XIV. CCCCR

The CCCC interface files (commonly pronounced "four cees") were developed by the Committee for Computer Code Coordination for the US Fast Breeder Reactor Program. When the members of this committee started work in 1970, they noted that because of the large variety of computers and computer systems, computer codes developed at one laboratory were often incompatible with computers at other laboratories. Major rewrites of codes or wasteful duplicate efforts were common. They hoped to create a system that would allow different laboratories to create codes that could be moved to other sites more easily. Moreover, they hoped that the codes developed at different laboratories could easily work together, thereby achieving larger and more capable calculational systems than any one laboratory could hope to develop by itself.

They approached this problem in two ways. First, they tried to establish general programming standards that would make computer codes more portable. And second, they tried to establish standard interface files for reactor physics codes that would make it easier for computer codes to communicate with each other. The results of this work appeared in fullest form as the CCCC-III and CCCC-IV standards.[1, 2]

The MINX code,[3] which was the predecessor of NJOY, was able to produce libraries that used the CCCC-III interface formats.[4] The LINX and BINX library management codes[5] and the CINX group collapse code[6] were also released during this period. Major codes that used data in CCCC-format included SPHINX[7] from Westinghouse, TDOWN[8] from General Electric, DIF3D[9] from Argonne National Laboratory, and ONEDANT[10] from Los Alamos. It was indeed found that codes could be moved more easily than before. Analysts could use ONEDANT and DIF3D on similar problems; they could even use one code to generate utility files (for example, mixture and geometry files) that would work with the other code! When NJOY was developed, it first produced version III formats and was later upgraded to the CCCC-IV standard.

With the demise of the breeder reactor program, development of the CCCC system has stopped. However, many good programs are still available that make use of CCCC files and programming standards. The Los Alamos DANDE system[11] is an example of how the use of standard interface files can be used to couple several reactor physics programs together into an easy-to-use and powerful product. In areas where the CCCC standards were not very successful, such as gamma ray cross sections and cross sections for the fusion energy range, the MATXS format is available as an alternative. This generalized material cross section library format uses CCCC-type techniques. Thus, the CCCC spirit is not dead.

A. CCCC Procedures and Programming Standards

Although the CCCC programming standards went so far as to give advice on program structure, documentation, and good coding practice, their main purpose was to make it easier to move computer codes from one machine to another. The main problems in those days were the slightly different implementations of input/output on CDC and IBM machines, the different word size on CDC and IBM machines, and the relatively small size of the main memory on the CDC 7600.

The last of these problems was attacked by limiting the maximum memory requirements for CCCC-compliant codes. This problem has essentially disappeared for the current generation of large computers.

The word-size problem has three components. First, it is often necessary to change the statements that allocate space for variables and arrays [for example, "`DIMENSION A(10)`" might have to be changed to "`REAL*8 A(10)`" when moving from a long-word machine (CDC, Cray) to a short-word machine (IBM, VAX, Sun)]. Second, the names of functions that work with double-precision variables normally must be changed (for example, `ALOG10` to `DLOG10`). And third, the word boundaries of double-precision variables must be properly aligned in common blocks and equivalenced arrays. The standard CCCC method for handling name changes has been based on using standard control cards. As an example, a code for a long-word machine might contain the following code fragment:

```
CSW
C     REAL*8 HA(10)
CSW
CLW
      INTEGER HA(10)
CLW   .
```

The variable `HA` is intended to hold 10 words of Hollerith information using the standard CCCC 6-character word length. Such a variable must be declared as double precision on short-word machines, which typically allow four Hollerith characters per word. To change this code to its short-word version, a special utility code reads through each line removing the comment "C" from lines bracketed by the "SW" comments and inserting a "C" in column 1 for all lines bracketed by "LW" comments. Previous versions of NJOY used this scheme; this version uses UPD[12] conditional statements instead. For example, the source file contains

```
*IF SW
      REAL*8 HA(10)
*ELSE
      INTEGER HA(10)
*ENDIF   ,
```

and the compile file produced by UPD has only one of the two alternatives activated, depending on whether SW has been set or not.

The word-alignment problem requires that some care be used in allocating arrays and common blocks. For example,

```
REAL*8 HA
COMMON/BAD/IA(3),HA(10)
```

should be avoided; it would be OK with IA(4). Most CCCC records contain mixtures of Hollerith, floating-point, and integer variables. The desired data is normally extracted by making use of equivalenced arrays. For example, a code could contain the following declarations:

```
REAL*8 HA(10)
DIMENSION A(20),IA(20)
EQUIVALENCE (HA(1),A(1)),(IA(1),A(1))   .
```

Assume that a record containing 2 Hollerith variables (which require two single-precision variables each), 2 floating-point numbers (at single precision), and 2 integers has been read into array A. How do you extract the first of the integers? The solution depends on defining a CCCC-standard quantity called MULT, which is 1 for long-word machines and 2 for short-word machines. Now, the desired value can be obtained with an expression of the form

```
I1=IA(2*MULT+3)   .
```

The second Hollerith variable would be extracted using the simple expression

```
H2=HA(2)   .
```

Changing the value of MULT when transporting a code to a different machine is easily handled using control-card brackets or UPD conditionals as described above.

The remaining feature of the CCCC programming standards that is used in NJOY is the concept of standardized input/output subroutines. The CCCC interface files are sequential binary files (binary for efficiency and sequential for simplicity). The interface formats are arranged so that the length of any record can be calculated using parameters already read from previous records. It is convenient to insulate CCCC input/output from system variations by defining two standard routines:

`REED(NREF,IREC,ARRAY,NWDS,MODE)`
: Read record `IREC` from unit `NREF` into `ARRAY`. The record has length `NWDS` in single-precision words. The `MODE` parameter is used to control I/O buffering, and it is not used in NJOY. Records can be read out of sequence; the routine does any record skipping (forward or backward) needed to arrive at record number `IREC`.

`RITE(NREF,IREC,ARRAY,NWDS,MODE)`
: Write record `IREC` onto unit `NREF` using the data in `ARRAY`. The first `NWDS` single-precision words will be written. The `MODE` parameter is ignored. The records `NREF` must be written in sequence. The unit will be rewound if `IREC=1`.

When transporting a code between different computer systems, it is only necessary to have (or prepare) operational versions of `REED` and `RITE` for the target machine.

B. The Standard Interface Files

The CCCCR module produces data libraries that use three of the CCCC-IV standard interface files, namely:

ISOTXS for nuclide (isotope)-ordered multigroup neutron cross sections including cross section versus energy functions for the principal cross sections, group-to-group scattering matrices, and fission neutron production and spectra tables;

BRKOXS for Bondarenko-type self-shielding factors versus energy group, temperature, and background cross section for the reactions with major resonance contributions; and

DLAYXS for delayed-neutron precursor yields, emission spectra, and decay constants for the major fissionable isotopes.

The format of each of these files, the definition of the types of data included, and the uses and weaknesses of these three standard file formats are discussed in the following three sections.

As mentioned in the preceding section, the normal form of the CCCC files is binary and sequential. CCCCR writes its output in this binary mode. Of course, coded versions (BCD, ASCII, EBCDIC, etc.) are needed to move library files between different machines, and the formats used for the coded versions are given in the file descriptions below. A separate program, BINX,[5] is used to convert back and forth between coded and binary modes. BINX can also be used to prepare an interpreted listing of a library. CCCCR can prepare an entire multimaterial library in one run if a multimaterial GENDF file is available. It can also be used to prepare an interface file containing only one material. These one-material files can be merged into multimaterial libraries using the LINX code.[5]

C. ISOTXS

The format for the ISOTXS material (isotope)-ordered cross section file is given below. This computer-text format is standard for the CCCC interface files.

```
C***********************************************************************
C                        REVISED 11/30/76                              -
C                                                                      -
CF          ISOTXS-IV                                                  -
CE          MICROSCOPIC GROUP NEUTRON CROSS SECTIONS                   -
C                                                                      -
CN                       THIS FILE PROVIDES A BASIC BROAD GROUP        -
CN                       LIBRARY, ORDERED BY ISOTOPE                   -
CN                       FORMATS GIVEN ARE FOR FILE EXCHANGE PURPOSES  -
CN                       ONLY.                                         -
C                                                                      -
C***********************************************************************

C-----------------------------------------------------------------------
CS          FILE STRUCTURE                                             -
CS                                                                     -
CS             RECORD TYPE                       PRESENT IF            -
CS             ==============================    ===============       -
CS             FILE IDENTIFICATION               ALWAYS                -
CS             FILE CONTROL                      ALWAYS                -
CS             FILE DATA                         ALWAYS                -
CS             FILE-WIDE CHI DATA                ICHIST.GT.1           -
CS    ***************(REPEAT FOR ALL ISOTOPES)                         -
CS    *        ISOTOPE CONTROL AND GROUP                               -
CS    *                       INDEPENDENT DATA   ALWAYS                -
CS    *        PRINCIPAL CROSS SECTIONS          ALWAYS                -
CS    *        ISOTOPE CHI DATA                  ICHI.GT.1             -
CS    *  **********(REPEAT TO NSCMAX SCATTERING BLOCKS)                -
CS    *  *  *******(REPEAT FROM 1 TO NSBLOK)                           -
CS    *  *  *   SCATTERING SUB-BLOCK             LORD(N).GT.0          -
CS    *************                                                    -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FILE IDENTIFICATION                                        -
C                                                                      -
CL    HNAME,(HUSE(I),I=1,2),IVERS                                      -
C                                                                      -
CW    1+3*MULT=NUMBER OF WORDS                                         -
C                                                                      -
```

```
CB    FORMAT(11H 0V ISOTXS  ,1H*,2A6,1H*,I6)                           -
C                                                                      -
CD    HNAME       HOLLERITH FILE NAME - ISOTXS -                       -
CD    HUSE(I)     HOLLERITH USER IDENTIFICATION (A6)                   -
CD    IVERS       FILE VERSION NUMBER                                  -
CD    MULT        DOUBLE PRECISION PARAMETER                           -
CD                    1- A6 WORD IS SINGLE WORD                        -
CD                    2- A6 WORD IS DOUBLE PRECISION WORD              -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FILE CONTROL   (1D RECORD)                                 -
C                                                                      -
CL    NGROUP,NISO,MAXUP,MAXDN,MAXORD,ICHIST,NSCMAX,NSBLOK              -
C                                                                      -
CW    8=NUMBER OF WORDS                                                -
C                                                                      -
CB    FORMAT(4H 1D ,8I6)                                               -
C                                                                      -
CD    NGROUP        NUMBER OF ENERGY GROUPS IN FILE                    -
CD    NISO          NUMBER OF ISOTOPES IN FILE                         -
CD    MAXUP         MAXIMUM NUMBER OF UPSCATTER GROUPS                 -
CD    MAXDN         MAXIMUM NUMBER OF DOWNSCATTER GROUPS               -
CD    MAXORD        MAXIMUM SCATTERING ORDER (MAXIMUM VALUE OF         -
CD                     LEGENDRE EXPANSION INDEX USED IN FILE).         -
CD    ICHIST        FILE-WIDE FISSION SPECTRUM FLAG                    -
CD                     ICHIST.EQ.0,      NO FILE-WIDE SPECTRUM         -
CD                     ICHIST.EQ.1,      FILE-WIDE CHI VECTOR          -
CD                     ICHIST.GT.1,      FILE-WIDE CHI MATRIX          -
CD    NSCMAX        MAXIMUM NUMBER OF BLOCKS OF SCATTERING DATA        -
CD    NSBLOK        SUBBLOCKING CONTROL FOR SCATTER MATRICES. THE      -
CD                     SCATTERING DATA ARE SUBBLOCKED INTO NSBLOK      -
CD                     RECORDS (SUBBLOCKS) PER SCATTERING BLOCK.       -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FILE DATA   (2D RECORD)                                    -
C                                                                      -
CL    (HSETID(I),I=1,12),(HISONM(I),I=1,NISO),                         -
CL   1(CHI(J),J=1,NGROUP),(VEL(J),J=1,NGROUP),                         -
CL   2(EMAX(J),J=1,NGROUP),EMIN,(LOCA(I),I=1,NISO)                     -
C                                                                      -
CW    (NISO+12)*MULT+1+NISO                                            -
CW    +NGROUP*(2+ICHIST*(2/ICHIST+1)))=NUMBER OF WORDS                 -
C                                                                      -
CB    FORMAT(4H 2D ,1H*,11A6,1H*/     HSETID,HISONM                    -
CB   11H*,A6,1H*,9(1X,A6)/(10(1X,A6)))                                 -
CB    FORMAT(6E12.5)                  CHI (PRESENT IF ICHIST.EQ.1)     -
CD    FORMAT(6E12.5)                  VEL,EMAX,EMIN                    -
CD    FORMAT(12I6)                    LOCA                             -
C                                                                      -
```

```
CD    HSETID(I)     HOLLERITH IDENTIFICATION OF FILE (A6)                -
CD    HISONM(I)     HOLLERITH ISOTOPE LABEL FOR ISOTOPE I (A6)           -
CD    CHI(J)        FILE-WIDE FISSION SPECTRUM(PRESENT IF ICHIST.EQ.1) -
CD    VEL(J)        MEAN NEUTRON VELOCITY IN GROUP J (CM/SEC)            -
CD    EMAX(J)       MAXIMUM ENERGY BOUND OF GROUP J (EV)                 -
CD    EMIN          MINIMUM ENERGY BOUND OF SET (EV)                     -
CD    LOCA(I)       NUMBER OF RECORDS TO BE SKIPPED TO READ DATA FOR   -
CD                     ISOTOPE I.  LOCA(1)=0                             -
C                                                                        -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FILE-WIDE CHI DATA   (3D RECORD)                             -
C                                                                        -
CC        PRESENT IF ICHIST.GT.1                                         -
C                                                                        -
CL    ((CHI(K,J),K=1,ICHIST),J=1,NGROUP),(ISSPEC(I),I=1,NGROUP)        -
C                                                                        -
CW    NGROUP*(ICHIST+1)=NUMBER OF WORDS                                  -
C                                                                        -
CB    FORMAT(4H 3D ,5E12.5/(6E12.5))   CHI                               -
CB    FORMAT(12I6)                     ISSPEC                            -
C                                                                        -
CD    CHI(K,J)      FRACTION OF NEUTRONS EMITTED INTO GROUP J AS A     -
CD                     RESULT OF FISSION IN ANY GROUP,USING SPECTRUM K -
CD    ISSPEC(I)     ISSPEC(I)=K IMPLIES THAT SPECTRUM K IS USED          -
CD                     TO CALCULATE EMISSION SPECTRUM FROM FISSION     -
CD                     IN GROUP I                                        -
C                                                                        -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          ISOTOPE CONTROL AND GROUP INDEPENDENT DATA   (4D RECORD)   -
C                                                                        -
CL    HABSID,HIDENT,HMAT,AMASS,EFISS,ECAPT,TEMP,SIGPOT,ADENS,KBR,ICHI, -
CL   1IFIS,IALF,INP,IN2N,IND,INT,LTOT,LTRN,ISTRPD,                       -
CL   2(IDSCT(N),N=1,NSCMAX),(LORD(N),N=1,NSCMAX),                        -
CL   3((JBAND(J,N),J=1,NGROUP),N=1,NSCMAX),                              -
CL   4((IJJ(J,N),J=1,NGROUP),N=1,NSCMAX)                                 -
C                                                                        -
CW    3*MULT+17+NSCMAX*(2*NGROUP+2)=NUMBER OF WORDS                      -
C                                                                        -
CB    FORMAT(4H 4D ,3(1X,A6)/6E12.5/                                     -
CB   1(12I6))                                                            -
C                                                                        -
CD    HABSID        HOLLERITH ABSOLUTE ISOTOPE LABEL - SAME FOR ALL    -
CD                            VERSIONS OF THE SAME ISOTOPE IN FILE (A6)-
CD    HIDENT        IDENTIFIER OF LIBRARY FROM WHICH BASIC DATA          -
CD                            CAME (E.G. ENDF/B) (A6)                    -
CD    HMAT          ISOTOPE IDENTIFICATION (E.G. ENDF/B MAT NO.) (A6)  -
CD    AMASS         GRAM ATOMIC WEIGHT                                   -
CD    EFISS         TOTAL THERMAL ENERGY YIELD/FISSION (W.SEC/FISS)    -
CD    ECAPT         TOTAL THERMAL ENERGY YIELD/CAPTURE (W.SEC/CAPT)    -
```

```
CD    TEMP          ISOTOPE TEMPERATURE (DEGREES KELVIN)               -
CD    SIGPOT        AVERAGE EFFECTIVE POTENTIAL SCATTERING IN          -
CD                            RESONANCE RANGE (BARNS/ATOM)             -
CD    ADENS         DENSITY OF ISOTOPE IN MIXTURE IN WHICH ISOTOPE     -
CD                            CROSS SECTIONS WERE GENERATED (A/BARN-CM)-
CD    KBR           ISOTOPE CLASSIFICATION                             -
CD                     0=UNDEFINED                                     -
CD                     1=FISSILE                                       -
CD                     2=FERTILE                                       -
CD                     3=OTHER ACTINIDE                                -
CD                     4=FISSION PRODUCT                               -
CD                     5=STRUCTURE                                     -
CD                     6=COOLANT                                       -
CD                     7=CONTROL                                       -
CD    ICHI          ISOTOPE FISSION SPECTRUM FLAG                      -
CD                      ICHI.EQ.0,     USE FILE-WIDE CHI               -
CD                      ICHI.EQ.1,     ISOTOPE CHI VECTOR              -
CD                      ICHI.GT.1,     ISOTOPE CHI MATRIX              -
CD    IFIS          (N,F) CROSS SECTION FLAG                           -
CD                     IFIS=0, NO FISSION DATA IN PRINCIPAL CROSS      -
CD                                       SECTION RECORD                -
CD                         =1, FISSION DATA PRESENT IN PRINCIPAL       -
CD                                       CROSS SECTION RECORD          -
CD    IALF          (N,ALPHA) CROSS SECTION FLAG                       -
CD                     SAME OPTIONS AS IFIS                            -
CD    INP           (N,P) CROSS SECTION FLAG                           -
CD                     SAME OPTIONS AS IFIS                            -
CD    IN2N          (N,2N) CROSS SECTION FLAG                          -
CD                     SAME OPTIONS AS IFIS                            -
CD    IND           (N,D) CROSS SECTION FLAG                           -
CD                     SAME OPTIONS AS IFIS                            -
CD    INT           (N,T) CROSS SECTION FLAG                           -
CD                     SAME OPTIONS AS IFIS                            -
CD    LTOT          NUMBER OF MOMENTS OF TOTAL CROSS SECTION PROVIDED  -
CD                     IN PRINCIPAL CROSS SECTIONS RECORD              -
CD    LTRN          NUMBER OF MOMENTS OF TRANSPORT CROSS SECTION       -
CD                     PROVIDED IN PRINCIPAL CROSS SECTION RECORD      -
CD    ISTRPD        NUMBER OF COORDINATE DIRECTIONS FOR WHICH          -
CD                     COORDINATE DEPENDENT TRANSPORT CROSS SECTIONS   -
CD                     ARE GIVEN, IS ISTRPD=0, NO COORDINATE DEPENDENT -
CD                     TRANSPORT CROSS SECTIONS ARE GIVEN.             -
CD    IDSCT(N)      SCATTERING MATRIX TYPE IDENTIFICATION FOR          -
CD                     SCATTERING BLOCK N, SIGNIFICANT ONLY IF         -
CD                     LORD(N).GT.0                                    -
CD                     IDSCT(N)=000 + NN, TOTAL SCATTERING, (SUM OF    -
CD                         ELASTIC, INELASTIC, AND N2N SCATTERING      -
CD                         MATRIX TERMS),                              -
CD                             =100 + NN, ELASTIC SCATTERING           -
CD                             =200 + NN, INELASTIC SCATTERING         -
CD                             =300 + NN, (N,2N) SCATTERING,----SEE    -
CD                              NOTE BELOW----                         -
CD                     WHERE NN IS THE LEGENDRE EXPANSION INDEX OF THE -
CD                     FIRST MATRIX IN BLOCK N                         -
```

```
CD    LORD(N)       NUMBER OF SCATTERING ORDERS IN BLOCK N.  IF        -
CD                     LORD(N)=0, THIS BLOCK IS NOT PRESENT FOR THIS   -
CD                     ISOTOPE.  IF NN IS THE VALUE TAKEN FROM         -
CD                     IDSCT(N), THEN THE MATRICES IN THIS BLOCK       -
CD                     HAVE LEGENDRE EXPANSION INDICES OF NN,NN+1,     -
CD                     NN+2,...,NN+LORD(N)-1                           -
CD    JBAND(J,N)    NUMBER OF GROUPS THAT SCATTER INTO GROUP J,        -
CD                     INCLUDING SELF-SCATTER, IN SCATTERING BLOCK N.  -
CD                     IF JBAND(J,N)=0, NO SCATTER DATA IS PRESENT IN  -
CD                     BLOCK N                                         -
CD    IJJ(J,N)      POSITION OF IN-GROUP SCATTERING CROSS SECTION IN   -
CD                     SCATTERING DATA FOR GROUP J, SCATTERING BLOCK   -
CD                     N, COUNTED FROM THE FIRST WORD OF GROUP J DATA. -
CD                     IF JBAND(J,N).NE.0 THEN IJJ(J,N) MUST SATISFY   -
CD                     THE RELATION 1.LE.IJJ(J,N).LE.JBAND(J,N)        -
C                                                                      -
CD                  NOTE- FOR N,2N SCATTER, THE MATRIX CONTAINS TERMS  -
CD                     SCAT(J TO G), WHICH ARE EMISSION (PRODUCTION)-  -
CD                     BASED, I.E., ARE DEFINED SUCH THAT MACROSCOPIC  -
CD                     SCAT(J TO G) TIMES THE FLUX IN GROUP J GIVES    -
CD                     THE RATE OF EMISSION (PRODUCTION) OF NEUTRONS   -
CD                     INTO GROUP G.                                   -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          PRINCIPAL CROSS SECTIONS   (5D RECORD)                     -
C                                                                      -
CL    ((STRPL(J,L),J=1,NGROUP),L=1,LTRN),                              -
CL   1((STOTPL(J,L),J=1,NGROUP),L=1,LTOT),(SNGAM(J),J=1,NGROUP).       -
CL   2(SFIS(J),J=1,NGROUP),(SNUTOT(J),J=1,NGROUP),                     -
CL   3(CHISO(J),J=1,NGROUP),(SNALF(J),J=1,NGROUP),                     -
CL   4(SNP(J),J=1,NGROUP),(SN2N(J),J=1,NGROUP),                        -
CL   5(SND(J),J=1,NGROUP),(SNT(J),J=1,NGROUP),                         -
CL   6((STRPD(J,I),J=1,NGROUP),I=1,ISTRPD)                             -
C                                                                      -
CW   (1+LTRN+LTOT+IALF+INP+IN2N+IND+ISTRPD+2*IFIS+                     -
CW   ICHI*(2/(ICHI+1)))*NGROUP=NUMBER OF WORDS                         -
C                                                                      -
CB   FORMAT(4H 5D ,5E12.5/(6E12.5)) LENGTH OF LIST AS ABOVE            -
C                                                                      -
CD    STRPL(J,L)   PL WEIGHTED TRANSPORT CROSS SECTION                 -
CD                    THE FIRST ELEMENT OF ARRAY STRPL IS THE          -
CD                    CURRENT (P1) WEIGHTED TRANSPORT CROSS SECTION    -
CD                    THE LEGENDRE EXPANSION COEFFICIENT FACTOR (2L+1) -
CD                    IS NOT INCLUDED IN STRPL(J,L).                   -
CD    STOTPL(J,L)  PL WEIGHTED TOTAL CROSS SECTION                     -
CD                    THE FIRST ELEMENT OF ARRAY STOTPL IS THE         -
CD                    FLUX (P0) WEIGHTED TOTAL CROSS SECTION           -
CD                    THE LEGENDRE EXPANSION COEFFICIENT FACTOR (2L+1) -
CD                    IS NOT INCLUDED IN STOTPL(J,L).                  -
CD    SNGAM(J)     (N,GAMMA)                                           -
CD    SFIS(J)      (N,F)         (PRESENT IF IFIS.GT.0)                -
```

```
CD    SNUTOT(J)    TOTAL NEUTRON YIELD/FISSION (PRESENT IF IFIS.GT.0)  -
CD    CHISO(J)I    ISOTOPE CHI  (PRESENT IF ICHI.EQ.1)                 -
CD    SNALF(J)     (N,ALPHA)    (PRESENT IF IALF.GT.0)                 -
CD    SNP(J)       (N,P)        (PRESENT IF INP.GT.0)                  -
CD    SN2N(J)      (N,2N)       (PRESENT IF IN2N.GT.0)  ----SEE        -
CD                    NOTE----                                         -
CD    SND(J)       (N,D)        (PRESENT IF IND.GT.0)                  -
CD    SNT(J)       (N,T)        (PRESENT IF INT.GT.0)                  -
CD    STRPD(J,I)   COORDINATE DIRECTION I TRANSPORT CROSS SECTION      -
CD                              (PRESENT IF ISTRPD.GT.0)               -
C                                                                      -
CN                 NOTE - THE PRINCIPAL N,2N CROSS SECTION SN2N(J)     -
CN                    IS DEFINED AS THE N,2N REACTION CROSS SECTION,   -
CN                    I.E., SUCH THAT MACROSCOPIC SN2N(J) TIMES THE    -
CN                    FLUX IN GROUP J GIVES THE RATE AT WHICH N,2N     -
CN                    REACTIONS OCCUR IN GROUP J.  THUS, FOR N,2N      -
CN                    SCATTERING, SN2N(J) = 0.5*(SUM OF SCAT(J TO G)   -
CN                    SUMMED OVER ALL G).                              -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          ISOTOPE CHI DATA   (6D RECORD)                             -
C                                                                      -
CC          PRESENT IF ICHI.GT.1                                       -
C                                                                      -
CL    ((CHIISO(K,J),K=1,ICHI),J=1,NGROUP),(ISOPEC(I),I=1,NGROUP)       -
C                                                                      -
CW    NGROUP*(ICHI+1)=NUMBER OF WORDS                                  -
C                                                                      -
CB    FORMAT(4H 6D ,5E12.5/(6E12.5))   CHIISO                          -
CB    FORMAT(12I6)                     ISOPEC                          -
C                                                                      -
CD    CHIISO(K,J)   FRACTION OF NEUTRONS EMITTED INTO GROUP J AS       -
CD                     RESULT OF FISSION IN ANY GROUP,USING SPECTRUM K -
CD    ISOPEC(I)     ISOPEC(I)=K IMPLIES THAT SPECTRUM K IS USED        -
CD                     TO CALCULATE EMISSION SPECTRUM FROM FISSION     -
CD                     IN GROUP I                                      -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          SCATTERING SUB-BLOCK   (7D RECORD)                         -
C                                                                      -
CC          PRESENT IF LORD(N).GT.0                                    -
C                                                                      -
CL    ((SCAT(K,L),K=1,KMAX),L=1,LORDN)                                 -
C                                                                      -
CC    KMAX=SUM OVER J OF JBAND(J,N) WITHIN THE J-GROUP RANGE OF THIS   -
CC       SUB-BLOCK.  IF M IS THE INDEX OF THE SUB-BLOCK, THE J-GROUP   -
CC       RANGE CONTAINED WITHIN THIS SUB-BLOCK IS                      -
CC       JL=(M-1)*((NGROUP-1)/NSBLOK+1 TO JU=MIN0(NGROUP,JUP),         -
CC       WHERE JUP=M*((NGROUP-1)/NSBLOK+1).                            -
```

```
C                                                                          -
CC     LORDN=LORD(N)                                                       -
CC     N IS THE INDEX FOR THE LOOP OVER NSCMAX (SEE FILE STRUCTURE)        -
C                                                                          -
CW     KMAX*LORDN=NUMBER OF WORDS                                          -
C                                                                          -
CB     FORMAT(4H 7D ,5E12.5/(6E12.5))                                      -
C                                                                          -
CD     SCAT(K,L)      SCATTERING MATRIX OF SCATTERING ORDER L, FOR         -
CD                       REACTION TYPE IDENTIFIED BY IDSCT(N) FOR THIS     -
CD                       BLOCK, JBAND(J,N) VALUES FOR SCATTERING INTO      -
CD                       GROUP J ARE STORED AT LOCATIONS K=SUM FROM 1      -
CD                       TO (J-1) OF JBAND(J,N) PLUS 1 TO K-1+JBAND(J,N).-
CD                       THE SUM IS ZERO WHEN J=1, J-TO-J SCATTER IS       -
CD                       THE IJJ(J,N)-TH ENTRY IN THE RANGE JBAND(J,N),    -
CD                       VALUES ARE STORED IN THE ORDER (J+JUP),           -
CD                       (J+JUP-1),...,(J+1),J,(J-1),...,(J-JDN),          -
CD                       WHERE JUP=IJJ(J,N)-1 AND JDN=JBAND(J,N)-IJJ(J,N)-
C                                                                          -
C--------------------------------------------------------------------------
```

Most of the variables in the "File Identification and File Control" record are taken from the user's input. Note that MAXUP is always set to zero. CCCCR does not process the NJOY thermal data at the present time. The ICHIST parameter will always be zero. CCCCR does not produce a file-wide fission spectrum or matrix. The old practice of using a single fission spectrum for all calculations is inaccurate and obsolete. Actually, the effective fission spectrum depends on the mixture of isotopes and the flux. Any file-wide spectrum would have to be at least problem dependent, and it should also be region dependent. The parameters NSCMAX and NSBLOK in the "File Control" record will be discussed in connection with the scattering matrix format.

In the "File Data" record, the Hollerith set identification and the isotope names are taken from the user's input. As mentioned above, the file-wide fission spectrum CHI never appears. The mean neutron velocities by group (VEL) are obtained from the inverse velocities computed by GROUPR:

$$\left\langle \frac{1}{v} \right\rangle_g = \frac{\displaystyle\int_g \frac{1}{v}\,\phi(E)\,dE}{\displaystyle\int_g \phi(E)\,dE} \,, \tag{1}$$

where g is the group index, $\phi(E)$ is the GROUPR weighting spectrum, and v is the neutron velocity, which is computed from the neutron mass and energy using $v{=}\sqrt{2E/m}$. The units of these quantities are s/m; they are converted to cm/s for ISOTXS by inverting and multiplying by 100. The group structure [see

EMAX(J) and EMIN] is obtained directly from MF1,MT451 on the GENDF tape. Note that GROUPR energy groups are given in order of increasing energy and ISOTXS energy groups are given in order of decreasing energy. CCCCR handles the conversion.

The "File-Wide Chi Data" record never appears; see the discussion above for the reasons.

In the "Isotope Control and Group Independent Data" record, the first ten parameters are taken from the user's input. The gram atomic weight for the material (AMASS) can be computed from the ENDF AWR parameter available on the GENDF file using the gram atomic weight of the neutron as a multiplier. The energy-release parameters EFISS and ECAPT must also be computed by the user. The ECAPT values are normally based on the ENDF Q values given in File 3, but, in some cases, it is also necessary to add additional decay energy coming from short-lived activation steps. For example, the ECAPT value for ^{238}U should include the energy for the ^{239}U β-decay step, and perhaps even the energy from the ^{239}Np β decay. The values for EFISS should be based on the total non-neutrino energy release, which can be obtained from MF3,MT18 or MF1,MT458 on the ENDF tape. The TEMP parameter is normally set to 300 K. The value of SIGPOT can be computed from the scattering-radius parameter AP in File 2 of the ENDF tape using σ_p=$4\pi a^2$. The parameter ADENS is usually set to zero to imply infinite dilution. KBR can be chosen based on the normal use of the material by the community for which the library is being produced.

The ICHI parameter is related to the ICHIX parameter in the user's input. As discussed above, the option ICHI=0 is never used by CCCCR. Beyond that, the NJOY user has the option of producing a fission χ vector using the default GROUPR flux (which is available on the GENDF tape) or a user-supplied weighting flux SPEC. This enables the user to produce an ISOTXS library appropriate to a class of problems with a flux similar to SPEC. In general, the incident-energy dependence of the fission spectrum is weak, so the choice of this weighting spectrum is not critical. Noticeable differences might be expected between a thermal spectrum on the one hand and a fast-reactor or fusion-blanket spectrum on the other. The χ vector is defined as follows:

$$\chi_{g'} = \frac{\sum\limits_{g} \sigma_{fg\to g'}\,\phi_g}{\sum\limits_{g'}\sum\limits_{g} \sigma_{fg\to g'}\,\phi_g}\,, \qquad (2)$$

where σ_f is the fission group-to-group matrix from GROUPR, ϕ_g is either the model flux or `SPEC`, and the denominator assures that $\chi_{g'}$ will be normalized. Actually, the calculation is more complicated than that because of the necessity to include delayed-neutron production. A "steady-state" value for the fission spectrum can be obtained as follows:

$$\chi_{g'}^{SS} = \frac{\sum_g \sigma_{fg\to g'}\,\phi_g + \chi_{g'}^D \sum_g \bar{\nu}_g^D \sigma_{fg}\,\phi_g}{\sum_{g'} \sum_g \sigma_{fg\to g'}\,\phi_g + \sum_g \bar{\nu}_g^D \sigma_{fg}\,\phi_g}\ , \tag{3}$$

where $\bar{\nu}_g^D$ is the delayed-neutron yield obtained from MF3,MT455 on the GENDF tape, χ_g^D is the total delayed-neutron spectrum obtained by summing over the 6 time groups in MF5,MT455, and σ_{fg} is the fission cross section for group g obtained from MF3,MT18.

This is still not the end of the complications of fission. If the partial fission reactions MT19, 20, 21, and 38 are present, the fission matrix term in the above equations is obtained by adding the contributions from all the partial reactions found. In these cases, a matrix for MT18 will normally not be present on the GENDF tape. If it is, it will be ignored. Beginning with NJOY 91.0, a new and more efficient representation is used for the fission matrix computed in GROUPR. It is well known that the shape of the fission spectrum is independent of energy up to energies of several hundred keV. GROUPR takes advantage of this by computing this low-energy spectrum only once. It then computes a fission neutron production cross section for all the groups up to the energy at which significant energy dependence starts. At higher energies, the full group-to-group fission matrix is computed as in earlier versions of NJOY. Therefore, it is now necessary to compute the values of $\sigma_{fg\to g'}$ as used in the above equations using

$$\sigma_{fg\to g'} = \chi_{g'}^{LE} (\bar{\nu}\sigma_f)_g^{LE} + \sigma_{fg\to g'}^{HE}\ , \tag{4}$$

where LE stands for low energy, HE stands for high energy; the low-energy production cross sections written as $\nu\sigma_f$ will be found on the GENDF tape using the special flag `IG2LO=0`, and the low-energy χ will be found on the GENDF tape with `IG=0`.

In order to obtain still better accuracy, CCCCR can produce a fission χ matrix instead of the vector. Using the above notation, the full χ matrix becomes

$$\chi_{g\to g'}^{SS} = \frac{\chi_{g'}^{LE} (\bar{\nu}\sigma_f)_g^{LE} + \sigma_{fg\to g'}^{HE} + \chi_{g'}^D \bar{\nu}_g^D \sigma_{fg}}{\text{NORM}}\ , \tag{5}$$

where NORM is just the value that normalizes the χ matrix; that is, the sum of the numerator over all g'. Note that the "Isotope Chi Data" record allows for a rectangular fission matrix similar to the one produced by GROUPR. It is obtained by using the input `SPEC` array to define the range of groups that will be averaged into each of the final `ICHIX` spectra. For example, to collapse a ten-group χ matrix into a five-group matrix, `SPEC` might contain the ten values 1, 2, 3, 4, 5, 5, 5, 5, 5, 5. More formally,

$$\chi^{SS}_{k\rightarrow g'} = \frac{\sum\limits_{s(g)=k} (\chi^{LE}_{g'}(\bar{\nu}\sigma_f)^{LE}_g + \sigma^{HE}_{fg\rightarrow g'} + \chi^D_{g'}\bar{\nu}^D_g\sigma_{fg})\,\phi_g}{\mathrm{NORM}} \;, \tag{6}$$

where ϕ_g is the default weighting function from the GENDF tape, $s(g)$ is the `SPEC` array provided by the user, and the summation is over all groups g satisfying the condition that $s(g)=k$. Future versions of CCCCR could construct the `SPEC` array automatically using the information in the new GENDF format.

Continuing with the description of the "Isotope Control and Group Independent Data" record, the next 9 parameters are flags that tell what reactions will be described in the "Principal Cross Sections" record. They will be described below. Similarly, the parameters `IDSCT`, `LORDN`, `JBAND`, and `IJJ` will be described later in connection with the "Scattering Sub-Block" records.

The ISOTXS format allows for a fixed set of principal cross sections that was chosen based on the needs of fission reactor calculations. This is one of its main defects; the list does not allow for other reactions that become important above 6–10 MeV, and it does not allow for other quantities of interest, such as gas production, KERMA factors, and radiation damage production cross sections. Most of the reactions are simply copied from MF3 on the GENDF tape with the group order inverted—this is true for `SNGAM`, the (n,γ) cross section, which is taken from MT102; for `SFIS`, the (n,f) cross section, which is taken from MT18; for `SNALF`, the (n,α) cross section, which is taken from MT107; for `SNP`, the (n,p) cross section, which is taken from MT103; for `SND`, the (n,d) cross section, which is taken from MT104; and for `SNT`, the (n,t) cross section, which is taken from MT105. The (n,2n) cross section, `SN2N`, is normally taken from MT16. However, earlier versions of ENDF represented the sequential (n,2n) reaction in ^{9}Be using MT6, 7, 8, and 9. If present, these partial (n,2n) reactions are added into `SN2N`. The flags `IFIS`, `IALF`, `INP`, `IN2N`, `IND`, and `INT` in the "Isotope Control and Group Independent Data" record are set to indicate which of these reactions have been found for this material.

In going from version III of the CCCC specifications to version IV, there was some controversy over the appropriate definition for the (n,2n) cross section and matrix. It was decided that the quantity in `SN2N` would be the (n,2n) reaction cross section; that is, it would define the probability that an (n,2n) reaction takes place. The (n,2n) matrix would be defined such that the sum over all secondary groups would produce the (n,2n) production cross section, which is two times larger than the reaction cross section.

The `CHISO` vector, which contains the fission spectrum vector (if any), was discussed above. A complete calculation of the fission source also requires the fission yield, `SNUTOT`, which can be used together with the fission cross section to calculated the fission neutron production cross section, $\bar{\nu}\sigma_f$. The fission yield can be calculated from the GROUPR fission matrix using

$$\bar{\nu}_g = \frac{\sum_{g'} \sigma_{fg\to g'}}{\sigma_{fg}} \ . \tag{7}$$

Adding delayed neutron contributions and accounting for the partition of the fission matrix into low-energy and high-energy parts (see the discussion of χ above) gives the equation actually used by CCCCR:

$$\bar{\nu}_g^{SS} = \frac{\sum_{g'} \sigma_{fg\to g'}^{HE} + (\bar{\nu}\sigma_f)_g^{LE} + \bar{\nu}_g^D \sigma_{fg}}{\sigma_{fg}} \ . \tag{8}$$

The total cross section produced by GROUPR contains two components: the flux-weighted or P_0 total cross section, and the current-weighted or P_1 total cross section. The P_0 part is stored into `STOTPL`, and the `LTOT` flag is set to 1. `STRPL` contains the transport cross section used by diffusion codes; this is,

$$\sigma_{tr,g} = \sigma_{t1,g} - \sum_{g'} \sigma_{e1,g\to g'} \ , \tag{9}$$

where $\sigma_{t1,g}$ is the P_1 total cross section and $\sigma_{e1,g\to g'}$ is the P_1 component of the elastic scattering matrix, which is obtained from MF6,MT2 on the GENDF tape from GROUPR. The flag `LTRN` is set to 1; that is, no higher-order transport corrections are provided. Direction-dependent transport cross sections are not computed by CCCCR; therefore, `ISTRPD` is always zero, and the `STRPD` vectors are missing.

As discussed above, the "Isotope Chi Data" record may be present if the user set `ICHIX>1` and supplied a `SPEC` vector to define how the full χ matrix is to be collapsed into a rectangular χ matrix.

The treatment of scattering matrices in the ISOTXS format is complex and has lots of possible variations. Only the variations supported by CCCCR will be described here. First of all, the scattering data is divided into blocks and subblocks. A block is either one of the designated scattering reactions [that is, total, elastic, inelastic, or (n,2n)] and contains all the group-to-group elements and Legendre orders for that reaction (`IFOPT=1`), or it is one particular Legendre order for one of the designated reactions and contains all the group-to-group elements for that order and reaction (`IFOPT=2`). Its actual content is determined by `IDSCT` and `LORDN`. If `IFOPT=1` has been selected, `IDSCT(1)=100` and `LORDN(1)=4` would designate a block for the elastic scattering matrix of order P_3 that contains all 4 Legendre orders and all group-to-group elements. If `IFOPT=2` has been selected, `IDSCT(1)=100` with `LORDN(1)=1` would designate a block containing all group-to-group elements for the P_0 elastic matrix, `IDSCT(2)=101` with `LORDN(2)=1` would designate a block containing the P_1 elastic matrix, and so on. In CCCCR, `LORDN` is always equal to 1 for `IFOPT=2`.

The ISOTXS format attempts to pack scattering matrices efficiently. First, all the scattering matrices treated here are triangular because only downscatter is present. And second, because of the limited range of elastic downscatter, only a limited range of groups above the inscatter group will contribute to the scattering into a given secondary-energy group. Therefore, ISOTXS removes zero cross sections by defining bands of incident energy groups that contribute to each final energy group. The bands are defined by `JBAND`, the number of initial energy groups in the band, and `IJJ`, an index to identify the position of the ingroup element in the band. The following table illustrates banding for a hypothetical elastic scattering reaction:

Band	Element	JBAND	IJJ
1	1→1	1	1
2	2→2	2	1
	1→2		
3	3→3	2	1
	2→3		
4	4→4	2	1
	3→4		

Note that `IJJ` is always 1 in the absence of upscatter. This scheme is efficient for elastic scattering, but it is not efficient for threshold reactions because the ingroup element must always be included in the band. This means that lots of zeros must be given for final energy groups below the threshold group. An improved and simplified scheme is used in the MATXS format.

For `IFOPT=2`, the elements in the table above would be stored in the sequence shown, top to bottom. Each Legendre order would have its own block arranged in the same order. For `IFOPT=1`, the Legendre order data are intermixed with the group-to-group data. In each band, the elements for all initial groups for P_0 are given, then all initial groups for P_1, and so on through `LORDN` Legendre orders.

Scattering matrices can be very large. For example, an 80-group elastic matrix can have as many as $80 \times 79/2 = 3160$ elements per Legendre order. That would be 12 640 words for a P_3 block using `IFOPT=1`, or four blocks of 3160 words each for `IFOPT=2`. The latter is practical; the former is not. The corresponding numbers for 200 groups would be 79 600 and 19 900. Both of these numbers are clearly impractical as record sizes. This is where subblocking comes in. If each block is divided up so that there is one subblock for each energy group, the maximum record size is reduced substantially. For `IFOPT=1`, the maximum record size is equal to the number of groups times the number of Legendre orders, or 800 for the 200-group P_3 case. For `IFOPT=2`, the maximum record size is just equal to the number of groups. Although the ISOTXS formats allows subblocks to contain several groups, CCCCR does not. The possible values of `NSBLOK` are limited to 1 and `NGROUP`. In summary, the CCCCR user has four matrix blocking options:

1. *IFOPT=1 and NSBLOK=1.* This produces a single block and a single subblock for each reaction. It is probably the best choice for small group structures (up to about 30 groups). The maximum record size is $n_\ell \times n_g(n_g-1)/2$.

2. *IFOPT=1 and NSBLOK=NGROUP.* This produces a block for each reaction, and each block contains n_g subblocks. The maximum record size is $n_\ell \times n_g$. This is a good choice for larger group structures because it keeps the record size up as compared with option 4 below.

3. *IFOPT=2 and NSBLOK=1.* This produces n_ℓ blocks and subblocks for each reaction. The maximum record size is $n_g(n_g-1)/2$. It has only a modest advantage in the maximum number of groups over option 1. Unless the application that uses the library finds it convenient to read one Legendre order at a time, the user might just as well choose option 2 if option 1 produces records that are too large.

4. *IFOPT=2 and NSBLOK=NGROUP.* This produces n_ℓ blocks for each reaction, each with n_g subblocks. The maximum record size is n_g. The number of groups would have to be on the order of 1000 before this option would be preferred to option 2.

If CCCCR does not have enough memory to process option 1 or 3, the code automatically sets `NSBLOK` to `NGROUP`, thereby activating option 2 or 4, respectively.

Note that the ISOTXS format specifies that the total scattering matrix is the sum of the elastic, inelastic, and (n,2n) matrices [see the definition of `IDSCT(N)`]. This implies that the inelastic matrix must contain the normal (n,n′) reactions from MT51–91, and also any other neutron-producing reactions that might be present. Examples are (n,n′α), (n,n′p), and (n,3n).

D. BRKOXS

The format for the BRKOXS Bondarenko-type self-shielding factor file is given below in the standard format.

```
C***********************************************************************
C                       REVISED 11/30/76                               -
C                                                                      -
CF          BRKOXS-IV                                                  -
CE          MICROSCOPIC GROUP DELAYED NEUTRON PRECURSOR DATA           -
C                                                                      -
CN                      THIS FILE PROVIDES DATA NECESSARY FOR          -
CN                      BONDARENKO TREATMENT IN ADDITION TO            -
CN                      THOSE DATA IN FILE ISOTXS                      -
CN                      FORMATS GIVEN ARE FOR FILE EXCHANGE PURPOSES   -
CN                      ONLY.                                          -
C                                                                      -
C***********************************************************************

C-----------------------------------------------------------------------
CS          FILE STRUCTURE                                             -
CS                                                                     -
CS             RECORD TYPE                          PRESENT IF         -
CS             ==============================       ===============    -
CS             FILE IDENTIFICATION                  ALWAYS             -
CS             FILE CONTROL                         ALWAYS             -
CS             FILE DATA                            ALWAYS             -
CS   **************(REPEAT FROM 1 TO NISOSH)                           -
CS   *         SELF-SHIELDING FACTORS               ALWAYS             -
CS   *         CROSS SECTIONS                       ALWAYS             -
CS   **************                                                    -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FILE IDENTIFICATION                                        -
C                                                                      -
CL    HNAME,(HUSE(I),I=1,2),IVERS                                      -
C                                                                      -
CW    1+3*MULT=NUMBER OF WORDS                                         -
C                                                                      -
CB    FORMAT(11H OV BRKOXS  ,1H*,2A6,1H*,I6)                           -
C                                                                      -
CD    HNAME       HOLLERITH FILE NAME - BRKOXS -                       -
```

```
CD    HUSE(I)     HOLLERITH USER IDENTIFICATION (A6)                    -
CD    IVERS       FILE VERSION NUMBER                                   -
CD    MULT        DOUBLE PRECISION PARAMETER                            -
CD                    1- A6 WORD IS SINGLE WORD                         -
CD                    2- A6 WORD IS DOUBLE PRECISION WORD               -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FILE CONTROL   (1D RECORD)                                  -
C                                                                       -
CL    NGROUP,NISOSH,NSIGPT,NTEMPT,NREACT,IBLK                           -
C                                                                       -
CW    6 = NUMBER OF WORDS                                               -
C                                                                       -
CB    FORMAT(4H 1D ,6I6)                                                -
C                                                                       -
CD    NGROUP        NUMBER OF ENERGY GROUPS IN SET                      -
CD    NISOSH        NUMBER OF ISOTOPES WITH SELF-SHIELDING FACTORS      -
CD    NSIGPT        TOTAL NUMBER OF VALUES OF VARIABLE X (SEE FILE DATA-
CD                     RECORD) WHICH ARE GIVEN.  NSIGPT IS EQUAL TO     -
CD                     THE SUM FROM 1 TO NISOSH OF NTABP(I)             -
CD    NTEMPT        TOTAL NUMBER OF VALUES OF VARIABLE TB (SEE FILE     -
CD                     DATA RECORD) WHICH ARE GIVEN.  NTEMPT IS EQUAL   -
CD                     TO THE SUM FROM 1 TO NISOSH OF NTABT(I)          -
CD    NREACT        NUMBER OF REACTION TYPES FOR WHICH SELF-SHIELDING   -
CD                     FACTORS ARE GIVEN (IN PREVIOUS VERSIONS OF THIS  -
CD                     FILES NREACT HAS BEEN IMPLICITLY SET TO 5).      -
CD    IBLK          BLOCKING OPTION FLAG FOR SELF-SHIELDING FACTORS,    -
CD                     IBLK=0, FACTORS NOT BLOCKED BY REACTION TYPE,    -
CD                     IBLK=1, FACTORS ARE BLOCKED BY REACTION TYPE.    -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FILE DATA   (2D RECORD)                                     -
C                                                                       -
CL    (HISONM(I),I=NISOSH),(X(K),K=1,NSIGPT),(TB(K),K=1,NTEMPT),        -
CL   1(EMAX(J),J=1,NGROUP),EMIN,(JBFL(I),I=1,NISOSH),                   -
CL   2(JBFH(I),I=NISOSH),(NTABP(I),I=1,NISOSH),(NTABT(I),I=1,NISOSH)    -
C                                                                       -
CW    (4+MULT)*NISOSH+NSIGPT+NTEMPT+NGROUP+1=NUMBER OF WORDS            -
C                                                                       -
CB    FORMAT(4H 2D ,9(1X,A6)/          HISONM                           -
CB   1(10(1X,A6)))                                                      -
CB    FORMAT(6E12.5)                   X,TB,EMAX,EMIN                   -
CB    FORMAT(12I6)                     JBFL,JBFH,NTABP,NTABT            -
C                                                                       -
CD    HISONM(I)     HOLLERITH ISOTOPE LABEL FOR ISOTOPE I (A6).  THESE  -
CD                     LABELS MUST BE A SUBSET OF THOSE IN FILE ISOTXS  -
CD                     OR GRUPXS, IN THE CORRESPONDING ARRAY.           -
CD    X(K)          ARRAY OF LN(SIGP0)/LN(10) VALUES FOR ALL ISOTOPES,  -
CD                     WHERE SIGP0 IS THE TOTAL CROSS SECTION OF THE    -
```

```
CD                      OTHER ISOTOPES IN THE MIXTURE IN BARNS PER ATOM -
CD                      OF THIS ISOTOPE.  FOR ISOTOPE I, THE NTABP(I)   -
CD                      VALUES OF X FOR WHICH SELF-SHIELDING FACTORS    -
CD                      ARE GIVEN ARE STORED STARTING AT LOCATION L=1+  -
CD                      SUM FROM 1 TO I-1 OF NTABP(K).                  -
CD    TB(K)          ARRAY OF TEMPERATURES (DEGREES C) FOR ALL ISOTOPES.-
CD                      FOR ISOTOPE I, THE NTBT(I) VALUES OF TB FOR     -
CD                      WHICH SELF-SHIELDING FACTORS ARE GIVEN ARE      -
CD                      STORED AT LOCATION L=1+SUM FROM 1 TO I-1 OF     -
CD                      NTABT(K).                                       -
CD    EMAX(J)        MAXIMUM ENERGY BOUND OF GROUP J (EV)               -
CD    EMIN           MINIMUM ENERGY BOUND OF SET (EV)                   -
CD    JBFL(I)        LOWEST NUMBERED OF HIGHEST ENERGY GROUP FOR WHICH  -
CD                      SELF-SHIELDING FACTORS ARE GIVEN                -
CD    JBFH(I)        HIGHEST NUMBERED OR LOWEST ENERGY GROUP FOR WHICH  -
CD                      SELF-SHIELDING FACTORS ARE GIVEN                -
CD    NTABP(I)       NUMBER OF SIGPO VALUES FOR WHICH SELF-SHIELDING    -
CD                      FACTORS ARE GIVEN FOR ISOTOPE I.                -
CD    NTABT(I)       NUMBER OF TEMPERATURE VALUES FOR WHICH SELF-       -
CD                      SHIELDING FACTORS ARE GIVEN FOR ISOTOPE I.      -
C                                                                       -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          SELF-SHIELDING FACTORS   (3D RECORD)                        -
C                                                                       -
CL    ((((FFACT(N,K,J,M),N=1,NBINT),K=1,NBTEM),J=JBFLI,JBFHI),M=ML,MU) -
CL                   ------ SEE DESCRIPTION BELOW ------                -
C                                                                       -
CC    NBINT=NTABP(I)                                                    -
CC    NBTEM=NTABT(I)                                                    -
CC    JBFLI=JBFL(I)                                                     -
CC    JBFHI=JBFH(I)                                                     -
CC    FOR ML, MU SEE STRUCTURE BELOW                                    -
C                                                                       -
CW    NBINT*NBTEM*(JBFHI-JBFLI+1)*(MU-ML+1) = NUMBER OF WORDS           -
C                                                                       -
CB    FORMAT(4H 3D ,5E12.5/(6E12.5))                                    -
C                                                                       -
CC    DO 1 L=1,NBLOK                                                    -
CC  1 READ(N) *LIST AS ABOVE*                                           -
C                                                                       -
CC          IF IBLK=0, NBLOK=1, ML=1, MU=NREACT                         -
CC          IF IBLK=1, NBLOK=NREACT, ML=MU=L, WHERE L IS THE BLOCK      -
C                                                                       -
CD    FFACT(N,K,J,M)    SELF-SHIELDING FACTOR EVALUATED AT X(N) AND     -
CD                         TB(K) FOR ENERGY GROUP J, THE M INDEX IS     -
CD                         A DUMMY INDEX TO DENOTE THE REACTION TYPE,   -
CD                         THE FIRST FIVE REACTION TYPES ARE, IN        -
CD                         ORDER, TOTAL, CAPTURE, FISSION, TRANSPORT,   -
CD                         AND ELASTIC.                                 -
C                                                                       -
CB          NOTE THAT IS IBLK=1, EACH REACTION TYPE WILL CONSTITUTE     -
```

```
CB             A SEPARATE DATA BLOCK.                                    -
C                                                                        -
C-------------------------------------------------------------------------

C-------------------------------------------------------------------------
CR          CROSS SECTIONS   (4D RECORD)                                 -
C                                                                        -
CL    (XSPO(J),J=1,NGROUP),(XSIN(J),J=1,NGROUP),(XSE(J),J=1,NGROUP),     -
CL   1(XSMU(J),J=1,NGROUP),(XSED(J),J=1,NGROUP),(XSX(J),J=1,NGROUP)      -
C                                                                        -
CW    6*NGROUP=NUMBER OF WORDS                                           -
C                                                                        -
CB    FORMAT(4H 4D ,5E12.5/(6E12.5))                                     -
C                                                                        -
CD    XSPO(J)       POTENTIAL SCATTERING CROSS SECTION (BARNS)           -
CD    XSIN(J)       INELASTIC CROSS SECTION (BARNS)                      -
CD    XSE(J)        ELASTIC CROSS SECTION (BARNS)                        -
CD    XSMU(J)       AVERAGE COSINE OF ELASTIC SCATTERING ANGLE           -
CD    XSED(J)       ELASTIC DOWN-SCATTERING TO ADJACENT GROUP            -
CD    XSXI(J)       AVERAGE ELASTIC SCATTERING LETHARGY INCREMENT        -
C                                                                        -
C-------------------------------------------------------------------------
```

The BRKOXS file is used to supply self-shielding factors for use with the Bondarenko method[13] for calculating effective macroscopic cross sections for the components of nuclear systems. As discussed in detail in the GROUPR chapter of this manual, this system is based on using a model flux for isotope i of the form

$$\phi_\ell^i(E,T) = \frac{C(E)}{[\sigma_0^i + \sigma_t^i(E,T)]^{\ell+1}} , \tag{10}$$

where $C(E)$ is a smooth weighting flux, $\sigma_t^i(E,T)$ is the total cross section for material i at temperature T, ℓ is the Legendre order, and σ_0^i is a parameter that can be used to account for the presence of other materials and the possibility of escape from the absorbing region (heterogeneity). GROUPR uses this model flux to calculate effective multigroup cross sections for the resonance-region reactions (total, elastic, fission, capture) for several values of σ_0 and several values of T.

When σ_0 is large with respect to the highest peaks in σ_t, the flux is essentially proportional to $C(E)$. This is called infinite dilution, and the corresponding cross sections are appropriate for an absorber in a dilute mixture or for a very thin sample of the absorber. As σ_0 decreases, the flux $\phi(E)$ develops dips where σ_t has peaks. These dips cancel out part of the effect of the corresponding peaks in the resonance cross sections, thereby reducing, or self-shielding the reaction rate. It is convenient to represent this effect as a self-shielding factor; that is,

$$\sigma_{xg}(T,\sigma_0) = f_{xg}(T,\sigma_0) \times \sigma_{xg}(300K,\infty)\ . \tag{11}$$

In the CCCC system, the f-factors are stored in the BRKOXS file and the infinitely dilute cross sections are stored in the ISOTXS file. A code that prepares effective cross sections, such as SPHINX[7] or 1DX,[14] determines the appropriate T and σ_0 values for each region and group in a reactor problem, using equivalence theory together with the user's specifications for composition and geometry. It then reads in the cross sections and f-factors from the ISOTXS and BRKOXS files, interpolates in the T and σ_0 tables to obtain the desired f-factors, and multiplies to obtain the effective cross sections.

In the BRKOXS file specification given above, the components of the "File Identification" record are the same as for ISOTXS. The parameters in the "File Control" record are used to calculate the sizes and locations of data in the records to follow. The "File Data" record contains all the isotope names, all the σ_0 values for every isotope, all the T values for every isotope, the group structure, and several arrays used for unpacking the other data. The Hollerith material names in `HISONM` are the same as those used in ISOTXS, and they are obtained from the user's input. The σ_0 values are packed into `X(K)` using `NTABP(I)`. Note that the base-10 logarithm of σ_0 is stored. Therefore, a typical library might contain the following:

material `I`	`NTABP(I)`	`X(K)`
1	3	3.0 2.0 1.0
2	7	4.0 3.0 2.0 1.477 1. 0. -1.
3	5	4.0 3.0 2.0 1.0 0.0
...	...	...

Similarly, the T values are stored in `TB(K)` using `NTABT(I)`. The absolute temperatures used by GROUPR must be changed to degrees C before being stored. The energy bounds for the group structure found on the GENDF tape are stored in `EMAX(J)` and `EMIN`. As discussed in connection with the ISOTXS format, group boundaries are stored in order of decreasing energy in the BRKOXS file.

The self-shielding factor approach is designed to account for resonance self-shielding. It is not necessarily appropriate for low energies if only broad resonance features are apparent, or for high energies where only small residual fluctuations in the cross section are seen. For this reason, the BRKOXS format provides the `JBFL(I)` and `JBFH(I)` arrays in the "File Data" record. They are used to limit the range of the numbers given in the "Self-Shielding Factors" record. The reactions that are active in the resonance energy range usually include only the total, elastic, fission, and capture channels. The total cross section is usually computed for the two Legendre orders ℓ=0 and ℓ=1. This second value is often called the current-weighted total cross section, and it is needed to compute the self-shielded diffusion coefficient. GROUPR also computes a self-shielded elastic scattering matrix. It can be used to provide two quantities for the BRKOXS file. First, the diffusion coefficient requires the calculation of a transport cross section for diffusion. The relationships are as follows:

$$D_g = \frac{1}{3\sigma_{tr,g}} \ , \tag{12}$$

and

$$\sigma_{tr,g} = \sigma_{t1,g} - \sum_{g'} \sigma_{e1,g\to g'} \ . \tag{13}$$

Therefore, the current-weighted P_1 elastic cross section contributes to the transport self-shielding factor. The second use for the self-shielded elastic scattering matrix is to compute a self-shielding factor for elastic removal. For heavy isotopes, the energy lost in elastic scattering is small, and all the removal is normally to one group. The format requires that at least the five standard reactions be given in a specified order. NJOY is able to add one more as follows:

1. total (P_0 weighted),
2. capture (P_0),
3. fission (P_0),
4. transport (P_1),
5. elastic (P_0), and
6. elastic removal (P_0).

The normal pattern for the BRKOXS file expects that there will be one record of self-shielding factors for each material. Such a record could get quite large. For example, with 6 reactions, 6 temperatures, 6 σ_0 values, and 100 resonance groups, a "Self-Shielding Factors" record could have over 20 000 words. This number can be made more manageable by setting the `IBLK` flag in the "File Control" record to 1. Then there will be a separate record of self-shielding factors for each reaction; this would reduce the record size for the example to a more reasonable 3600 words.

The actual self-shielding factors are computed from the cross sections given on the GENDF tape and stored into the `FFACT(N,K,J,M)` array of the "Self-Shielding Factors" record with group order converted to the standard decreasing-energy convention. Following the FORTRAN convention, `N` is the fastest varying index in this array, `K` is the next fastest varying index, and so on. The identities of these indices are

`N` σ_0,

`K` temperature T,

`J` group, and

`M` reaction.

The "Cross Sections" record contains some additional cross sections and special parameters that are often used in self-shielding codes and are not included in the ISOTXS file. The `XSPO` cross section is taken to be constant and equal to the CCCCR input parameter `XSPO`, which is computed as $4\pi a^2$. The `XSIN` cross section is obtained by summing over the final group index for every group-to-group matrix in File 6 except elastic, (n,2n), and fission. Therefore, it may contain effects of multiplicities greater than 1 if reactions like (n,3n) or (n,2nα) are active for the material. It may be slightly larger in high-energy groups than the cross section that would be obtained using the same sum over reactions in File 3. The `XSE` cross section is obtained from MF6,MT2 on the GENDF tape by summing over final groups. The parameters for continuous slowing down theory, `XSMU` and `XSXI`, are obtained from MT251 and MT252, respectively. The methods used for calculating these quantities are described in the GROUPR section of this report. Finally, the elastic downscattering cross section is obtained from the elastic matrix on the GENDF tape (MF6,MT2).

E. DLAYXS

The format for the DLAYXS delayed-neutron data file is given below in the standard format.

```
C***********************************************************************
C                       REVISED 11/30/76                               -
C                                                                      -
CF          DLAYXS-IV                                                  -
CE          MICROSCOPIC GROUP DELAYED NEUTRON PRECURSOR DATA           -
C                                                                      -
CN                      THIS FILE PROVIDES PRECURSOR YIELDS,           -
CN                      EMISSION SPECTRA, AND DECAY CONSTANTS          -
CN                      ORDERED BY ISOTOPE.  ISOTOPES ARE IDENTIFIED   -
CN                      BY ABSOLUTE ISOTOPE LABELS FOR RELATION TO     -
CN                      ISOTOPES IN EITHER FILE ISOTXS OR GRUPXS.      -
CN                      FORMATS GIVEN ARE FOR FILE EXCHANGE PURPOSES   -
CN                      ONLY.                                          -
C                                                                      -
```

```
C***********************************************************************

C-----------------------------------------------------------------------
CS          FILE STRUCTURE                                             -
CS                                                                     -
CS             RECORD TYPE                          PRESENT IF         -
CS             ===============================    ===============      -
CS             FILE IDENTIFICATION                  ALWAYS             -
CS             FILE CONTROL                         ALWAYS             -
CS             FILE DATA, DECAY CONSTANTS, AND                         -
CS                EMISSION SPECTRA                  ALWAYS             -
CS   *************(REPEAT TO NISOD)                                    -
CS   *         DELAYED NEUTRON PRECURSOR                               -
CS   *            YIELD DATA                        ALWAYS             -
CS   *************                                                     -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FILE IDENTIFICATION                                        -
C                                                                      -
CL    HNAME,(HUSE(I),I=1,2),IVERS                                      -
C                                                                      -
CW    1+3*MULT=NUMBER OF WORDS                                         -
C                                                                      -
CB    FORMAT(11H OV DLAYXS  ,1H*,2A6,1H*,I6)                           -
C                                                                      -
CD    HNAME       HOLLERITH FILE NAME - DLAYXS -                       -
CD    HUSE(I)     HOLLERITH USER IDENTIFICATION (A6)                   -
CD    IVERS       FILE VERSION NUMBER                                  -
CD    MULT        DOUBLE PRECISION PARAMETER                           -
CD                    1- A6 WORD IS SINGLE WORD                        -
CD                    2- A6 WORD IS DOUBLE PRECISION WORD              -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FILE CONTROL   (1D RECORD)                                 -
C                                                                      -
CL    NGROUP,NISOD,NFAM,IDUM                                           -
C                                                                      -
CW    4=NUMBER OF WORDS                                                -
C                                                                      -
CB    FORMAT(4H 1D ,4I6)                                               -
C                                                                      -
CD    NGROUP        NUMBER OF NEUTRON ENERGY GROUPS IN SET             -
CD    NISOD         NUMBER OF ISOTOPES IN DELAYED NEUTRON SET          -
CD    NFAM          NUMBER OF DELAYED NEUTRON FAMILIES IN SET          -
CD    IDUM          DUMMY TO MAKE UP FOUR-WORD RECORD                  -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
```

```
CR          FILE DATA, DECAY CONSTANTS, AND EMISSION SPECTRA          -
C                             (2D RECORD)                              -
C                                                                      -
CL    (HABSID(I),I=1,NISOD),(FLAM(N),N=1,FAM),((CHID(J,N),J=1,NGROUP), -
CL    N=1,NFAM),(EMAX(J),J=1,NGROUP),EMIN,(NKFAM(I),I=1,NISOD),        -
CL    (LOCA(I),I=1,NISOD)                                              -
C                                                                      -
CW    (2+MULT)*NISOD+(NGROUP+1)*(NFAM+1)=NUMBER OF WORDS               -
C                                                                      -
CB    FORMAT(4H 2D ,9(1X,A6))          HABSID                          -
CB   1(10(1X,A6)))                                                     -
CB    FORMAT(6E12.5)                   FLAM,CHID,EMAX,EMIN             -
CB    FORMAT(12I6)                     NKFAM,LOCA                      -
C                                                                      -
CD    HABSID(I)     HOLLERITH ABSOLUTE ISOTOPE LABEL FOR ISOTOPE I (A6)-
CD    FLAM(N)       DELAYED NEUTRON PRECURSOR DECAY CONSTANT           -
CD                     FOR FAMILY N                                    -
CD    CHID(J,N)     FRACTION OF DELAYED NEUTRONS EMITTED INTO NEUTRON  -
CD                     ENERGY GROUP J FROM PRECURSOR FAMILY N          -
CD    EMAX(J)       MAXIMUM ENERGY BOUND OF GROUP J (EV)               -
CD    EMIN          MINIMUM ENERGY BOUND OF SET (EV)                   -
CD    NKFAM(I)      NUMBER OF FAMILIES TO WHICH FISSION IN ISOTOPE I   -
CD                     CONTRIBUTES DELAYED NEUTRON PRECURSORS          -
CD    LOCA(I)       NUMBER OF RECORDS TO BE SKIPPED TO READ DATA FOR   -
CD                     ISOTOPE I, LOCA(1)=0                            -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          DELAYED NEUTRON PRECURSOR YIELD DATA   (3D RECORD)         -
C                                                                      -
CL    (SNUDEL(J,K),J=1,NGROUP),K=1,NKFAMI),(NUMFAM(K),K=1,NKFAMI)      -
C                                                                      -
CC    NKFAMI=NKFAM(I)                                                  -
C                                                                      -
CW    (NGROUP+1)*NKFAMI=NUMBER OF WORDS                                -
C                                                                      -
CB    FORMAT(4H 3D ,5E12.5/(6E12.5))  SNUDEL                           -
CB    FORMAT(12I6)                    NUMFAM                           -
C                                                                      -
CD    SNUDEL(J,K)   NUMBER OF DELAYED NEUTRON PRECURSORS PRODUCED IN   -
CD                     FAMILY NUMBER NUMFAM(K) PER FISSION IN          -
CD                     GROUP J                                         -
CD    NUMFAM(K)     FAMILY NUMBER OF THE K-TH YIELD VECTOR IN          -
CD                     ARRAY SNUDEL(J,K)                               -
C                                                                      -
C-----------------------------------------------------------------------
```

This file is used to communicate delayed-neutron data to reactor kinetics codes. The ENDF files give a total delayed-neutron yield $\bar{\nu}_d$ in the section labeled MF1,MT455.

GROUPR averages this yield for each neutron group g using

$$\bar{\nu}_g^D = \frac{\displaystyle\int_g \nu_d(E)\sigma_f(E)\phi(E)\,dE}{\displaystyle\int_g \sigma_f(E)\phi(E)\,dE} \,. \tag{14}$$

This same section of the ENDF tape contains the decay constants for six delayed-neutron time groups. These numbers are passed on to the GROUPR routine that averages the delayed-neutron spectra, and they end up in the MF5 record on the GENDF tape. The ENDF evaluations give the delayed-neutron spectra for the six time groups in MF5,MT455. These spectra are not separately normalized. Rather, the sum over all six time groups is normalized, but the integral of any one of the spectra gives the "delayed fraction" for that time group. GROUPR simply averages these six spectra using the specified neutron group structure. The resulting group spectra (and the decay constants from File 1) are written onto the GENDF tape.

Returning to the DLAYXS format description, the parameters in the "File Identification" record are obtained from the user's input, just as for ISOTXS and BRKOXS. The parameter `NGROUP` is also a user input quantity. `NISOD` is determined after the entire GENDF tape has been searched for isotopes that are on the user's list of `NISO` materials and that have delayed-neutron data. The `NFAM` parameter needs some additional explanation. A "family" for the DLAYXS file is actually an index that selects one particular spectrum from the `CHID` array. It could correspond to an actual delayed-neutron precursor isotope left after a fission event. In such a case, there would be many "families" corresponding to the many possible fission fragment isotopes. The `SNUDEL` yields would be analogous to fission product yields. The ENDF evaluations take a more macroscopic approach. Spectra are chosen to include all the emissions from a group of delayed-neutron precursors for a particular fissioning nucleus with similar decay constants. In this representation, the DLAYXS "family" corresponds to a particular decay constant and spectrum for a particular target isotope. Therefore, the number of families is simply six times the number of isotopes, or `NFAM=6*NISOD`.

In the "File Data, Decay Constants, and Emission Spectra" record, the Hollerith isotope names `HABSID` are obtained from the names in the user's input. The `FLAM` values come directly from the decay constant values originally extracted from File 1 of the ENDF tape. The family index for isotope `ISO` and time group `I` is simply computed as `6*(ISO-1)+I`. The `CHID` array is loaded from the MF5,MT455 section on the GENDF tape using the family index and the group index. As usual, the order of groups has to be changed from the GROUPR convention with increasing-energy order to the CCCC convention with decreasing-energy order. The group structure itself is obtained from the GENDF header record and stored into `EMAX` and `EMIN` in the conventional order. The value of `NKFAM` is simply 6 for every isotope. The `LOCA` values are also easy to compute; they are just `ISO` minus 1.

The delayed-neutron yields versus incident neutron energy group and family index are given in the "Delayed Neutron Precursor Yield Data" record. As mentioned above, the total yield is given in MF3 of the GENDF tape, and the delayed fractions can be computed by summing the spectrum for each time group over the energy group index. The array `SNUDEL` in this DLAYXS record contains the product of these values. Note that there is one of these yield records for each delayed-neutron isotope, and each record contains six families. The `NKFAM` vector is used to establish the correspondence between these families and the entire list of families used in the file data record. As an example, `NUMFAM(1)` would contain 1, 2, 3, 4, 5, 6; `NUMFAM(2)` would contain 7, 8, 9, 10, 11, 12, and so on.

F. Coding Details

The main subroutine of CCCCR starts by initializing some variables and the storage system. Note that the CCCC standards specify that Hollerith variables contain 6 characters. This means that they must be declared to be double-precision variables on short-word machines, which normally allow up to 4 characters per word. Long-word machines usually allow from 8 to 10 characters per word. This requirement is handled by using the letter "h" to start every Hollerith word and by activating the statement "`IMPLICIT REAL*8 (H)`" on short-word machines. For use in calculating data pointers, the value of `MULT` is set to 2 on short-word machines. In order to make sure that dynamic arrays allocated by `RESERV` will have correct word alignment for short-word machines, a 2-word array called `DUM` is allocated. If its pointer `LZERO` is even, one of the words is released. This assures that the next array assigned by `RESERV` will have an odd pointer.

Next, the unit numbers for input and output are read. The signs given for CCCC units are ignored; they are opened as binary files. The subroutine continues by reading input cards 2 through 5. All integers are converted from the `Z` array of `FREE` using the FORTRAN nearest-integer function `NINT` to avoid round-off problems that occur in some machines. All Hollerith variables are moved into variables whose names start with "h" by making use of the equivalence between the arrays Z and HZ. The MULT parameter is used to calculate the addresses in the equivalenced array.

At this point, CCCCR branches to different subroutines for each of the three interface file types that have been requested (see CISOTX, CBRKXS, and CDLYXS). Each of these routines is paired with a print routine that is called if the IPRINT flag has been set to 1 (see PISOTX, PBRKXS, and PDLYXS). When the last of these routines returns, CCCCR closes its active I/O units, writes a report, and terminates.

1. ISOTXS File Preparation. The CISOTX routine starts by calling RUINIS to read in the portion of the user's input specific to the ISOTXS file. It then calls ISXDAT to read through the input GENDF file and extract the ISOTXS data.

Subroutine ISXDAT reads the GENDF header record for the first material and extracts the group boundary energies. If the group structure found does not match the one requested in the user's input, an error message is issued. Otherwise, the order of the groups is changed from the GROUPR/ENDF convention of increasing energy to the CCCC convention of decreasing energy (which is the normal ordering for application programs). The routine then begins a loop over all the materials (isotopes) requested (see DO 300 I=1,NISO). It searches through the input GENDF tape for the first material with the requested MAT number (that is, the first temperature for the MAT) and copies it to a scratch file. Note that materials are written in the order requested by the user's input material list, not in the order that they are found on the GENDF tape.

This scratch tape is scanned for the ISOTXS principal cross section data in PRINXS. This process is fairly simple for most of the ENDF File 3 cross sections. Each MT number in File 3 is compared to the list of desired principal cross sections in NSTX; if a match is found, the corresponding element of IFLAG is set, and the cross section table is copied into memory using a pointer from the IPTR array. The (n,2n) reaction is a special case. In addition to MT16, the routine watches for the partial (n,2n) representation used in the ENDF/B-IV and -V evaluations for ^{9}Be (namely, MT6, 7, 8, and 9), and adds them into the appropriate memory locations. Fission is obtained from MT18, but if the partial fission reactions are present (MT19, 20, 21, 38), the flag MT19 is set. Average neutron velocities are obtained from the special GROUPR-produced section labeled by MT259. These are inverse velocities in s/m, and PRINXS inverts them and multiplies by 100 to get velocities in cm/s. In addition to the normal flux-weighted total cross section, the routine also stores the current-weighted, or P_1, cross section for use in calculating the transport cross section (see below). Finally, File 3 may also contain MT455, the delayed-neutron $\bar{\nu}$ parameter. The GENDF record for this parameter also contains σ_f and the flux for each group. The delayed-neutron production rate $\bar{\nu}_d\sigma_f$ is stored for use in calculating the total $\bar{\nu}$ parameter, and $\bar{\nu}_d\sigma_f\phi$ is added into the `DNORM` array for later use in normalizing the total fission spectrum, χ. Note that there are two options for the flux used in this normalization: it can be the default library flux found on each record of the GENDF file, or it can be a flux spectrum `SPEC` provided by the user.

While reading through the scratch tape, `PRINXS` also watches for the elastic scattering matrix (MF6, MT2). The total P_1 elastic cross section is calculated by summing over all secondary neutron groups, and the result is subtracted from the current-weighted total cross section to obtain the transport cross section.

The processing of the fission matrix (MF6, MT18) and the delayed-fission spectra (MF5, MT455) depend on the `ICHIX` option. The $\bar{\nu}$ parameter `SNUTOT` is always calculated for fissionable isotopes. `CHISO` is only calculated if the vector representation was requested; in addition, it can be calculated using the flux from GENDF or using the input flux in `SPECT`. Starting with NJOY 91.0, the fission matrix is represented by a real group-to-group matrix at high energies, and by a single spectrum (with `IG=0`) and an associated production cross section (with `IG2LO=0`) at low energies. This representation can lead to great savings for libraries with many low-energy groups. The contributions to `SNUTOT` from the low-energy range are easily obtained by adding in the production cross section. At high energies, the sum of the group-to-group matrix over all secondary-energy groups is added in. After MF3,MT455 and MF6,MT18 have been processed, it is only necessary to divide the total production rate in memory by the fission cross section to obtain the required total $\bar{\nu}$ values (see statement number 242).

The prompt part of the fission χ vector or matrix is obtained from MF6,MT18, or if the `MT19` flag was set while reading File 3, from MT19, 20, 21, and 38. The code starts at statement number 207, and it is fairly complicated because it has to cope with the following options:

1. χ vector versus χ matrix,
2. default weighting for the vector versus input weighting,
3. square matrix versus collapsed rectangular matrix, and
4. constant and matrix parts of MF6 GENDF record.

Note that separate normalization sums are accumulated in `CNORM(ISPEC)` for the chi vector or for each column of the matrix while the χ elements are being stored. The delayed contributions to the fission χ vector or matrix are taken from

MF5,MT455 (see statement number 230). The spectra for all of the six time groups are added and multiplied by the delayed neutron production rate DNORM (which can be incident energy dependent through the ISPEC index if a matrix is being constructed). The delayed contributions to the normalization sum for the χ vector or for each column of the χ matrix are added into CNORM during this step. After all the components of the fission spectrum have been read from the GENDF file, the χ vector or the columns of the χ matrix are normalized in the DO 249 loop.

When all sections of the scratch tape have been processed, PRINXS goes through the principal cross section block in memory removing any parts that have zero cross sections, and it writes the resulting block on scratch file NSCRT2. Finally, it writes the chi matrix data, if any, to the same scratch file and returns to ISXDAT.

Subroutine ISOMTX is then called to read through the scratch tape and process the group-to-group matrices into CCCC format. In order to allow large matrices to be processed on machines with limited memory, one or more passes can be made through the scratch tape (see DO 400 NJ=1,NPASS). The number of passes used depends upon the amount of space available in scratch array B and on the subblocking option requested by the user. The four options supported by CCCCR were discussed in connection with the ISOTXS format description. Only one pass is required for the first option. In the other cases, the length of one subblock is divided into the length of the scratch array to determine the number of subblocks that can be accumulated on one pass (NREC) and the number of passes required (NPASS).

Four matrix reactions are extracted from the scratch tape (see DO 500 I=1,4). The total matrix is obtained by adding all matrices found on the GENDF tape except the fission matrices. The elastic matrix is obtained from MT2 only. The (n,2n) matrix is normally obtained from MT16, but the sum of MT6, 7, 8, 9, 46, 47, 48, and 49 will be used for the old ^{9}Be representation, if found. The inelastic matrix is the sum of everything else; that is, it includes the normal inelastic reactions MT51–91, and it also includes other neutron-producing reactions like (n,3n), (n,n$'$p), and (n,n$'\alpha$). Each GENDF section found is passed to SHUFFL, which rearranges the input data into the CCCC order in scratch array B, and then to WRTMTX, which repacks the data into banded form and writes the results to NSCRT2.

Subroutine SHUFFL reads each of the group-to-group cross sections for a given reaction (MT) and calculates a location for each cross section in the scratch array (NOLOC). Different formulas are used for the location of the two allowed values of IFOPT. For IFOPT=1, the data are stored with incident group index JG1 changing fastest, then Legendre index IL, and with final group index JG2 changing slowest.

Note that the indexing scheme only stores the triangle of the matrix corresponding to ingroup scattering and downscatter (that is, JG2≥JG1). In addition, the first group in a subblocking range NG2Z is used. This means that values of JG2 less than NG2Z will result in storage locations less than IRSIZE, and they will not be stored (see statement 200). Groups with JG2 above the subblock might be stored in memory, or they might end up above the upper limit of the memory area and be suppressed by statement number 200. Similarly, the data for IFOPT=2 are stored with JG1 as the fastest varying index, then JG2, and finally with IL as the slowest varying index. Here also, the storage pointer NOLOC is calculated so that only elements with JG2≥JG1 are stored, and elements that are outside of a given subblock are removed if they fall outside the bounds of the memory array.

Subroutine WRTMTX searches through the memory area loaded in SHUFFL to find the bands of group-to-group elements that will be written on the final ISOTXS file. The calculation of locations in the memory array depends on the blocking and subblocking options selected. In general, the routine calculates locations NOLOCA and tests the cross section found there against the value EPS=1.E-10. The highest index that violates this test for a given final energy group determines the bandwidth for that group. (Remember that the inscattering group is always kept, even if it has zero cross section.) Once the band limits have been found, the subroutine loops back through the memory area and squeezes out the locations that are not included in the bands. At this point, all the elements of the "Scattering Sub-Block" are in their final locations, and the record is written out to scratch tape NSCRT2.

When ISOMTX returns to ISXDAT, the "Isotope Control and Group Independent Data" record is completed by filling in the values of IDSCT and IJJ, and the record is written to scratch tape NSCRT3. The LOCA values for the "File Date" record are also calculated at this point. They remain in memory at L19. Once the "DO 300" loop over the requested isotopes has finished, the ISXDAT routine returns.

Back in CISOTX, all the data needed for the ISOTXS file are now in memory or on one of the CCCC-style scratch files NSCRT2 or NSCRT3. The routine simply steps through the ISOTXS records and either constructs them or copies them from a scratch file. When the file has been written, the routine returns to CCCCR, which checks the print flag, and calls \cwordPISOTX—, if requested.

PISOTX is a fairly simple routine. It reads through the ISOTXS file produced by CCCCR and prepares an interpreted listing of the data.

2. BRKOXS File Preparation. Subroutine `CBRKXS` is used to prepare the BRKOXS file, if requested. Following the same pattern as CISOTX, it calls `RUINBR` to read the user's input, then it calls `BRKDAT` to extract the desired data from the GENDF file, and finally it writes the output BRKOXS file using data stored in memory and on a scratch tape by `BRKDAT`.

The storage locations used by `BRKDAT` are outlined in the comment cards at the beginning of the subroutine. Note that `L1` is the pointer to dynamic array `FLID` reserved in `CBRKXS`. Pointers down through `L8` are not really independent; they are defined relative to `L1` and are used to load data from the general CCCCR input plus the σ_0 and T counts from the BRKOXS input section. Next, dynamic arrays are reserved using pointers `L9` through `L17` for data arrays of known length. The dynamic array `IRINP` is reserved using all of the remaining memory (`NWD=-1`). The subroutine now opens the input GENDF file and reads in the header record. After checking for possibly incompatible group structures, it reverses the order of the group bounds and loads them into the `EMAX` and `EMIN` arrays. The number of words required for reading the rest of the GENDF records is computed as `N19`, and the rest of the `IRINP` array is released. The dynamic array `INFX` with pointer `L19` is reserved to hold 13 infinitely dilute cross section vectors that will either be needed during the processing (vectors 1 through 7) or will be written into the "Cross Sections" record. These 13 quantities are

1. P_0 total cross section,
2. capture cross section,
3. fission cross section,
4. P_1 total - P_1 elastic,
5. elastic cross section,
6. P_1 total cross section,
7. P_1 flux,
8. `XSPO`,
9. inelastic cross section,
10. elastic cross section,
11. average elastic scattering cosine $\bar{\mu}$,
12. elastic downscatter to adjacent group, and
13. average elastic lethargy increment ξ.

Now the entire remaining memory is reserved for the array SCRT with pointer L20.

The next step is to determine whether it is necessary to subblock the self-shielding factor record. The amount of space available in dynamic array SCRT is compared with the maximum amount of memory required for the f-factors. If there is not enough space, NSBLK is increased to NREACT; otherwise, it is left at 1. The value of NSBLK is stored into the IBLK field of the BRKOXS "File Control" record.

The isotope loop is complicated because CCCCR allows the materials on the GENDF tape to be in any order, but it arranges things so that the materials on the BRKOXS files are in the order that the materials are named in the user's input. The main loop is controlled by DO 370 I=1,NISO. For each pass, the input GENDF tape is rewound and searched for isotope I (see DO 170 J=1,NISO). Once a desired material has been found, the σ_0 list in the header record is examined. Either the first abs(NZI) values are extracted (for NZI negative), or the particular values that occur on the input ASIG list are extracted (for NZI positive). In either case, NZJ is the number of σ_0 values found, ISIG contains the pointers to the values selected, and CSIG contains the actual values of σ_0.

GENDF tapes contain one of more temperatures for each material recorded as consecutive MATs. Starting at statement number 190, BRKDAT reads through all the materials with the current MAT number selecting the desired temperatures and copying them to a scratch file NSCRT1. The procedure used to select temperatures is similar to the one used to select σ_0 values. If NTI is negative, the first abs(NTI) temperatures are extracted. If NTI is positive, only temperatures on the list in ATEM are extracted. In either case, NTJ is the number of temperatures found for this material, ITEM contains indices to those temperatures, and CTEM contains the actual temperature values. When all the desired temperatures have been copied (see statement number 260), the space used for GENDF input is released, and a new block is reserved with a size appropriate for reading in the desired data. In addition, INFX and SCRT are reserved to hold the BRKOXS cross sections and f-factors, respectively.

In the loop beginning at DO 340 NSB=1,NSBLK, a pass through the scratch tape is made for each subblock (1 or NREACT). Each section of the GENDF format is located, and either XSPROC (for MF3) or MXPROC (for MF6) is called to process the data in the section.

Subroutine XSPROC is called once for each reaction in File 3 of the GENDF tape. It reads in all the data, checks which reaction is present, and stores the data in one of the 13 cross section locations (see L19), or in one of the f-factor locations (see L20). If the denominator for the f-factor calculation is zero, the division is skipped, and a warning message is issued.

Subroutine MXPROC is called once for each reaction in File 6 of the GENDF tape. It loops through statement number 120 to read all of the incident groups, and then it uses different sections of coding to fill in or fix up the rest of the 13 elements in the infinitely dilute cross section block at L19. These quantities include the elastic and inelastic cross sections, the transport cross section, and the removal cross section. This routine also computes the elastic removal self-shielding factors from MF6,MT2, and stores the results in the f-factor area at L20.

Back in BRKDAT, the self-shielded transport cross sections are converted into f-factors. A check is then made to see if the transport values were properly computed. This requires that a self-shielded elastic matrix was available for all the higher temperatures. A warning message is issued if the required data were not present. The last 6 of the 13 vectors stored starting at L19 are the data needed for the "Cross Sections" record; that block is written to scratch file NSCRT2. Next, the accumulated f-factor data at L20 are written to NSCRT2, and the NTABP and NTABT arrays are stored at L14 and L15, respectively.

The last step inside the isotope loop is to call THNWRT to thin out the f-factor data and write the results onto scratch file NSCRT3. It starts by reading the cross section data from NSCRT2 into memory. Then it reads the f-factor data into memory and repacks it to take account of the group range for interesting self-shielding factors, namely, JBFL to JBFH. When this is finished, it writes the f-factor array out to NSRT3, and then it writes the unchanged cross section block out to NSCRT3. Note that these two records are now in the correct order to be copied to the BRKOXS file.

Subroutine THNWRT now returns control to BRKDAT. When the "DO 370" loop has finished, the routine cleans up the "File Data" information in memory and returns to the main BRKOXS routine. At this point, all the information required to construct the output file is present in memory or on scratch tape NSCRT3. The routine steps through the records of the BRKOXS format constructing them or copying them from the CCCC-style scratch file. It then returns to CCCCR, which checks to see whether PBRKXS should be called.

Subroutine PBRKXS is a fairly simple routine. It reads through the BRKOXS file produced by CCCCR and prepares an interpreted listing of the data.

3. DLAYXS File Preparation. Subroutine CDLYXS is used to prepare the DLAYXS file, if requested. It starts by calling DLDATA to extract the delayed-neutron data from the input GENDF file. Since all the data are stored into memory, CDLYXS continues by simply writing out the required "File Identification," "File Control," "File Data, Decay Constants, and Emission Spectra," and "Delayed Neutron Precursor Yield Data" records. If no delayed-neutron data are found, CDLYXS issues a fatal error message.

Subroutine DLDATA starts by reserving space for the dynamic arrays used to store the delayed-neutron data; the purpose for each of these arrays is summarized in the comment block at the beginning of the subroutine. ENDF delayed-neutron files are based on the traditional 6 time groups; therefore, CCCCR makes each time group for each isotope correspond to one DLAYXS "delayed-neutron family" (see NFAM=6*NISOD). Next, DLDATA starts reading through the materials on the GENDF tape and looking at each material requested in the user's input (the material loop goes through statement 110). For the first material, it reads the header record, checks that the group structure is compatible with the user's input value NGROUP, and stores the structure in EMAX and EMIN in the conventional decreasing-energy order. For all materials, it watches for sections with MF3,MT455 or MF5,MT455.

When MF3/MT455 is found (see statement 310), DLDATA stores the total delayed-neutron yield from GROUPR in the SNUDEL array (pointer L8) using an offset computed from the time group index (which varies from 1 to 6), the group index, and the isotope index. (The group index goes through statement 130). For the present, the same value is stored for every time group.

When MF5/MT455 is found (see statement 410), the rest of the data for this isotope are stored into memory. The HABSID field is obtained from the isotope name in the user's input. The LOCA field is easy to calculate from the isotope index. The decay constants for each of the time groups are copied into FLAM from the GENDF record. The number of families for this isotope is simply 6; this number is loaded into the location corresponding to NKFAM. Finally, the actual delayed-neutron spectra for each time group are loaded into the CHID area using energy group and family number as indexes. At this point, the spectrum for each time group is summed over group index to determine the delayed fraction for that time group [see FRACT(I)]. Then this fraction is used to change the total delayed-neutron yield for each time group in the SNUDEL area into the fractional delayed-neutron yield for that time group (family).

When all the isotopes containing delayed-neutron data have been processed, DLDATA returns to CDLYXS. When CDLYXS returns to the main subroutine of CCCCR after writing the DLAYXS file, the print routine `PDLYXS` may be called. This is a fairly simple routine that reads through a file in DLAYXS format and prepares an interpreted listing.

G. User Input

The user input instructions copied from the comment cards at the beginning of the CCCCR source code are given below. It is always a good idea to check the comments cards in the current version of the code in case there have been any changes.

```
*---INPUT SPECIFICATIONS (FREE FORMAT)---------------------------*
*                                                               *
*-CCCCR-                                                        *
* CARD 1 UNITS                                                  *
*    NIN      INPUT UNIT FOR DATA FROM GROUPR                   *
*    NISOT    OUTPUT UNIT FOR ISOTXS (0 IF ISOTXS NOT WANTED)   *
*    NBRKS    OUTPUT UNIT FOR BRKOXS (0 IF BRKOXS NOT WANTED)   *
*    NDLAY    OUTPUT UNIT FOR DLAYXS (0 IF DLAYXS NOT WANTED)   *
* CARD 2 IDENTIFICATION                                         *
*    LPRINT    PRINT FLAG (0/1=NOT PRINT/PRINTED)               *
*    IVERS     FILE VERSION NUMBER (DEFAULT=0)                  *
*    HUSE      USER IDENTIFICATION (12 CHARACTERS)              *
*              DELIMITED BY *, ENDED BY /.                      *
*              (DEFAULT=BLANK)                                  *
* CARD 3                                                        *
*    HSETID    HOLLERITH IDENTIFICATION OF SET (12 CHARACTERS)  *
*              DELIMITED BY *, ENDED BY /.                      *
*              (DEFAULT=BLANK)                                  *
* CARD 4 FILE CONTROL                                           *
*    NGROUP    NUMBER OF NEUTRON ENERGY GROUPS                  *
*    NGGRUP    NUMBER OF GAMMA ENERGY GROUPS                    *
*    NISO      NUMBER OF ISOTOPES DESIRE                        *
*    MAXORD    MAXIMUM LEGENDRE ORDER                           *
*    IFOPT     MATRIX BLOCKING OPTION (1/2=BLOCKING BY          *
*                                  REACTION/LEGENDRE ORDER)     *
* CARD 5 ISOTOPE PARAMETERS (ONE CARD PER ISOTOPE)              *
*       (FIRST FOUR WORDS ARE HOLLERITH, UP TO SIX CHARACTERS   *
*       EACH, DELIMITED BY *)                                   *
*    HISNM     HOLLERITH ISOTOPE LABEL                          *
*    HABSID    HOLLERITH ABSOLUTE ISOTOPE LABEL                 *
*    HIDENT    IDENTIFIER OF DATA SOURCE LIBRARY (ENDF/B)       *
*    HMAT      ISOTOPE IDENTIFICATION                           *
*    IMAT      NUMERICAL ISOTOPE IDENTIFIER (ENDF/B MAT NUMBER) *
*    XSPO      AVERAGE POTENTIAL SCATTERING CROSS SECT. (BRKOXS) *
*                                                               *
*-CISOTX- (ONLY IF NISOT.GT.0)                                  *
* CARD 1 FILE CONTROL                                           *
*    NSBLOK    SUBBLOCKING OPTION FOR SCATTERING MATRIX         *
*              (1 OR NGRUP SUB-BLOCKS ALLOWED)                  *
```

```
*    MAXUP     MAXIMUM NUMBER OF UPSCATTER GROUPS (ALWAYS ZERO)  *
*    MAXDN     MAXIMUM NUMBER OF DOWNSCATTER GROUPS              *
*    ICHIX     FISSION CHI REPRESENTATION                        *
*                   -1   VECTOR (USING GROUPR FLUX)              *
*                    0   NONE                                    *
*                   +1   VECTOR (USING INPUT FLUX)               *
*                .GT.1   MATRIX                                  *
* CARD 2 CHI VECTOR CONTROL (ICHIX=1 ONLY)                       *
*    SPEC      NGROUP FLUX VALUES USED TO COLLAPSE THE GROUPR    *
*              FISSION MATRIX INTO A CHI VECTOR                  *
* CARD 3 CHI MATRIX CONTROL (ICHIX.GT.1 ONLY)                    *
*    SPEC      NGROUP VALUES OF SPEC(I)=K DEFINE THE RANGE OF    *
*              GROUPS I TO BE AVERAGED TO OBTAIN SPECTRUM K.     *
*              INDEX K RANGES FROM 1 TO ICHI.                    *
*              THE MODEL FLUX IS USED TO WEIGHT EACH GROUP I.    *
* CARD 4 ISOTOPE CONTROL (ONE CARD PER ISOTOPE)                  *
*    KBR       ISOTOPE CLASSIFICATION                            *
*    AMASS     GRAM ATOMIC WEIGHT                                *
*    EFISS     TOTAL THERMAL ENERGY/FISSION                      *
*    ECAPT     TOTAL THERMAL ENERGY/CAPTURE                      *
*    TEMP      ISOTOPE TEMPERATURE                               *
*    SIGPOT     AVERAGE EFFECTIVE POTENTIAL SCATTERING           *
*    ADENS     DENSITY OF ISOTOPE IN MIXTURE                     *
*                                                                *
*-CBRKXS- (ONLY IF NBRKS.GT.0)                                   *
* CARD 1 (2I6) FILE DATA                                         *
*    NTI       NUMBER OF TEMPERATURES DESIRED                    *
*              (-N MEANS ACCEPT FIRST N TEMPERATURES)            *
*    NZI       NUMBER OF SIGPO VALUES DESIRE                     *
*              (-N MEANS ACCEPT FIRST N DILUTION FACTORS)        *
* CARD 2 (NOT NEEDED IF NTI.LT.0)                                *
*    ATEM(NTI) VALUES OF DESIRED TEMPERATURES                    *
* CARD 3 (NOT NEEDED IF NZI.LT.0)                                *
*    ASIG(NZI) VALUES OF DESIRED SIGPO                           *
*                                                                *
*-CDLAYX-- NO INPUT REQUIRED                                     *
*                                                                *
******************************************************************
```

These instructions are divided into four parts. First, there is a general section that applies to all three interface files following `-CCCCR-`. Second, there is a section of special parameters for ISOTXS following `-CISOTX-`. Third, there is a section of special parameters for BRKOXS following `-CBRKXS-`. And fourth, there is a comment following `-CDLYXS-` noting that no special input is required for the DLAYXS file.

In the `-CCCCR-` section, Card 1 is used to read in the unit numbers for input and output. `NIN` must be a GENDF tape prepared using GROUPR, and it can have either binary (`NIN>0`) or BCD (`NIN<0`) mode. The units for the output ISOTXS, BRKOXS, and DLAYXS files are all binary, but either sign can be used on the unit numbers. If any unit number is given as zero, the corresponding CCCC interface file will not be generated. On Card 2, the LPRINT=1 is used to request a full printout of all the CCCC files generated. The file version number IVERS can be used to distinguish between different libraries generated using NJOY. The user identification field HUSE can contain any desired 12-character string. An example of Card 2 might be

```
0  4  *T2 LANL NJOY*/  .
```

Card 3 contains a description of the library using up to 72 characters (12 standard CCCC words of 6 characters each). For example,

```
*LIB-IV 50-GROUP LMFBR LIBRARY FROM ENDF/B-IV (1976)*/  .
```

On Card 4, the values given for NGROUP must agree with the number of groups on the input GENDF tape or a fatal error message will be issued. NGGROUP is not used. NISO is the total number of materials or isotopes to be searched for on the GENDF tape. The value of MAXORD should be less than or equal to the maximum Legendre order used in the GROUPR run. The use of the matrix blocking parameter IFOPT was discussed in detail in connection with the description of the ISOTXS format above. A value of 1 has been normally used for Los Alamos libraries.

A line using the Card 5 format is given for each of the NISO isotopes or materials to be processed. The Hollerith isotope label and the Hollerith absolute isotope label have normally been set to the conventional isotope name at Los Alamos; for example, U235 or FENAT. The library name in HABSID can vary quite a lot now that many other libraries are available in ENDF format. The values of HMAT and IMAT will normally be derived from the MAT number characteristic of all libraries in ENDF format. Unfortunately, XSPO, the average potential scattering cross section, must be entered by hand. It can be obtained from MF2,MT151 on the ENDF file for the material by determining the scattering radius a from the AP field and computing $\sigma_p{=}4\pi a^2$. The following fragment of an ENDF/B evaluation shows the vicinity of AP:

```
 ...
                                                                 9228 0  0  572
 9.223500+4 2.330250+2          0          0          1          09228 2151  573
 9.223500+4 1.000000+0          0          1         11          09228 2151  574
 1.000000-5 1.100000+2          1          3          0          09228 2151  575
 3.500000+0 1.001760+0          0          0          1          29228 2151  576
 2.330250+2 0.000000+0          0          0       1416        2369228 2151  577
-9.997600+1 3.000000+0 3.771300-3 3.980000-2 1.861800-1 4.700200-19228 2151  578
 ...
```

The scattering radius is the second number on the third card in the section MF2,MT151. Using it as a gives $4\pi(1.00176)^2 = 12.611$ barns for the value of `XSPO`. An example of Card 5 follows:

```
U235 U235 ENDF6 *9228* 9228 12.611
```

Note that the Hollerith string "9228" had to be delimited by stars because it does not begin with a letter. The delimiters are optional for the other Hollerith variables.

The next block of input cards is specific to ISOTXS and only appears if ISOTXS processing was requested with a nonzero value for `NISOT`. The first parameter on Card 1 is `NSBLOK`, which was discussed in connection with matrix blocking and subblocking. `NSBLOK` and `IFOPT` work together to control how a large scattering matrix is broken up into smaller records on the ISOTXS interface file. The important factor is the maximum size of the binary records. They should be small enough to fit into a reasonable amount of memory in any application codes that use ISOTXS files, but they should be large enough to keep the number of I/O operations to a minimum. The maximum record size for each option is repeated below for the convenience of the reader:

1. *IFOPT=1 and NSBLOK=1*: $n_\ell \times n_g(n_g-1)/2$,
2. *IFOPT=1 and NSBLOK=NGROUP*: $n_\ell \times n_g$,
3. *IFOPT=2 and NSBLOK=1*: $n_g(n_g-1)/2.$,
4. *IFOPT=2 and NSBLOK=NGROUP*: n_g,

where n_ℓ is the number of Legendre orders and n_g is the number of groups. If the user specifies `NSBLOK=1` and the resulting output record is too large for the available memory, `NSBLOK` will be changed to `NGROUP` automatically.

Card 1 of the ISOTXS section continues with `MAXUP`. This parameter is always zero for CCCCR; thermal upscatter matrices are not processed. The normal value of `MAXDN` is `NGROUP`, but it can be made smaller to reduce the size of the matrices. The cross section for any removed downscatter groups will be lumped into the last group in order to preserve the production cross section. The `ICHIX` is used to control the generation of fission χ vectors and matrices. The representations allowed were discussed above in connection with the description of the ISOTXS format (see Section XIV.C). The most commonly used option has been `ICHIX=-1` because most application codes cannot handle fission χ matrices. The GROUPR flux is normally chosen to be characteristic of the class of problems a given library is intended to treat; therefore, it is rarely necessary to supply an input weighting spectrum (see `ICHIX=+1` and `SPEC`). The following scenario illustrates a case where this option might be useful. Assume that an 80-group library is made using the GROUPR fast reactor weight function (`IWT=8`), which contains a shape in the fission range typical of both fast reactors and fusion blankets plus a fusion peak at 14 MeV. This GENDF library could be used to generate two different ISOTXS libraries, one using the default flux and useful for fusion problems, and one using a spectrum `SPEC` from which the fusion peak has been removed. The latter would be better for fast reactor analysis because the χ vectors would not contain the component of high-energy fission from the 14 MeV range. Card 2 is used to input the user's choice for `SPEC`.

CCCCR can also produce fission χ matrices for codes that can use them. These matrices can be rectangular to take advantage of the fact that the $\chi_{g \rightarrow g'}$ function is basically independent of g at low energies (large values of g). Taking the GROUPR 30-group structure as an example, if the energy at which significant incident-energy dependence begins is taken to be about 100 keV, then groups 16 through 30 will have identical χ vectors. The value of `ICHIX` should be set to 16, and the `SPEC` vector of Card 3 should be set to

```
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 15R16/  .
```

The resulting χ matrix will be rectangular with 16×30 elements.

Card 4 completes the input specific to ISOTXS. The value of `KBR` can be set to reflect the normal use of this material in the applications that this library is intended to treat. The `AMASS` parameter has units of gram atomic weight. It can be calculated from the normal ENDF AWR parameter (the atomic weight ratio to the neutron) by multiplying by the gram atomic weight of the neutron. `TEMP` is normally 300 K for NJOY libraries. The same value can be used for `SIGPOT` and `XSPO` (see above). The `ADENS` parameter has no meaning for CCCCR; it can be set to zero to imply infinite dilution.

The choice of values for `EFISS` and `ECAPT` is more complicated. As discussed in Section XIV.C, `EFISS` is basically the total non-neutrino energy released by a fission reaction. It is available in eV as the pseudo Q value in MF3,MT18 (the energy release from fission is given in more detail in MF1,MT458). The following fragment of the ENDF/B-VI evaluation for ^{235}U shows how to find the Q value:

```
 ...
                                                                   9228 3  0 4413
9.223500+4 2.330250+2          0          0          0          09228 3 18 4414
1.937200+8 1.937200+8          0          0          1        3339228 3 18 4415
       333          2                                           9228 3 18 4416
1.000000-5 0.000000+0 7.712960+1 0.000000+0 2.250000+3 0.000000+09228 3 18 4417
2.250000+3 5.362770+0 2.300000+3 5.396710+0 2.500000+3 5.957280+09228 3 18 4418
 ...
```

The Q value is the second number on the second card of the section MF3,MT18. Converting to CCCC units gives

$193.72{\times}10^6$ eV $\times$ $1.602{\times}10^{-13}$ watt-s/eV = $.31034{\times}10^{-10}$ watt-s/fission

The value for `ECAPT` is determined from the Q value for MF3,MT102, the radiative capture reaction. However, if the isotope remaining after capture has a relatively short half-life, the energy of the decays leading to the final stable daughter should be added onto the capture Q value. (The meaning of "stable" may vary from application to application). As an example, consider aluminum. The ^{28}Al capture product decays with a half-life of 2.24 minutes producing 9.31 MeV of β^- energy and a 1.779 MeV photon. Therefore, the actual value of `ECAPT` should be calculated as follows:

7.724 MeV	MT102 prompt Q value
9.310 MeV	β^- energy
1.779 MeV	delayed-γ energy
18.813 MeV	
$\times 1.602 \times 10^{-13}$	
$.3014 \times 10^{-11}$	in watt-s/capture

The next section of the input file is specific to BRKOXS. Card 1 enables the user to just accept all or part of the temperatures and sigma-zero values on the input GENDF tape. If the value of `NTI` is negative, the first abs(`NTI`) T values for each material will be used. If fewer values are available, only those will be used. If `NTI` is positive, input Card 2 will be read for a list of T values, and only data with temperatures on that list will be extracted from the GENDF tape. The parameter `NZI` and the list of σ_0 values on Card 3 work in the same way.

No additional input is required for DLAYXS files.

H. Error Messages

`ERROR IN ISXDAT***INCOMPATIBLE GROUP STRUCTURES`

The number of groups on the input GENDF tape must match the number of groups specified in the CCCCR input. Check whether the correct input file was mounted.

`ERROR IN ISOMTX***INPUT RECORD TOO LARGE`

There is not enough space in the scratch array `B` to read in the input records from the GENDF tape. The only solution is to increase the size of the main container array. See `COMMON/CSTORE/A(25000)` and `ISIZA=25000` in subroutine CCCCR.

`ERROR IN ISOMTX***OUTPUT RECORD TOO LARGE`

There is not enough space in the scratch array `B` for the output subblock record, even with `NSBLOK` changed to `NGROUP`. The only solution is to increase the size of the main container array. See `COMMON/CSTORE/A(25000)` and `ISIZA=25000` in subroutine CCCCR.

`ERROR IN SHUFFL***INPUT RECORD OVERRAN OUTPUT`

This shouldn't happen because of the checks in `ISOMTX`. It may reflect a problem in the input data record.

`ERROR IN PISOTX***INPUT RECORD TOO LARGE`

One of the binary records on the ISOTXS file is too large for the memory available to `PRINXS`. This should not occur because there was enough memory to create the record in the first place.

`ERROR IN BRKDAT***INCOMPATIBLE GROUP STRUCTURES`

The number of groups on the input GENDF tape must match the number of groups specified in the CCCCR input. Check whether the correct input file was mounted.

`MESSAGE FROM BRKDAT---ALL AVAILABLE MATS HAVE BEEN PROCESSED`

This message is issued when all the materials on the GENDF file have been processed, but one or more of the materials requested in the user's input were not found. Check the input material list, and check which materials were written onto the input GENDF file.

`MESSAGE FROM BRKDAT---NO TEMPERATURES FOR MAT=nnnn`

This means that none of the requested temperatures were found for this MAT. This makes it impossible to include the material in the BRKOXS file. The warning message is issued, and all references to this material are thinned out of the BRKOXS records.

`MESSAGE FROM BRKDAT---NEED ELASTIC MATRICES AT HIGHER TEMPERATURES`

The self-shielded transport cross section requires self-shielded P_1 elastic scattering matrices for accurate results. This means that MF6,MT2 should be available on the GENDF tape for all temperatures. If this scattering matrix is missing for the higher temperatures, this warning message is issued.

`MESSAGE FROM XSPROC---INFINITE F-FACTOR mt jg jz temp`

The calculation of an f-factor requires division by the infinitely dilute cross section. This message means that the divisor was zero for reaction *mt*, group *jg*, background cross section *jz*, and temperature *temp*. The division is skipped, and the numerator is used unchanged.

`ERROR IN MXPROC***NOT ENOUGH STORAGE FOR INPUT`

There is not enough space in the dynamic array `RINP` with pointer `L18` for the data for one incident group of a scattering matrix. The only solution is to increase the size of the main container array. See `COMMON/CSTORE/A(25000)` and `ISIZA=25000` in subroutine CCCCR.

`ERROR IN PBRKXS***INPUT RECORD TOO LARGE`

One of the binary records on the BRKOXS file is too large for the memory available to `PBRKXS`. This should not occur because there was enough memory to create the record in the first place.

`MESSAGE FROM CDLYXS---NO DELAYED NEUTRON DATA FOUND`

There was no delayed-neutron data found by `DLDATA`. Make sure that MF3,MT455 and MF5,MT455 were requested during the GROUPR run and that the delayed-neutron isotopes were included in the material list given in the CCCCR input.

`ERROR IN DLDATA***INCOMPATIBLE GROUP STRUCTURES`

The number of groups on the input GENDF tape must match the number of groups specified in the CCCCR input. Check whether the correct input file was mounted.

`ERROR IN PDLYXS***INPUT RECORD TOO LARGE`

One of the binary records on the DLAYXS file is too large for the memory available to `PDLYXS`. This should not occur because there was enough memory to create the record in the first place.

I. References

1. B. M. Carmichael, "Standard Interface Files and Procedures for Reactor Physics Codes, Version III," Los Alamos Scientific Laboratory report LA-5486-MS (February 1974).

2. R. Douglas O'Dell, "Standard Interface Files and Procedures for Reactor Physics Codes, Version IV," Los Alamos Scientific Laboratory report LA-6941-MS (September 1977).

3. C. R. Weisbin, P. D. Soran, R. E. MacFarlane, D. R. Harris, R. J. LaBauve, J. S. Hendricks, J. E. White, and R. B. Kidman, "MINX: A Multigroup Interpretation of Nuclear X-Sections from ENDF/B," Los Alamos Scientific Laboratory report LA-6486-MS (ENDF-237) (September 1976).

4. R. B. Kidman and R. E. MacFarlane, "LIB-IV: A Library of Group Constants for Nuclear Reactor Calculations," Los Alamos Scientific Laboratory report LA-6260-MS (March 1976).

5. R. E. MacFarlane and R. B. Kidman, "LINX and BINX: CCCC Utility Codes for the MINX Multigroup Processing Code," Los Alamos Scientific Laboratory report LA-6219-MS (February 1976).

6. "CINX: Collapsed Interpretation of Nuclear X Sections," Los Alamos Scientific Laboratory report LA-6287-MS (April 1976).

7. W. J. Davis, M. B. Yarbrough, and A. B. Bortz, "SPHINX: A One Dimensional Diffusion and Transport Nuclear Cross Section Processing Code," Westinghouse Advanced Reactors Division report WARD-XS-3045-17 (August 1977).

8. C. L. Cowan, B. A. Hutchins, and J. E. Turner, "TDOWN – A Code to Generate Composition and Spatially Dependent Cross Sections," General Electric report GEAP-13740 (August 1971).

9. K. L. Derstine, "DIF3D: A Code to Solve One-, Two-, and Three-Dimensional Finite-Difference Diffusion Theory Problems," Argonne National Laboratory report ANL-82-64 (April 1984).

10. R. Douglas O'Dell, Forrest W. Brinkley, Jr., Duane R. Marr, and Raymond E. Alcouffe, "Revised User's Manual for ONEDANT: A Code Package for One-Dimensional, Diffusion-Accelerated, Neutral-Particle Transport," Los Alamos National Laboratory report LA-9184-M, Rev. (December 1989).

11. R. J. LaBauve, T. R. England, D. C. George, R. E. MacFarlane, and W. B. Wilson, "DANDE—A Linked Code System for Core Neutronics/Depletion Analysis," Los Alamos National Laboratory report LA-10412-MS (June 1985).

12. R. E. MacFarlane and D. C. George, "UPD: A Portable Version-Control Program," Los Alamos National Laboratory report LA-12057-MS (April 1991).

13. I. I. Bondarenko, Ed., *Group Constants for Nuclear Reactor Calculation* (Consultants Bureau, New York, 1964).

14. R. W. Hardie and W. W. Little, Jr., "1DX, A One-Dimensional Diffusion Code for Generating Effective Nuclear Cross Sections," Battelle Northwest Laboratories report BNWL-954 (1969).

CONTENTS