**=======================================================================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 SAMESIGMA1**

 **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-6 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 ROUNDINGSIGMA1**

 **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 CHANGESIGMA1**

 **\*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-6, NOT 5, 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-6. 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 (OVERSIGMA1**

 **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 MANYSIGMA1**

 **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 changedSIGMA1**

 **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 scatteringSIGMA1**

 **radius for all resonance types (see, SIGMA1**

 **the above comments). SIGMA1**

 **VERS. 2018-1 (Nov. 2018) \*Added on-line report for ALL ENDERRORSIGMA1**

 **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**

 **VERS. 2020-1 (Dec. 2020) \*Complete Re-write of convergence SIGMA1**

 **\*Replaced INCORE9 by INCORE10. SIGMA1**

 **\*Updated minimum/maximum convergence SIGMA1**

 **procedure. SIGMA1**

 **\*Added Target Isomer State SIGMA1**

 **\*Check Atomic Weight > 0 SIGMA1**

 **VERS. 2021-1 (Mar. 2021) \*Updated for FORTRAN 2018 SIGMA1**

 **\*Minimum Cross Section is no longer SIGMA1**

 **an input option - set to 1.0d-30. 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 CONSIDEREDSIGMA1**

 **THE LATEST DOCUMENTATION INCLUDING ALL RECENT IMPROVEMENTS. PLEASESIGMA1**

 **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 COMPUTERSIGMA1**

 **INDEPENDENT PROGRAMS THAT CAN EASILY BE IMPLEMENTED ON ANY ONE SIGMA1**

 **OF A WIDE VARIETY OF COMPUTERS. IN ORDER TO ASSIST IN THIS PROJECTSIGMA1**

 **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-1, 2, 3, 4, 5, 6 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 TABULATEDSIGMA1**

 **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 INTERPOLABLESIGMA1**

 **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 SECTIONSSIGMA1**

 **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 DEPENDENTSIGMA1**

 **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 (2021-1) \*\*\*\*\*\*\*\*\*\*\*\*\*\*\* 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 FORMATSIGMA1**

 **OF THE HOLLERITH SECTION IN ENDF/B-5 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 WASSIGMA1**

 **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 PROGRAMSIGMA1**

 **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 LEFTSIGMA1**

 **AT ITS ORIGINAL VALUE. SIGMA1**

 **SIGMA1**

 **MULTIPLE FINAL TEMPERATURES SIGMA1**

 **--------------------------- SIGMA1**

 **THE PRESENT VERSION ONLY DOPPLER BROADENS TO ONE FINAL TEMPERATURESIGMA1**

 **(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 OUTPUTSIGMA1**

 **TAPE. SIGMA1**

 **SIGMA1**

 **ALLOWABLE ERROR SIGMA1**

 **--------------- SIGMA1**

 **AFTER DOPPLER BROADENING THE CROSS SECTION IN THE RESONANCE REGIONSIGMA1**

 **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 THINNEDSIGMA1**

 **WITH ESSENTIALLY NO LOSE OF INFORMATION. SIGMA1**

 **SIGMA1**

 **THE ALLOWABLE ERROR MAY BE ENERGY INDEPENDENT (CONSTANT) OR ENERGYSIGMA1**

 **DEPENDENT. THE ALLOWABLE ERROR IS DESCRIBED BY A TABULATED SIGMA1**

 **FUNCTION OF UP TO 20 (ENERGY,ERROR) PAIRS AND LINEAR INTERPOLATIONSIGMA1**

 **BETWEEN TABULATED POINTS. IF ONLY ONE TABULATED POINT IS GIVEN THESIGMA1**

 **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 EVSIGMA1**

 **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**