groupie
			DEPENDENT WEIGHTING SPECTRUM S(E).	Groupie
			= -2 - MAXWELLIAN - UP TO 0.1 EV	Groupie
			1/E - 0.1 EV TO 67 KEV	Groupie
			FISSION - ABOVE 67 KEV	Groupie
			= -1 - 1/E	Groupie
			= 0 OR 1- ENERGY INDEPENDENT (SO CALLED FLAT	Groupie
			WEIGHTING SPECTRUM).	Groupie
			= .GT.1 - READ THIS MANY POINTS FROM INPUT	Groupie
			TO DESCRIBE WEIGHTING SPECTRUM.	Groupie
			NO LIMIT TO THE NUMBER OF POINTS	Groupie
			USED TO DESCRIBE WEIGHTING.	Groupie
1	45-55	D11.4	MULTI-BAND CONVERGENCE CRITERIA.	Groupie
			ONLY USED FOR 3 OR MORE BANDS. THE NUMBER OF	Groupie
			BANDS IN EACH GROUPS IS SELECTED TO INSURE	Groupie
			THAT THE ENTIRE SELF-SHIELDING CURVE CAN BE	Groupie
			REPRODUCED TO WITHIN THIS FRACTIONAL ERROR.	Groupie
			= .LT. 0.0001 - USE STANDARD 0.001	Groupie
			(0.1 PER-CENT)	Groupie
			= .GE. 0.0001 - USE AS CONVERGENCE CRITERIA	Groupie
1	56-66	I11	SIGMA-0 DEFINITION SELECTOR.	Groupie
			< 0 - 21 VALUES OF SIGMA0 ARE READ INPUT AND	Groupie
			INTERPRETED AS FIXED VALUES = SAME AS	Groupie
			= 1 DESCRIPTION BELOW	Groupie
			INPUT VALUES MUST ALL BE,	Groupie
			1) GREATER THAN 0	Groupie
			2) IN DESCENDING VALUE ORDER	Groupie

12

EXAMPLE INPUT NO. 1

EXPLICITLY SPECIFY THE STANDARD FILENAMES.

THE FOLLOWING 7 INPUT LINES ARE REQUIRED.

EXAMPLE INPUT NO. 2

THE SAME EXAMPLE 1, AS ABOVE, ONLY THE ENDF/B DATA WILL BE READ FROM \ENDFB6\SIGMA1\K300\ZA092238 (U-238 AT 300 KELVIN) AND WRITTEN TO \ENDFB6\GROUPIE\K300\ZA092238

THE FOLLOWING 7 INPUT LINES ARE REQUIRED.

```

      0      0      -2      0 1.00000-03      0
\ENDFB6\SIGMA1\K300\ZA092238
\ENDFB6\GROUPIE\K300\ZA092238
      1      1      1      1      1
TART 175 GROUP, 2 BAND LIBRARY TO 0.1 PER-CENT ACCURACY
      1 1 1 9999 0 0
      (BLANK CARD TERMINATES REQUEST LIST)

```

EXAMPLE INPUT NO. 3

PROCESS ALL DATA. USE 1/V WEIGHTING IN ORDER TO CALCULATE
UNSHIELDED ONE GROUP CROSS SECTIONS OVER THE ENERGY RANGE 0.5 EV
TO 1 MEV (NOTE THAT THE RESULTS ARE SIMPLY PROPORTIONAL TO THE
RESONANCE INTEGRAL FOR EACH REACTION). OUTPUT UNSHIELDED LISTING.

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

THE FOLLOWING 7 INPUT CARDS ARE REQUIRED.

```

0          0          1          -1          0
      (USE STANDARD FILENAME = ENDFB.IN)
      (USE STANDARD FILENAME = ENDFB.OUT)
0          0          0          0          1
RESONANCE INTEGRAL CALCULATION (FROM 0.5 EV TO 1 MEV)
      (RETRIEVE ALL DATA, TERMINATE REQUEST LIST)
5.00000-01 1.00000+06

```

=====