**======================================================================= Sigma1**

 **Sigma1**

 **PROGRAM SIGMA1 Sigma1**

 **============== Sigma1**

 **VERSION 73-1 (MARCH 1973) Sigma1**

 **VERSION 76-1 (FEBRUARY 1976) Sigma1**

 **VERSION 76-2 (OCTOBER 1976) Sigma1**

 **VERSION 77-1 (JANUARY 1977) Sigma1**

 **VERSION 78-1 (JULY 1978) Sigma1**

 **VERSION 79-1 (JULY 1979) CDC-7600 AND CRAY-1 VERSION. Sigma1**

 **VERSION 80-1 (MAY 1980) IBM, CDC AND CRAY VERSION Sigma1**

 **VERSION 80-2 (DECEMBER 1980)IMPROVED BASED ON USER COMMENTS. Sigma1**

 **VERSION 81-1 (MARCH 1981) DOUBLE PRECISION IBM VERSION Sigma1**

 **VERSION 81-2 (AUGUST 1981) IMPROVED IBM SPEED AND STABILITY Sigma1**

 **VERSION 82-1 (JANUARY 1982) IMPROVED COMPUTER COMPATIBILITY Sigma1**

 **VERSION 83-1 (JANUARY 1983)\*MAJOR RE-DESIGN. Sigma1**

 **\*PAGE SIZE INCREASED - 1002 TO 2004. Sigma1**

 **\*ELIMINATED COMPUTER DEPENDENT CODING. Sigma1**

 **\*NEW, MORE COMPATIBLE I/O UNIT NUMBER. Sigma1**

 **\*ADDED STANDARD ALLOWABLE ERROR OPTION Sigma1**

 **(CURRENTLY 0.1 PER-CENT). Sigma1**

 **\*UNRESOLVED RESONANCE REGION COPIED. Sigma1**

 **\*1/V EXTENSION OF CROSS SECTIONS Sigma1**

 **OUTSIDE OF TABULATED ENERGY RANGE AND Sigma1**

 **INTO UNRESOLVED ENERGY RANGE. Sigma1**

 **VERSION 83-2 (OCTOBER 1983)\*IMPROVED BASED ON USER COMMENTS. Sigma1**

 **VERSION 84-1 (APRIL 1984) \*IMPROVED NUMERICAL STABILITY. Sigma1**

 **\*PARTIAL EVALUATION TREATMENT. Sigma1**

 **VERSION 85-1 (APRIL 1985) \*ITERATE TO CONVERGENCE (USING THE SAME Sigma1**

 **ENERGY GRID FOR HOT CROSS SECTION AS Sigma1**

 **COLD CROSS SECTIONS WAS FOUND TO BE Sigma1**

 **INACCURATE). Sigma1**

 **\*NEW FASTER HIGH ENERGY BROADENING. Sigma1**

 **\*UPDATED FOR ENDF/B-VI FORMATS. Sigma1**

 **\*SPECIAL I/O ROUTINES TO GUARANTEE Sigma1**

 **ACCURACY OF ENERGY. Sigma1**

 **\*DOUBLE PRECISION TREATMENT OF ENERGY Sigma1**

 **(REQUIRED FOR NARROW RESONANCES). Sigma1**

 **VERSION 85-2 (AUGUST 1985) \*FORTRAN-77/H VERSION Sigma1**

 **VERSION 86-1 (JANUARY 1986)\*ENERGY DEPENDENT SCATTERING RADIUS Sigma1**

 **VERSION 88-1 (JULY 1988) \*OPTION...INTERNALLY DEFINE ALL I/O Sigma1**

 **FILE NAMES (SEE, SUBROUTINE FILEIO Sigma1**

 **FOR DETAILS). Sigma1**

 **\*IMPROVED BASED ON USER COMMENTS. Sigma1**

 **VERSION 89-1 (JANUARY 1989)\*PSYCHOANALYZED BY PROGRAM FREUD TO Sigma1**

 **INSURE PROGRAM WILL NOT DO ANYTHING Sigma1**

 **CRAZY. Sigma1**

 **\*UPDATED TO USE NEW PROGRAM CONVERT Sigma1**

 **KEYWORDS. Sigma1**

 **\*ADDED LIVERMORE CIVIC COMPILER Sigma1**

 **CONVENTIONS. Sigma1**

 **VERSION 90-1 (JUNE 1990) \*UPDATED BASED ON USER COMMENTS Sigma1**

 **\*ADDED FORTRAN SAVE OPTION Sigma1**

 **\*NEW MORE CONSISTENT ENERGY OUTPUT Sigma1**

 **ROUTINES Sigma1**

 **VERSION 91-1 (JULY 1991) \*WARNING...INPUT PARAMETER FORMAT Sigma1**

 **HAS BEEN CHANGED - SEE BELOW FOR Sigma1**

 **DETAILS. Sigma1**

 **\*ADDED CHARGED PARTICLE PROJECTILES Sigma1**

 **\*OUTPUT ENERGY RANGE IS ALWAYS AT Sigma1**

 **LEAST AS LARGE AS INPUT ENERGY RANGE. Sigma1**

 **\*NO 1/V EXTENSION OF CROSS SECTIONS Sigma1**

 **FROM UNRESOLVED ENERGY RANGE. Sigma1**

 **VERSION 92-1 (JANUARY 1992)\*INSURE MINIMUM AND MAXIMUM CROSS Sigma1**

 **SECTIONS ARE ALWAYS KEPT (NOT THINNED) Sigma1**

 **\*MT=19 (FIRST CHANCE FISSION) TREATED Sigma1**

 **THE SAME AS FISSION. Sigma1**

 **\*VARIABLE MINIMUM CROSS SECTION OF Sigma1**

 **INTEREST - TO ALLOW SMALL CROSS Sigma1**

 **SECTIONS NEAR THRESHOLDS TO BE Sigma1**

 **TREATED PROPERLY. Sigma1**

 **\*ALL ENERGIES INTERNALLY ROUNDED PRIOR Sigma1**

 **TO CALCULATIONS. Sigma1**

 **\*COMPLETELY CONSISTENT I/O AND ROUNDING Sigma1**

 **ROUTINES - TO MINIMIZE COMPUTER Sigma1**

 **DEPENDENCE. Sigma1**

 **VERSION 92-2 (JULY 1992) \*CORRECTED BUG ASSOCIATED WITH Sigma1**

 **THRESHOLD REACTIONS. Sigma1**

 **\*UNRESOLVED REGION COPIED WITHOUT Sigma1**

 **THINNING (IT SHOULD BE EXACTLY THE Sigma1**

 **SAME AT ALL TEMPERATURES). Sigma1**

 **\*NO THINNING OF REACTIONS (MT) THAT Sigma1**

 **WERE NOT BROADENED. Sigma1**

 **VERSION 93-1 (APRIL 1993) \*INCREASED PAGE SIZE FROM 2004 Sigma1**

 **TO 24000 ENERGY PONTS. Sigma1**

 **VERSION 94-1 (JANUARY 1994)\*VARIABLE ENDF/B DATA FILENAMES Sigma1**

 **TO ALLOW ACCESS TO FILE STRUCTURES Sigma1**

 **(WARNING - INPUT PARAMETER FORMAT Sigma1**

 **HAS BEEN CHANGED) Sigma1**

 **\*CLOSE ALL FILES BEFORE TERMINATING Sigma1**

 **(SEE, SUBROUTINE ENDIT) Sigma1**

 **VERSION 96-1 (JANUARY 1996) \*COMPLETE RE-WRITE Sigma1**

 **\*IMPROVED COMPUTER INDEPENDENCE Sigma1**

 **\*ALL DOUBLE PRECISION Sigma1**

 **\*ON SCREEN OUTPUT Sigma1**

 **\*UNIFORM TREATMENT OF ENDF/B I/O Sigma1**

 **\*IMPROVED OUTPUT PRECISION Sigma1**

 **\*DEFINED SCRATCH FILE NAMES Sigma1**

 **\*ALWAYS INCLUDE THERMAL VALUE Sigma1**

 **VERSION 97-1 (APRIL 1997) \*OPTIONALLY SET NEGATIVE CROSS Sigma1**

 **SECTIONS = 0 ON INPUT AND Sigma1**

 **OUTPUT. Sigma1**

 **\*INCREASED PAGE SIZE FROM 24000 Sigma1**

 **TO 60000 ENERGY POINTS. Sigma1**

 **VERSION 99-1 (MARCH 1999) \*CORRECTED CHARACTER TO FLOATING Sigma1**

 **POINT READ FOR MORE DIGITS Sigma1**

 **\*UPDATED TEST FOR ENDF/B FORMAT Sigma1**

 **VERSION BASED ON RECENT FORMAT CHANGE Sigma1**

 **\*TREAT LOW ENERGY INITIAL CROSS Sigma1**

 **SECTIONS AS LOG-LOG INTERPOLABLE Sigma1**

 **\*CONSTANT (RATHER THAN 1/V) EXTENSION Sigma1**

 **TO HIGHER ENERGY. Sigma1**

 **\*UPDATED CONSTANTS BASED ON CSEWG Sigma1**

 **SUBCOMMITTEE RECOMMENDATIONS Sigma1**

 **\*GENERAL IMPROVEMENTS BASED ON Sigma1**

 **USER FEEDBACK Sigma1**

 **VERSION 99-2 (JUNE 1999) \*EXTENDED RANGE OF INTEGRALS FROM 4 Sigma1**

 **TO 5 UNITS ON EACH SIDE OF ENERGY Sigma1**

 **POINT TO ALLOW FOR LARGER VARIATION Sigma1**

 **IN THE LOCAL CROSS SECTION Sigma1**

 **\*ASSUME ENDF/B-VI, NOT V, IF MISSING Sigma1**

 **MF=1, MT-451. Sigma1**

 **VERSION 99-3 (OCTOBER 1999))\*IMPROVED ERFC FUNCTION DEFINITION. Sigma1**

 **I THANK BOB MACFARLANE (LANL) FOR Sigma1**

 **SUPPLYING A MORE ACCURATE ERFC Sigma1**

 **FUNCTION. Sigma1**

 **VERS. 2000-1 (FEBRUARY 2000)\*CORRECTED LOW ENERGY INTERPOLATION Sigma1**

 **FOR NON-POSITIVE CROSS SECTIONS Sigma1**

 **\*GENERAL IMPROVEMENTS BASED ON Sigma1**

 **USER FEEDBACK Sigma1**

 **VERS. 2002-1 (MAY 2002) \*OPTIONAL INPUT PARAMETERS Sigma1**

 **VERS. 2004-1 (JAN. 2004) \*OPTIONALLY IGNORE UNRESOLVED REGION Sigma1**

 **\*CORRECTED PROBLEM AT THE RESOLVED/ Sigma1**

 **UNRESOLVED ENERGY BOUNDARY. Sigma1**

 **\*CORRECTED HIGH ENERGY CONSTANT CROSS Sigma1**

 **SECTION EXTENSION. Sigma1**

 **\*TIGHTER CRITERIA FOR INITIAL ENERGY Sigma1**

 **POINT SPACING Sigma1**

 **\*TEMPERATURE DEPENDENT ENERGY POINT Sigma1**

 **SPACING. Sigma1**

 **\*ADDED NEW REICH-MOORE (LRF=7) TO Sigma1**

 **FILE2 TO ALLOW COPY TO FIND ANY Sigma1**

 **FOLLOWING UNRESOLVED PARAMETERS Sigma1**

 **VERS. 2005-1 (JUNE 2005) \*CORRECTED ERROR IN EHOT3 EQUIVALENCE Sigma1**

 **TO EHOT - THIS ONLY EFFECTS VERY BIG Sigma1**

 **OUTPUT FILES. Sigma1**

 **VERS. 2007-1 (JAN. 2007) \*CHECKED AGAINST ALL ENDF/B-VII. Sigma1**

 **\*INCREASED PAGE SIZE FROM 60,000 Sigma1**

 **TO 360,000 ENERGY POINTS. Sigma1**

 **VERS. 2008-1 (APRIL 2008) \*1/2 INITIAL ENERGY POINT SPACING Sigma1**

 **\*72 CHARACTER FILE NAMES. Sigma1**

 **VERS. 2010-1 (Apr. 2010) \*ASSUME LOW ENERGY LOG-LOG VARIATION Sigma1**

 **UP TO 1/A (eV) FOR ALL BUT TOTAL AND Sigma1**

 **ELASTIC. Sigma1**

 **\*CHANGED DEFAULT UNCERTAINTY TO 0.01% Sigma1**

 **FROM 0.1% Sigma1**

 **\*ALLOW MULTIPLE, ADJACENT UNRESOLVED Sigma1**

 **RESONANCE REGIONS = COMBINE INTO ONE Sigma1**

 **LARGER ENERGY RANGE TO COPY. Sigma1**

 **\*DO NOT BROADEN SECTIONS THAT START Sigma1**

 **ABOVE 1 MILLION KT - PREVIOUSLY IT Sigma1**

 **WAS ASSUMED TOTAL, ELASTIC, CAPTURE Sigma1**

 **AND FISSION, AND LARGE SECTIONS (OVER Sigma1**

 **10,000 ENERGY POINTS) WOULD BROADEN. Sigma1**

 **VERS. 2012-1 (Aug. 2012) \*CHANGE COPY CRITERIA TO HANDLE NEW Sigma1**

 **(N,N') DATA = THRESHOLD MAY BE VERY Sigma1**

 **HIGH (OLD CRITERIA) BUT INCLUDES MANY Sigma1**

 **TABULATED ENERGY POINTS (NEW ADDED Sigma1**

 **CRITERIA). Sigma1**

 **\*ADDED STOP IF INCIDENT PARTICLE DATA Sigma1**

 **CANNOT BE DOPPLER BROADENED, E.G., Sigma1**

 **PHOTON INCIDENT. Sigma1**

 **\*Added CODENAME Sigma1**

 **\*32 and 64 bit Compatible Sigma1**

 **\*Added ERROR stop Sigma1**

 **VERS. 2013-1 (Nov. 2013) \*Added NO broadening above 10 MeV - Sigma1**

 **this is to handle newer evaluations Sigma1**

 **that extend to higher energies and Sigma1**

 **may do "strange" things to stop one Sigma1**

 **MT and then include it as part of Sigma1**

 **a sum at higher energies, e.g. this Sigma1**

 **change will copy ALL points above Sigma1**

 **10 MeV, thus avoiding problems near Sigma1**

 **transistion energies at 20. 30, etc. Sigma1**

 **MeV or higher energies. Sigma1**

 **VERS. 2015-1 (Jan. 2015) \*Replaced ALL 3 way IF Statements. Sigma1**

 **\*Replaced ALL LOGICAL by INTEGER. Sigma1**

 **\*Extended OUT9. Sigma1**

 **VERS. 2017-1 (May 2017) \*For MF=2 only use MT=151 = Defines Sigma1**

 **Unresolved Resonance Region (URR). Sigma1**

 **Ignore - NJOY created MT=152 and 153. Sigma1**

 **\*Increased page size to 1,2000,000. Sigma1**

 **\*All floating input parameters changed Sigma1**

 **to character input + IN9 conversion. Sigma1**

 **\*Added NRO = energy dependent scatter Sigma1**

 **radius to copying FILE2 parameters Sigma1**

 **to define unresolved energy range. Sigma1**

 **\*Corrected energy dependent scattering Sigma1**

 **radius for all resonance types (see, Sigma1**

 **the above comments). Sigma1**

 **VERS. 2018-1 (Nov. 2018) \*Added on-line report for ALL ENDERROR Sigma1**

 **VERS. 2019-1 (June 2019) \*Terminate if MF=3 Point Count and Sigma1**

 **Interpolation Law do not agree. Sigma1**

 **\*Terminate if MF=3 Background Sigma1**

 **Interpolation is NOT Linear. Sigma1**

 **\*Terminate if MF/MT=1/451 Input Sigma1**

 **temperature exceeds requested Sigma1**

 **Temperature - otherwise the output Sigma1**

 **by this code to MF=3 would appear Sigma1**

 **to be at the WRONG temperature. Sigma1**

 **\*Additional Interpolation Law Tests Sigma1**

 **\*Check consistency of Maximum Sigma1**

 **Tabulated cross sections for ALL MT Sigma1**

 **processed - print WQARNING if NOT Sigma1**

 **the same for ALL MTs. Sigma1**

 **Sigma1**

 **Sigma1**

 **OWNED, MAINTAINED AND DISTRIBUTED BY Sigma1**

 **------------------------------------ Sigma1**

 **THE NUCLEAR DATA SECTION Sigma1**

 **INTERNATIONAL ATOMIC ENERGY AGENCY Sigma1**

 **P.O. BOX 100 Sigma1**

 **A-1400, VIENNA, AUSTRIA Sigma1**

 **EUROPE Sigma1**

 **Sigma1**

 **ORIGINALLY WRITTEN BY Sigma1**

 **------------------------------------ Sigma1**

 **Dermott E. Cullen Sigma1**

 **Sigma1**

 **PRESENT CONTACT INFORMATION Sigma1**

 **--------------------------- Sigma1**

 **Dermott E. Cullen Sigma1**

 **1466 Hudson Way Sigma1**

 **Livermore, CA 94550 Sigma1**

 **U.S.A. Sigma1**

 **Telephone 925-443-1911 Sigma1**

 **E. Mail RedCullen1@Comcast.net Sigma1**

 **Website RedCullen1.nedt/HOMEPAGE.NEW Sigma1**

 **Sigma1**

 **Acknowledgement 2004 Sigma1**

 **-------------------- Sigma1**

 **Currently almost all improvements to this code are based upon Sigma1**

 **feedback from code users who report problems. This feedback Sigma1**

 **benefits ALL users of this code, and ALL users are encouraged Sigma1**

 **to report problems. Sigma1**

 **Sigma1**

 **Improvements on the 2004 version of this code based on user Sigma1**

 **feedback including, Sigma1**

 **1) Bret Beck - reported a problem at the resolved/unresolved Sigma1**

 **energy boundary. Sigma1**

 **2) S. Ganesan - reported a problem for small temperature changes. Sigma1**

 **Sigma1**

 **AUTHORS MESSAGE Sigma1**

 **--------------- Sigma1**

 **THE REPORT DESCRIBED ABOVE IS THE LATEST PUBLISHED DOCUMENTATION Sigma1**

 **FOR THIS PROGRAM. HOWEVER, THE COMMENTS BELOW SHOULD BE CONSIDERED Sigma1**

 **THE LATEST DOCUMENTATION INCLUDING ALL RECENT IMPROVEMENTS. PLEASE Sigma1**

 **READ ALL OF THESE COMMENTS BEFORE IMPLEMENTATION, PARTICULARLY Sigma1**

 **THE COMMENTS CONCERNING MACHINE DEPENDENT CODING. Sigma1**

 **Sigma1**

 **AT THE PRESENT TIME WE ARE ATTEMPTING TO DEVELOP A SET OF COMPUTER Sigma1**

 **INDEPENDENT PROGRAMS THAT CAN EASILY BE IMPLEMENTED ON ANY ONE Sigma1**

 **OF A WIDE VARIETY OF COMPUTERS. IN ORDER TO ASSIST IN THIS PROJECT Sigma1**

 **IT WOULD BE APPECIATED IF YOU WOULD NOTIFY THE AUTHOR OF ANY Sigma1**

 **COMPILER DIAGNOSTICS, OPERATING PROBLEMS OR SUGGESTIONS ON HOW TO Sigma1**

 **IMPROVE THIS PROGRAM. HOPEFULLY, IN THIS WAY FUTURE VERSIONS OF Sigma1**

 **THIS PROGRAM WILL BE COMPLETELY COMPATIBLE FOR USE ON YOUR Sigma1**

 **COMPUTER. Sigma1**

 **Sigma1**

 **PURPOSE Sigma1**

 **------- Sigma1**

 **THIS PROGRAM IS DESIGNED TO DOPPLER BROADEN NEUTRON INDUCED Sigma1**

 **CROSS SECTIONS. EACH SECTION OF CROSS SECTIONS (FILE 3) IS READ Sigma1**

 **FROM THE ENDF/B FORMAT. THE DATA IS DOPPLER BROADENED, THINNED Sigma1**

 **AND OUTPUT IN THE ENDF/B FORMAT. Sigma1**

 **Sigma1**

 **IN THE FOLLOWING DISCUSSION FOR SIMPLICITY THE ENDF/B TERMINOLOGY Sigma1**

 **---ENDF/B TAPE---WILL BE USED. IN FACT THE ACTUAL MEDIUM MAY BE Sigma1**

 **TAPE, CARDS, DISK OR ANY OTHER MEDIUM. Sigma1**

 **Sigma1**

 **ENDF/B FORMAT Sigma1**

 **------------- Sigma1**

 **THIS PROGRAM ONLY USES THE ENDF/B BCD OR CARD IMAGE FORMAT (AS Sigma1**

 **OPPOSED TO THE BINARY FORMAT) AND CAN HANDLE DATA IN ANY VERSION Sigma1**

 **OF THE ENDF/B FORMAT (I.E., ENDF/B-I, II, III, IV OR V FORMAT). Sigma1**

 **Sigma1**

 **IT IS ASSUMED THAT THE DATA IS CORRECTLY CODED IN THE ENDF/B Sigma1**

 **FORMAT AND NO ERROR CHECKING IS PERFORMED. IN PARTICULAR IT IS Sigma1**

 **ASSUMED THAT THE MAT, MF AND MT ON EACH CARD IS CORRECT. SEQUENCE Sigma1**

 **NUMBERS (COLUMNS 76-80) ARE IGNORED ON INPUT, BUT WILL BE Sigma1**

 **CORRECTLY OUTPUT ON ALL CARDS. THE FORMAT OF SECTION MF=1, MT=451 Sigma1**

 **AND ALL SECTIONS OF MF=3 MUST BE CORRECT. THE PROGRAM COPIES ALL Sigma1**

 **OTHER SECTION OF DATA AS HOLLERITH AND AS SUCH IS INSENSITIVE TO Sigma1**

 **THE CORRECTNESS OR INCORRECTNESS OF ALL OTHER SECTIONS. Sigma1**

 **Sigma1**

 **ALL CROSS SECTIONS THAT ARE USED BY THIS PROGRAM MUST BE TABULATED Sigma1**

 **AND LINEARLY INTERPOLABLE IN ENERGY AND CROSS SECTION (ENDF/B Sigma1**

 **INTERPOLATION LAW 2). FILE 3 CROSS SECTIONS MAY BE MADE LINEARLY Sigma1**

 **INTERPOLABLE BY USING PROGRAM LINEAR (UCRL-50400, VOL.17, PART A). Sigma1**

 **FILE 2 RESONANCE PARAMETERS MAY BE USED TO RECONSTRUCT ENERGY Sigma1**

 **DEPENDENT CROSS SECTIONS AND ADD IN FILE 3 BACKGROUND CROSS Sigma1**

 **SECTIONS TO DEFINE LINEARLY INTERPOLABLE CROSS SECTIONS BY USING Sigma1**

 **PROGRAM RECENT (UCRL-50400, VOL. 17, PART C). IF THIS PROGRAM Sigma1**

 **FINDS THAT THE FILE 3 CROSS SECTIONS ARE NOT LINEARLY INTERPOLABLE Sigma1**

 **THIS PROGRAM WILL TERMINATE EXECUTION. Sigma1**

 **Sigma1**

 **UNRESOLVED RESONANCE REGION Sigma1**

 **--------------------------- Sigma1**

 **IN THE UNRESOLVED RESONANCE REGION IT IS NOT POSSIBLE TO EXACTLY Sigma1**

 **DEFINE THE ENERGY DEPENDENCE OF THE CROSS SECTIONS. THE AVERAGE Sigma1**

 **WIDTHS AND SPACINGS GIVEN IN ENDF/B ARE ONLY ADEQUATE TO DEFINE Sigma1**

 **AVERAGE VALUES OF THE CROSS SECTIONS. THEREFORE ALL CROSS SECTIONS Sigma1**

 **IN THE ENDF/B FORMAT FOR THE UNRESOLVED REGION ARE REALLY AVERAGE Sigma1**

 **VALUES WHICH CANNOT BE DOPPLER BROADENED USING THE SIGMA1 METHOD Sigma1**

 **(WHICH REQUIRES TABULATED, LINEARLY INTERPOLABLE, ENERGY DEPENDENT Sigma1**

 **CROSS SECTIONS. Sigma1**

 **Sigma1**

 **THEREFORE, Sigma1**

 **(1) ALL TABULATED POINTS WITHIN THE UNRESOLVED RESONANCE REGION Sigma1**

 **WILL BE COPIED, WITHOUT MODIFICATION OR BROADENING. ADOPTION OF Sigma1**

 **THIS CONVENTION WILL ALLOW SUBSEQUENT PROGRAMS TO PROPERLY DEFINE Sigma1**

 **SELF-SHIELDED, DOPPLER BROADENED CROSS SECTIONS IN THE UNRESOLVED Sigma1**

 **RESONANCE REGION. Sigma1**

 **(2) CROSS SECTIONS WILL BE EXTENDED AS 1/V ABOVE THE UPPER ENERGY Sigma1**

 **LIMIT OF THE RESOLVED RESONANCE REGION AND BELOW THE LOWER ENERGY Sigma1**

 **LIMIT OF THE CONTINUUUM REGION (I.E. INTO THE UNRESOLVED Sigma1**

 **RESONANCE REGION). THIS CONVENTION WILL GUARANTEE A SMOOTH Sigma1**

 **BEHAVIOR CLOSE TO THE UNRESOLVED RESONANCE REGION BOUNDARIES. Sigma1**

 **Sigma1**

 **OUTPUT FORMAT Sigma1**

 **------------- Sigma1**

 **IN THIS VERSION OF SIGMA1 ALL FILE 3 ENERGIES WILL BE OUTPUT IN Sigma1**

 **F (INSTEAD OF E) FORMAT IN ORDER TO ALLOW ENERGIES TO BE WRITTEN Sigma1**

 **WITH UP TO 9 DIGITS OF ACCURACY. IN PREVIOUS VERSIONS THIS WAS AN Sigma1**

 **OUTPUT OPTION. HOWEVER USE OF THIS OPTION TO COMPARE THE RESULTS Sigma1**

 **OF ENERGIES WRITTEN IN THE NORMAL ENDF/B CONVENTION OF 6 DIGITS Sigma1**

 **TO THE 9 DIGIT OUTPUT FROM THIS PROGRAM DEMONSTRATED THAT FAILURE Sigma1**

 **TO USE THE 9 DIGIT OUTPUT CAN LEAD TO LARGE ERRORS IN THE DATA Sigma1**

 **JUST DUE TO TRANSLATION OF THE ENERGIES TO THE ENDF/B FORMAT. Sigma1**

 **Sigma1**

 **CONTENTS OF OUTPUT Sigma1**

 **------------------ Sigma1**

 **ENTIRE EVALUATIONS ARE OUTPUT, NOT JUST THE BROADENED FILE 3 Sigma1**

 **CROSS SECTIONS, E.G. ANGULAR AND ENERGY DISTRIBUTIONS ARE ALSO Sigma1**

 **INCLUDED. Sigma1**

 **Sigma1**

 **DOCUMENTATION Sigma1**

 **------------- Sigma1**

 **THE FACT THAT THIS PROGRAM HAS OPERATED ON THE DATA IS DOCUMENTED Sigma1**

 **BY THE ADDITION OF THREE COMMENTS CARDS AT THE END OF EACH Sigma1**

 **HOLLERITH SECTION IN THE FORM Sigma1**

 **Sigma1**

 **\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* PROGRAM SIGMA1 (2019-1) \*\*\*\*\*\*\*\*\*\*\*\*\*\*\* Sigma1**

 **DATA DOPPLER BROADENED TO 300.0 KELVIN AND Sigma1**

 **DATA THINNED TO WITHIN AN ACCURACY OF 0.1 PER-CENT Sigma1**

 **Sigma1**

 **THE ORDER OF ALL SIMILAR COMMENTS (FROM LINEAR,RECENT AND GROUPY) Sigma1**

 **REPRESENTS A COMPLETE HISTORY OF ALL OPERATIONS PERFORMED ON Sigma1**

 **THE DATA. Sigma1**

 **Sigma1**

 **THESE COMMENT CARDS ARE ONLY ADDED TO EXISTING HOLLERITH SECTIONS, Sigma1**

 **I.E., THIS PROGRAM WILL NOT CREATE A HOLLERITH SECTION. THE FORMAT Sigma1**

 **OF THE HOLLERITH SECTION IN ENDF/B-V DIFFERS FROM THE THAT OF Sigma1**

 **EARLIER VERSIONS OF ENDF/B. BY READING AN EXISTING MF=1, MT=451 Sigma1**

 **IT IS POSSIBLE FOR THIS PROGRAM TO DETERMINE WHICH VERSION OF Sigma1**

 **THE ENDF/B FORMAT THE DATA IS IN. WITHOUT HAVING A SECTION OF Sigma1**

 **MF=1, MT=451 PRESENT IT IS IMPOSSIBLE FOR THIS PROGRAM TO Sigma1**

 **DETERMINE WHICH VERSION OF THE ENDF/B FORMAT THE DATA IS IN, AND Sigma1**

 **AS SUCH IT IS IMPOSSIBLE FOR THE PROGRAM TO DETERMINE WHAT FORMAT Sigma1**

 **SHOULD BE USED TO CREATE A HOLLERITH SECTION. Sigma1**

 **Sigma1**

 **REACTION INDEX Sigma1**

 **-------------- Sigma1**

 **THIS PROGRAM DOES NOT USE THE REACTION INDEX WHICH IS GIVEN IN Sigma1**

 **SECTION MF=1, MT=451 OF EACH EVALUATION. Sigma1**

 **Sigma1**

 **THIS PROGRAM DOES NOT UPDATE THE REACTION INDEX IN MF=1, MT=451. Sigma1**

 **THIS CONVENTION HAS BEEN ADOPTED BECAUSE MOST USERS DO NOT Sigma1**

 **REQUIRE A CORRECT REACTION INDEX FOR THEIR APPLICATIONS AND IT WAS Sigma1**

 **NOT CONSIDERED WORTHWHILE TO INCLUDE THE OVERHEAD OF CONSTRUCTING Sigma1**

 **A CORRECT REACTION INDEX IN THIS PROGRAM. HOWEVER, IF YOU REQUIRE Sigma1**

 **A REACTION INDEX FOR YOUR APPLICATIONS, AFTER RUNNING THIS PROGRAM Sigma1**

 **YOU MAY USE PROGRAM DICTIN TO CREATE A CORRECT REACTION INDEX. Sigma1**

 **Sigma1**

 **SECTION SIZE Sigma1**

 **------------ Sigma1**

 **SINCE THIS PROGRAM USES A LOGICAL PAGING SYSTEM THERE IS NO LIMIT Sigma1**

 **TO THE NUMBER OF POINTS IN ANY SECTION, E.G., THE TOTAL CROSS Sigma1**

 **SECTION MAY BE REPRESENTED BY 200,000 DATA POINTS. Sigma1**

 **Sigma1**

 **SELECTION OF DATA Sigma1**

 **----------------- Sigma1**

 **THE PROGRAM SELECTS MATERIALS TO BE BROADENED BASED EITHER ON Sigma1**

 **MAT (ENDF/B MAT NO.) OR ZA. THE PROGRAM ALLOWS UP TO 100 MAT OR Sigma1**

 **ZA RANGES TO BE SPECIFIED. THE PROGRAM WILL ASSUME THAT THE Sigma1**

 **ENDF/B TAPE IS IN EITHER MAT OR ZA ORDER, WHICHEVER CRITERIA IS Sigma1**

 **USED TO SELECT MATERIALS, AND WILL TERMINATE WHEN A MAT OR ZA Sigma1**

 **IS FOUND THAT IS ABOVE THE RANGE OF ALL REQUESTS. Sigma1**

 **Sigma1**

 **ENERGY GRID OF BROADENED DATA Sigma1**

 **----------------------------- Sigma1**

 **THE ENERGY GRID FOR THE DOPPLER BROADENED CROSS SECTIONS IS Sigma1**

 **SELECTED TO INSURE THAT THE BROADENED DATA IS LINEAR-LINEAR Sigma1**

 **INTERPOLABLE. AS SUCH THE ENERGY GRID FOR THE BROADENED DATA Sigma1**

 **MAY NOT BE THE SAME AS THE ENERGY GRID FOR THE ORIGINAL Sigma1**

 **UNBROADENED DATA. GENERALLY AFTER BROADENING THERE WILL BE Sigma1**

 **FEWER DATA POINTS IN THE RESONANCE REGION, BUT AT LOW ENERGY Sigma1**

 **THERE MAY BE MORE POINTS, DUE TO THE 1/V LOW ENERGY EFFECT Sigma1**

 **CREATED BY DOPPLER BROADENING. Sigma1**

 **Sigma1**

 **EFFECTIVE TEMERATURE INCREASE Sigma1**

 **----------------------------- Sigma1**

 **IF THE ORIGINAL DATA IS NOT AT ZERO KELVIN THE PROGRAM WILL Sigma1**

 **BROADEN THE DATA BY THE EFFECTIVE TEMPERATURE DIFFENCE TO THE Sigma1**

 **FINAL TEMPERATURE. IF THE DATA IS ALREADY AT A TEMPERATURE THAT Sigma1**

 **IS HIGHER THAN THE FINAL TEMPERATURE DOPPLER BROADENING IS Sigma1**

 **NATURALLY NOT PERFORMED AND THE TEMPERATURE IN THE SECTION IS LEFT Sigma1**

 **AT ITS ORIGINAL VALUE. Sigma1**

 **Sigma1**

 **MULTIPLE FINAL TEMPERATURES Sigma1**

 **--------------------------- Sigma1**

 **THE PRESENT VERSION ONLY DOPPLER BROADENS TO ONE FINAL TEMPERATURE Sigma1**

 **(IF THERE IS SUFFICIENT INTEREST EXPRESSED BY USERS FUTURE Sigma1**

 **VERSION MAY BROADEN TO MULTIPLE TEMPERATURES. PLEASE Sigma1**

 **CONTACT THE AUTHOR IF YOU ARE INTERESTED IN A MULTIPLE Sigma1**

 **TEMPERATURE OPTION). Sigma1**

 **Sigma1**

 **PROGRAM OPERATION Sigma1**

 **----------------- Sigma1**

 **EACH SECTION OF FILE 3 DATA IS CONSIDERED SEPERATELY. THE DATA Sigma1**

 **IS READ AND DOPPLER BROADENED A PAGE AT A TIME (ONE PAGE IS Sigma1**

 **60000 DATA POINTS). UP TO THREE PAGES OF DATA MAY BE IN THE CORE Sigma1**

 **AT ANY GIVEN TIME, THE PAGE BEING BROADENED, THE PAGE BELOW IT Sigma1**

 **IN ENERGY AND THE PAGE ABOVE IT IN ENERGY. AFTER A PAGE HAS BEEN Sigma1**

 **BROADENED IT IS THINNED, IF THE ENTIRE SECTION CONTAINS ONLY Sigma1**

 **ONE PAGE OR LESS, IT WILL STILL BE CORE RESIDENT AND WILL BE Sigma1**

 **WRITTEN DIRECTLY FROM CORE TO THE OUTPUT TAPE. IF THE BROADENED, Sigma1**

 **THINNED SECTION IS LARGER THAN A PAGE, AFTER A PAGE HAS BEEN Sigma1**

 **BROADENED AND THINNED IT IS WRITTEN TO A SCRATCH FILE. AFTER THE Sigma1**

 **ENTIRE SECTION HAS BEEN BROADENED AND THINNED THE DATA IS READ Sigma1**

 **FROM SCRATCH TO CORE, ONE PAGE AT A TIME, THE OUTPUT TO THE OUTPUT Sigma1**

 **TAPE. Sigma1**

 **Sigma1**

 **ALLOWABLE ERROR Sigma1**

 **--------------- Sigma1**

 **AFTER DOPPLER BROADENING THE CROSS SECTION IN THE RESONANCE REGION Sigma1**

 **WILL GENERALLY BE MUCH SMOOTHER THAN THE UNBROADENED DATA AND CAN Sigma1**

 **BE REPRESENTED TO THE SAME ACCURACY BY A SMALLER NUMBER OF ENERGY Sigma1**

 **POINTS. THEREFORE AFTER DOPPLER BROADENING THE DATA CAN BE THINNED Sigma1**

 **WITH ESSENTIALLY NO LOSE OF INFORMATION. Sigma1**

 **Sigma1**

 **THE ALLOWABLE ERROR MAY BE ENERGY INDEPENDENT (CONSTANT) OR ENERGY Sigma1**

 **DEPENDENT. THE ALLOWABLE ERROR IS DESCRIBED BY A TABULATED Sigma1**

 **FUNCTION OF UP TO 20 (ENERGY,ERROR) PAIRS AND LINEAR INTERPOLATION Sigma1**

 **BETWEEN TABULATED POINTS. IF ONLY ONE TABULATED POINT IS GIVEN THE Sigma1**

 **ERROR WILL BE CONSIDERED CONSTANT OVER THE ENTIRE ENERGY RANGE. Sigma1**

 **WITH THIS ENERGY DEPENDENT ERROR ONE MAY OPTIMIZE THE OUTPUT FOR Sigma1**

 **ANY GIVEN APPLICATION BY USING A SMALL ERROR IN THE ENERGY RANGE Sigma1**

 **OF INTEREST AND A LESS STRINGENT ERROR IN OTHER ENERGY RANGES. Sigma1**

 **Sigma1**

 **INPUT FILES Sigma1**

 **----------- Sigma1**

 **UNIT DESCRIPTION Sigma1**

 **---- ----------- Sigma1**

 **2 INPUT CARDS (BCD - 80 CHARACTERS/RECORD) Sigma1**

 **10 ORIGINAL ENDF/B DATA (BCD - 80 CHARACTERS/RECORD) Sigma1**

 **Sigma1**

 **OUTPUT FILES Sigma1**

 **------------ Sigma1**

 **UNIT DESCRIPTION Sigma1**

 **---- ----------- Sigma1**

 **3 OUTPUT REPORT (BCD - 120 CHARACTERS/RECORD) Sigma1**

 **11 FINAL ENDF/B DATA (BCD - 80 CHARACTERS/RECORD) Sigma1**

 **Sigma1**

 **SCRATCH FILES Sigma1**

 **------------- Sigma1**

 **UNIT DESCRIPTION Sigma1**

 **---- ----------- Sigma1**

 **12 SCRATCH FILE FOR BROADENED DATA Sigma1**

 **(BINARY - 180000 WORDS/RECORD - DOUBLE PRECISION/ Sigma1**

 **42000 WORDS/RECORD - SINLGE PRECISION) Sigma1**

 **Sigma1**

 **OPTIONAL STANDARD FILE NAMES (SEE SUBROUTINE FILEIO) Sigma1**

 **---------------------------------------------------- Sigma1**

 **UNIT FILE NAME Sigma1**

 **---- ---------- Sigma1**

 **2 SIGMA1.INP Sigma1**

 **3 SIGMA1.LST Sigma1**

 **10 ENDFB.IN Sigma1**

 **11 ENDFB.OUT Sigma1**

 **12 (SCRATCH) Sigma1**

 **Sigma1**

 **INPUT CARDS Sigma1**

 **----------- Sigma1**

 **CARD COLS. DESCRIPTION Sigma1**

 **---- ----- ----------- Sigma1**

 **1 1-11 SELECTION CRITERIA (0=MAT, 1=ZA) Sigma1**

 **12-22 MONITOR MODE SELECTOR Sigma1**

 **= 0 - NORMAL OPERATION Sigma1**

 **= 1 - MONITOR PROGRESS OF DOPPLER BROADENING OF DATA. Sigma1**

 **EACH TIME A PAGE OF DATA POINTS IS WRITTEN TO Sigma1**

 **THE SCRATCH FILE PRINT OUT THE TOTAL NUMBER OF Sigma1**

 **POINTS ON SCRATCH AND THE LOWER AND UPPER Sigma1**

 **ENERGY LIMITS OF THE PAGE (THIS OPTION MAY BE Sigma1**

 **USED IN ORDER TO MONITOR THE EXECUTION SPEED Sigma1**

 **OF LONG RUNNING JOBS). Sigma1**

 **23-33 KELVIN TEMPERATURE Sigma1**

 **34-44 MINIMUM CROSS SECTION OF INTEREST Sigma1**

 **(DEFAULT VALUE = 1.0E-10 BARNS). Sigma1**

 **45-55 NEGATIVE CROSS SECTION TREATMENT Sigma1**

 **= 0 - O.K. Sigma1**

 **= 1 - SET = 0 Sigma1**

 **56-66 UNRESOLVED RESONANCE REGION TREATMENT Sigma1**

 **= 0 - COPY (NO BROADENING) Sigma1**

 **= 1 - IGNORE (BROADEN) Sigma1**

 **2 1-72 ENDF/B INPUT DATA FILENAME Sigma1**

 **(STANDARD OPTION = ENDFB.IN) Sigma1**

 **3 1-72 ENDF/B OUTPUT DATA FILENAME Sigma1**

 **(STANDARD OPTION = ENDFB.OUT) Sigma1**

 **4-N 1-11 LOWER MAT OR ZA LIMIT Sigma1**

 **12-22 UPPER MAT OR ZA LIMIT Sigma1**

 **UP TO 100 MAT OR ZA RANGES MAY BE SPECIFIED, ONE Sigma1**

 **RANGE PER CARD. THE LIST OF RANGES IS TERMINATED BY Sigma1**

 **A BLANK CARD. IF THE UPPER LIMIT IS LESS THAN THE Sigma1**

 **LOWER LIMIT THE UPPER LIMIT WILL BE SET EQUAL TO THE Sigma1**

 **LOWER LIMIT. IF THE FIRST REQUEST CARD IS BLANK IT Sigma1**

 **WILL TERMINATE THE LIST OF REQUESTS AND CAUSE ALL Sigma1**

 **DATA TO BE RETRIEVED (SEE EXAMPLE INPUT). Sigma1**

 **VARY 1-11 ENERGY FOR ERROR LAW Sigma1**

 **12-22 ERROR FOR ERROR LAW Sigma1**

 **THE ACCEPTABLE LINEARIZING ERROR CAN BE GIVEN AS AN Sigma1**

 **ENERGY DEPENDENT FUNCTION SPECIFIED BY UP TO 20 Sigma1**

 **(ENERGY,ERROR) PAIRS AND LINEAR INTERPOLATION Sigma1**

 **TABULATE POINTS. ENERGIES MUST BE IN ASCENDING ORDER. Sigma1**

 **THE ERROR LAW IS TERMINATED BY A BLANK CARD. IF THE Sigma1**

 **FIRST ERROR LAW CARD IS BLANK IT WILL TERMINATE THE Sigma1**

 **ERROR LAW AND THE ERROR WILL BE TREATED AS ENERGY Sigma1**

 **INDEPENDENT, EQUAL TO ZERO, WHICH INDICATES THAT THE Sigma1**

 **BROADENED DATA SHOULD NOT BE THINNED. Sigma1**

 **Sigma1**

 **EXAMPLE INPUT NO. 1 Sigma1**

 **------------------- Sigma1**

 **BROADEN ALL URANIUM ISOTOPES AND THORIUM-232 TO 300 KELVIN. FROM Sigma1**

 **0 TO 100 EV THIN OUTPUT DATA TO 0.1 PER-CENT ACCURACY. FROM 100 EV Sigma1**

 **TO 1 KEV VARY THE ERROR BETWEEN 0.1 AND 1 PER-CENT. ABOVE 1 KEV Sigma1**

 **USE 1 PER-CENT ACCURACY. Sigma1**

 **Sigma1**

 **EXPLICITLY SPECIFY THE STANDARD FILENAMES. Sigma1**

 **Sigma1**

 **THE FOLLOWING 11 CARDS ARE REQUIRED Sigma1**

 **Sigma1**

 **1 0 3.00000+ 2 Sigma1**

 **ENDFB.IN Sigma1**

 **ENDFB.OUT Sigma1**

 **92000 92999 Sigma1**

 **90232 (UPPER LIMIT WILL AUTOMATICALLY BE DEFINED) Sigma1**

 **(BLANK CARD INDICATES END OF REQUEST LIST) Sigma1**

 **0.00000+ 0 1.00000-03 Sigma1**

 **1.00000+ 2 1.00000-03 Sigma1**

 **1.00000+ 3 1.00000-02 Sigma1**

 **1.00000+ 9 1.00000-02 Sigma1**

 **(BLANK CARD INDICATES END OF ERROR LAW) Sigma1**

 **Sigma1**

 **EXAMPLE INPUT NO. 2 Sigma1**

 **------------------- Sigma1**

 **BROADEN ALL DATA TO 300 KELVIN AND DO NOT THIN THE BROADEN DATA. Sigma1**

 **ALL OF THE STANDARD OPTION MAY BE INVOKED MERELY BY SPECIFYING Sigma1**

 **THE KELVIN TEMPERATURE ON THE FIRST CARD. ALL OTHER FIELDS MAY Sigma1**

 **BE LEFT BLANK. Sigma1**

 **Sigma1**

 **LEAVE THE DEFINITION OF THE FILENAMES BLANK - THE PROGRAM WILL Sigma1**

 **THEN USE STANDARD FILENAMES. Sigma1**

 **Sigma1**

 **THE FOLLOWING 5 CARDS ARE REQUIRED Sigma1**

 **Sigma1**

 **3.00000+ 2 Sigma1**

 **(USE STANDARD FILENAME = ENDFB.IN) Sigma1**

 **(USE STANDARD FILENAME = ENDFB.OUT) Sigma1**

 **(RETRIEVE ALL DATA, TERMINATE REQUEST LIST) Sigma1**

 **(0.0 ALLOWABLE ERROR, TERMINATE ERROR LAW) Sigma1**

 **Sigma1**

 **EXAMPLE INPUT NO. 3 Sigma1**

 **------------------- Sigma1**

 **THE SAME AS ABOVE, ONLY DEFINE THE MINIMUM CROSS SECTION OF Sigma1**

 **INTEREST TO BE 1.0E-30 BARNS (INSTEAD OF THE DEFAULT VALUE OF Sigma1**

 **1.0E-10). Sigma1**

 **Sigma1**

 **READ ENDF/B DATA FROM \ENDFB6\RECENT\ZA092238 AND WRITE ENDF/B Sigma1**

 **DATA TO \ENDFB\SIGMA1\ZA092238 Sigma1**

 **Sigma1**

 **THE FOLLOWING 5 CARDS ARE REQUIRED Sigma1**

 **Sigma1**

 **3.00000+ 2 1.00000-30 Sigma1**

 **\ENDFB6\RECENT\ZA092238 Sigma1**

 **\ENDFB6\SIGMA1\ZA092238 Sigma1**

 **(RETRIEVE ALL DATA, TERMINATE REQUEST LIST) Sigma1**

 **(0.0 ALLOWABLE ERROR, TERMINATE ERROR LAW) Sigma1**

 **Sigma1**

 **======================================================================= Sigma1**