DKDATA: SUBROUTINE FOR RETRIEVING RADIONUCLIDE GAMMA-RAY DECAY DATA FROM RSIC DATA SET DLC-19/DECAYGAM

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Nucleonuclide Gamma-ray Decay Data from
RSIC Data Set DLC-19/DECAYGAM

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ABSTRACT

DKDATA is a subroutine written in Fortran IV which returns to the calling program information concerning the gamma-ray decay characteristics of a nuclide of specified atomic number and mass. This data is initially read from the Radiation Shielding Information Center Data Set DLC-19/DECAYGAM on first entry to the subroutine, and the pertinent data for all nuclides of interest are stored for use in subsequent calls.
INTRODUCTION

The DECAYGAM data set of the Radiation Shielding Information Center contains a large amount of information on the characteristics of radionuclides. This report describes one subroutine useful for retrieving this information for use in the calling program. The specific routine described here reads from the data tape all information concerning each nuclide, and selects for retention and subsequent return to the calling program only two quantities. These are the half-life of the nuclide (if gamma-active) and a weighting factor which is a measure of the average total energy emitted by the nuclide as photons. For other applications, the choice of what information read from the data tape is to be retained and what is to be discarded can be changed with little programming effort.

Use of the subroutine requires three steps: First, the subroutine call must be inserted into the main program with arguments Z and A set. Second, the namelist statements described below must be inserted into the standard input data set (assumed to be 5) such that it can be read by DKKDATA on first entry. Third, data set DECAYGAM must be accessed with appropriate JCL cards, or in card form immediately following the namelist.
USAGE OF SUBROUTINE

The following subroutine call must be inserted into the calling program:

```
CALL DKDATA(Z,A,WEIGHT,HALFLF)
```

where the calling arguments are the following:

- **Z** - atomic number of the nuclide for which the decay gamma-ray information is sought. Z must be the floating point representation of an integer.

- **A** - atomic mass of the nuclide. A must be the floating point representation of an integer.

- **WEIGHT** - a measure of the importance of the nuclide as a gamma-ray emitter found by summing the product of the gamma-ray energy and the branching ratio for each possible decay gamma ray.

- **HALFLF** - halflife of the nuclide in minutes.

The first execution of this subroutine call causes the namelist 6DKGAM to be read from the standard input to determine the parameters to be considered in calculating the
weight. In addition, the amount of printed output to be listed during the reading of the data tape and the logical numbers of the input and output data set are specified. The arguments of the namelist RDKGAM are the following:

NTIN - Data set number for the RSIC Data Set DECAYGAM.
Default: NTIN=5.

NTOU - Output data set number for the listing of information during the reading of the DECAYGAM data. In addition, a listing of the data retained by the subroutine is made after the end of the tape has been reached. If NTOU is less than or equal to 0, all printed output is suppressed.
Default: NTOU=6

MAXZ - Maximum value of \( Z \) required by the calling program. Since the DECAYGAM tape has the radionuclides ordered in \( Z \), scanning of the data is halted when a radionuclide having \( Z=\text{MAXZ}+1 \) is encountered.
Default: MAXZ=400.

HALFLO - Lowest value of halflife (in minutes) to be considered in calculating the weight. If
HALFLO is assigned a value in the namelist input data, nuclides of lower halflife will be assigned a WEIGHT of zero. The correct halflife will still be returned in the argument HALFLF.
Default: HALFLO=0.

HALFHI - Highest value of the halflife (in minutes) to be considered in calculating the weight. If HALFHI is assigned a value in the namelist input data, nuclides of higher halflife will be tagged by a WEIGHT of zero and the correct value of HALFLF.
Default: HALFHI=33.33 mins.

ELOW - Lowest gamma-ray energy (in MeV) that is to be considered in computing the weight. If a value for ELOW appears in the namelist input data, gamma rays of energy less than ELOW will not be included in the computation of WEIGHT. If the printed output is enabled, each gamma-ray omitted from the calculation will be flagged.
Default: ELOW=0.

EHIGH - Highest gamma-ray energy (in MeV) that is to be considered in calculating the weight. If EHIGH
is assigned a value in the namelist input data, gamma rays of energy higher than EHIGH will not be included in the computation of WEIGHT. If the printed output is enabled, each gamma-ray so ignored by the computation will be flagged. Default: EHIGH=33.3E33 MeV.

LIST - Logical variable to control the output of subroutine DKDATA only during the actual reading of the DECAYGAM data. In the namelist data, set LIST=.FALSE. or LIST=F to suppress listing. The final summary of stored information is not affected, and the limits of output controlled by LIST is printed in the full output listing, whenever listing is enabled.
Default: LIST=.TRUE.

The namelist data is inserted into the data cards of the standard input data set so as to be in position to be read on first entry to DKDATA. The customary rules regarding namelist data entry apply (column 1 not used, columns 73-80 may be used, commas separate data entries, blanks are ignored, etc.). An example of these cards is:
in which the values of all the variables is explicitly specified, with the exception of \textit{EHIGH}, which is taken to be infinite, by default. The data set:

\begin{verbatim}
&DKGAM ELOW=2 &END
\end{verbatim}

results in the rejection of gamma-ray energies below 2 MeV and, by default, specifies \textit{NTIN}=5, \textit{NTOU}=6, \textit{LIST}=.TRUE., \textit{HALFLO}=0, and \textit{HALPHI} infinite.

Because the namelist input statement causes all input cards of the standard data set to be skipped through until the \&DKGAM card is encountered, it must be inserted at the correct place. Even if standard options are desired, the following card \textbf{must} appear:

\begin{verbatim}
&DKGAM &END
\end{verbatim}

with at least one space preceding the \&END.

After reading the namelist, the subroutine reads the \texttt{DECAYGAM} input from data set \texttt{NTIN}. All the data entries on the tape for a single radionuclide are read into the common
region /DKCOM/, which is not used after the original reading of the tape. Upon return to the calling program, /DKCOM/ contains all the information concerning the last radionuclide read from the DECAYGAM tape. The data on the tape are indentified within the subroutine as follows:

KILL - flag to indicate end of DECAYGAM data tape.
SYM - chemical symbol of element in Hollerith.
TA - atomic mass of nuclide.
STATE - state of radionuclide:
  0 - ground state
  M - metastable
IZ - atomic number of nuclide.
HALF - halflife of radionuclide in units given in IUNIT.
COEFU - prefix of units of halflife:
  M - milli
  6 - \(10^{**6}\)
  9 - \(10^{**9}\)
IUNIT - units of halflife:
  S - seconds
  M - minutes
  H - hours
  D - days
  Y - years
MODE - mode of decay:
B- - negative beta (negatron) emission.
B+ - positive beta (positron) emission.
EC - orbital electron capture.
K - orbital electron capture from K-shell.

- chemical symbol of radionuclide precursor.
- atomic mass of radionuclide precursor.
- natural abundance of radionuclide precursor.
- thermal (2200 m/s) thermal cross section for \((n, \gamma)\) reaction.

- method by which radionuclide can be made:
  0 - \((n, \gamma)\) product
  1 - fission product
  2 - both \((n, \gamma)\) and fission product
  3 - charged particle or cyclotron-produced
  4 - natural radionuclide
  5 - other

- fission yield.
- number of gamma-ray energies tabulated.

- status of gamma-ray branching ratio data:
  A - absolute
  R - relative
  D - based on referenced decay scheme.

- resonance integral of radionuclide precursor.
- first reference from which data are taken.
- second reference.
- the gamma-ray energies and the corresponding
branching ratios, a total of \( \text{IMAX} \) pairs.

After reading these data for a radionuclide, the energies are converted to MeV and the halflives to minutes. The variables \( Z, A, \) and \( \text{HALF} \) are then transferred into \( \text{ZVEC}, \) \( \text{AVEC} \) and \( \text{HAFVEC} \) to be saved for subsequent calls. The weight is calculated from the formula:

\[
\text{WEIGHT} = \sum_{I=1}^{\text{IMAX}} (E(I) \times 0.01 \times \text{PCT}(I))
\]

ignoring gamma-ray energies having \( E \) less than \( \text{ELOW} \) or greater than \( \text{EHIGH} \). If the halflife falls outside the limits defined by \( \text{HALFLO} \) and \( \text{HALFHI} \), the weight is cleared to zero. The resulting \( \text{WEIGHT} \) is entered into the \( \text{WTVEC} \) array and data for a new nuclide is read from the \( \text{DECAYGAM} \) tape.

When the data set has been completely read up to the end of the tape or to \( \text{MAXZ}+1 \), the stored data vectors \( \text{ZVEC}, \) \( \text{AVEC} \) and \( \text{WTVEC} \) are listed and the information sought by the calling routine looked up in the data arrays.

Since some radionuclides have metastable states, the arrays are always searched fully on first and subsequent entries and the value of halflife and weight returned is that for the entry of highest weight.
SUBROUTINE CKDATA(Z,A,WEIGHT,HALFLF)

C-----------------------------
C
C SUBROUTINE CKDATA
C
C PURPOSE
C TO RETURN TO THE CALLING PROGRAM DATA THAT HAS
C BEEN RETRIEVED FROM THE GAMMA DECAY DATA TAPE DESIGNATED
C RSIC NUMBER DLC-19. THE DATA IS READ FROM THE TAPE ON THE
C FIRST ENTRY TO THE SUBROUTINE AND STORED FOR USE
C IN SUBSEQUENT ENTRIES.
C
USAGE
C (1) INSERT INTO THE MAIN PROGRAM THE STATEMENT:
C  CALL CKDATA(Z,A,WEIGHT,HALFLF)
C  WHOSE ARGUMENTS ARE DESCRIBED BELOW.
C (2) ENTER DATA INTO THE STANDARD INPUT DATA SET
C IN THE FORM OF A NAMELIST, DESCRIBED BELOW, WHICH
C IS READ BY SUBROUTINE CKDATA ON FIRST ENTRY.
C (3) MOUNT THE DATA TAPE RSIC DLC-19 WITH A DATA SET
C LOGICAL NUMBER GIVEN TO SUBROUTINE CKDATA VIA THE
C NAMELIST.
C
DESCRIPTION OF CALLING ARGUMENTS
C Z - ATOMIC NUMBER OF ELEMENT, SET BY CALLING PROGRAM
C A - NUCLEAR MASS OF NUCLIDE, SET BY CALLING PROGRAM
C WEIGHT - A MEASURE OF THE IMPORTANCE OF THE NUCLIDE FOUND
C BY SUMMING THE PRODUCT OF THE GAMMA ENERGY
C AND THE BRANCHING RATIO FOR EACH POSSIBLE
C DECAY GAMMA
C HALFLF - HALFLIFE OF THE NUCLIDE IN MINUTES.
C
DESCRIPTION OF THE NAMELIST VARIABLES IN NAMELIST 6DKGA
C NTOU - OUTPUT DATA SET NO. FOR LIST OF INFORMATION AS
C TAKEN FROM THE DATA TAPE AND AS SUMMARIZED
C AFTER THE ENTIRE TAPE HAS BEEN READ. IF
C NTOU IS NOT SPECIFIED IN THE NAMELIST, IT
C IS SET TO NTOU=0. IF NTOU IS LESS THAN OR
C EQUAL 0, ALL OUTPUT IS SUPPRESSED.
C MAXZ - MAXIMUM VALUE OF Z REQUIRED. SCANNING OF THE
C TAPE IS TERMINATED WHEN AN ENTRY HAVING Z=MAXZ+1 IS
C ENCOUNTERED. AS DEFAULT, Z=400
C HALFLO - LOWEST VALUE OF HALFLIFE TO BE CONSIDERED IN
C COMPUTING THE WEIGHT. NUCLIDES OF SMALLER
C HALFLIFE WILL BE ASSIGNED A WEIGHT OF 0.0, BUT
C THE HALFLIFE WILL BE RETURNED TO THE CALLING
C PROGRAM.
C HALFHI - HIGHEST VALUE OF HALFLIFE TO BE CONSIDERED IN
C COMPUTING THE WEIGHT. (CF. HALFLO).
C LOW - LOWEST ENERGY OF GAMMA TO BE CONSIDERED IN
C COMPUTING THE WEIGHT. GAMMAS OF LOWER ENERGY
C ARE IGNORED.
C EHIGH - HIGHEST ENERGY OF GAMMA TO BE CONSIDERED IN
C COMPUTING THE WEIGHT.
C LIST - LOGICAL VARIABLE TO CONTROL THE OUTPUT OF
C SUBROUTINE CKDATA DURING READING OF THE DATA
C TAPE. SET LIST=.FALSE. OR LIST=F TO SUPPRESS
C LIST OF TAPE DATA EXCEPT AS FINAL STORED DATA.
SUBROUTINES AND FUNCTION PROGRAMS REQUIRED

METHOD

ON FIRST ENTRY, THE NAMELIST DKGAM IS READ FROM
THE STANDARD INPUT TO DETERMINE THE PARAMETERS TO
BE CONSIDERED IN CALCULATING THE WEIGHT, TO CONTROL THE OUT-
PUT, AND FIND THE DATA SET HAVING THE GAMA DATA. THE TAPE
IS SCANNED AND THE VALUE OF WEIGHT COMPUTED. THE
RESULTANT WEIGHT AND THE HALFLIFE ARE STORED IN COMBINATION
WITH THE Z AND A OF THE NUCLIDE IN A 600 X 4 ARRAY.
WHEN THE END OF THE TAPE IS ENCOUNTERED, OR WHEN
Z EXCEEDS MAXZ, THE WEIGHT AND HALFLIFE FOR THE INITIAL
CALL ARE Sought IN THE STORAGE ARRAY. BECAUSE THE ARRAY MAY
INCLUDE MULTIPLE ENTRIES FOR THE SAME Z AND A, BECAUSE
OF ISOMERIC STATES, THE ENTIRE ARRAY IS SCANNED
AND THE GREATEST WEIGHT DETERMINES WHICH DATA IS RETURNED.

LOGICAL ENTERD / .FALSE. /
LOGICAL LIST / .TRUE. /  
INTEGER UNITS(5) /
'SECS','MINS','HOUR','DAYS','YEAR' /
REAL CONV(5) / 1.667E-2, 1., 1.44E3, 5.256E5 /
REAL*8 MODE

DIMENSION ZVEC(600),AVEC(600),HALFVEC(600),WTVEC(600)
DIMENSION E(200),PCT(200)
DIMENSION REF1(20),REP2(20)
COMMON /DKCCM/ SM,IA,STATE,IZ,HALF,COEPU,IUNIT,
* MODE,PRECUR,MASSP,ABUND,CRSSEC,
* MADE,IFYIELD,IMAX,STATUS,RESINT,
* REP1,REP2,E,PCT

NAMELIST /DKGAM/ HALFLO,HALPHI,NTIN,NTOU,MAXZ,
1 LIST,ELow,EHIGH

IF(ENTERD) GO TO 140

INITIAL ENTRY

SET PARAMETERS TO THEIR DEFAULT VALUES, READ
THE VARIABLES OF THE NAMELIST FROM STANDARD INPUT
AND LIST THE CURRENT VALUES (UNLESS NTOU=0).

ENTERD=.TRUE.
NTIN=5
NTOU=6
HALFLO=0.0
HALPHI=33.3E33
ELow=0.0
EHIGH=33.3E33
MAXZ=400

READ NAMELIST DKGAM FROM TAPE 5

READ(5,DKGAM)
IF(NTOU.LE.0) LIST=.FALSE.
WRITE(NTOU,9000)
9000 FORMAT('1 **** INITIALIZATION OF DATA *****')
WRITE(NTOU,9001)HALPLO
9001 FORMAT('0 REJECTING NUCLIDES OF HALF-LIFE (IN MINS) .LT. ',G14.7)
WRITE(NTOU,9002)HALPHI
9002 FORMAT('0 REJECTING NUCLIDES OF HALF-LIFE (IN MINS) .GT. ',G14.7)
WRITE(NTOU,9003)LOW
9003 FORMAT('0 WEIGHT IGNORES GAMMAS OF ENERGY .LT. ',G14.7)
WRITE(NTOU,9004)HIGH
9004 FORMAT('0 WEIGHT IGNORES GAMMAS OF ENERGY .GT. ',G14.7)
WRITE(NTOU,9005)MAXZ
9005 FORMAT('0 REJECTING NUCLIDES OF ATOMIC NUMBER .GT. ',G14.7)
WRITE(NTOU,9006)NTIN
9006 FORMAT('0 READING GAMMA DECAY DATA FROM TAPE NR ',I4)
WRITE(NTOU,9007)NTOU
9007 FORMAT('0 WRITING INITIALIZATION DATA ON TAPE ',I4)
IF(.NOT.LIST) WRITE(NTOU,9008)
9008 FORMAT('0 LIST = .FALSE., ALL PRINT-OUT EXCEPT SUMMARY WILL BE
SUPPRESSED. )
WRITE(NTOU,9009)
9009 FORMAT('1 **** BEGIN OUTPUT INVOKED BY SETTING LIST=.TRUE./1X)
C
NOW READ THE GAMMA DECAY DATA TAPE FROM NTIN
C
CONTINUE
C
IGNORE THE FIRST 100 RECORDS CONTAINING NORMAL DENSITIES
C
DO 20 I=1,100
20 READ(NTIN,9010)SYM,HALF
9010 FORMAT(A2,F8.4)
K=0
C
BEGINNING CP LCP HANDLING THE RECORDS PERTAINING TO
C A SINGLE RADIO-NUClide. THE NUMBER OF RECORDS IS DEFINED
C BY THE NUMBER OF GAMMAS, GIVEN BY I MAX IN THE FIRST RECORD.
C
CONTINUE
READ(NTIN,9011)KILL,SYM,IA,STATE,IZ,HALF,COEFU,IUNIT, 
*MDDE,PRCUR,MASSP,ABUND,CRSSEC,EADE,FYIHL,IMAX, 
*STATUS,RESINT
9011 FORMAT(I2,A2,I3,1X,A1,2X,I2,1X,E10.3,A1,A1,1X, 
IF(HILL.NE.0) GO TO 130
IF(I2.GT.MAXZ) GO TO 120
C
COEFU IS THE PREFIX ON THE HALFLIFE.
C
M - MILLI
C
6 - 10**6
C
9 - 10**9
C
THE UNITS FOR HALF-LIFE ARE GIVEN BY IUNIT. CONVERT TO MINUTES.

M DENOTES MINUTES
S SECONDS
Y YEAR
D DAYS

IF (ICOMP(A(IUNIT,'S',1).EQ.0) J=1
IF (ICOMP(A(IUNIT,'M',1).EQ.0) J=2
IF (ICOMP(A(IUNIT,'H',1).EQ.0) J=3
IF (ICOMP(A(IUNIT,'D',1).EQ.0) J=4
IF (ICOMP(A(IUNIT,'Y',1).EQ.0)
IUNIT=UNITS (J)
HPLIFE=HALF*CCNV(J)
IF (.NOT.LIST) GO TO 40

40 CONTINUE

LOAD Z, A, AND HALFLIFE INTO THE STORAGE VECTORS

K=K+1
ZVEC(K)=IZ
AVEC(K)=IA
HALFVEC(K)=HPLIFE

NOW READ THE REFERENCES AND THE GAMMA ENERGIES AND PCTS.

READ (NTIN,9013) REF1,REF2
9013 FORMAT (20A4)
READ (NTIN,9014) (E(I),PCT(I),I=1,1MAX)
9014 FORMAT (8F10.4)
DO 50 I=1,1MAX
E(I)=E(I)*0.001
PCT(I)=E(I)*0.001
50 CONTINUE

PROD((MAX,LB,C) GO TO 110
IF (.NOT.LIST) GO TO 60
WRITE (NTOU,9015)
9015 FORMAT (980,9016) (PCT(I),I=1,1MAX)
WRITE (NTOU,9016) (F(I),PCT(I),I=1,1MAX)
9016 FORMAT (12X,3X,980,9017) REF1
9017 FORMAT (100,9018) (REFERENCE: ' ,20A4)
9018 FORMAT (100,9019) WRITE (NTOU,9017) REF1
9019 FORMAT (1X)
60 CONTINUE
C COMPUTE THE WEIGHT, IGNORING GAMMAS OUTSIDE THE ENERGY LIMITS
C
C WEIGHT=0.0
DO 80 I=1,IMAX
IF(E(I).LT.ELOW) GO TO 70
IF(E(I).GT.EHIG) GO TO 70
WEIGHT=WEIGHT+E(I)*0.01*PCT(I)
GO TO 80
70 CONTINUE
IF (.NOT. LIST) GO TO 80
WRITE(NTOU,9020)E(I)
9020 FORMAT(12X,'WEIGHTING OMIITS GAMMA OF ENERGY = ',G14.7)
80 CONTINUE
WTVEC(K)=WEIGHT
IF (.NOT. LIST) GO TO 90

C PRINT OUT THE WEIGHT BEFORE ANY REJECTION TEST
C
C IF HALFLIFE TOO HIGH OR TOO LOW, REVISE WEIGHT TO 0.0.
C
C WRITE(NTOU,9021) WEIGHT
9021 FORMAT(1H0,15X,'WEIGHT = ',F10.3)
90 CONTINUE
IF (HFLIFE.GE.HALFLO) GO TO 100
WTVEC(K)=0.0
IF (.NOT. LIST) GO TO 30
WRITE(NTOU,9022)
9022 FORMAT('0 **** REJECTED ****')
WRITE(NTOU,9023) WTVEC(K)
9023 FORMAT('0 HALF-LIFE TOO LOW. NEW WEIGHT= ',G14.7)
GO TO 110
100 CONTINUE
IF (HFLIFE.LE.HALPHI) GO TO 110
WTVEC(K)=0.0
IF (.NOT. LIST) GO TO 30
WRITE(NTOU,9022)
WRITE(NTOU,9024) WTVEC(K)
9024 FORMAT('0 HALF-LIFE TOO HIGH. NEW WEIGHT= ',G14.7)
110 CONTINUE
IF (.NOT. LIST) GO TO 30
WRITE(NTOU,9025)
9025 FORMAT(1H /11X,50(1H-)/1H )

C END OF LOOP TO HANDLE ONE NUCLIDE, GO BACK TO HEAD TAPE
C
C GO TO 30
120 CONTINUE
C
C STOP READING TAPE AND PUBLISH STORED INFORMATION (IF NTOU.GT.0)
C
C IF (NTOU.LE.0) GO TO 140
WRITE(NTOU,9031)
WRITE(NTOU, 9026) MAXZ
9026 FORMAT(10 *** READING TERMINATED -- Z .GT. 114)
130 CONTINUE
WRITE(NTOU, 9027)
9027 FORMAT(1 SUMMARY OF STORED INFORMATION/1X)
WRITE(NTOU, 9028)
9028 FORMAT(5X,1HI,7X,1HZ,13X,1HA,8X,'HALF-LIFE',9X,'WEIGHT'/1X)
WRITE(NTOU, 9029) (I,ZVEC(I),AVEC(I),HAFVEC(I),WTVEC(I),
 1 I=1,K)
9029 FORMAT(1X,16,4G14.7)
WRITE(NTOU, 9030)
9030 FORMAT('1 ***** END INITIALIZATION OF DKEATA *****')
9031 FORMAT('1 ***** END OUTPUT CONTROLLED BY LOGICAL VARIABLE LIST')
C----------------------------------------------------------
C----------------------------------------------------------
C BEGINNING OF NON-INITIAL ENTRIES
C----------------------------------------------------------
C SEARCH THE STORED Z AND A VALUES FOR THE Z AND A
C PASSED IN THE CALLING ARGUMENTS. CHOOSE THE WEIGHT AND
C HALFLIFE CORRESPONDING TO THE NUCLIDE OF GREATEST WEIGHT.
C----------------------------------------------------------
C----------------------------------------------------------
C 140 CONTINUE
WEIGHT=0.0
HALFL=0.0
DO 150 I=1,K
  IF(ZVEC(I) .NE. A) GO TO 150
  IF(AVEC(I) .NE. A) GO TO 150
  IF(WEIGHT.GT.WTVEC(I)) GO TO 150
WEIGHT=WTVEC(I)
HALFL=HAFVEC(I)
150 CONTINUE
RETURN
END
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