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Implementation of a General Treatment of Photoelectric-Related Phenomena for Compounds or Mixtures in EGS4

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ABSTRACT

Various modifications of the EGS4 system were performed for a general treatment of photoelectric-related phenomena for compounds or mixtures.

PEGS4 was modified to produce piece-wise linear-fitted data of a branching ratio for each element in a compound or a mixture. `SUBROUTINE HATCH` was modified in order to read thus-created data.

Various atomic data related to the photoelectric effect, such as the K and L X-ray energies; their intensities; K and L Auger electron energies etc. are prepared as `BLOCK DATA ATOMIC`.

`SUBROUTINE PHOTO` was modified to determine an element which interacts with an incident photon and to sample a secondary particle, such as photoelectron, K or L X-ray or Auger electron, from the data prepared for all elements. An energy-dependent branching ratio of the L-subshell was also introduced.

Contents

1. Introduction

Standard EGS4[1] does not create or transport fluorescent photons. However, a substitute sampling routine, `SUBROUTINE PHOTO`, allows for the generation of K_α and K_β fluorescent photons for an element. It, along with the auxiliary `SUBROUTINE EDGSET` (extended by Keith Weaver of the University of California at San Francisco to 100 elements) are provided with the EGS4 distribution in the example code `UCEDGE.MOR`. This method was extended by Hirayama et al.[2] to treat K_{α_1}, K_{α_2}, K_{β_1} and K_{β_2} and to include an L-shell photoelectron and an L X-ray.

It is not easy to extend this treatment to compounds or mixtures, because a compound or a mixture is treated like an element in EGS4 to increase the computational speed. Del Guerra *et al.*[3] have developed a K-edge sampling scheme for compounds by using the material data of each element constituting the compound.

It is desired to develop a method which can treat fluorescence X-rays for compounds or mixtures generally, due to increased interest regarding low-energy photon transport.

It is necessary to create a branching ratio of the photoelectric effect of each element included in a compound or mixture in the general way. PEGS4 was modified to provide piece-wise linear-fitted data, like other data used in EGS4. This modification was checked by comparing the fitted branching ratio of Na and I for NaI at various energies with the basic data.

For a general treatment, it is reasonable to provide various atomic data related to the photoelectric effect, like K and L X-ray energies, their intensities, K and L Auger electron energies etc. as the `BLOCK DATA`, rather than to calculate from the basic data each time in the user code. `BLOCK DATA ATOM` was created from this point of view using various published data.

`SUBROUTINE HATCH` was modified to read piece-wise linear-fitted data created by PEGS4. A modification was also made so as to be able to use the material data created by the current PEGS4.

New routines were added to `SUBROUTINE PHOTO` to determine an element at which an incident photon interacts using data created by PEGS4. The following statements were modified so as to treat a thus-determined element.

The new method mentioned above was checked by comparing the sampled K X-rays yields from CsI with the probabilities obtained from the basic data at 40 keV.

For the case of L X-rays, the branching ratio of each sub-shell depends on the photon energy[4]. This is introduced by fitting from the data provided for limited materials.

2. Modifications of PEGS4 to Produce the Branching Ratio of Each Element in a Compound or a Mixture

An element which can interact with a photon at a photoelectric interaction must be determined in a general treatment for a compound or a mixture. PEGS4 was modified so as to produce the branching ratio of each element as a cumulative distribution function, which is calculated by

$$P_I(E) = \frac{\sum_{i=1}^{I} p_i \mu_{photo,i}(E)}{\sum_{i=1}^{\mathtt{NELM}} p_i \mu_{photo,i}(E)}, \tag{1}$$

where

$P_I(E)$ = the cumulative distribution function of the branching ratio for the I-th element at photon energy E,

p_i = proportion by number of the i-th element in a material,

$\mu_{photo,i}(E)$ = photoelectric interaction cross-section of i-th element at photon energy E, and

`NELM` = number of elements in the material.

```
"*********************************************************************"
"PWLF for branching ration of each element at photoelectric.          "
"                                              H.Hirayama(KEK) 29DEC1997"
"*********************************************************************"
IF(IXRAY.NE.0) [
"PWLF for branching ratio of each element at photoelectric"
OUTPUT;(' Do PWLF To Photoelectric data'/);
DELTAE=EXP(ALOG(UP/AP)/$MXGE);
"At first check data which are not 0"
"PWLF for all elements included by one PWLF1. 99/12/28 YN and HH"
"PWLF for all elements included by one PWLF1. 99/12/28 YN and HH"
EE=AP;
UPE=UP;
DO I=1,$MXGE [
EE=EE*DELTAE;
PHOTS=PHOTTE(EE);
IF(PHOTS.EQ.0.0) [UPE=EE/DELTAE; EXIT;]
]

"Modified 99/12/28  YN and HH"
CALL PWLF1(NGX,NALG,AP,UPE,EBINDA-0.0001,EPG,ZTHRG,ZEPG,NIPG,ALOG,EXP,
AXX,BXX,$MXGE,$MXEL,AFX,BFX,XRFUNS);
] "End of photoelectric branching ration PWLF"

"     THAT'S ALL FOLKS---PWLF DOES ALL THE WORK."
GOTO :OPTION:;


"Following SUBROUTINE added by H. Hirayama to create branching     "
"ration of photoelectric for each element"
"*********************************************************************"
"                      High Energy Accelerator Research Organization"
SUBROUTINE XRFUNS(E,V);
"                                VERSION 4.00  --  29 DEC 1997/1900"
"*********************************************************************"
"*****SUBROUTINE TO COMPUTE PHOTON FUNCTIONS TO BE FIT               "
"     IN A WAY THAT AVOIDS REPETITION.                              "
;COMIN/MIXDAT/;
REAL V(1);

"Modified to PWLF for all elements included by once call of XRFUNS"
"                                  99/12/28 YN and HH"
DO I=1,NE [V(I)=1.0;]
PHOT=PHOTTE(E);
IF(PHOT.EQ.0.0) [RETURN;]

DO I=1,NE-1 [
RNELM=I;
PHOTS=PHOTTS(E,RNELM);
V(I)=PHOTS/PHOT;
]

RETURN;
END; "END OF SUBROUTINE XRFUNS"

"Following FUNCTION is added by H. Hirayama to get branching ratio  "
"of element.                                    12/29/97             "
"*********************************************************************"
"                      High Energy Accelerator Research Organization"
FUNCTION PHOTFR(K,RNEL);
"                                VERSION 4.00  --  29 DEC 1997/1900"
"*********************************************************************"

"***'E' FOR EMPIRICAL OR EXPERIMENTAL PHOTOEFFECT CROSS-SECTION.   "
"   THIS FUNCTION GIVE THE PROPER SUMMATION TO NEL OF PHOTTZ'S.    "
REAL K;
COMIN/MIXDAT/;
NEL=RNEL;
PHOT=PHOTTE(K);
PHOTS=PHOTTS(K,RNEL);
PHOTFR=PHOTS/PHOT;
RETURN;
END;   "END OF FUNCTION PHOTFR"

"Following FUNCTION is added by H. Hirayama to get branching ratio "
"of element.                                   12/29/97              "
"*********************************************************************"
"                      High Energy Accelerator Research Organization"
FUNCTION PHOTTS(K,RNEL);
"                                VERSION 4.00  --  29 DEC 1997/1900"
```

```
"*****************************************************************"

"***'E' FOR EMPIRICAL OR EXPERIMENTAL PHOTOEFFECT CROSS-SECTION.   "
"   THIS FUNCTION GIVE THE PROPER SUMMATION TO NEL OF PHOTTZ'S.    "
REAL K;
COMIN/MIXDAT/;
NEL=RNEL;
PHOTTS=0.0;
DO I=1,NEL[PHOTTS=PHOTTS+PZ(I)*PHOTTZ(Z(I),K);]
RETURN;
END;   "END OF FUNCTION PHOTTS"
```

2.1. **Order of elements in PEGS4 input data**

The branching ratio of each element is piece-wise linear fitted in PEGS4, like other data. Therefore, if a compound or mixture includes an element of which the composition is very small, like Tl in CsI(Tl), this element must first be defined in the input data of PEGS4 in order to obtain correct data.

The following are the input data of PEGS4 for CsI(Tl) which includes 600ppm (in weight percent) of Tl.

```
COMP
 &INP NE=3, RHO=4.53, IRAYL=1, IXRAY=1, PZ=7.6E-4,1,1, IAPRIM=1 &END
CSI(TL)-IAPRIM-XRAY           CSI
TL CS I
```

2.2. **Check of fitted results**

The fitted branching ratios of I and Na for NaI are compared with theoretical data to check the new function of PEGS4. The results are given in Table 1.

Table 1. Comparison of the fitted and theoretical branching ratio of I and Na for NaI.

	Na		I	
Energy(MeV)	Fitted	Theoretical	Fitted	Theoretical
0.005	2.4992E-2	2.4934E-2	0.97496	0.97507
0.01	1.6754E-2	1.6753E-2	0.98325	0.98325
0.05	1.4286E-3	1.4282E-3	0.99857	0.99857
0.1	1.0312E-3	1.0308E-3	0.99897	0.99897
0.2	7.9958E-4	7.9944E-4	0.99920	0.99920
0.3	7.1008E-4	7.0979E-4	0.99929	0.99929
0.4	6.6382E-4	6.6358E-4	0.99934	0.99934
0.5	6.3670E-4	6.3650E-4	0.99936	0.99936
1.0	0.0	0.0	1.0	1.0

3. BLOCK DATA ATOM

`BLOCK DATA ATOM` includes various atomic data, like the K-, L-binding energies, X-ray energies, their relative intensities etc., of all elements necessary for photoelectric-related phenomena. These data are taken from various published data, and are summarized in Table 1.

Table 1 Atomic data included in `BLICK DATA ATOM`.

Kind of data	Explanation
K edge energy	Table 2 of Table of Isotopes, Eighth Edition[5]
Probability of X-ray emission at K- and L-Shell absorption	Table 3 of Table of Isotopes, Eighth Edition
K X-ray energy	Table 7 Table of Isotopes, Eighth Edition
K X-ray emission probability	Table 7 Table of Isotopes, Eighth Edition Adjusted to experimental data by Salem et al.[6]
K-shell contribution to photoelectric cross section	Table 8 from Storm and Israel [7]
L1, L2, and L3 edge energy	Table 2 of Table of Isotopes, Eighth Edition
L X-ray energy	Table 7b of Table of Isotopes, Eighth Edition
Relative L-shell contribution to photoelectric cross section at EDGE	Table 8 from Storm and Israel
Probability of Coster-Kronig L1- and L2-Shell absorption	Table 3 of Table of Isotopes, Eighth Edition
L X-ray emission probability	Theoretical data by J.M. Scofield[8] Adjusted to experimental data by Salem et al.
Average M edge energy	Calculated subshell binding energy in Table 2 of Table of Isotopes, Eighth Edition
Auger electron energy	Calculated neglecting correction term by using Atomic-Electron Binding Energy in Table 2 of Table of Isotopes, Eighth Edition
K-Auger Intensity	Z=12-17 Table 1 of Assad[9] Z>17 Table 8 of Table of Isotopes, Eighth Edition
L-Auger Intensity	Table 2 from McGuire[10]

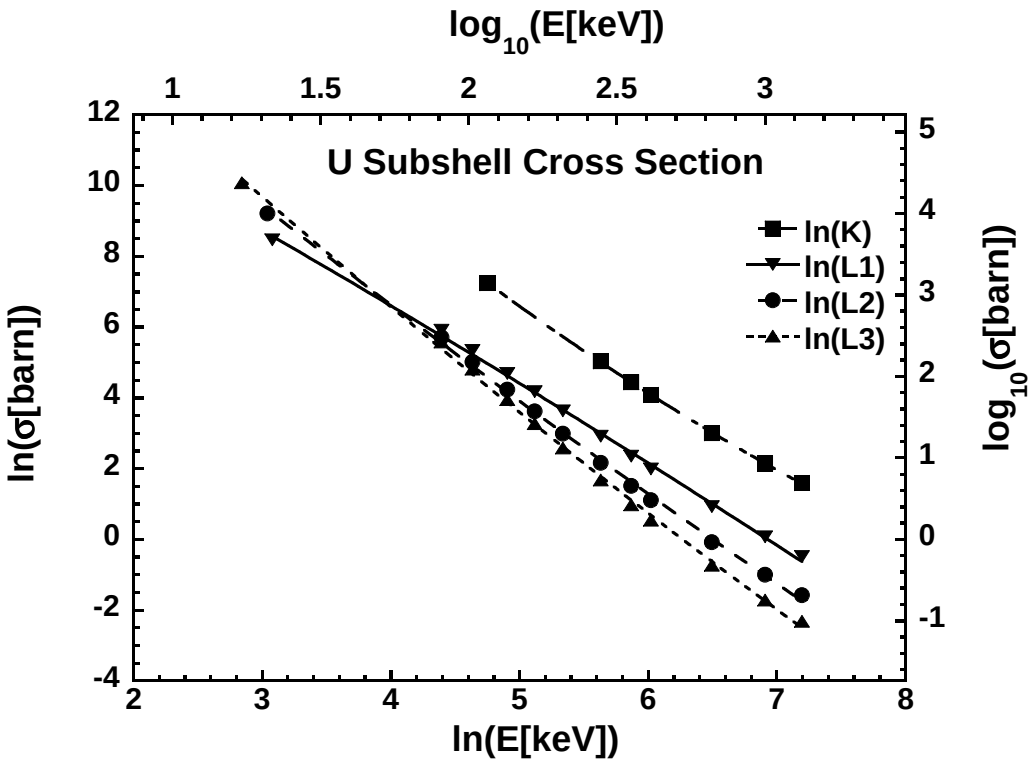

Figure 1: Subshell photoelectric cross section of U.

3.1. Energy Dependence of the Ratio of the L-Sub-Shell Photoelectric Effect Cross Sections

L-sub-shell cross sections of Ag, Pb and U were taken from two data;

- Photoelectric cross sections at energies above/blow the L1-, L2- and L3-edges.
- Matase and Jonson[4] (1965).

These L-sub-shell cross sections were fitted to a quadratic function in a log-log plot:

$$ln(\sigma) = M_0 + M_1 \ln(k_0) + M_2 \ln(k_0)^2, \tag{2}$$

where k_0 denotes photon energy. As shown Figs. 1-3, a quadratic function fitted to the data very well.

M_1 and M_2 for other elements were obtained by a linear interpolation along Z. The interpolated values of M_1 and M_2 are shown in Figs. 4 and 5, respectively.

The photoelectric-effect cross sections at energies above/blow L1-, L2- and L3-edges for all elements were taken from `PHOTX`[11]. These data are shown in Fig. 6. The L1-sub-shell cross sections at 1 keV (M_0) were calculated as

$$\ln(\sigma_1) = \ln(\sigma_{L1}) - M_1 \ln(E_{L1}(keV)) - M_2(\ln(E_{L1}(keV))^2. \tag{3}$$

The L2-subshell and the L3-subshell cross sections were calculated in the same way. The thus obtained M_0 values are shown in Fig. 7.

The M_0, M_1, M_2 values of each subshell for all elements are also included in `BLOCK DATA ATOM`.

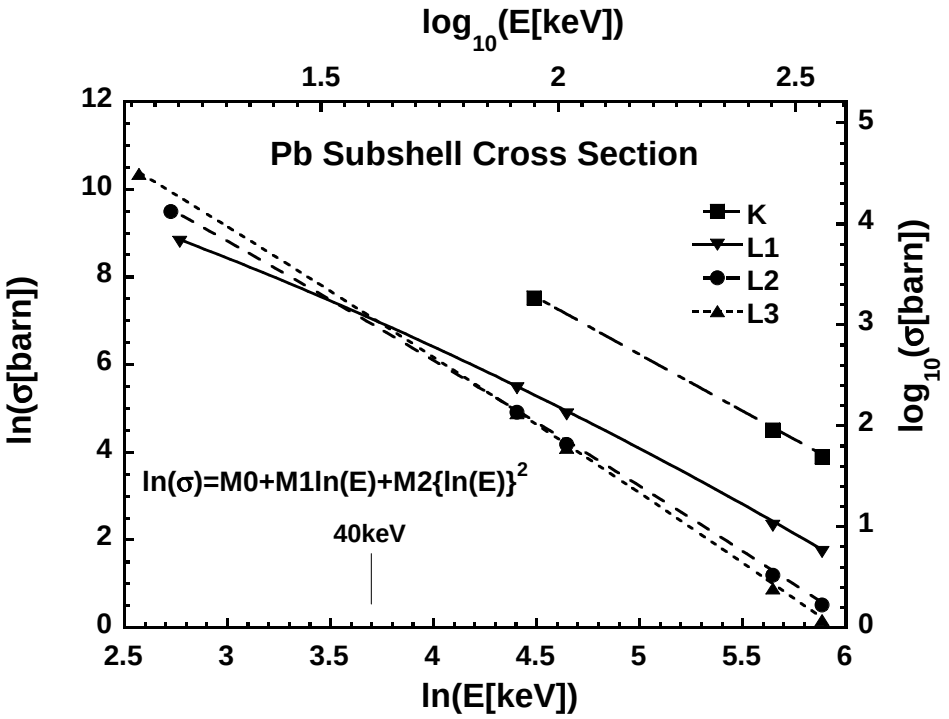

Figure 2: Subshell photoelectric cross section of Pb.

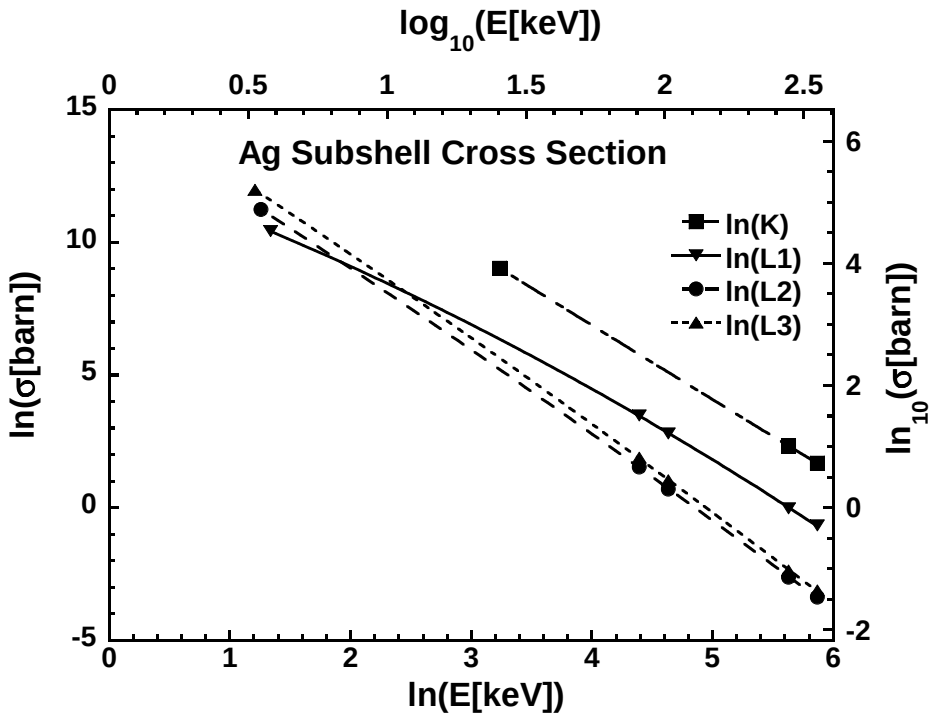

Figure 3: Subshell photoelectric cross section of Ag.

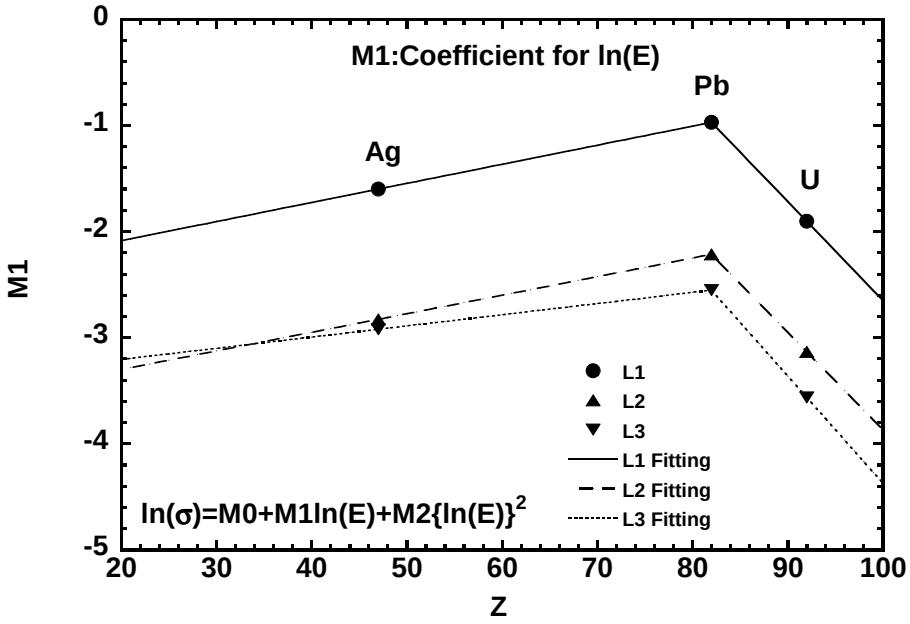

Figure 4: Interpolated values of M_1.

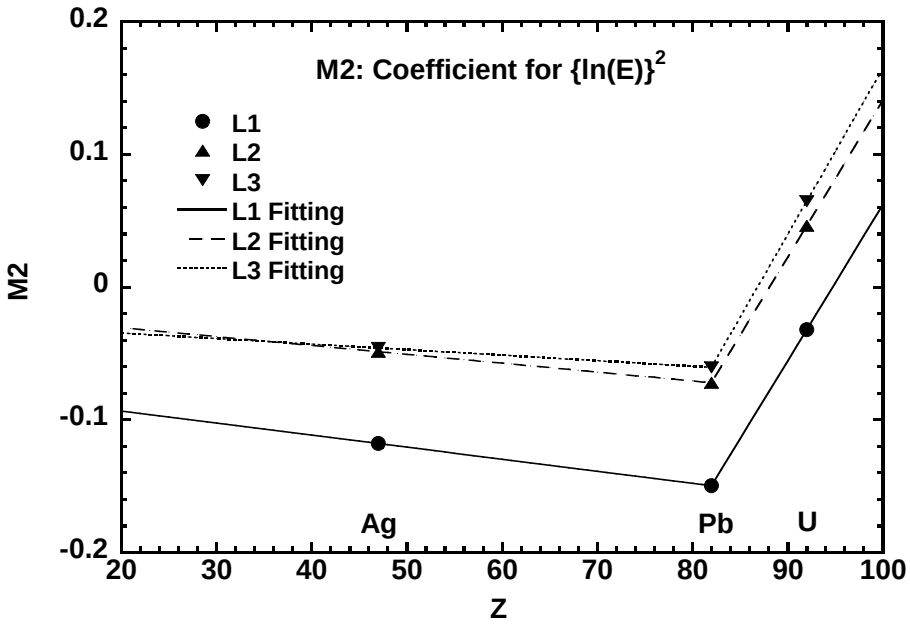

Figure 5: Interpolated values of M_2.

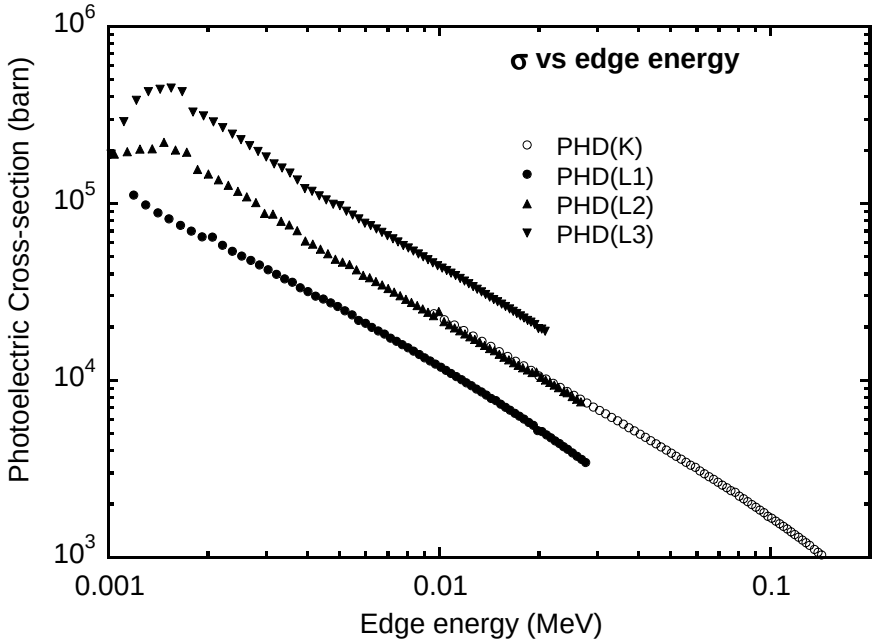

Figure 6: Photoelectric cross sections at the edge energies.

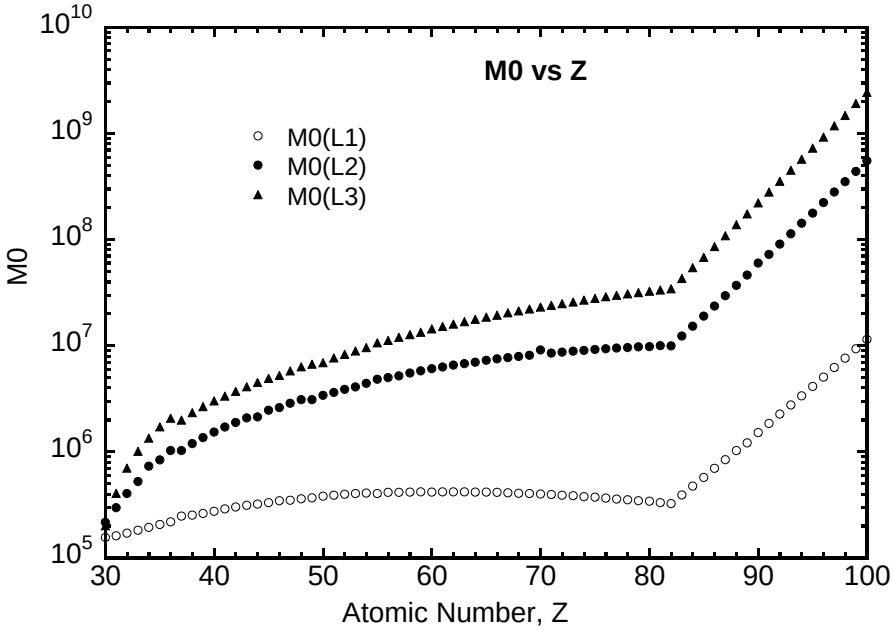

Figure 7: M_0 values for the L1-, L2- and L3-subshell cross sections.

4. Over-ride Macros (see kek4macn.mor)

The following over-ride macros are used in EGS4.
Various names of variables are changed to reflect their meanings.

```
"Over-ride to treat K-edge correctly.    H. Hirayama 12/29/97"
PARAMETER $MXGE=1000;      "GAMMA MAPPED ENERGY INTERVALS"

REPLACE {$COMIN-HATCH;} WITH {;COMIN/DEBUG,BOUNDS,BREMPR,
  EDGE,ELECIN,MEDIA,MISC,PHOTIN,STACK,THRESH,UPHIIN,
  UPHIOT,USEFUL,USER,RANDOM/;}
" PHOTIN added by H. Hirayama 12/29/97          "

"THIS EXTENSION IS NEEDED FOR THE PHOTOELECTRON ANGLE SELECTION"
REPLACE {$COMIN-PHOTO;} WITH {;COMIN/BOUNDS,DEBUG,EDGE,EPCONT,MEDIA,
  MISC,PHOTIN,STACK,UPHIOT,USEFUL,USER,RANDOM/;}
" ====     Added by H. Hirayama 12/29/97       "

PARAMETER $MXEPERMED=20;   "Maximum number of element in medium"
" Introduced to treat photoelectric phenomena of a compound or "
" mixture corresponding to $MXEL in pegs4. H. Hirayama 12/29/97"




"-------------------------------------------------------------------"
"*** PHOTIN--PHOTON TRANSPORT DATA                                  "
"-------------------------------------------------------------------"
REPLACE {;COMIN/PHOTIN/;} WITH
   {;COMMON/PHOTIN/
     EBINDA(100),
     $LGN(GE($MXMED)/0,1/),
     $LGN(GMFP,GBR1,GBR2($MXGE,$MXMED)/0,1/),
     $LGN(RCO($MXMED)/0,1/),
     $LGN(RSCT($MXRAYFF,$MXMED)/0,1/),
     $LGN(COHE($MXGE,$MXMED)/0,1/),
     MPGEM($MXSGE,$MXMED),
     NGR($MXMED);}
"    EBINDA(100) is modified by H. Hirayama.  12/29/97              "
```

```
REPLACE {;COMIN/EDGE/;} WITH
{;COMMON/EDGE/NAUGER,IEDGFL($MXREG),IAUGER($MXREG),$LGN(EKALPH,EKBETA,
BKPHOT,OMEGAK,EMBIND,OMEGAL1,OMEGAL2,OMEGAL3,F12,F13,F23,PHOTK,RSCL1,
RSCL2,RSCL3(100)),EEDGE(4,100),EKX(10,100),DFKX(9,100),ELX1(8,100),
ELX2(5,100),ELX3(7,100),DFLX1(7,100),DFLX2(4,100),DFLX3(6,100),
PM0(3,100),PM1(3,100),PM2(3,100),EKAUG(14,100),DFKAUG(13,100),
EL1AUG(6,100),EL2AUG(6,100),EL3AUG(6,100),DFL1AUG(5,100),
DFL2AUG(5,100),DFL3AUG(5,100),LEDGB(80,$MXMED),IZE($MXEPERMED,$MXMED),
NGX($MXMED),UPE($MXMED),$LGN(PHO($MXEPERMED)/0,1/),
$LGN(PHOTBR($MXGE,$MXEPERMED,$MXMED)/0,1/),EDGB(80,$MXMED),
EXRAY(10),EAUGER(10),NEPM($MXEPERMED),NEDGB($MXMED),NXRAY,NPHOTO,
NAL1,NAL2,NBE1,NBE2,NBLK,NNOK,IZ,IEXTP,EBIND;}
"NOTE :ABOVE MACROS OVER-RIDED TO TREAT L-X  FLUORESCENT PHOTON "
"BY H.Hirayama                                          6/21/96"
"Modified to include Auger electron by H. Hirayama      10/7/96"
"Modified to treat photoelectric phenomena for a compound or    "
"mixture.       H. Hirayama   12/29/97                          "
"Modified to make SUBROUTINE version.   H. Hirayama 8/17/98     "
"Add EMBIND (average M-shell binding energy in keV),            "
"    EKAUG (K-Auger electron energy, in keV),                  "
"    DFKAUG (K-Auger PDF) are added to treat K-Auger.          "
"                           H. Hirayama    1/23/99             "
"Add PM0, PM1 and  PM2 to calculate energy dependent L subshell "
"cross section.  ln(Sigma)=PM0+PM1*ln(E in keV)+PM2*ln(E)*ln(E) "
"Delete BSHL1 and BSHL2.                  3/31/99 Y.N. & H.H.    "
"Add BKR1(1), BKR2(1) to avoid error in original PHOT0 11/20/99 YN"
"Modified corresponding to modification of PEGS4. 99/12/28 YN HH"
```

5. Modification of SUBROUTINE HATCH (see kek4n.mor)

SUBROUTINE HATCH was modified as follows so as to include data related to the branching ratio of each element and to keep the possibility using the material data created by the current PEGS4.

1. EFECZ=EFECZ+PZ(IM,IE)*ZELEM(IM,IE); was added at the end of the DO-loop of :GASP-NOT-THERE: and IZE(1,IM)=EFECZ at the outside of this DO-loop to use the material data produced by the current PEGS4.

2. IXRAY was added like $ECHO READ(KMPI,:INT:) $LGN(MSGE, MGE,MSEKE,MEKE, MLEKE,MCMFP,MRANGE(IM)),IRAYL,IXRAY;.

3. Change EBINDA(IM) to TEBINDA(IM) in the part of PHOTIN $ECHO READ.

```
"   PHOTIN"
"$ECHO READ(KMPI,:FLT:)EBINDA(IM),$LGN(GE(IM)/0,1/);"
$ECHO READ(KMPI,:FLT:)TEBINDA,$LGN(GE(IM)/0,1/);
"    EBINDA(IM) modified to TEBINDA.  H. Hirayama 12/29/97   "
```

4. Following statements were added after the RAYLEIGH related data read.

```
"Following statements are added to read photoelectric related"
"data by H. Hirayama.      12/29/97                          "
"Modified related to the modification of PEGS4.  YN and HH"
IF (IXRAY.EQ.1) [
$ECHO READ(KMPI,:INT:) NEPM(IM);
NER=NEPM(IM);
NER1=NER-1;
$ECHO READ(KMPI,:INT:) (IZE(I,IM),I=1,NER);
$ECHO READ(KMPI,:INT:) NGX(IM);
READ(KMPI,:FLT:) PHO0(IM),PHO1(IM);
WRITE(KMPO,:FLT:) PHO0(IM),PHO1(IM);
READ(KMPI,:FLT:)
((PHOTBR0(I,IFUN,IM),PHOTBR1(I,IFUN,IM),IFUN=1,NER1),I=1,NGX(IM));
WRITE(KMPO,:FLT:)
((PHOTBR0(I,IFUN,IM),PHOTBR1(I,IFUN,IM),IFUN=1,NER1),I=1,NGX(IM));
]
```

Full listings of SUBROUTINE HATCH (LSCAT version[12]) are given in Appendix 1.

6. Modification of SUBROUTINE PHOTO (see kek4n.mor)

The SUBROUTINE PHOTO was modified to decide an element at which a photon interacted. Following statements were added at the top of the SUBROUTINE.

```
IRL=IR(NP);
PEIG=E(NP);
EIG=PEIG; "ENERGY OF INCIDENT GAMMA"
PHOL=ALOG(EIG);"GLE IS GAMMA LOG ENERGY"

MEDIUM=MED(IRL);
IF(NEPM(MEDIUM).EQ.1) [IZ=IZE(1,MEDIUM);GO TO :K-EDGE:;]
ELSE [
$RANDOMSET PBRAT;
DO I=1,NEPM(MEDIUM)-1 [
$SETINTERVAL PHOL,PHO; "SET PWLF INTERVAL"
PBRAN=PHOTBR1(LPHOL+IEXTP,I,MEDIUM)*PHOL+PHOTBR0(LPHOL+IEXTP,I,MEDIUM);
IF(PBRAT.LE.PBRAN) [IZ=IZE(I,MEDIUM);GO TO :K-EDGE:;]
]]
IZ=IZE(NEPM(MEDIUM),MEDIUM);

"After this 'MEDIUM' is changed to 'IZ' to treat K , L X-rays"
"for each element.   H. Hirayama  12/29/97.                  "
:PNEWENERGY:
```

The parts that determine the type of emitted particle (fluorescence photon or Auger electron) at the K- or L-absorption and the energy of the emitted photon or electron are written in the form of SUBROUTINE.

The full listings of SUBROUTINE PHOTO and other related SUBROUTINEs and the flow charts of these are given as Appendix 2 and 3, respectively.

7. Check of a General Treatment of Photoelectric Reaction for Compound

K X-rays for 40 keV photons from CsI were calculated to check this new general treatment for photoelectric-related phenomena. For this energy, 53.04% of the photoelectric reaction occurs with Cs. Sampled each K X-rays both from Cs and I for 5,000,000 incident photons were compared with the theoretical ones (Table 2).

From this table, it is clear that this new treatment can correctly produce K X-rays of CsI.

Table 2. Comparison of K X-rays from CsI for 40 keV photons.

	Cs			I		
	Energy(keV)	Sampled	Theory	Energy(keV)	Sampled	Theory
K_{α_1}	31.0	0.20726	0.20730	28.6	0.18288	0.18301
K_{α_2}	30.6	0.11251	0.11253	28.3	0.09848	0.09860
K_{β_1}	35.0	0.06185	0.06119	32.3	0.05327	0.05328
K_{β_2}	35.8	0.01382	0.01382	33.0	0.01105	0.01107

8. How to get Files Related to the General Treatment of Photoelectric-Related Phenomena

8.1. How to get files

Get following files using anonymous ftp from ftp.kek.jp (130.87.34.28);

`/kek/kek_egs4/kek_improve/kek_improve.tar.Z`	for unix.
`/kek/kek_egs4/kek_improve/kek_improve.exe`	for PC.
`/kek/kek_egs4/kek_improve/scp31.tar.Z`	Shell-wise Compton profile for unix.
`/kek/kek_egs4/kek_improve/scp31.exe`	Shell-wise Compton profile for PC.

On unix machine, Uncompress and extract files by

```
uncompress kek_improve.tar.Z
tar xvf - < kek_improve.tar
```

On PC, extract files by

```
kek_improve
```

This is a self-extraction file.
Send e-mail when you take these files, writing

- Your name, institute and e-mail address.
- A brief paragraph on the purpose you are using LSCAT.

e-mail: hideo.hirayama@kek.jp or yoshihito.namito@kek.jp
Fax: 81-298-64-1993.

8.2. Contents of the files

- `bcomp.dat`

  Bound total Compton cross section (σ_{bC}) for all elements ($Z = 1 \sim 100$). `pegs4nb.mor` automatically picks up this as an input file (unit= 11). Made using DLC-99 [13].

- `cic3.dat`

  An example of the output of `pegs4nb.mor` and an example input for `ucbcomp4.mor`.

- `cic3.inp`

  An example of an input for `pegs4nb.mor` (unit=5). See the description on `pegs4nb.mor` for the meaning of additional flags in namelist INP.

- `csitl.dat`

  Input for `ucphotol.mor`.

- `egs4blkn.mor`

  Added initialization for flags.

- `egs4n.mor`

  Subroutine edgset and photo were removed.

- `ics_x.dat`

  Coherent scattering cross section with an interference effect. x is the first letter of materials (Water, PMMA, Fat, Muscle, Kidney, Liver and Blood).

- `iff_x.dat`

  Form factor with an interference effect, which are named in the same fashion as the coherent scattering cross section files.

- `incoh.dat`

  Incoherent scattering function ($S(x, Z)$) for all elements ($Z = 1 \sim 100$). `pegs4nb.mor` automatically pick up this

  as an input file (unit= 12). Made using DLC-99 [13].

- `kek4macn.mor`

  Includes macros for lscat. `negs4run` automatically pick it up.

- `kek4n.mor`
  Includes subroutines for lscat. `negs4run` automatically pick it up.
- `makescpr.mor`
  Short program to prepare Compton profile for a compound and mixture.
- `negs4run` (unix) or `negs4run.bat` (PC)
  C-shell script (unix) or batch file (PC) to run EGS4 user's code. `kek4macn.mor` and `kek4n.mor` are automatically added to the user's code.
- `pegs4nbcompile` (unix) or `pegs4nbcom.bat` (PC)
  C-shell script (unix) or batch file (PC) to compile `pegs4nb.mor` and make `pegs4nb.exe`.
- `pegs4nbrun` (unix) or `pegs4nbrun.bat` (PC)
  C shell script (unix) or batch file (PC) to run `pegs4nb.exe`.
- `pegs4nb.mor`
  `pegs4nb.mor` is made from `pegs4.mor` (NRCC-unix version). Bound Compton cross section(σ_{bC}), incoherent scattering function ($S(x, Z)/Z$), Doppler broadening and EII were added.
- `sn.dat`
  Material data for `ucbrem.mor`. EII/Moller ratio using Casnati's formula was contained.
- `ucbcomp4.mor`
  An EGS4 user code used to calculate the spectra of a scattered
  photon with photon scattering part of LSCAT.
- `ucbrem.mor`
  An example user's code to calculate with EII.
- `ucphotol.mor`
  EGS4 user code to calculate L-X rays from first element to check L-X ray emission.

9. How to Implement in Your System

9.1. PEGS4 and material data

Compile pegs4nb.mor with pegs4nbcompile (pegs4nb_com.bat). Create material data with `IXRAY=1` option by running pegs4nb with pegs4nbrun (pegs4nbrun.bat). In the case of element, it is not necessary to re-create the material data.

9.2. EGS4 related

The procedure to run EGS4 with this implementation depends on the current system.

1. Running EGS4 in KEK-way
   By using negs4run (negs4run.bat and negs4runp.bat), following things are automatically performed.
   - Replace kek4mac.mortran (kek4mac.mor) with kek4macn.mor.
   - Replace kek4.mortran (kek4.mor) with kek4n.mor.
   - Replace egs4block.mortran (egs4blok.mor) with egs4blkn.mor.
   - Replace egs4.mortran (egs4.mor) with egs4n.mor.
   - Delete `SUBROUTINE`s related `PHOTO` those are not included in the original EGS4 and ones related to `LSCAT`.
2. Running EGS4 in another way
   - Put kek4macn.mor after egs4mac.mortran (egs4mac.mor)
   - Put kek4n.mor after your user code.

- Replace egs4block.mortran (egs4blok.mor) with egs4blkn.mor.
- Replace egs4.mortran (egs4.mor) with egs4n.mor.
- Delete `SUBROUTINE`s related `PHOTO` those are not included in the original EGS4 and ones related to `LSCAT`.

9.3. User code

- Delete macros and `SUBROUTINES`s copied from the previous version of `LSCAT` and `SUBROUTINE`s related to `PHOTO` from the user code.
- Change the value of IEDGFL flag to 1 like IEDGFL(1)=1;.
- Delete a statement including `CALL EDGSET(NREG)` like

```
DO I=1,NREG [IF(IEDGFL(I).NE.0) [CALL EDGSET(NREG); EXIT;]]
```

- If it is necessary to print out the energies of K- and L-X-rays, insert the following statements after `HATCH CALL` (see ucphoto.mor for an example).

```
OUTPUT;(/' INFORMATION OF MEDIUM AND CUT-OFFFOR EACH REGION'//);
DO I=1,NREG [
IF(MED(I).EQ.0) [OUTPUT I,ECUT(I),PCUT(I);
(' MEDIUM(',I3,')=VACUUM',18X,'ECUT=',G10.5,' MEV, PCUT=',G10.5,' MEV');
]
ELSE [OUTPUT I,(MEDIA(II,MED(I)),II=1,24),ECUT(I),PCUT(I);
(' MEDIUM(',I3,')=',24A1,'ECUT=',G10.5,' MEV, PCUT=',G10.5,' MEV');
"Statements to print out energy information of K- and L-X-rays"
IF(IEDGFL(I).NE.0) ["Output X-ray energy"
NER=NEPM(MED(I));
DO IIZ=1,NER [IZN=IZE(IIZ,MED(I));"Atomic number of this element"
OUTPUT IZN;(' X-ray information for Z=',I3);
OUTPUT (EKX(II,IZN),II=1,10);
('     K-X-ray energy in keV'/
4G15.5/4G15.5/2G15.5);
OUTPUT (EKAUG(II,IZN),II=1,14);
('     K-Auger energy in keV'/
3(4G15.5/),2G15.5);
OUTPUT (ELX1(II,IZN),II=1,8);
(3X,' L-1 X-ray in keV'/4G15.5/4G15.5);
OUTPUT (EL1AUG(II,IZN),II=1,6);
(3X,' L-1 Auger in keV'/4G15.5/2G15.5);
OUTPUT (ELX2(II,IZN),II=1,5);
(3X,' L-2 X-ray in keV'/5G15.5);
OUTPUT (EL2AUG(II,IZN),II=1,6);
(3X,' L-2 Auger in keV'/4G15.5/2G15.5);
OUTPUT (ELX3(II,IZN),II=1,7);
(3X,' L-3 X-ray in keV'/4G15.5/3G15.5);
OUTPUT (EL3AUG(II,IZN),II=1,6);
(3X,' L-3 Auger in keV'/4G15.5/2G15.5);
] "end of IIZ-loop"
] "end of IEDGFL.EQ.1"
"End of print out related to X-ray"
]
]
```

References

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[13] Hugo

Appendix 1 Full listings of SUBROUTINE HATCH (included in kekphoto_ls.tar.Z or kek_improve.exe).

```
"*****************************************************************"
"                                STANFORD LINEAR ACCELERATOR CENTER"
SUBROUTINE HATCH;
"                                VERSION 4.00  --  26 JAN 1986/1900"
"*****************************************************************"
"================================================================="
"MODIFIED BY Y.NAMITO(KEK)                          20 OCT 1994/1830"
"                                                                 "
"  - READ S(X,Z)/Z IN.                                            "
"  - INVOLVES NRCC EXPANSION IN EGS4/UNIX.                        "
"  - READ J(Q) IN.                                                "
"  - READ Ji(Q) IN. Ji is Compton Profile for each shell.         "
"================================================================="
"   SETUP WHICH THE USER IS EXPECTED TO DO BEFORE CALLING HATCH IS:"
"     1. SET 'NMED' TO THE NUMBER OF MEDIA TO BE USED."
"     2. SET THE ARRAY 'MEDIA', WHICH CONTAINS THE NAMES OF THE"
"        MEDIA THAT ARE DESIRED.  THE CHARACTER FORMAT IS A1, SO"
"        THAT MEDIA(IB,IM) CONTAINS THE IB'TH BYTE OF THE NAME OF"
"        THE IM'TH MEDIUM IN A1 FORMAT."
"     3. SET 'DUNIT', THE DISTANCE UNIT TO BE USED."
"        DUNIT.GT.0 MEANS VALUE OF DUNIT IS LENGTH OF DISTANCE UNIT"
"        CENTIMETERS.  DUNIT.LT.0 MEANS USE THE RADIATION LENGTH OF"
"        THE ABS(DUNIT)'TH MEDIUM FOR THE DISTANCE UNIT."
"     4. FILL THE ARRAY 'MED' WITH THE MEDIUM INDICES FOR THE"
"        REGIONS."
"     5. FILL ARRAYS 'ECUT' AND 'PCUT' WITH THE ELECTRON AND PHOTON"
"        CUT-OFF ENERGIES FOR EACH REGION RESPECTIVELY.  SETUP WILL"
"        RAISE THESE IF NECESSARY TO MAKE THEM AT LEAST AS LARGE AS"
"        THE REGION'S MEDIUM'S AE AND AP RESPECTIVELY."
"     6. FILL 'MED' ARRAY.  MED(IR) IS THE MEDIUM INDEX FOR REGION"
"        IR.  A ZERO MEDIUM INDEX MEANS THE REGION IS IN A VACUUM."
"     7. FILL THE ARRAY 'IRAYLR' WITH 1 FOR EACH REGION IN WHICH"
"        RAYLEIGH (COHERENT) SCATTERING IS TO BE INCLUDED."
"     8. FILL THE ARRAY 'INCOHR' WITH 1 FOR EACH REGION IN WHICH"
"        INCOHERENT SCATTERING IS TO BE INCLUDED."
"     9. NRCC EXPANSION ABOUT BREMS INCLUDED."
"    10. FILL THE ARRAY 'IPROFR' WITH 1 FOR EACH REGION IN WHICH"
"        COMPTON PROFILE IS TO BE INCLUDED."
"*****************************************************************"
$TYPE MBUF(72),MDLABL(8);
DIMENSION ZEROS(3),LOK($MXMED);
"NOTE: ABOVE IS ZEROS OF SINE, 0,PI,TWOPI"
DIMENSION NGS($MXMED),NGC($MXMED),NEII($MXMED);
;$COMIN-HATCH;    "DEFAULT REPLACEMENT PRODUCES THE FOLLOWING:     "
"COMIN/DEBUG,BOUNDS,BREMPR,ELECIN,MEDIA,MISC,PHOTIN,STACK,        "
"  THRESH,UPHIIN,UPHIOT,USEFUL,USER,RANDOM/;                      "
COMIN/BCOMP,EIICOM/;
DATA MDLABL/$S' MEDIUM='/,LMDL/8/,LMDN/24/,DUNIT0/1./;
DATA I1ST/1/,NSINSS/37/,MXSINC/$MXSINC/,ISTEST/0/,NRNA/1000/;

"   FORMAT STATEMENTS USED MULTIPLE TIMES IN SETUP"
:INT:FORMAT(1X,14I5);
:FLT:FORMAT(1X,1PE14.5,4E14.5);
:BYTE:FORMAT(72A1);

IF (I1ST.NE.0)[ I1ST=0;"RESET FIRST TIME FLAG"
"   DO FIRST TIME INITIALIZATION"

$HATCH-USER-INPUT-INIT;
" DEFAULT FOR $HATCH-USER-INPUT-INIT; IS ; (NULL)"

"   SET UP ENERGY PRECISION VARIABLES"
PRM=RM; "PRECISE REST MASS"
PRMT2=2.D0*PRM;  "TWICE THE PRECISION REST MASS"
PZERO=0.0D0; "PRECISE ZERO"

"   NOW CONSTRUCT PIECEWISE LINEAR FIT TO SINE FUNCTION OVER THE"
"   INTERVAL (0,5*PI/2).  DIVIDE THIS INTERVAL INTO MXSINC SUB-"
"   INTERVALS.  EACH OF THESE SUBINTERVALS IS THEN SUBDIVIDED INTO"
"   NSINSS SUB-SUB-INTERVALS.  THE ANGLES AT THE BOUNDARIES OF"
"   THESE SUB-SUB-INTERVALS AND THEIR SINES ARE USED TO COMPUTE"
"   LEAST SQUARES COEFFICIENTS FOR THE SUBINTERVAL.  AN EXTRA"
"   SUBINTERVAL ON EACH SIDE OF THE INTERVAL (0,5*PI/2) IS INCLUDED"
"   FOR GOOD MEASURE."
NISUB=MXSINC-2;FNSSS=NSINSS;
WID=PI5D2/FLOAT(NISUB);
WSS=WID/(FNSSS-1.0);
ZEROS(1)=0.;ZEROS(2)=PI; ZEROS(3)=TWOPI;
```

```
DO ISUB=1,MXSINC ["LOOP OVER SUBINTERVALS"
SX=0.;SY=0.;SXX=0.;SXY=0.;"ZERO SUMS"

XS0=WID*FLOAT(ISUB-2);XS1=XS0+WID;"LOWER & UPPER LIMITS"
"   NOW CHECK TO SEE IF ANY ZEROS ARE IN THE INTERVAL"
IZ=0; DO IZZ=1,3 [
IF ((XS0.LE.ZEROS(IZZ)).AND.(ZEROS(IZZ).LE.XS1))[IZ=IZZ;EXIT;]
] "END OF LOOP OVER ZEROS"
IF (IZ.EQ.0)[XSI=XS0;]ELSE[XSI=ZEROS(IZ);]
DO ISS=1,NSINSS ["LOOP OVER SUB-SUBINTERVALS"
XS=WID*FLOAT(ISUB-2)+WSS*FLOAT(ISS-1)-XSI; "ANGLE VALUE"
YS=SIN(XS+XSI); "SINE OF ANGLE"
SX=SX+XS; "ACCUMULATE SUMS"
SY=SY+YS;
SXX=SXX+XS*XS;
SXY=SXY+XS*YS;
] "END SUB-SUBINTERVAL LOOP"

"   NOW COMPUTE LEAST SQUARES COEFFICIENTS"
IF (IZ.NE.0)["FORCE FIT THROUGH SINES' ZEROS,"
"             FOR SMALL REL.ERR.&GOOD"
"   VALUES OF SINTHE/THETA NEAR ZERO"
SIN1(ISUB)=SXY/SXX;
SIN0(ISUB)=-SIN1(ISUB)*XSI;]
ELSE["DO FULL LEAST SQUARES"
DEL=FNSSS*SXX-SX*SX;
SIN1(ISUB)=(FNSSS*SXY-SY*SX)/DEL;
SIN0(ISUB)=(SY*SXX-SX*SXY)/DEL - SIN1(ISUB)*XSI ; ]
] "END SUB-INTERVAL LOOP"

SINC0=2.0 ;"SET COEFFICIENTS WHICH DETERMINE INTERVAL"
SINC1=1.0/WID;

"   NOW TEST FIT, IF REQUESTED"
IF (ISTEST.NE.0)[
"   FIRST TEST AT POINTS PREVIOUSLY COMPUTED, EXCLUDING"
"   END SUBINTERVALS"
ADEV=0.;RDEV=0.;S2C2MN=10.;S2C2MX=0.;
DO ISUB=1,NISUB [ DO ISS=1,NSINSS [
THETA=WID*FLOAT(ISUB-1)+WSS*FLOAT(ISS-1);
CTHET=PI5D2-THETA;
$SET INTERVAL THETA,SINC;$SET INTERVAL CTHET,SINC;
$EVALUATE SINTHE USING SIN(THETA);
$EVALUATE COSTHE USING SIN(CTHET);
SINT=SIN(THETA); COST=COS(THETA);
ASD=ABS(SINTHE-SINT); ACD=ABS(COSTHE-COST);
ADEV=AMAX1(ADEV,ASD,ACD);
IF (SINT.NE.0.0)RDEV=AMAX1(RDEV,ASD/ABS(SINT));
IF (COST.NE.0.0)RDEV=AMAX1(RDEV,ACD/ABS(COST));
S2C2=SINTHE**2+COSTHE**2;
S2C2MN=AMIN1(S2C2MN,S2C2);
S2C2MX=AMAX1(S2C2MX,S2C2);
IF (ISUB.LT.11)[
OUTPUT THETA,SINTHE,SINT,COSTHE,COST;(1PE20.7,4E20.7);]
] ] "END OF FIXED INTERVAL TEST-OUTPUT RESULTS"
OUTPUT MXSINC,NSINSS;(' SINE TESTS,MXSINC,NSINSS=',2I5);
OUTPUT ADEV,RDEV,S2C2MN,S2C2MX;
(' ADEV,RDEV,S2C2(MN,MX) =',1PE16.8,3E16.8);
"   NOW DO RANDOM TEST"
ADEV=0.;RDEV=0.;S2C2MN=10.;S2C2MX=0.;
DO IRN=1,NRNA[ $RANDOMSET THETA;THETA=THETA*PI5D2;
CTHET=PI5D2-THETA;
$SET INTERVAL THETA,SINC;$SET INTERVAL CTHET,SINC;
$EVALUATE SINTHE USING SIN(THETA);
$EVALUATE COSTHE USING SIN(CTHET);
SINT=SIN(THETA); COST=COS(THETA);
ASD=ABS(SINTHE-SINT); ACD=ABS(COSTHE-COST);
ADEV=AMAX1(ADEV,ASD,ACD);
IF (SINT.NE.0.0)RDEV=AMAX1(RDEV,ASD/ABS(SINT));
IF (COST.NE.0.0)RDEV=AMAX1(RDEV,ACD/ABS(COST));
S2C2=SINTHE**2+COSTHE**2;
S2C2MN=AMIN1(S2C2MN,S2C2);
S2C2MX=AMAX1(S2C2MX,S2C2);
] "END RANDOM ANGLE LOOP"
OUTPUT NRNA;(' TEST AT ',I7,' RANDOM ANGLES IN (0,5*PI/2)');
OUTPUT ADEV,RDEV,S2C2MN,S2C2MX;
(' ADEV,RDEV,S2C2(MN,MX) =',1PE16.8,3E16.8);
] "END OF SINE TABLE TEST"

"   NOW FILL IN POWER OF TWO TABLE.  PWR2I(I)=1/2**(I-1)"
P=1.; DO I=1,$MXPWR2I [PWR2I(I)=P; P=P/2.;]
```

```
] "END OF FIRST TIME INITIALIZATION"

"FILL IRAYLM ARRAY BASED ON IRAYLR INPUTS"

DO J=1,NMED [
:LOOP-OVER-REGIONS:  DO I=1,$MXREG [
IF(IRAYLR(I).EQ.1.AND.MED(I).EQ.J) [
"REGION I = MEDIUM J AND WE WANT RAYLEIGH SCATTERING, SO"
"SET FLAG TO PICK UP DATA FOR MEDIUM J AND TRY NEXT MEDIUM."
IRAYLM(J)=1; EXIT :LOOP-OVER-REGIONS:;]
"END OF REGION-LOOP"]
"END OF MEDIA-LOOP"]

"FILL INCOHM ARRAY BASED ON INCOHR INPUTS"

DO J=1,NMED [
:LOOP-OVER-REGIONS2:  DO I=1,$MXREG [
IF(INCOHR(I).EQ.1.AND.MED(I).EQ.J) [
"REGION I = MEDIUM J AND WE WANT INCOHERENT SCATTERING, SO"
"SET FLAG TO PICK UP DATA FOR MEDIUM J AND TRY NEXT MEDIUM."
INCOHM(J)=1; EXIT :LOOP-OVER-REGIONS2:;]
"END OF REGION-LOOP"]
"END OF MEDIA-LOOP"]

"FILL IPROFM ARRAY BASED ON IPROFR INPUTS"

DO J=1,NMED [
:LOOP-OVER-REGIONS3:  DO I=1,$MXREG [
IF(IPROFR(I).EQ.1.AND.MED(I).EQ.J) [
"REGION I = MEDIUM J AND WE WANT COMPTON PROFILE, SO       "
"SET FLAG TO PICK UP DATA FOR MEDIUM J AND TRY NEXT MEDIUM."
IPROFM(J)=1; EXIT :LOOP-OVER-REGIONS3:;]
"END OF REGION-LOOP"]
"END OF MEDIA-LOOP"]

"FILL IMPACM ARRAY BASED ON IMPACR INPUTS"

DO J=1,NMED [
:LOOP-OVER-REGIONS4:  DO I=1,$MXREG [
IF(IMPACR(I).EQ.1.AND.MED(I).EQ.J) [
"REGION I = MEDIUM J AND WE WANT e- IMPACT IONIZATION, SO  "
"SET FLAG TO PICK UP DATA FOR MEDIUM J AND TRY NEXT MEDIUM."
IMPACM(J)=1; EXIT :LOOP-OVER-REGIONS4:;]
"END OF REGION-LOOP"]
"END OF MEDIA-LOOP"]

"   NOW SEARCH FILE FOR DATA FOR REQUESTED MATERIALS"
REWIND KMPI;
"For use with NRCC-way setup PC-egs4, uncomment out following 2 lines"
"OPEN (UNIT=KMPI,FILE='PEGS4.DAT',STATUS='OLD'); PC FILE NAME ADDITION"
"OPEN (UNIT=KMPO,FILE='ECHO.DAT',STATUS='NEW');"
"ABOVE ALLOWS SEVERAL USERS TO READ THE FILE AT ONCE"
"ABOVE STATEMENT WAS COMMENTED OUT BY Y.NAMITO AND H.HIRAYAMA"
"TO AVOID I/O ERROR on PERSONAL DEC/Station 11 MAY 1992"
IUECHO=KMPO;
NM=0; "NUMBER OF MEDIA FOUND"
DO IM=1,NMED [LOK(IM)=0;"SET FLAG TELLING WHICH MEDIA ARE OK"
"NOW TELL USER IF RAYLEIGH OPTION HAS BEEN REQUESTED"
IF(IRAYLM(IM).EQ.1) [
OUTPUT IM;
(' RAYLEIGH OPTION REQUESTED FOR MEDIUM NUMBER',I3,/);
]
]
DO IM=1,NMED [
"NOW TELL USER IF INCOHERENT OPTION HAS BEEN REQUESTED"
IF(INCOHM(IM).EQ.1) [
OUTPUT IM;
(' INCOHERENT OPTION REQUESTED FOR MEDIUM NUMBER',I3,/);
]
]

DO IM=1,NMED [
"NOW TELL USER IF COMPTON PROFILE OPTION HAS BEEN REQUESTED"
IF(IPROFM(IM).EQ.1) [
OUTPUT IM;
(' COMPTON PROFILE OPTION REQUESTED FOR MEDIUM NUMBER',I3,/);
]
]

DO IM=1,NMED [
"NOW TELL USER IF e- IMPACT IONIZATION OPTION HAS BEEN REQUESTED"
IF(IMPACM(IM).EQ.1) [
```

```
OUTPUT IM;
(' E- IMPACT IONIZATION OPTION REQUESTED FOR MEDIUM NUMBER',I3,/);
]
]

:MEDIUM:
LOOP["MEDIUM SEARCH LOOP"

:MDLOOK:
LOOP["MEDIUM HEADER SEARCH LOOP"
"   FIRST LOOK FOR MEDIUM HEADER"
READ(KMPI,:BYTE:,END=:MDNOMORE:)MBUF;
DO IB=1,LMDL [IF (MBUF(IB).NE.MDLABL(IB))NEXT:MDLOOK:;]
"   HEADER MATCHES. NOW SEE IF IT IS ONE OF REQUESTED MEDIA"
:MDNAME:
DO IM=1,NMED [
DO IB=1,LMDN [IL=LMDL+IB; IF (MBUF(IL).NE.MEDIA(IB,IM))NEXT:MDNAME:;
IF (IB.EQ.LMDN)EXIT:MDLOOK:; ]
] "END :MDNAME: DO"
"   NOT IN NAME TABLE, SO IGNORE IT"
]REPEAT "MDLOOK"

"   'IM' IS THE INDEX OF THE MEDIUM READY TO BE READ"
IF (LOK(IM).NE.0)GO TO :MDLOOK:;"WE ALREADY HAVE THIS ONE"
LOK(IM)=1;NM=NM+1;"SET FOUND FLAG AND STEP MEDIUM COUNTER"

"   NOW READY TO READ IN DATA FOR THIS MEDIUM"
$UOUTPUT(KMPO)IM,MBUF;(' DATA FOR MEDIUM #',I3,', WHICH IS:',72A1);

"   NOW PUT OUT LINES SHOWING COMPOSITION OF MEDIUM"
"THE FOLLOWING LINE WAS CHANGED TO STORE THE ELEMENTAL COMPOSITION"
"AFB 88/05/31"
"$UINPUT(KMPI)(MBUF(I),I=1,5),RHO(IM),NE;"
"The next two lines were line prior to Dec 89 mods to get IUNRST"
"$UINPUT(KMPI)(MBUF(I),I=1,5),RHO(IM),NNE(IM);"
"(5A1,5X,F11.0,4X,I2);"
"following used to pick up IUNRST, IAPRIM and EPSTFL"
"Problem is that GASP may or may not be printed, so we make"
"a kludge which will work with all old data files"
"FIRST WE ASSUME THERE IS NO GASP VALUE IN THE LINE"
READ(KMPI,1,ERR=:GASP-THERE:)
(MBUF(I),I=1,5),RHO(IM),NNE(IM),IUNRST(IM),EPSTFL(IM),IAPRIM(IM);
1   FORMAT(5A1,5X,F11.0,4X,I2,9X,I1,9X,I1,9X,I1);
"IUNRST, EPSTFL AND IAPRIM ARE STORED IN COMIN ELECIN"
GO TO :GASP-NOT-THERE:;

:GASP-THERE:
"WE MUST REREAD THE LINE WITH THE CORRECT FORMAT"
BACKSPACE(KMPI);"THIS BACKS UP ONE RECORD TO RE-READ IT"
READ(KMPI,2)(MBUF(I),I=1,5),RHO(IM),NNE(IM),IUNRST(IM),EPSTFL(IM),
IAPRIM(IM);
2     FORMAT(5A1,5X,F11.0,4X,I2,26X,I1,9X,I1,9X,I1);

:GASP-NOT-THERE:

"THE FOLLOWING LINE WAS CHANGED AS WELL AFB 88/05/31"
"$UOUTPUT(KMPO)(MBUF(I),I=1,5),RHO(IM),NE;"
;$UOUTPUT(KMPO)(MBUF(I),I=1,5),RHO(IM),NNE(IM);
(5A1,',RHO=',1PG11.4,',NE=',I2,',COMPOSITION IS :');
"THE FOLLOWING LINE WAS CHANGED AS WELL AFB 88/05/31"
"DO IE=1,NE["
EFECZ=0.0;
DO IE=1,NNE(IM)[
    "THE FOLLOWING LINE, COMMENTED OUT, WAS THE OLD WAY OF READING"
    "IN THE ELEMENTAL COMPOSITION OF EACH MEDIUM. THE INFORMATION "
    "WAS NOT PASSED ON TO EGS. IN THE PRESENT VERSION IT IS READ  "
    "IN AND STORED IN COMMON BREMPR. AFB 88/05/31.                "
    "READ(KMPI,:BYTE:)MBUF;WRITE(KMPO,:BYTE:)MBUF;"
    $UINPUT(KMPI)
    (MBUF(I),I=1,6),(ASYM(IM,IE,I),I=1,2),
    ZELEM(IM,IE),WA(IM,IE),PZ(IM,IE),RHOZ(IM,IE);
    (6A1,2A1,3X,F3.0,3X,F9.0,4X,F12.0,6X,F12.0);
    $UOUTPUT(KMPO)
    (MBUF(I),I=1,6),(ASYM(IM,IE,I),I=1,2),
    ZELEM(IM,IE),WA(IM,IE),PZ(IM,IE),RHOZ(IM,IE);
    (6A1,2A1,',Z=',F3.0,',A=',F9.3,',PZ=',1PE12.5,',RHOZ=',1PE12.5);
    EFECZ=EFECZ+PZ(IM,IE)*ZELEM(IM,IE);
"   Calculate effective Z for this material temporary to apply   "
"   previous  material data.       H. Hirayama   12/29/97        "
    ]
IZE(1,IM)=EFECZ;
"   Define effective Z for this material temporary to apply previous "
```

```
"   material data.       H. Hirayama   12/29/97                        "

"   MEDIA AND THRESH"
$ECHO READ(KMPI,:FLT:) $LGN(RLC,AE,AP,UE,UP(IM));
TE(IM)=AE(IM)-RM; THMOLL(IM)=TE(IM)*2. + RM ;

"   ACTUAL ARRAY SIZES FROM PEGS"
$ECHO READ(KMPI,:INT:)
$LGN(MSGE,MGE,MSEKE,MEKE,MLEKE,MCMFP,MRANGE(IM)),IRAYL,IBOUND,INCOH,
ICPROF(IM),IMPACT,IXRAY;
"ICPROF is changed as ICPROF(IM) by Y.Namito 16MAY1999"
"$LGN(MSGE,MGE,MSEKE,MEKE,MLEKE,MCMFP,MRANGE(IM)),IRAYL,IBOUND,INCOH,
ICPROF,IXRAY;      "
"IXRAY is added to read option related to photo-electric data.      "
"by H. Hirayama     12/29/97                                        "
"IMPACT is added to read data for Electron impact ionization data"

NSGE=MSGE(IM);NGE=MGE(IM);NSEKE=MSEKE(IM);NEKE=MEKE(IM);
NLEKE=MLEKE(IM);NCMFP=MCMFP(IM);NRANGE=MRANGE(IM);

"   BREMPR"
$ECHO READ(KMPI,:FLT:)($LGN(DL(I,IM)/1,2,3,4,5,6/),I=1,6);
$ECHO READ(KMPI,:FLT:)DELCM(IM),($LGN(ALPHI,BPAR,
   DELPOS(I,IM)),I=1,2);

"   ELECIN"
$ECHO READ(KMPI,:FLT:)$LGN(XR0,TEFF0,BLCC,XCC(IM));
$ECHO READ(KMPI,:FLT:)$LGN(EKE(IM)/0,1/);
$ECHO READ(KMPI,:FLT:)
($LGN(ESIG,PSIG,EDEDX,PDEDX,EBR1,PBR1,PBR2,
   TMXS(I,IM)/0,1/),I=1,NEKE);

"   PHOTIN"
"$ECHO READ(KMPI,:FLT:)EBINDA(IM),$LGN(GE(IM)/0,1/);"
$ECHO READ(KMPI,:FLT:)TEBINDA,$LGN(GE(IM)/0,1/);
"    EBINDA(IM) modified to TEBINDA.  H. Hirayama 12/29/97   "
$ECHO READ(KMPI,:FLT:)($LGN(GMFP,GBR1,GBR2(I,IM)/0,1/),I=1,NGE);

"   PHOTIN (CONTINUED)---OPTIONAL RAYLEIGH SCATTERING INPUT"

"IF(IRAYLM(IM).EQ.1.AND.IRAYL.NE.1) [OUTPUT IM; ORG"
IF(IRAYLM(IM).EQ.1.AND.(IRAYL.LT.1.OR.IRAYL.GT.3)) [OUTPUT IM;
(' STOPPED IN HATCH: REQUESTED RAYLEIGH OPTION FOR MEDIUM',I3,
  /,' BUT RAYLEIGH DATA NOT INCLUDED IN DATA CREATED BY PEGS.');
STOP;]

IF(INCOHM(IM).EQ.1.AND.INCOH.NE.1) [OUTPUT IM;
(' STOPPED IN HATCH: REQUESTED INCOHERENT OPTION FOR MEDIUM',I3,
  /,' BUT INCOHERENT DATA NOT INCLUDED IN DATA CREATED BY PEGS.');
STOP;]

IF(IPROFM(IM).EQ.1.AND.ICPROF(IM).EQ.0) [OUTPUT IM;
(' STOPPED IN HATCH: REQUESTED COMPTON PROFILE OPTION FOR MEDIUM',I3,
  /,' BUT COMPTON PROFILE DATA NOT INCLUDED IN DATA CREATED BY PEGS.');
STOP;]

IF(IMPACM(IM).EQ.1.AND.IMPACT.EQ.0) [OUTPUT IM;
(' STOPPED IN HATCH: REQUESTED e- IMPACT IONIZATION OPTION FOR MEDIUM',
I3,/,' BUT e- IMPACT IONIZATION DATA NOT INCLUDED IN DATA CREATED BY PEGS.');
STOP;]

IF (IRAYL.EQ.1.OR.IRAYL.EQ.2.OR.IRAYL.EQ.3) [
$ECHO READ(KMPI,:INT:) NGR(IM);
NGRIM=NGR(IM);
$ECHO READ(KMPI,:FLT:)$LGN(RCO(IM)/0,1/);
$ECHO READ(KMPI,:FLT:)($LGN(RSCT(I,IM)/0,1/),I=1,NGRIM);
$ECHO READ(KMPI,:FLT:)($LGN(COHE(I,IM)/0,1/),I=1,NGE);
IF(IRAYLM(IM).NE.1) [OUTPUT IM;
(' RAYLEIGH DATA AVAILABLE FOR MEDIUM',I3,
  ' BUT OPTION NOT REQUESTED.',/);]
]


IF (INCOH.EQ.1) [
$ECHO READ(KMPI,:INT:) NGS(IM);
NGSIM=NGS(IM);
$ECHO READ(KMPI,:FLT:)$LGN(SCO(IM)/0,1/);
$ECHO READ(KMPI,:FLT:)($LGN(SXZ(I,IM)/0,1/),I=1,NGSIM);
IF(INCOHM(IM).NE.1) [OUTPUT IM;
(' INCOHERENT DATA AVAILABLE FOR MEDIUM',I3,
  ' BUT OPTION NOT REQUESTED.',/);]
]
```

```
IF (ICPROF(IM).EQ.1.OR.ICPROF(IM).EQ.2) [
$ECHO READ(KMPI,:INT:) NGC(IM);
NGCIM=NGC(IM);
$ECHO READ(KMPI,:FLT:)$LGN(CCO(IM)/0,1/),CPIMEV;
$ECHO READ(KMPI,:FLT:)($LGN(CPR(I,IM)/0,1/),I=1,NGCIM);
IF(IPROFM(IM).NE.1) [OUTPUT IM;
(' TOTAL COMPTON PROFILE DATA AVAILABLE FOR MEDIUM',I3,
 ' BUT OPTION NOT REQUESTED.',/);]
]

IF (ICPROF(IM).EQ.3.OR.ICPROF(IM).EQ.4) [
$ECHO READ(KMPI,:INT:) MXSHEL(IM),NGC(IM);
NGCIM=NGC(IM);   MXSIM=MXSHEL(IM);
$ECHO READ(KMPI,:FLT:)(ELECNO(I,IM),I=1,MXSIM);
$ECHO READ(KMPI,:FLT:)(CAPIO(I,IM),I=1,MXSIM);
$ECHO READ(KMPI,:FLT:)$LGN(CCOS(IM)/0,1/);
$ECHO READ(KMPI,:FLT:)
(($LGN(CPRS(I,IS,IM)/0,1/),IS=1,MXSIM),I=1,NGCIM);

IF(IPROFM(IM).NE.1) [OUTPUT IM;
(' SHELL COMPTON PROFILE DATA AVAILABLE FOR MEDIUM',I3,
 ' BUT OPTION NOT REQUESTED.',/);]
]

"Following statements are added to read multi-element EII related"
"data by Y. Namito 20DEC1999"
IF(IMPACT.GE.1) [
$ECHO READ(KMPI,:INT:) NEPM(IM);
NER=NEPM(IM);
$ECHO READ(KMPI,:INT:) (IZEI(I,IM),I=1,NER);
$ECHO READ(KMPI,:INT:) NEII(IM);
$ECHO READ(KMPI,:FLT:) $LGN(EICO(IM)/0,1/);
$ECHO READ(KMPI,:FLT:) (($LGN(EII(I,IFUN,IM)/0,1/),IFUN=1,NER),
I=1,NEII(IM));

IF(IMPACM(IM).NE.1) [OUTPUT IM;
(' ELECTRON IMPACT IONIZATION DATA AVAILABLE FOR MEDIUM',I3,
 ' BUT OPTION NOT REQUESTED.',/);]
]

"Following statements are added to read photoelectric related"
"data by H. Hirayama.      12/29/97                              "
"Modified related to the modification of PEGS4.  YN and HH"
IF (IXRAY.EQ.1) [
$ECHO READ(KMPI,:INT:) NEPM(IM);
NER=NEPM(IM);
NER1=NER-1;
$ECHO READ(KMPI,:INT:) (IZE(I,IM),I=1,NER);
$ECHO READ(KMPI,:INT:) NGX(IM);
READ(KMPI,:FLT:) PHO0(IM),PHO1(IM);
WRITE(KMPO,:FLT:) PHO0(IM),PHO1(IM);
READ(KMPI,:FLT:)
((PHOTBR0(I,IFUN,IM),PHOTBR1(I,IFUN,IM),IFUN=1,NER1),I=1,NGX(IM));
WRITE(KMPO,:FLT:)
((PHOTBR0(I,IFUN,IM),PHOTBR1(I,IFUN,IM),IFUN=1,NER1),I=1,NGX(IM));
]


"   THAT'S ALL FOR THIS MEDIUM"
]UNTIL NM.GE.NMED; "LOOP UNTIL WE HAVE ENOUGH.  END :MEDIUM: LOOP"

"   WE NOW HAVE DATA FOR ALL MEDIA REQUESTED.  NOW DO DISTANCE UNIT"
"   CHANGE.  DATA FROM PEGS IS IN UNITS OF RADIATION LENGTHS."
"   EGS IS RUN IN UNITS OF 'DUNIT' CENTIMETERS, IF DUNIT.GT.0 "
"   OR IN UNITS OF RLC(-DUNIT) CENTIMETERS IF DUNIT.LT.0."
"   THAT IS, A NEGATIVE DUNIT MEANS UNIT IS TO BE THE RADIATION"
"   LENGTH OF THE MEDIUM WHOSE INDEX IS -DUNIT"
DUNITR=DUNIT; "SAVE REQUESTED"
IF(DUNIT.LT.0.0)[ID=MAX0(1,MIN0($MXMED,IFIX(-DUNIT)));
   DUNIT=RLC(ID);]
IF(DUNIT.NE.1.0) [
OUTPUT DUNITR,DUNIT;
(' DUNIT REQUESTED&USED ARE:',1PE14.5,E14.5,'(CM.)');
]
DO IM=1,NMED [
DFACT=RLC(IM)/DUNIT; "CONVERTS RL TO DUNITS"
DFACTI=1.0/DFACT;    "CONVERT RL**-1 TO DUNITS**-1"

FOR I=1 TO MEKE(IM) [
$SCALE $LGN(ESIG,PSIG,EDEDX,PDEDX(I,IM)/0,1/) BY DFACTI;
$SCALE $LGN(TMXS(I,IM)/0,1/) BY DFACT;]
```

```
FOR I=1 TO MLEKE(IM) [
$SCALE $LGN(ERANG,PRANG(I,IM)/0,1/) BY DFACT;]
$SCALE TEFF0(IM) BY DFACT;
$SCALE BLCC(IM) BY DFACTI;
$SCALE XCC(IM) BY SQRT(DFACTI);
RLDU(IM)=RLC(IM)/DUNIT;
FOR I=1 TO MGE(IM) [$SCALE $LGN(GMFP(I,IM)/0,1/) BY DFACT; ]
] "END IM DO"

"   SCALE VACDST.  UNDO PREVIOUS SCALE, THEN DO NEW."
VACDST=VACDST*DUNIT0/DUNIT;
DUNIT0=DUNIT; "SAVE OLD DUNIT"

"   NOW MAKE SURE ECUT AND PCUT ARE NOT LOWER THAN ANY AE OR AP"
"   ALSO SET DEFAULT DENSITIES"
DO JR=1,$MXREG [ MD=MED(JR);
IF ((MD.GE.1).AND.(MD.LE.NMED))["IT IS LEGAL NON-VACUUM MEDIUM."
ECUT(JR)=AMAX1(ECUT(JR),AE(MD));
PCUT(JR)=AMAX1(PCUT(JR),AP(MD));

"   USE STANDARD DENSITY FOR REGIONS NOT SPECIALLY SET UP"
IF (RHOR(JR).EQ.0.0)[RHOR(JR)=RHO(MD);]
]]

"BREMSSTRAHLUNG ANGULAR DISTRIBUTION INITIALIZATION - DEFAULT IS NULL"
"NEXT LINE ADDED AFB 88/05/31"
$INITIALIZE-BREMS-ANGLE;

"PAIR ANGULAR DISTRIBUTION INITIALIZATION - DEFAULT IS NULL"
"NEXT LINE ADDED AFB 91/05/31"
$INITIALIZE-PAIR-ANGLE;

"SETUP K-, L-edge information if X-rays or Augers are requested  "
"This is necessary to get piecewise fitting of photon related data."
"                                                    99/3/4 H.H. "
DO II=1,$MXREG [
IF(IEDGFL(II).NE.0.OR.IAUGER(II).NE.0) [
CALL EDGBIN; GO TO :END-SETUP:;]
]

:END-SETUP:
"   SETUP IS NOW COMPLETE"
IF (NMED.EQ.1)[OUTPUT;
(' EGS SUCCESSFULLY ''HATCHED'' FOR ONE MEDIUM.');]
ELSE[OUTPUT NMED;
(' EGS SUCCESSFULLY ''HATCHED'' FOR ',I5,' MEDIA.');]

"Comment out by Y.N to run on KEK-HITAC OCT 8,1992"
"Uncomment out following line for use with NRCC-way setup PC-EGS4"
"CLOSE (UNIT=KMPI, DISP='KEEP'); "
"FREE DATA INPUT FILE-NRCC VAX ADDITION"

RETURN;

:MDNOMORE:  OUTPUT KMPI; (' END OF FILE ON UNIT ',I2,//,
  ' PROGRAM STOPPED IN HATCH BECAUSE THE',/,
  ' FOLLOWING NAMES WERE NOT RECOGNIZED:',/);
DO IM=1,NMED [
IF(LOK(IM).NE.1) [
OUTPUT (MEDIA(I,IM),I=1,LMDN); (40X,'''',24A1,'''');
]
]
STOP;
"END OF SUBROUTINE HATCH"   END;
```

Appendix 2 Full listings of SUBROUTINE PHOTO and related SUBROUTINEs (including in kek_improve.tar.Z or kek_improve.exe)

```
"*****************************************************************"
"                              STANFORD LINEAR ACCELERATOR CENTER"
SUBROUTINE PHOTO;
"                       Include Auger electrons --  6 FEB 1999/1600"
"                            SUBROUTINE Version --  5 SEP 1998/1500"
"               General COMPOUND/MIXTURE VERSION -- 29 DEC 1997/1600"
"                              L-EDGE VERSION -- 16 FEB 1996/1600"
"                              K-EDGE VERSION -- 27 JUL 1988/2300"
"*****************************************************************"
"******* SPECIAL VERSION FOR TREATING K-EDGE FLUORESCENCE *********"
"*****************************************************************"
" Programmers:  W. R. Nelson and T. M. Jenkins (SLAC)              "
"               A.F. Bielajew (NRC) photoelectric angular distn   "
"               D.W.O. Rogers (NRC) document                      "
"               H. Hirayama (KEK) Produce photoelectrons below    "
"                                  K-Edge together with L-X rays  "
"                                  production.                    "
"                                 Modify to treat general treatment "
"                                 for a compound or a mixture.    "
"                                 Include Auger electrons.        "
"               Y. Namito (KEK) Modify sub-shell branching ratio  "
"                                 from total level width to relative "
"                                 shell contribution.             "
"*****************************************************************"
" The parts to determine Auger, fluorescence photon or Coster-Kronig"
" and those to decide fluorescence photon energy or Auger electron "
" energy are changed to SUBROUTINEs by H. Hirayama (KEK).          "
" This is a special L-edge version of an EGS4 subroutine that is   "
" based on a special K-edge version by H. Hirayama (KEK).          "
"                                                                  "
" A special K-edge version of an EGS4 subroutine is patterned      "
" after a method developed in 1978 by A. Clark (LBL) with the      "
" help of W. R. Nelson (SLAC).  It requires subroutine             "
" EDGSET (or equivalent for setting up the branching ratios and    "
" fluorescent photon energies).                                    "
"                                                                  "
" Original one treat 2 fluorescence photons. Modified by H. Hirayama"
" (KEK) to treat 4 fluorescence photons.                           "
"                                                                  "
" This version adds selection of photo-electron angle              "
"   see 'Photoelectron angle selection in the EGS4 code system'    "
"   A.F. Bielajew and D.W.O. Rogers, NRC Report PIRS-0052,Oct 86   "
"                                                                  "
"   This requires a redefinition of $COMIN-PHOTO which is done     "
"   in NRCC4MAC(P).MOR and definition of the macro                 "
"   $SELECT-PHOTOELECTRON-DIRECTION  (NRCC4MAC(P).MOR)             "
"   To select the A.D. in any region, one must set the variable    "
"   IPHTER(IR(NP))=1 passed in COMIN/USER;                         "
"                                                                  "
"  This version uses a simple model of K- and L-shell fluorescence."
"  To sample fluorescent x-rays from the K or L-shell in a given   "
"  region the flag IEDGFL(IR(NP)) (in COMIN/EDGE) must be set non- "
"  zero for each region; the value of IEDGFL is the value of Z used"
"  for that region - the model must treat the region as a single   "
"  element for the selection of the fluorescent x-ray.  IF IEDGFL  "
"  set to negative and its absolute value to Z, photoelectrons are "
"  produced below K edge without the fluorescent x-ray.            "
"  The routine EDGSET(NREG) must be called if IEDGFL is set at any "
"  region.  Otherwise, photoelectron below K-edge is treated as an "
"  absorption and does not followed.       "
"                                                                  "
"  The relevant arrays are all zeroed at the end of EGS4BLOK so    "
"  that if the user initializes nothing, the code is the same as   "
"  the EGS4 default system - i.e. no fluorescent x-rays and no     "
"  photo-electron A.D.                                             "
"                                                                  "
"  The output from this routine is complex.    99/2/6 H.H. revised."
"  E < L-III-BE  => EDEP = EMBIND, Average M-binding energy        "
"  E > K-BE   no K-, L-shell           with K- or L-shell          "
"             ENEW = PEIG-EBIND+RM ENEW = PEIG-EBIND+RM, and       "
"                                  K- or L-Xray and K-, or L-Auger "
"             EDEP = EBIND         EDEP = EBIND - ENEW            "
"             E(NP) = EDEP         E(NP) = EDEP                   "
"             EDIND is one of K-BE, L-I-, L-II-, L-III- or M-BE.   "
"       If K-alpha1,  K-alpha2 or K-alpha3 is selected for K-shell,"
```

```
"       L-shell sampling follows after determination of K X-ray.    "
"       If L-shell electron related to K-Auger-electron, L-shell    "
"       sampling follows after determination of K-Auger.            "
"  L-I < E <K-BE                                                    "
"             no L-shell               with L-shell                "
"             ENEW = PEIG-EBIND+RM ENEW = PEIG-EBIND+RM, and       "
"                                  L-Xray or L-Auger               "
"             EDEP = EBIND         EDEP = EBIND - ENEW            "
"             E(NP) = EDEP         E(NP) = EDEP                   "
"             EDIND is one of L-I-, L-II-, L-III- and M-BE.       "
"  L-II < E <L-I                                                    "
"             no L-shell               with L-shell                "
"             ENEW = PEIG-EBIND+RM ENEW = PEIG-EBIND+RM, and       "
"                                  L-II- or L-III-X-ray or Auger   "
"             EDEP = EBIND         EDEP = EBIND - ENEW            "
"             E(NP) = EDEP         E(NP) = EDEP                   "
"             EDIND is  one of L-II-, L-III- and M-BE.            "
"  L-III < E <L-II                                                  "
"             no L-shell               with L-shell                "
"             ENEW = PEIG-EBIND+RM ENEW = PEIG-EBIND+RM, and       "
"                                  L-III-X-ray or Auger            "
"             EDEP = EBIND         EDEP = EBIND - ENEW            "
"             E(NP) = EDEP         E(NP) = EDEP                   "
"             EDIND is  L-III- or M-BE.                           "
"  In the case of L-I and L-II, L X-ray from L-II or L-III subshell"
"  is sampled due to Coster-Kronig effect.                          "
"                                                                   "
"      THEN IARG = 4 CALL IS MADE i.e. energy discarded in middle  "
"                                                                   "
" THEN                                                             "
" E<L-III-BE  E(NP) = EBIND, EBIND is M-BE. E(NP)=Initial-EBIND+RM "
" E>L-III-BE  IQ(NP) = -1, E(NP) = Initial - EBIND+RM             "
"         and if flags on for Auger electron and/or fluorescence   "
"         and sampled, then NP => NP + 1 and electrons and/or gamma"
"         is set up                                                "
"                                                                  "
" This version is modified from the original one for an element    "
" to a compound or a mixture for a general treatments of           "
" photoelectric effect.                                            "
"                                                                  "
"******************************************************************"
$ENERGY PRECISION PEIG;
$COMIN-PHOTO; "the next line is the default replacement for this"
";COMIN/DEBUG,EDGE,EPCONT,MEDIA,PHOTIN,STACK,UPHIOT,USEFUL/;"
"but for the photo-electron angle selection, see definition in "
"NRCC4MAC(P)"

/NXRAY,NAUGER/=0.0; "Set to 0 at first"

"Following statements are added by H. Hirayama to determine "
"element interact.   12/29/97                                 "
IRL=IR(NP);
PEIG=E(NP);
EIG=PEIG; "ENERGY OF INCIDENT GAMMA"
PHOL=ALOG(EIG);"GLE IS GAMMA LOG ENERGY"
MEDIUM=MED(IRL);

IF(NEPM(MEDIUM).EQ.1) [IZ=IZE(1,MEDIUM);GO TO :K-EDGE:;]
ELSE [
$RANDOMSET PBRAT;
DO I=1,NEPM(MEDIUM)-1 [
$SETINTERVAL PHOL,PHO; "SET PWLF INTERVAL"
PBRAN=PHOTBR1(LPHOL+IEXTP,I,MEDIUM)*PHOL+PHOTBR0(LPHOL+IEXTP,I,MEDIUM);
IF(PBRAT.LE.PBRAN) [IZ=IZE(I,MEDIUM);GO TO :K-EDGE:;]
]]
IZ=IZE(NEPM(MEDIUM),MEDIUM);

"After this 'MEDIUM' is changed to 'IZ' to treat K , L X-rays"
"for each element.   H. Hirayama  12/29/97.                   "
:K-EDGE:
IF(E(NP).LE.EEDGE(1,IZ)*1.0E-3) [
  IF(E(NP).LE.EEDGE(4,IZ)*1.0E-3) ["below L3 edge and treat as "
"                                  M-absorption H. Hirayama 1/23/99."
    EBIND=EMBIND(IZ)*1.0E-3;EDEP=EBIND;
    GO TO :PHOTOELECTRON:; "below L3 edge"]
  ELSE [GO TO :L-ABSORPTION:; "between L3 edge to K edge"]]
ELSE [" 'K-EDGE P.E. IS POSSIBLE' LOOP"
  $RANDOMSET BR; "SAMPLE TO DECIDE K-EDGE PHOTON VERSUS EITHER"
  "                L-, M-EDGE etc. P.E. INTERACTION"
  IF(BR.GT.BKPHOT(IZ)) [GO TO :L-ABSORPTION:;]
```

```
  ELSE [CALL KSHELL; "Determine K-Xray or Auger"]

"END OF 'K-EDGE P.E. IS POSSIBLE' LOOP"]

"Set EBIND here for K-absorption"
EBIND=EEDGE(1,IZ)*1.0E-3;

GO TO :E(NP)-SET:;

:L-ABSORPTION:
"IF(EEDGE(4,IZ)*1.0E-3.EQ.0.0) [EDEP=PEIG; IBLOBE=1; must be EDGL1 H.H."
IF(EEDGE(2,IZ)*1.0E-3.EQ.0.0) ["Treat as M-absorption. 1/23/99 H.H."
  EBIND=EMBIND(IZ);EDEP=EBIND;
  GO TO :PHOTOELECTRON:;]

IF(E(NP).GT.EEDGE(2,IZ)*1.0E-3) ["Above L-I edge."
" Following check first.    2/26/99 H.H."
  $RANDOMSET BRL; "SAMPLE TO DECIDE L-EDGE PHOTON VERSUS EITHER"
  "                M- or N-EDGE P.E. INTERACTION"
  IF(BRL.GT.RSCL1(IZ))["Absorption below L. Treat as M-absorption."
"                        1/23/99 H. Hirayama                      "
    EBIND=EMBIND(IZ)*1.0E-3;EDEP=EBIND;
    GO TO :PHOTOELECTRON:;]
" L-photoelectric. Decide sub-shell.   2/26/99 H.H."
  $RANDOMSET SHELL;
"Calculate energy dependent sub-shell ratio.      3/31/99 Y.N. & H.H."
PEIGK=E(NP)*1000.0;
PHOLK=ALOG(PEIGK);  "ln(E), E in keV"
CROSL1=EXP(PM0(1,IZ)+PM1(1,IZ)*PHOLK+PM2(1,IZ)*PHOLK*PHOLK);
CROSL2=EXP(PM0(2,IZ)+PM1(2,IZ)*PHOLK+PM2(2,IZ)*PHOLK*PHOLK);
CROSL3=EXP(PM0(3,IZ)+PM1(3,IZ)*PHOLK+PM2(3,IZ)*PHOLK*PHOLK);
TCROS=CROSL1+CROSL2+CROSL3;
BSHL2=CROSL1/TCROS;
BSHL3=(CROSL1+CROSL2)/TCROS;
" IF(SHELL.GT.BSHL3) [GO TO :L3-SUBSHELL:;] changed 2/26/99 H.H"
  IF(SHELL.GT.BSHL3) [CALL LSHELL(3);
    GO TO :E(NP)-SET:;]
" IF(SHELL.GT.BSHL2) [GO TO :L1-L2:;] changed 2/26/99 H.H"
  ELSEIF(SHELL.GT.BSHL2) [CALL LSHELL(2);
    GO TO :E(NP)-SET:;]
  ELSE [CALL LSHELL(1); "L-1 hole is created"
    GO TO :E(NP)-SET:;]  "End of L1-hole"
  ] "End of above L-1 edge"

ELSEIF(E(NP).GT.EEDGE(3,IZ)*1.0E-3) ["Between L-1 to L-2."
  IF(EEDGE(3,IZ)*1.0E-3.EQ.0.0) ["Treat as M-absorption. 1/23/99 H.H."
    EBIND=EMBIND(IZ)*1.0E-3;EDEP=EBIND;
    GO TO :PHOTOELECTRON:;]
  GO TO :L1-L2:;]

ELSE ["Between L-2 to L-3." GO TO :L2-L3:;]

:L1-L2:
$RANDOMSET BRL; "SAMPLE TO DECIDE L-EDGE PHOTON VERSUS EITHER"
"                M-EDGE P.E. INTERACTION"
IF(BRL.GT.RSCL2(IZ)) ["Absorption below L. Treat as M-absorption."
"                        1/23/99 H. Hirayama                      "
    EBIND=EMBIND(IZ)*1.0E-3;EDEP=EBIND;
    GO TO :PHOTOELECTRON:;]
ELSE [ "L-photoelectric"
  $RANDOMSET SHELL;
"Calculate energy dependent sub-shell ratio.      3/31/99 Y.N. & H.H."
PEIGK=E(NP)*1000.0;
PHOLK=ALOG(PEIGK);  "ln(E), E in keV"
CROSL2=EXP(PM0(2,IZ)+PM1(2,IZ)*PHOLK+PM2(2,IZ)*PHOLK*PHOLK);
CROSL3=EXP(PM0(3,IZ)+PM1(3,IZ)*PHOLK+PM2(3,IZ)*PHOLK*PHOLK);
TCROS=CROSL2+CROSL3;
BSHL3=CROSL2/TCROS;
" IF(SHELL.GT.BSHL3) [GO TO :L3-SUBSHELL:;] changed 2/26/99 H.H"
  IF(SHELL.GT.BSHL3) ["L3 hole is created" CALL LSHELL(3);
    GO TO :E(NP)-SET:;]
  ELSE [CALL LSHELL(2); "L-2 hole is created"
    GO TO :E(NP)-SET:;]
  ]

:L2-L3:
$RANDOMSET BRL; "SAMPLE TO DECIDE L-EDGE PHOTON VERSUS EITHER"
"                AUGER ELECTRON OR M-EDGE P.E. INTERACTION"
IF(BRL.GT.RSCL3(IZ)) ["Absorption below L. Treat as M-absorption."
```

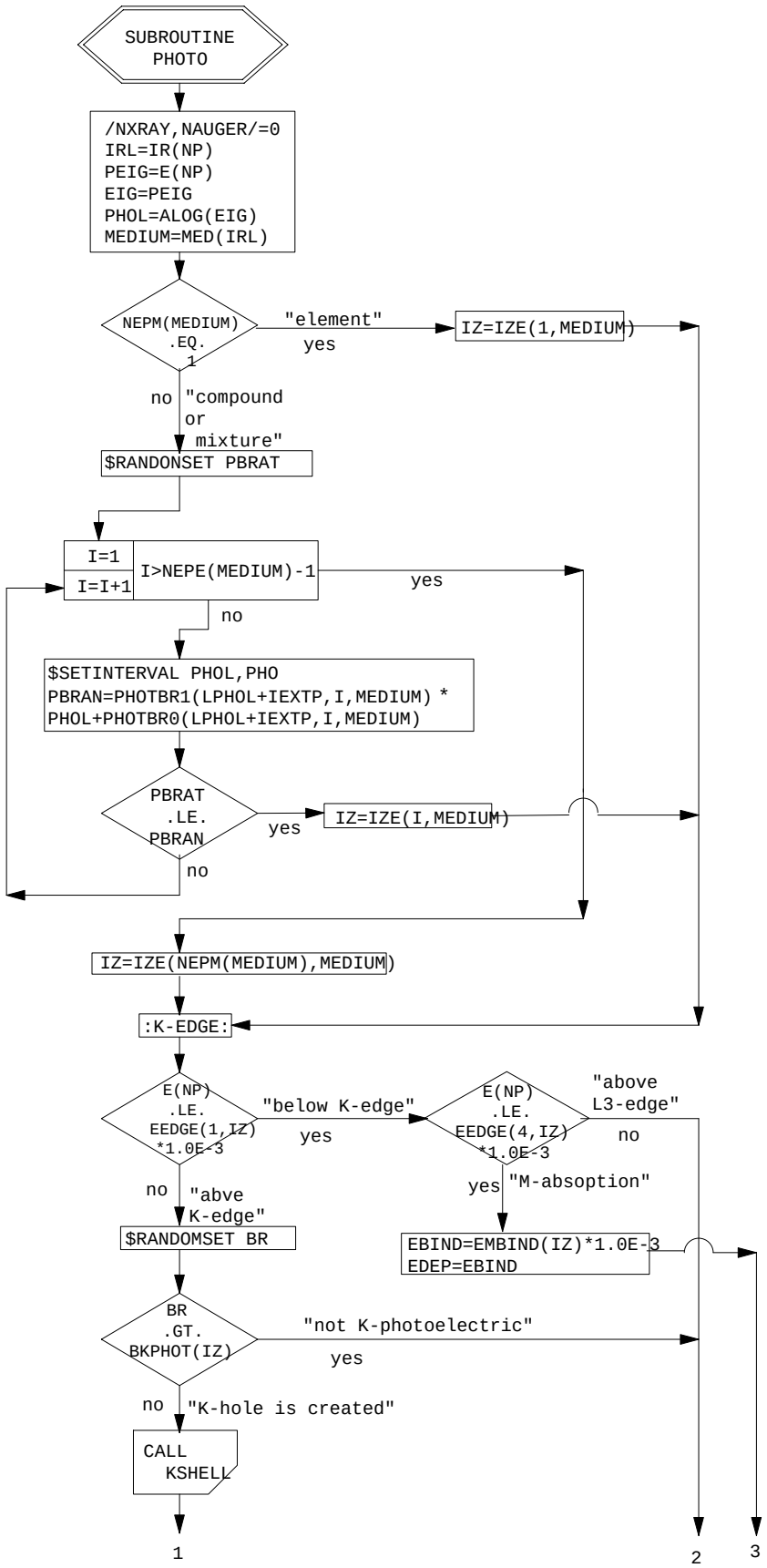
```
"                         1/23/99 H. Hirayama                           "
    EBIND=EMBIND(IZ)*1.0E-3;EDEP=EBIND;
    GO TO :PHOTOELECTRON:;]
ELSE [CALL LSHELL(3); "L-3 hole is created"]

:E(NP)-SET:
IF(IEDGFL(IRL).LE.0) [NXRAY=0;]
IF(IAUGER(IRL).LE.0) [NAUGER=0;]

EDEP=EBIND;
IF(NXRAY.GE.1) [
  DO IPHOT=1,NXRAY [
    EDEP=EDEP-EXRAY(IPHOT);]]

IF(NAUGER.GE.1) [
  DO IELEC=1,NAUGER [
    EDEP=EDEP-EAUGER(IELEC);]]

"Following statement is necessary not to treat negative energy"
"photons due to numerical precision"
IF(EDEP.LT.0.0.AND.ABS(EDEP).LT.1.0E-5) [EDEP=0.0;]

:PHOTOELECTRON:
E(NP)=EDEP;

$AUSCALL($PHOTXAUS);


" 'SET UP PARTICLE(S) LOOP"
IQ(NP)=-1; "PHOTOELECTRON (ALWAYS SET UP)"
E(NP)=PEIG-EBIND+PRM;
$SELECT-PHOTOELECTRON-DIRECTION; "defined in NRCC4MAC(P).MOR"
IF(NAUGER.NE.0) ["Set up Auger electrons"
  DO IELEC=1,NAUGER [
    NP=NP+1; E(NP)=EAUGER(IELEC)+PRM; IQ(NP)=-1;
    "Auger electrons comes off isotropically"
    $RANDOMSET RNISO;
    COSTHE=2.0*RNISO-1.0;
    SINTHE=SQRT(1.0-COSTHE*COSTHE);
    U(NP)=0.0; V(NP)=0.0; W(NP)=1.0; "MAKES THINGS EASIER IN UPHI"
    CALL UPHI(2,1);
    $TRANSFER PROPERTIES TO (NP) FROM (NP-1);]]

IF(NXRAY.NE.0) ["Set up fluorescent photons"
  DO IPHOT=1,NXRAY [
    NP=NP+1;
    E(NP)=EXRAY(IPHOT);
    IQ(NP)=0;

    "PHOTON COMES OFF ISOTROPICALLY"
    $RANDOMSET RNISO;
    COSTHE=2.0*RNISO-1.0;
    SINTHE=SQRT(1.0-COSTHE*COSTHE);
    U(NP)=0.0; V(NP)=0.0; W(NP)=1.0; "MAKES THINGS EASIER IN UPHI"
    CALL UPHI(2,1);
    $TRANSFER PROPERTIES TO (NP) FROM (NP-1);]]
"END OF 'SET UP PARTICLE(S)' LOOP"

RETURN;
"END OF SUBROUTINE PHOTO" END;


%E
"*****************************************************************"
"                    High Energy Accelerator Research Organization "
SUBROUTINE KSHELL;
"               Subroutine to determine Auger of K-Xray at K-P.E.   "
"               General COMPOUND/MIXTURE VERSION -- 2 Sep. 1998     "
"               Programmers:  H. Hirayama and Y. Namito (KEK)       "
"*****************************************************************"
$COMIN-PHOTO;

$RANDOMSET BRK; "Sample to decide K-edge photon versus either"
"                Auger electron"

IF(BRK.GT.OMEGAK(IZ)) [CALL KAUGER; "Auger electron will be emitted"]
ELSE [CALL KXRAY; " 'K X-ray will be emitted"]

RETURN;
"END OF SUBROUTINE KSHELL" END;
```

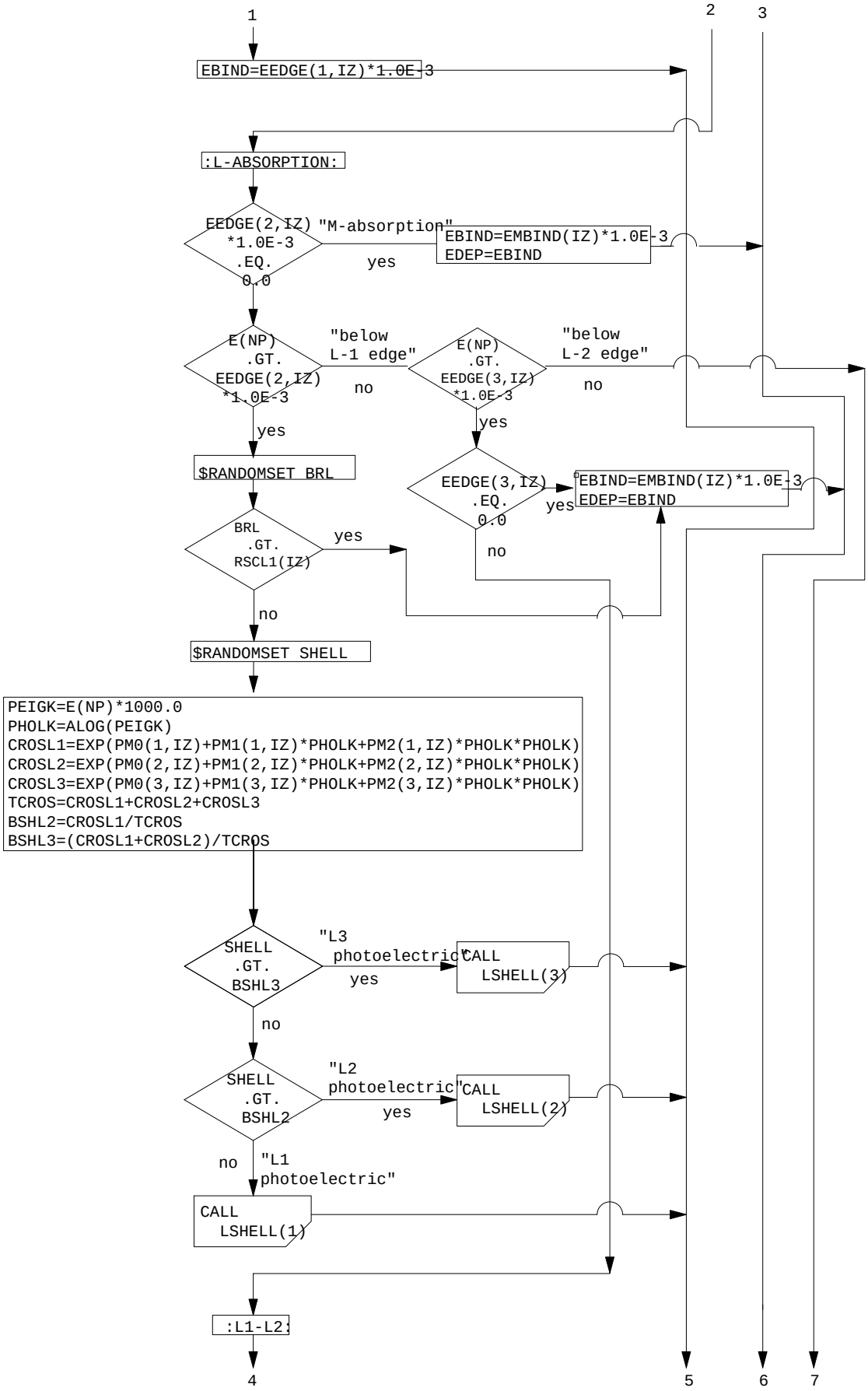
```
%E
"*****************************************************************"
"                     High Energy Accelerator Research Organization "
SUBROUTINE LSHELL(LL);
"               Subroutine to determine type at L-P.E.              "
"               General COMPOUND/MIXTURE VERSION -- 2 Sep. 1998     "
"               Programmers:  H. Hirayama and Y. Namito (KEK)       "
"*****************************************************************"
$COMIN-PHOTO;

ICKFLG=0;

IF(LL.EQ.2) [GO TO :L2-SUBSHELL:;]
IF(LL.EQ.3) [GO TO :L3-SUBSHELL:;]

$RANDOMSET BRL; "Sample to decide Coster-Kronig, Auger or L-X-ray"

EBIND=EEDGE(2,IZ)*1.0E-3;
IF(BRL.GT.OMEGAL1(IZ)) [
  IF(BRL.LE.OMEGAL1(IZ)+F12(IZ)) [
    ICKFLG=1; "Coster-Kronig f12" GO TO :L2-SUBSHELL:;]
  ELSEIF(BRL.LE.OMEGAL1(IZ)+F12(IZ)+F13(IZ)) [
    ICKFLG=1; "Coster-Kronig f13" GO TO :L3-SUBSHELL:;]
  ELSE [CALL LAUGER(1) "L1 Auger"]
  ]
ELSE [CALL LXRAY(1); "L1 X-ray"]
RETURN;

:L2-SUBSHELL:
$RANDOMSET BRL; "Sample to decide Coster-Kronig, Auger or L-X-ray"
IF(ICKFLG.EQ.0) [EBIND=EEDGE(3,IZ)*1.0E-3;]

IF(BRL.GT.OMEGAL2(IZ)) [
" IF(BRL.LE.OMEGAL2(IZ)+F13(IZ)) [ modified 2/26/99 H.H."
  IF(BRL.LE.OMEGAL2(IZ)+F23(IZ)) [
    ICKFLG=1; "Coster-Kronig f23" GO TO :L3-SUBSHELL:;]
  ELSE ["L2 Auger will be emitted"
    CALL LAUGER(2);" L2 Auger"]
  ]
ELSE [CALL LXRAY(2); "L2 X-ray"]
RETURN;

:L3-SUBSHELL:
IF(ICKFLG.EQ.0) [EBIND=EEDGE(4,IZ)*1.0E-3;]

$RANDOMSET BRL; "Sample to decide Coster-Kronig, Auger or L-X-ray"

IF(BRL.GT.OMEGAL3(IZ)) [CALL LAUGER(3); "L3 Auger"]
ELSE [CALL LXRAY(3); " L3 X-ray"]

RETURN;
"END OF SUBROUTINE LSHELL" END;

%E
"*****************************************************************"
"                     High Energy Accelerator Research Organization "
SUBROUTINE KXRAY;
"               Subroutine to determine energy of K-X-ray           "
"               General COMPOUND/MIXTURE VERSION -- 2 Sep. 1998     "
"               Programmers:  H. Hirayama and Y. Namito (KEK)       "
"*****************************************************************"
$COMIN-PHOTO;

IF(DFKX(9,IZ).EQ.0.0) ["No K-Xray" RETURN;]

NXRAY=NXRAY+1; " Determine K X-ray energy"

$RANDOMSET BRKX;

DO IK=1,9 [
IF(BRKX.LE.DFKX(IK,IZ)) [EXRAY(NXRAY)=EKX(IK,IZ)*1.0E-3;
GO TO :CASCADE:;]
]

EXRAY(NXRAY)=EKX(10,IZ)*1.0E-3;

"KX=1: K-alpha1 (K-L3)"
"   2: K-alpha2 (K-L2)"
```

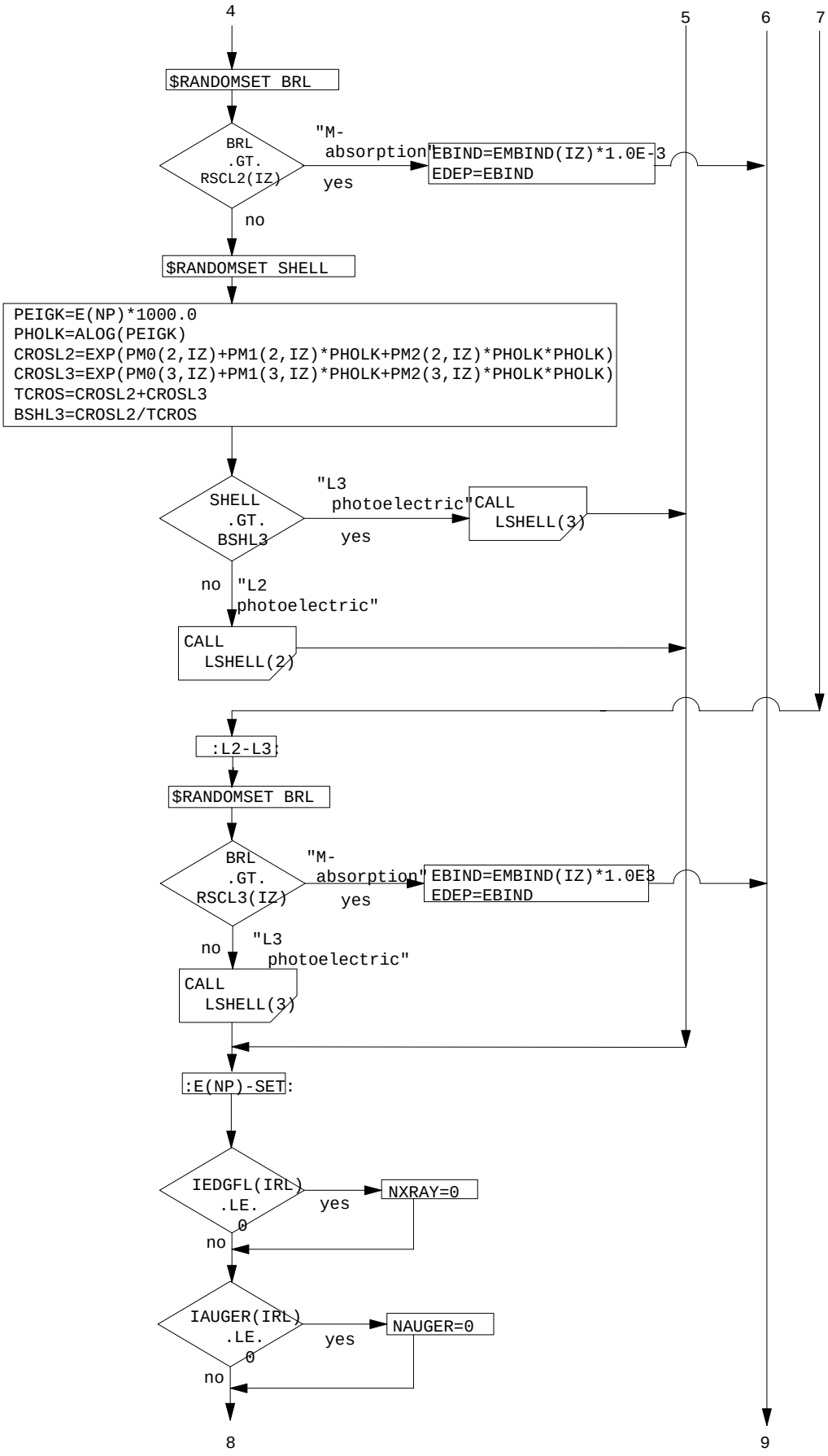
```
"   3: K-alpha3 (K-L1)"
"   4: K-beta1  (K-M3)"
"   5: K-beta2  (K-N2N3)"
"   6: K-beta3  (K-M2)"
"   7: K-beta4  (K-N4N5)"
"   8: K-beta5  (K-M4M5)"
"   9: K-O      (K-O2O3)"
"  10: L-P      (K-P2P3)"

:CASCADE:
IF(IK.EQ.1) [CALL LSHELL(3); "L3 hole is created"]
IF(IK.EQ.2) [CALL LSHELL(2); "L2 hole is created"]
IF(IK.EQ.3) [CALL LSHELL(1); "L1 hole is created"]
"End of cascade L-hole."

RETURN;
"END OF SUBROUTINE KXRAY" END;

%E
"*****************************************************************"
"                     High Energy Accelerator Research Organization "
SUBROUTINE LXRAY(LL);
"              Subroutine to determine energy of L-X-ray           "
"              General COMPOUND/MIXTURE VERSION -- 2 Sep. 1998     "
"              Programmers:  H. Hirayama and Y. Namito (KEK)       "
"*************************************************************"
$COMIN-PHOTO;

$RANDOMSET BRLX;

GO TO (:L1-XRAY:,:L2-XRAY:,:L3-XRAY:) LL;

:L1-XRAY:

IF(DFLX1(7,IZ).EQ.0.0) ["No L1-Xray" RETURN;]

NXRAY=NXRAY+1;
DO LX=1,7 [
  IF(BRLX.LE.DFLX1(LX,IZ)) [
    EXRAY(NXRAY)=ELX1(LX,IZ)*1.0E-3;
    RETURN;]
  ] "End of DO-loop"

EXRAY(NXRAY)=ELX1(8,IZ)*1.0E-3;
RETURN;

:L2-XRAY:

IF(DFLX2(4,IZ).EQ.0.0) ["No L2-Xray" RETURN;]

NXRAY=NXRAY+1;
DO LX=1,4 [
  IF(BRLX.LE.DFLX2(LX,IZ)) [
    EXRAY(NXRAY)=ELX2(LX,IZ)*1.0E-3;
    RETURN;]
  ] "End of DO-loop"

EXRAY(NXRAY)=ELX2(5,IZ)*1.0E-3;
RETURN;

:L3-XRAY:

IF(DFLX3(6,IZ).EQ.0.0) ["No L3-Xray" RETURN;]

NXRAY=NXRAY+1;
DO LX=1,6 [
  IF(BRLX.LE.DFLX3(LX,IZ)) [
    EXRAY(NXRAY)=ELX3(LX,IZ)*1.0E-3;
    RETURN;]
  ] "End of DO-loop"

EXRAY(NXRAY)=ELX3(7,IZ)*1.0E-3;
RETURN;
"END OF SUBROUTINE LXRAY"
END;

%E
```

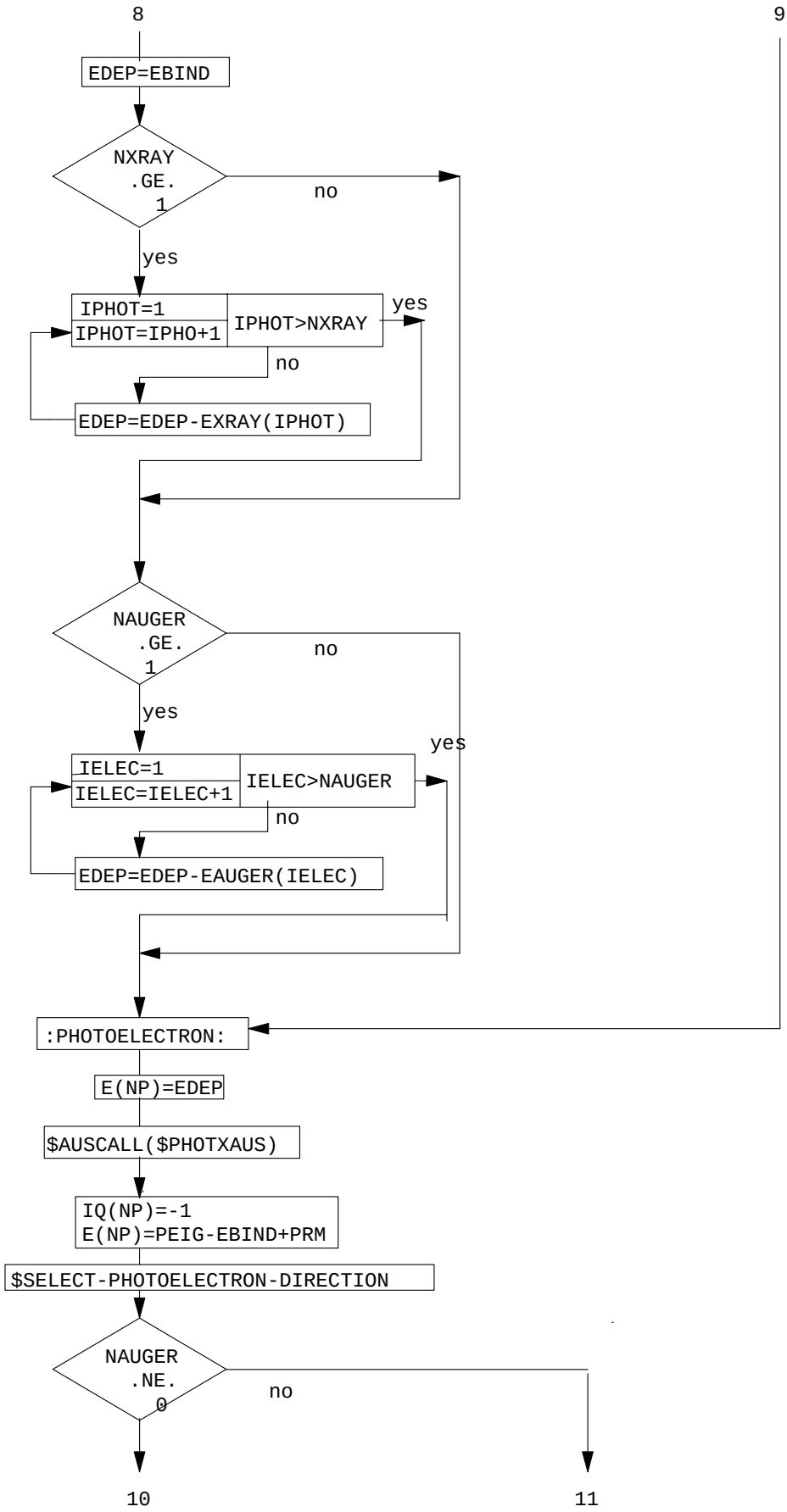
```
"*****************************************************************"
"                      High Energy Accelerator Research Organization "
SUBROUTINE KAUGER;
"               Subroutine to determine energy of K-Auger.           "
"               General COMPOUND/MIXTURE VERSION -- 2 Sep. 1998     "
"               Programmers:  H. Hirayama and Y. Namito (KEK)       "
"*****************************************************************"
$COMIN-PHOTO;

IF(DFKAUG(13,IZ).EQ.0.0) ["No K-Auger" RETURN;]

NAUGER=NAUGER+1;

$RANDOMSET EAUG;

DO KAUG=1,13 [
  IF(EAUG.LE.DFKAUG(KAUG,IZ)) [
    EAUGER(NAUGER)=EKAUG(KAUG,IZ)*1.0E-3;
    GO TO :CASCADE:;]
  ] "End of DO-loop"

EAUGER(NAUGER)=EKAUG(14,IZ)*1.0E-3;

:CASCADE:
IF(KAUG.EQ.1) [CALL LSHELL(1); CALL LSHELL(1);]
ELSEIF(KAUG.EQ.2) [CALL LSHELL(1); CALL LSHELL(2);]
ELSEIF(KAUG.EQ.3) [CALL LSHELL(1); CALL LSHELL(3);]
ELSEIF(KAUG.EQ.4) [CALL LSHELL(2); CALL LSHELL(2);]
ELSEIF(KAUG.EQ.5) [CALL LSHELL(2); CALL LSHELL(3);]
ELSEIF(KAUG.EQ.6) [CALL LSHELL(3); CALL LSHELL(3);]
ELSEIF(KAUG.EQ.7.OR.KAUG.EQ.10) [CALL LSHELL(1);]
ELSEIF(KAUG.EQ.8.OR.KAUG.EQ.11) [CALL LSHELL(2);]
ELSEIF(KAUG.EQ.9.OR.KAUG.EQ.12) [CALL LSHELL(3);]
ELSE [RETURN;]

"KAUG=1: K-L1L1"
"     2: K-L1L2"
"     3: K-L1L3"
"     4: K-L2L2"
"     5: K-L2L3"
"     6: K-L3L3"
"     7: K-L1M"
"     8: K-L2M"
"     9: K-L3M"
"    10: K-L1N"
"    11: K-L2N"
"    12: K-L3N"
"    13: K-MM"
"    14: K-MN"

RETURN;
"END OF SUBROUTINE KAUGER" END;

%E
"*****************************************************************"
"                      High Energy Accelerator Research Organization "
SUBROUTINE LAUGER(LL);
"               Subroutine to determine energy of L-Auger.           "
"               General COMPOUND/MIXTURE VERSION -- 2 Sep. 1998     "
"               Programmers:  H. Hirayama and Y. Namito (KEK)       "
"*****************************************************************"
$COMIN-PHOTO;

$RANDOMSET BRLA;

GO TO (:L1-AUGER:,:L2-AUGER:,:L3-AUGER:) LL;

:L1-AUGER:

IF(DFL1AUG(5,IZ).EQ.0.0) ["No L1-Auger" RETURN;]

NAUGER=NAUGER+1;
DO LAUG=1,5 [
  IF(BRLA.LE.DFL1AUG(LAUG,IZ)) [
    EAUGER(NAUGER)=EL1AUG(LAUG,IZ)*1.0E-3;
    RETURN;]
  ] "End of DO-loop"

EAUGER(NAUGER)=EL1AUG(6,IZ)*1.0E-3;
RETURN;
```

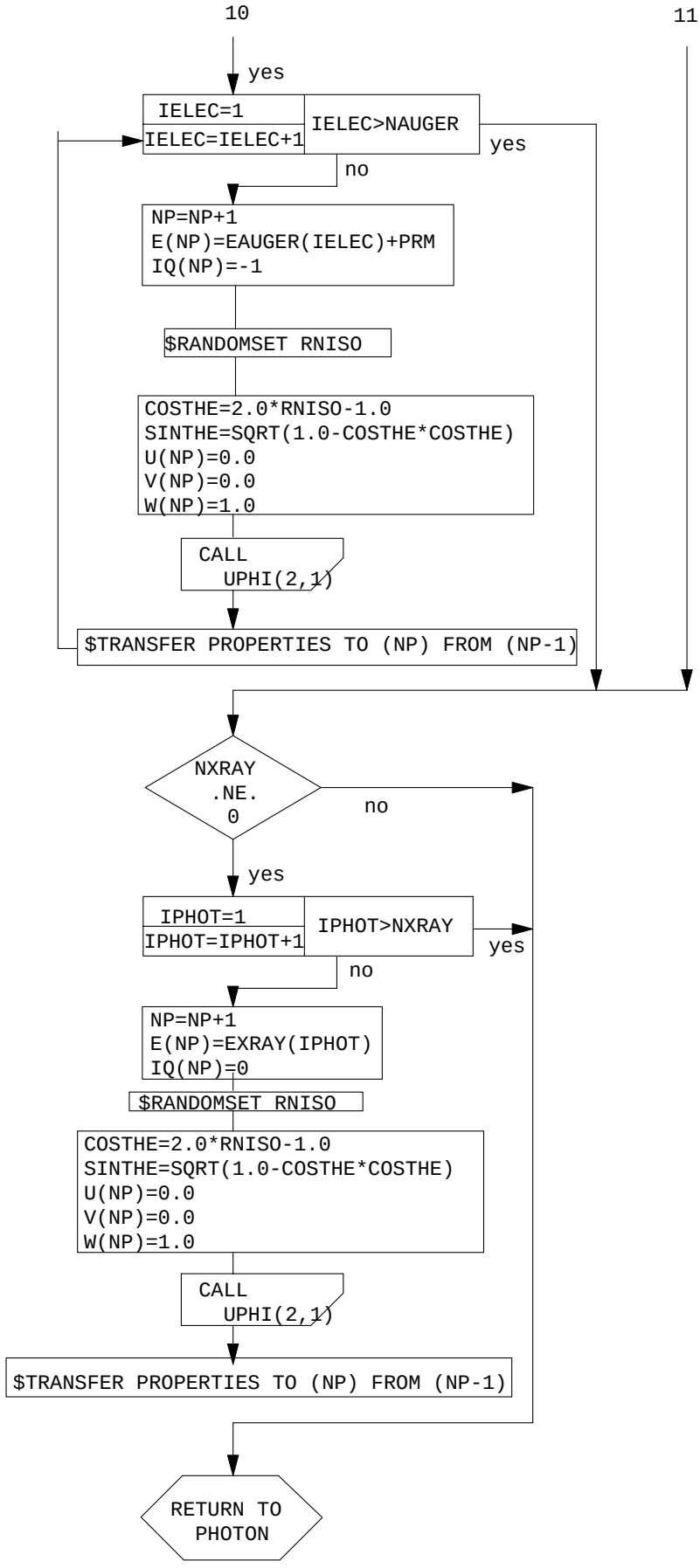
```
:L2-AUGER:

IF(DFL2AUG(5,IZ).EQ.0.0) ["No L1-Auger" RETURN;]

NAUGER=NAUGER+1;
DO LAUG=1,5 [
  IF(BRLA.LE.DFL2AUG(LAUG,IZ)) [
    EAUGER(NAUGER)=EL2AUG(LAUG,IZ)*1.0E-3;
    RETURN;]
  ] "End of DO-loop"

EAUGER(NAUGER)=EL2AUG(6,IZ)*1.0E-3;
RETURN;

:L3-AUGER:

IF(DFL3AUG(5,IZ).EQ.0.0) ["No L3-Auger" RETURN;]

NAUGER=NAUGER+1;
DO LAUG=1,5 [
  IF(BRLA.LE.DFL3AUG(LAUG,IZ)) [
    EAUGER(NAUGER)=EL3AUG(LAUG,IZ)*1.0E-3;
    RETURN;]
  ] "End of DO-loop"

EAUGER(NAUGER)=EL3AUG(6,IZ)*1.0E-3;

"LAUG=1: L1,2,3-MM"
"     2: L1,2,3-MN"
"     3: L1,2,3-MO"
"     4: L1,2,3-NN"
"     5: L1,2,3-NO"
"     6: L1,2,3-OO"

RETURN;
END;

%E
"*********************************************************************"
"                     High Energy Accelerator Research Organization "
SUBROUTINE EDGBIN;
"               Subroutine to calculate bin-number of K- and L-edge "
"               to check fitting parameter used near edge.          "
"               General COMPOUND/MIXTURE VERSION -- 2 Sep. 1998     "
"               Programmers:  H. Hirayama and Y. Namito (KEK)       "
"*********************************************************************"
$COMIN-PHOTO;
COMIN/THRESH/;

DO MEDIUM=1,NMED [
NER=NEPM(MEDIUM);
IF(NER.GT.20) [
OUTPUT;(' Number of elements in medium must be less than 20 !');
STOP;]

NEDGB(MEDIUM)=0;
DO IZN=1,NER [
IZ1=IZE(IZN,MEDIUM);
DO IKL=1,4 [EEE=EEDGE(IKL,IZ1)/1000.0;
IF(EEE.GT.AP(MEDIUM)) [NEDGB(MEDIUM)=NEDGB(MEDIUM)+1;
EIG=ALOG(EEE);
LEDGB(NEDGB(MEDIUM),MEDIUM)=GE1(MEDIUM)*EIG+GE0(MEDIUM);
EDGB(NEDGB(MEDIUM),MEDIUM)=EEE;]
]
]

IF(NEDGB(MEDIUM).GT.0) [
DO II=1,NEDGB(MEDIUM) [
DO JJ=1,NEDGB(MEDIUM) [
IF(II.NE.JJ) [
IF(LEDGB(II,MEDIUM).EQ.LEDGB(JJ,MEDIUM)) [OUTPUT MEDIUM;
(' K- or L-edge exists in the same fitting bin at MEDIUM=',I2,'!'/
' It is better to produce material having a small UE.');]
]]]]
] "end of MEDIUM-loop"

"END OF SUBROUTINE EDGBIN"
RETURN;
END;
```

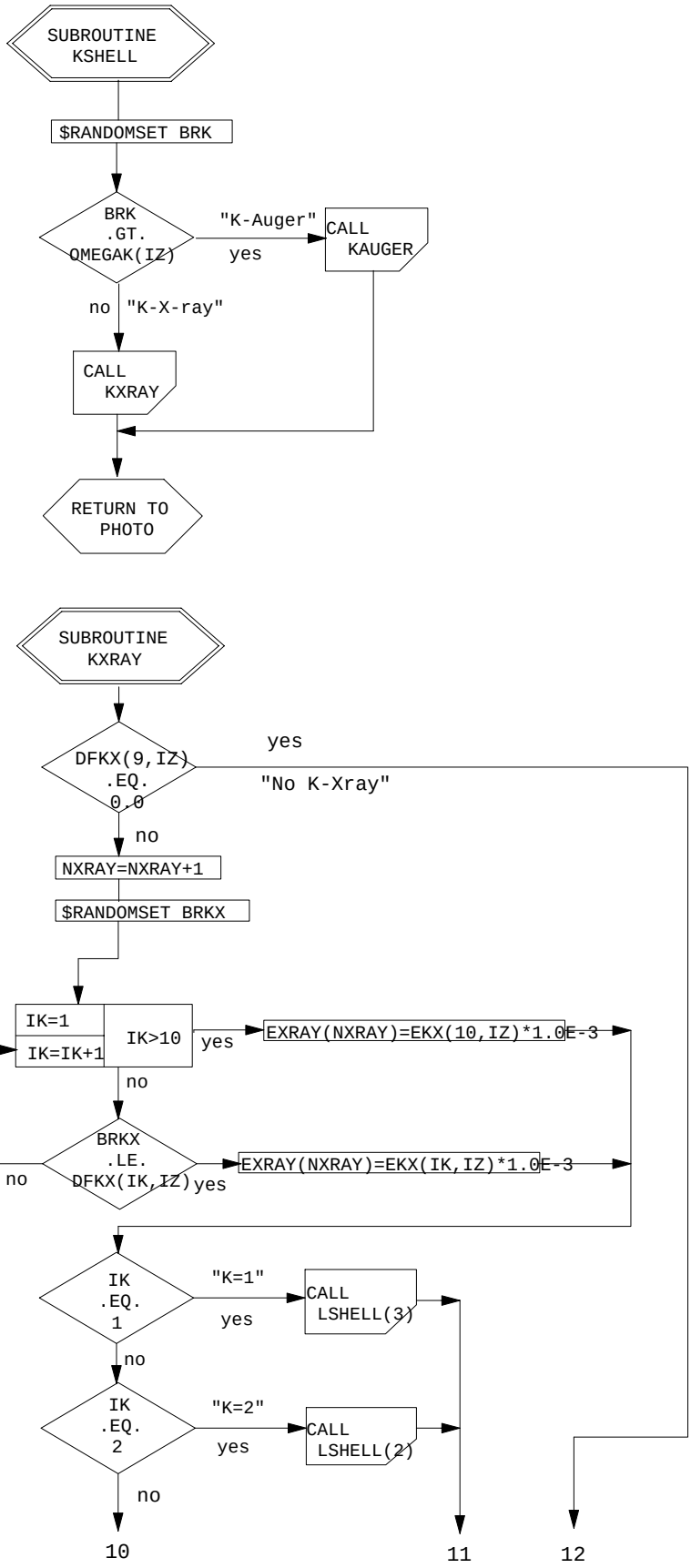

SUBROUTINE
PHOTO
/NXRAY,NAUGER/=0
IRL=IR(NP)
PEIG=E(NP)
EIG=PEIG
PHOL=ALOG(EIG)
MEDIUM=MED(IRL)
NEPM(MEDIUM)
.EQ.
1
"element"
yes
IZ=IZE(1,MEDIUM)
no
"compound
or
mixture"
$RANDONSET PBRAT
I=1
I=I+1
I>NEPE(MEDIUM)-1
yes
no
$SETINTERVAL PHOL,PHO
PBRAN=PHOTBR1(LPHOL+IEXTP,I,MEDIUM) *
PHOL+PHOTBR0(LPHOL+IEXTP,I,MEDIUM)
PBRAT
.LE.
PBRAN
yes
IZ=IZE(I,MEDIUM)
no
IZ=IZE(NEPM(MEDIUM),MEDIUM)
:K-EDGE:
E(NP)
.LE.
EEDGE(1,IZ)
*1.0E-3
"below K-edge"
yes
E(NP)
.LE.
EEDGE(4,IZ)
*1.0E-3
"above
L3-edge"
no
yes
"M-absoption"
no
"abve
K-edge"
$RANDOMSET BR
EBIND=EMBIND(IZ)*1.0E-3
EDEP=EBIND
BR
.GT.
BKPHOT(IZ)
"not K-photoelectric"
yes
no
"K-hole is created"
CALL
KSHELL
1
2
3

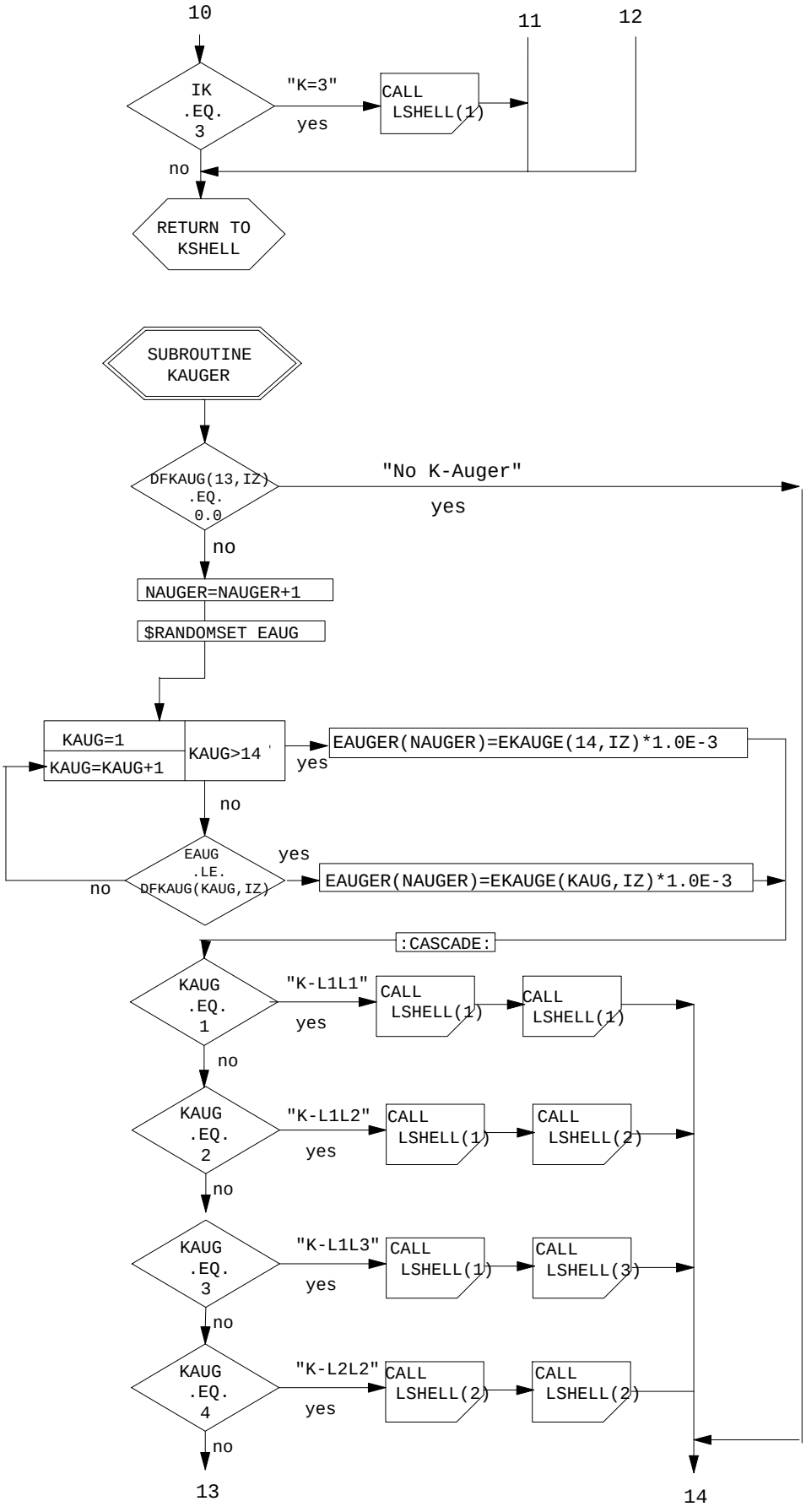

1
2
3
EBIND=EEDGE(1,IZ)*1.0E-3
:L-ABSORPTION:
EEDGE(2,IZ) *1.0E-3 .EQ. 0.0
"M-absorption"
yes
EBIND=EMBIND(IZ)*1.0E-3
EDEP=EBIND
E(NP) .GT. EEDGE(2,IZ) *1.0E-3
"below L-1 edge"
no
yes
E(NP) .GT. EEDGE(3,IZ) *1.0E-3
"below L-2 edge"
no
yes
$RANDOMSET BRL
EEDGE(3,IZ) .EQ. 0.0
yes
EBIND=EMBIND(IZ)*1.0E-3
EDEP=EBIND
BRL .GT. RSCL1(IZ)
yes
no
$RANDOMSET SHELL
PEIGK=E(NP)*1000.0
PHOLK=ALOG(PEIGK)
CROSL1=EXP(PM0(1,IZ)+PM1(1,IZ)*PHOLK+PM2(1,IZ)*PHOLK*PHOLK)
CROSL2=EXP(PM0(2,IZ)+PM1(2,IZ)*PHOLK+PM2(2,IZ)*PHOLK*PHOLK)
CROSL3=EXP(PM0(3,IZ)+PM1(3,IZ)*PHOLK+PM2(3,IZ)*PHOLK*PHOLK)
TCROS=CROSL1+CROSL2+CROSL3
BSHL2=CROSL1/TCROS
BSHL3=(CROSL1+CROSL2)/TCROS
SHELL .GT. BSHL3
"L3 photoelectric"
yes
CALL LSHELL(3)
no
SHELL .GT. BSHL2
"L2 photoelectric"
yes
CALL LSHELL(2)
no
"L1 photoelectric"
CALL LSHELL(1)
:L1-L2:
4
5
6
7

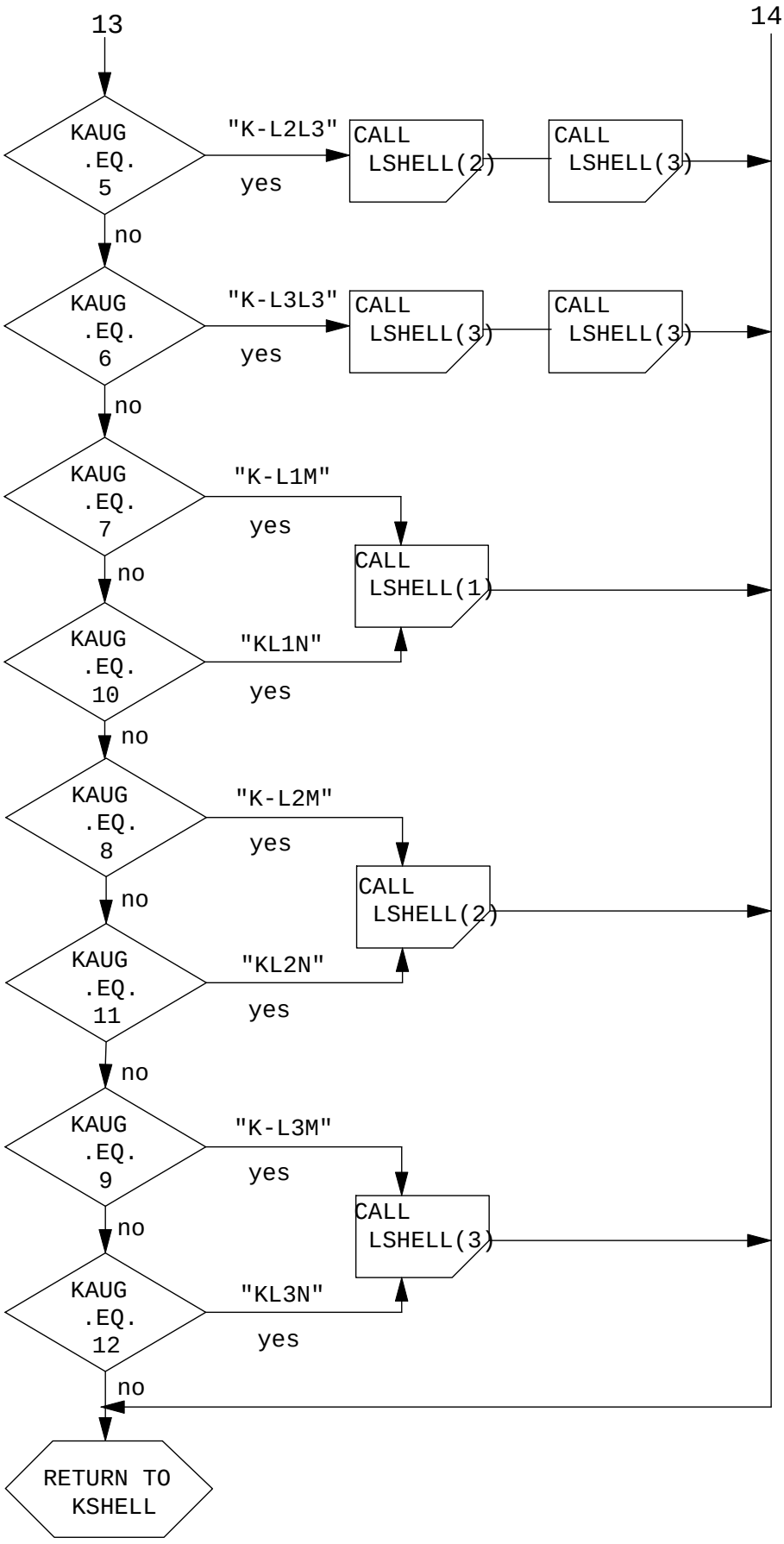

4
5
6
7
$RANDOMSET BRL
BRL .GT. RSCL2(IZ)
"M-absorption"
yes
EBIND=EMBIND(IZ)*1.0E-3
EDEP=EBIND
no
$RANDOMSET SHELL
PEIGK=E(NP)*1000.0
PHOLK=ALOG(PEIGK)
CROSL2=EXP(PM0(2,IZ)+PM1(2,IZ)*PHOLK+PM2(2,IZ)*PHOLK*PHOLK)
CROSL3=EXP(PM0(3,IZ)+PM1(3,IZ)*PHOLK+PM2(3,IZ)*PHOLK*PHOLK)
TCROS=CROSL2+CROSL3
BSHL3=CROSL2/TCROS
SHELL .GT. BSHL3
"L3 photoelectric"
yes
CALL LSHELL(3)
no
"L2 photoelectric"
CALL LSHELL(2)
:L2-L3:
$RANDOMSET BRL
BRL .GT. RSCL3(IZ)
"M-absorption"
yes
EBIND=EMBIND(IZ)*1.0E3
EDEP=EBIND
no
"L3 photoelectric"
CALL LSHELL(3)
:E(NP)-SET:
IEDGFL(IRL) .LE. 0
yes
NXRAY=0
no
IAUGER(IRL) .LE. 0
yes
NAUGER=0
no
8
9

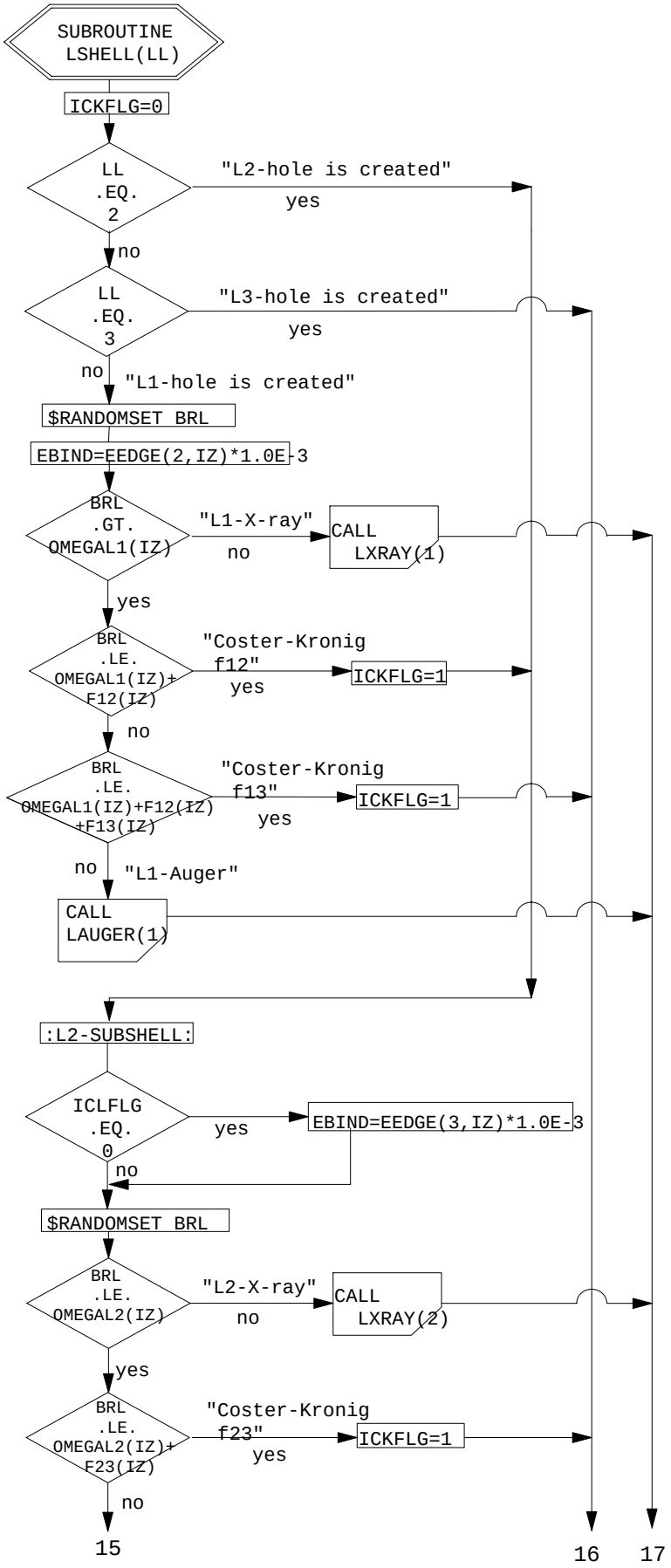

8
9
EDEP=EBIND
NXRAY
.GE.
1
no
yes
IPHOT=1
IPHOT=IPHO+1
IPHOT>NXRAY
yes
no
EDEP=EDEP-EXRAY(IPHOT)
NAUGER
.GE.
1
no
yes
IELEC=1
IELEC=IELEC+1
IELEC>NAUGER
yes
no
EDEP=EDEP-EAUGER(IELEC)
:PHOTOELECTRON:
E(NP)=EDEP
$AUSCALL($PHOTXAUS)
IQ(NP)=-1
E(NP)=PEIG-EBIND+PRM
$SELECT-PHOTOELECTRON-DIRECTION
NAUGER
.NE.
0
no
10
11

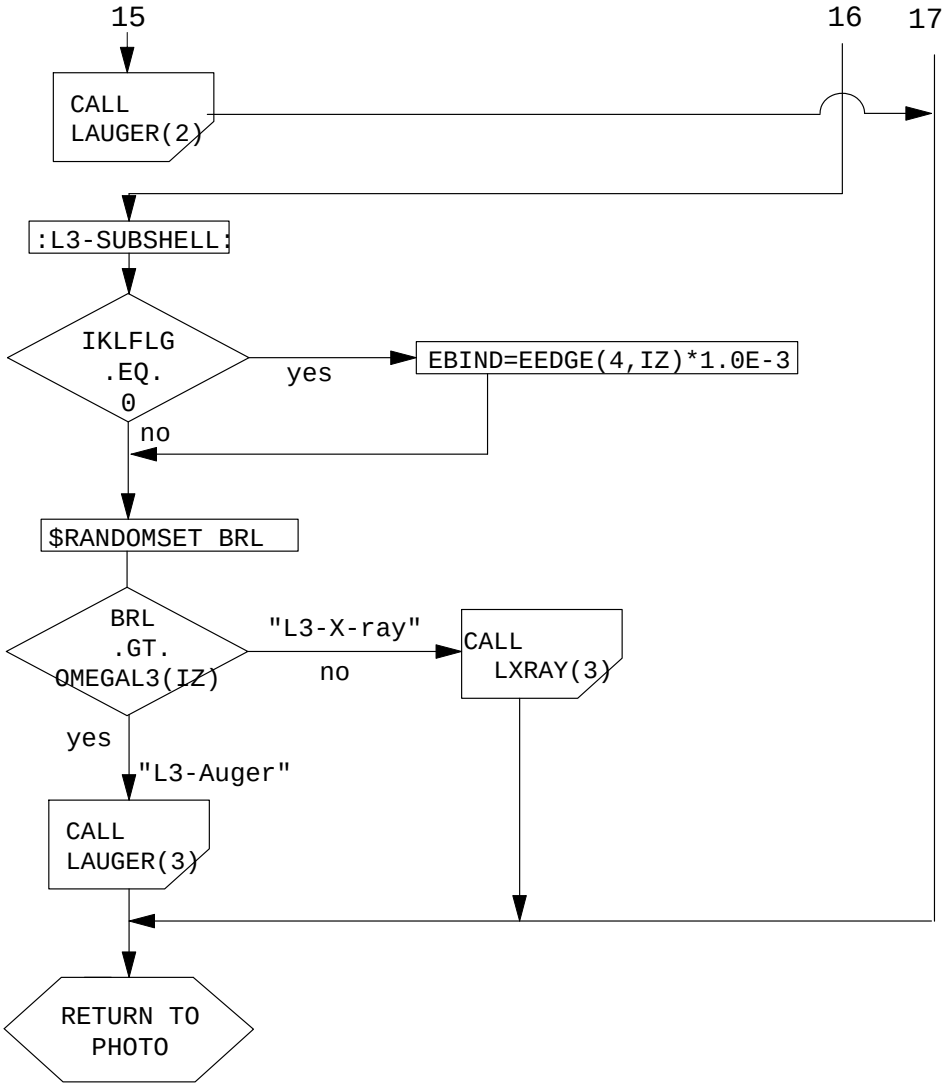

10
11
yes
IELEC=1
IELEC=IELEC+1
IELEC>NAUGER
yes
no
NP=NP+1
E(NP)=EAUGER(IELEC)+PRM
IQ(NP)=-1
$RANDOMSET RNISO
COSTHE=2.0*RNISO-1.0
SINTHE=SQRT(1.0-COSTHE*COSTHE)
U(NP)=0.0
V(NP)=0.0
W(NP)=1.0
CALL
UPHI(2,1)
$TRANSFER PROPERTIES TO (NP) FROM (NP-1)
NXRAY
.NE.
0
no
yes
IPHOT=1
IPHOT=IPHOT+1
IPHOT>NXRAY
yes
no
NP=NP+1
E(NP)=EXRAY(IPHOT)
IQ(NP)=0
$RANDOMSET RNISO
COSTHE=2.0*RNISO-1.0
SINTHE=SQRT(1.0-COSTHE*COSTHE)
U(NP)=0.0
V(NP)=0.0
W(NP)=1.0
CALL
UPHI(2,1)
$TRANSFER PROPERTIES TO (NP) FROM (NP-1)
RETURN TO
PHOTON

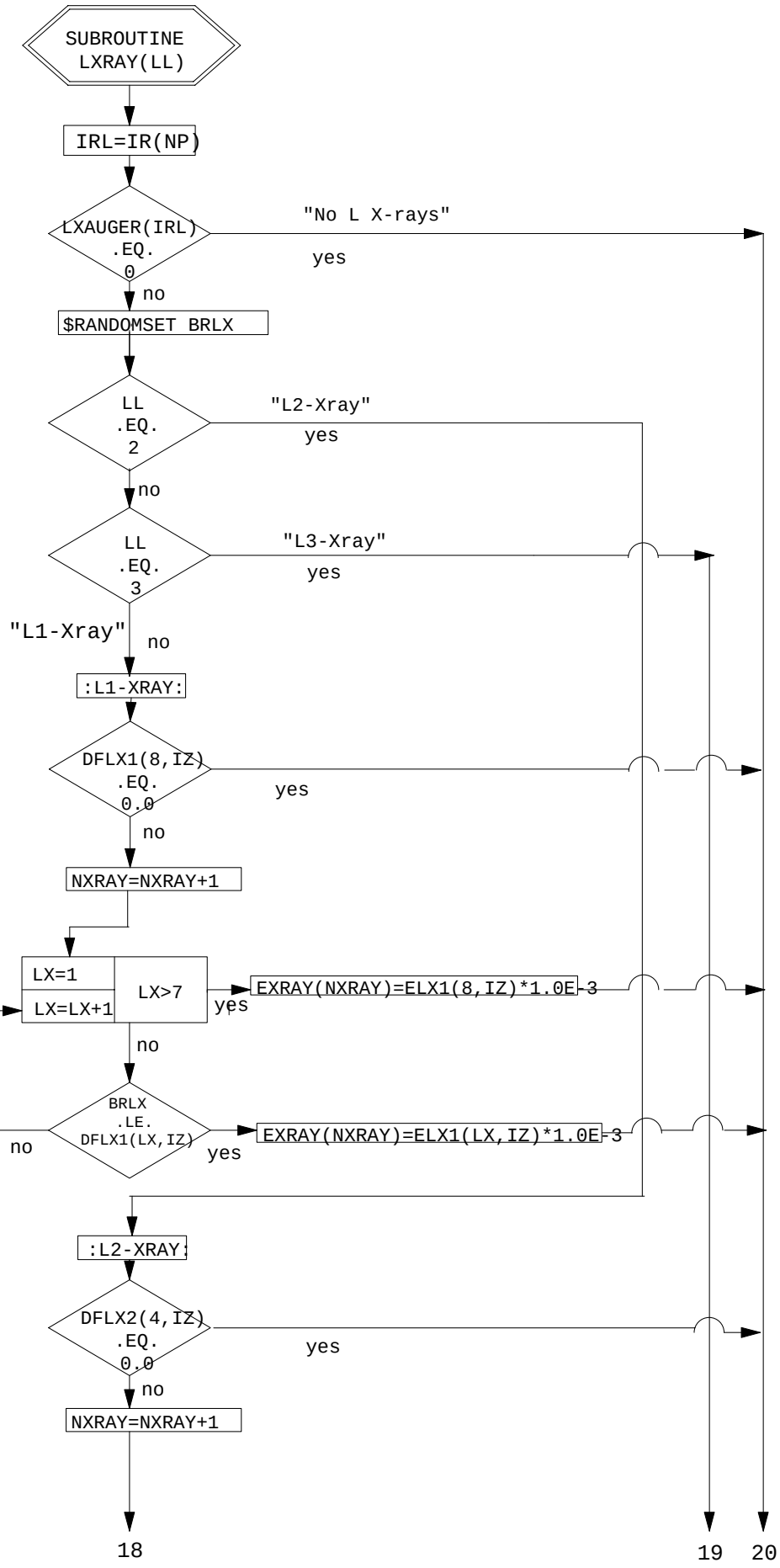

SUBROUTINE KSHELL
$RANDOMSET BRK
BRK .GT. OMEGAK(IZ)
"K-Auger"
yes
CALL KAUGER
no
"K-X-ray"
CALL KXRAY
RETURN TO PHOTO
SUBROUTINE KXRAY
DFKX(9,IZ) .EQ. 0.0
yes
"No K-Xray"
no
NXRAY=NXRAY+1
$RANDOMSET BRKX
IK=1
IK=IK+1
IK>10
yes
EXRAY(NXRAY)=EKX(10,IZ)*1.0E-3
no
BRKX .LE. DFKX(IK,IZ)
no
yes
EXRAY(NXRAY)=EKX(IK,IZ)*1.0E-3
IK .EQ. 1
"K=1"
yes
CALL LSHELL(3)
no
IK .EQ. 2
"K=2"
yes
CALL LSHELL(2)
no
10
11
12

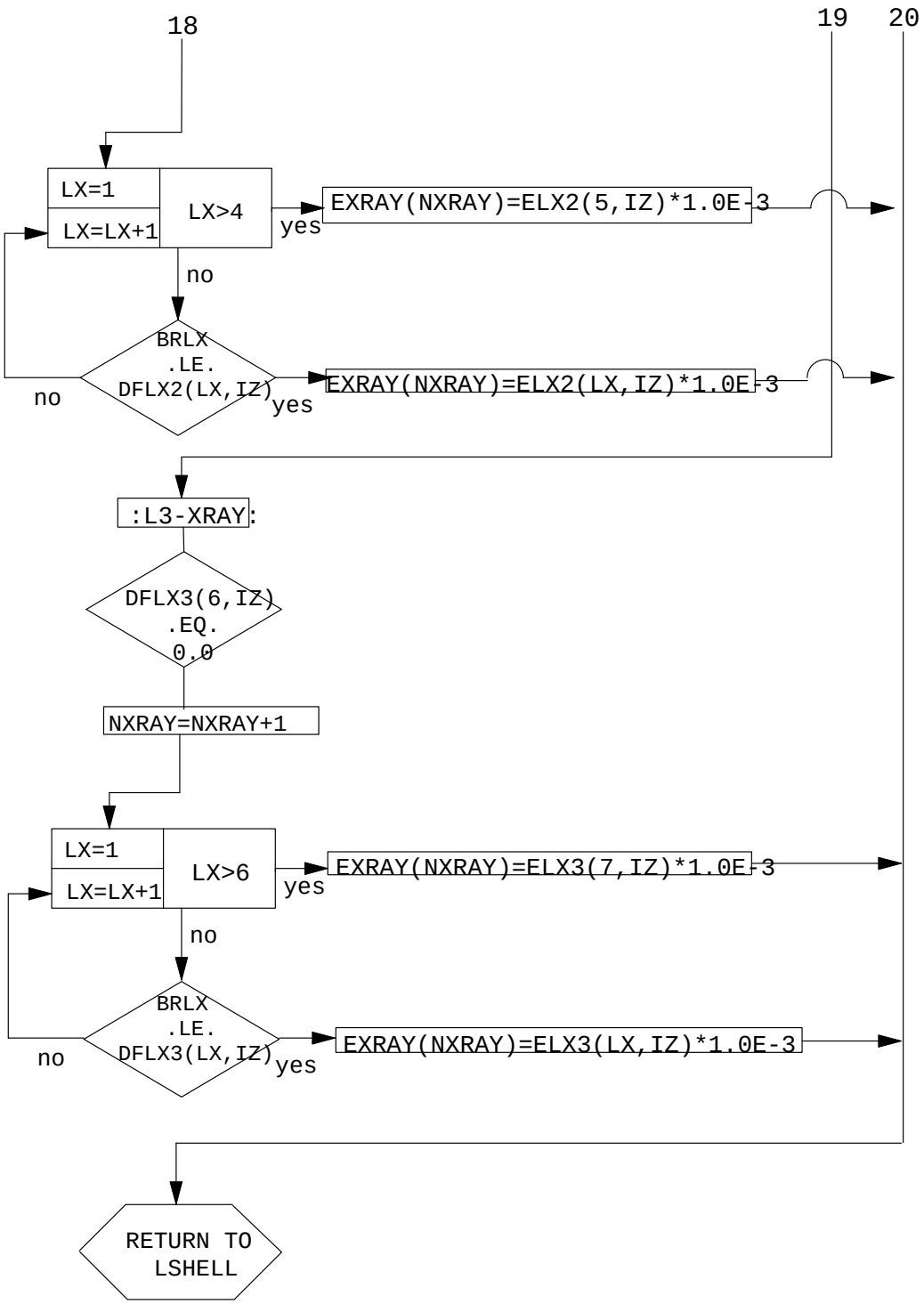

10
11
12
IK
.EQ.
3
"K=3"
yes
CALL
LSHELL(1)
no
RETURN TO
KSHELL
SUBROUTINE
KAUGER
DFKAUG(13,IZ)
.EQ.
0.0
"No K-Auger"
yes
no
NAUGER=NAUGER+1
$RANDOMSET EAUG
KAUG=1
KAUG=KAUG+1
KAUG>14
yes
EAUGER(NAUGER)=EKAUGE(14,IZ)*1.0E-3
no
EAUG
.LE.
DFKAUG(KAUG,IZ)
yes
no
EAUGER(NAUGER)=EKAUGE(KAUG,IZ)*1.0E-3
:CASCADE:
KAUG
.EQ.
1
"K-L1L1"
yes
CALL
LSHELL(1)
CALL
LSHELL(1)
no
KAUG
.EQ.
2
"K-L1L2"
yes
CALL
LSHELL(1)
CALL
LSHELL(2)
no
KAUG
.EQ.
3
"K-L1L3"
yes
CALL
LSHELL(1)
CALL
LSHELL(3)
no
KAUG
.EQ.
4
"K-L2L2"
yes
CALL
LSHELL(2)
CALL
LSHELL(2)
no
13
14

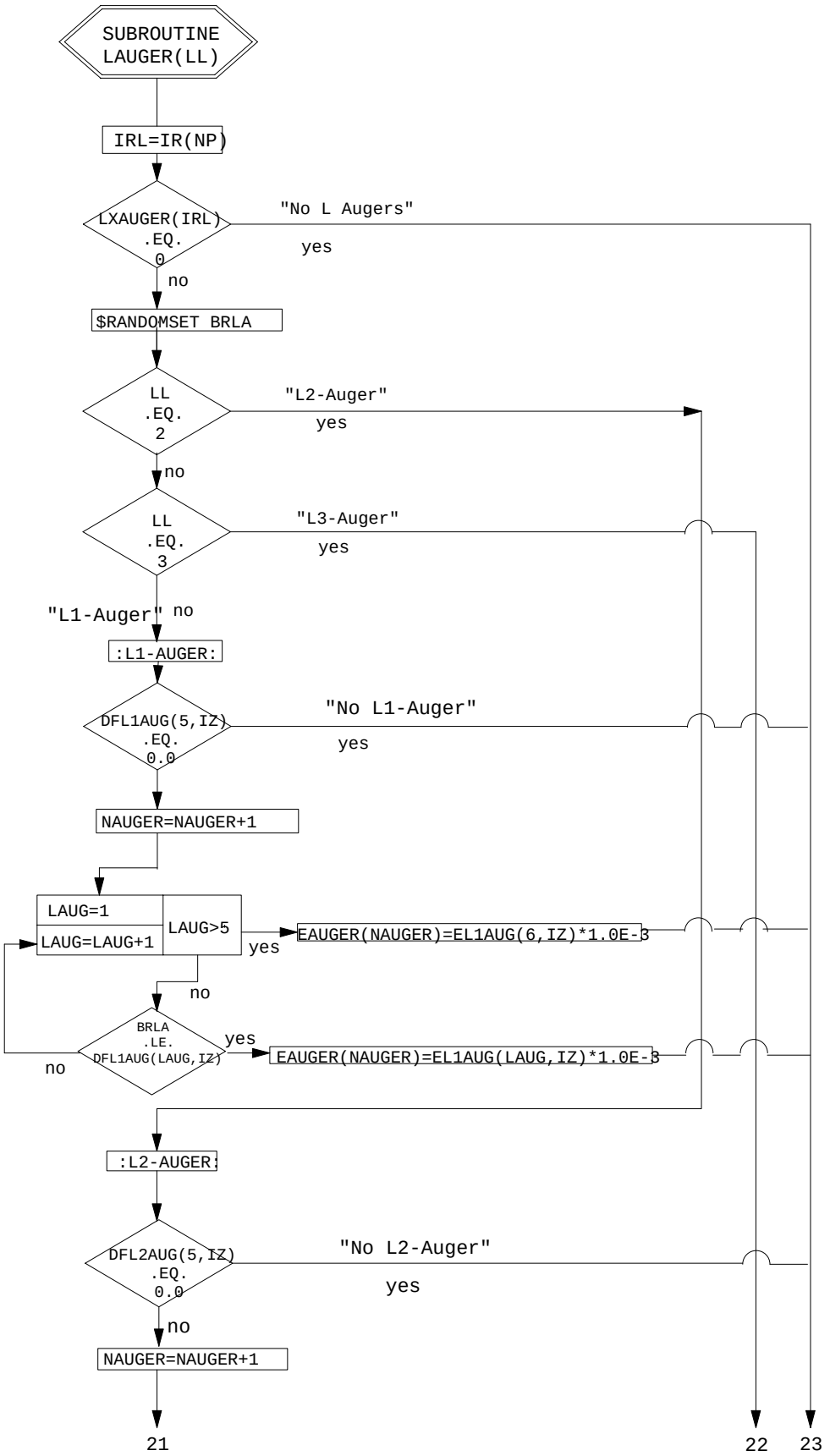

13
14
KAUG .EQ. 5
"K-L2L3"
yes
CALL LSHELL(2)
CALL LSHELL(3)
no
KAUG .EQ. 6
"K-L3L3"
yes
CALL LSHELL(3)
CALL LSHELL(3)
no
KAUG .EQ. 7
"K-L1M"
yes
CALL LSHELL(1)
no
KAUG .EQ. 10
"KL1N"
yes
no
KAUG .EQ. 8
"K-L2M"
yes
CALL LSHELL(2)
no
KAUG .EQ. 11
"KL2N"
yes
no
KAUG .EQ. 9
"K-L3M"
yes
CALL LSHELL(3)
no
KAUG .EQ. 12
"KL3N"
yes
no
RETURN TO KSHELL

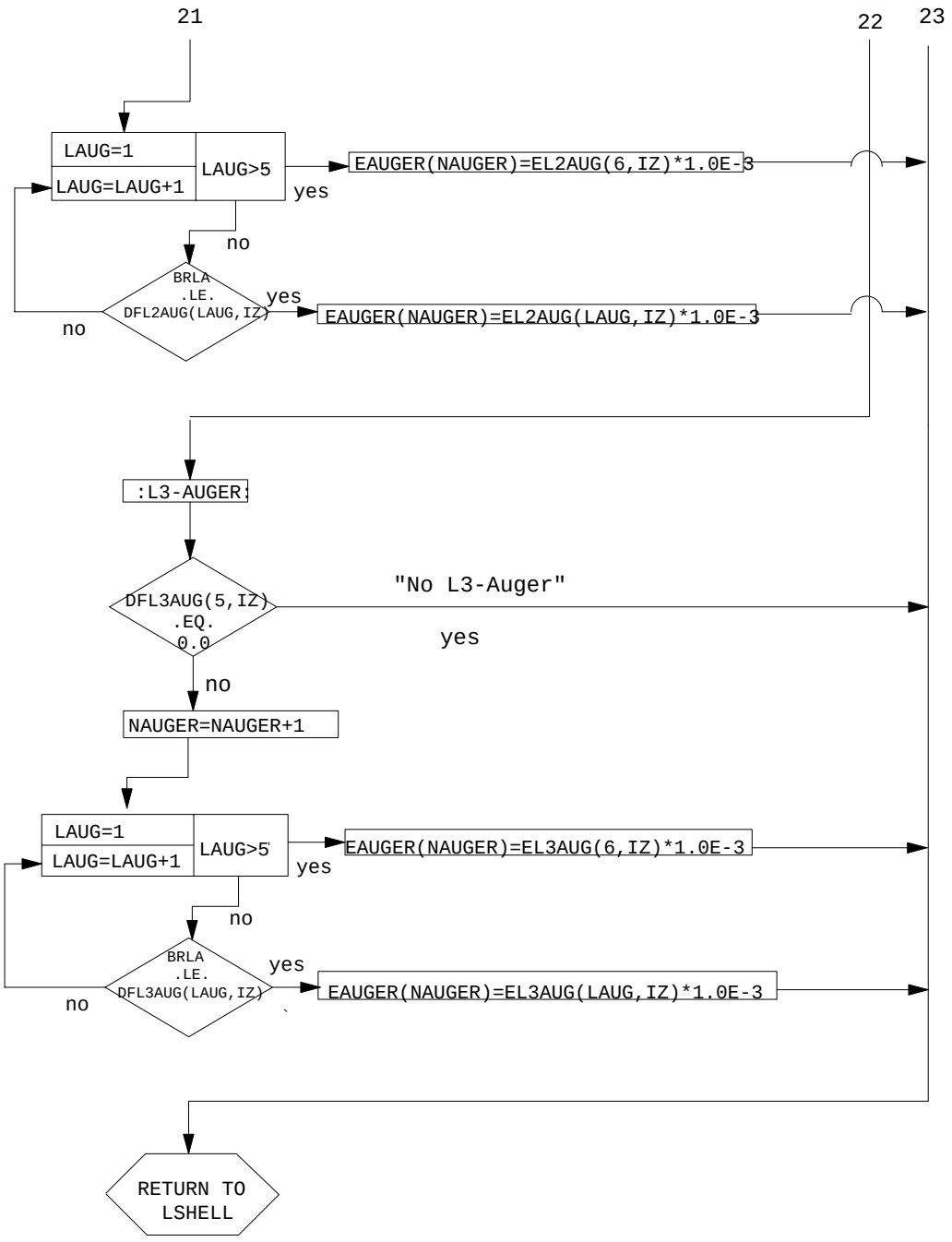

SUBROUTINE LSHELL(LL)
ICKFLG=0
LL .EQ. 2
"L2-hole is created"
yes
no
LL .EQ. 3
"L3-hole is created"
yes
no
"L1-hole is created"
$RANDOMSET BRL
EBIND=EEDGE(2,IZ)*1.0E-3
BRL .GT. OMEGAL1(IZ)
"L1-X-ray"
no
CALL LXRAY(1)
yes
BRL .LE. OMEGAL1(IZ)+ F12(IZ)
"Coster-Kronig f12"
yes
ICKFLG=1
no
BRL .LE. OMEGAL1(IZ)+F12(IZ) +F13(IZ)
"Coster-Kronig f13"
yes
ICKFLG=1
no
"L1-Auger"
CALL LAUGER(1)
:L2-SUBSHELL:
ICLFLG .EQ. 0
yes
EBIND=EEDGE(3,IZ)*1.0E-3
no
$RANDOMSET BRL
BRL .LE. OMEGAL2(IZ)
"L2-X-ray"
no
CALL LXRAY(2)
yes
BRL .LE. OMEGAL2(IZ)+ F23(IZ)
"Coster-Kronig f23"
yes
ICKFLG=1
no
15
16
17


15
16
17
CALL
LAUGER(2)
:L3-SUBSHELL:
IKLFLG
.EQ.
0
yes
EBIND=EEDGE(4,IZ)*1.0E-3
no
$RANDOMSET BRL
BRL
.GT.
OMEGAL3(IZ)
"L3-X-ray"
no
CALL
LXRAY(3)
yes
"L3-Auger"
CALL
LAUGER(3)
RETURN TO
PHOTO


SUBROUTINE
LXRAY(LL)
IRL=IR(NP)
LXAUGER(IRL)
.EQ.
0
"No L X-rays"
yes
no
$RANDOMSET BRLX
LL
.EQ.
2
"L2-Xray"
yes
no
LL
.EQ.
3
"L3-Xray"
yes
"L1-Xray"
no
:L1-XRAY:
DFLX1(8,IZ)
.EQ.
0.0
yes
no
NXRAY=NXRAY+1
LX=1
LX=LX+1
LX>7
EXRAY(NXRAY)=ELX1(8,IZ)*1.0E-3
yes
no
BRLX
.LE.
DFLX1(LX,IZ)
no
EXRAY(NXRAY)=ELX1(LX,IZ)*1.0E-3
yes
:L2-XRAY:
DFLX2(4,IZ)
.EQ.
0.0
yes
no
NXRAY=NXRAY+1
18
19
20


18
19
20
LX=1
LX=LX+1
LX>4
yes
EXRAY(NXRAY)=ELX2(5,IZ)*1.0E-3
no
BRLX
.LE.
DFLX2(LX,IZ)
no
yes
EXRAY(NXRAY)=ELX2(LX,IZ)*1.0E-3
:L3-XRAY:
DFLX3(6,IZ)
.EQ.
0.0
NXRAY=NXRAY+1
LX=1
LX=LX+1
LX>6
yes
EXRAY(NXRAY)=ELX3(7,IZ)*1.0E-3
no
BRLX
.LE.
DFLX3(LX,IZ)
no
yes
EXRAY(NXRAY)=ELX3(LX,IZ)*1.0E-3
RETURN TO
LSHELL


SUBROUTINE
LAUGER(LL)
IRL=IR(NP)
LXAUGER(IRL)
.EQ.
0
"No L Augers"
yes
no
$RANDOMSET BRLA
LL
.EQ.
2
"L2-Auger"
yes
no
LL
.EQ.
3
"L3-Auger"
yes
"L1-Auger" no
:L1-AUGER:
DFL1AUG(5,IZ)
.EQ.
0.0
"No L1-Auger"
yes
NAUGER=NAUGER+1
LAUG=1
LAUG=LAUG+1
LAUG>5
yes
EAUGER(NAUGER)=EL1AUG(6,IZ)*1.0E-3
no
BRLA
.LE.
DFL1AUG(LAUG,IZ)
yes
EAUGER(NAUGER)=EL1AUG(LAUG,IZ)*1.0E-3
no
:L2-AUGER:
DFL2AUG(5,IZ)
.EQ.
0.0
"No L2-Auger"
yes
no
NAUGER=NAUGER+1
21
22
23


21
22
23
LAUG=1
LAUG=LAUG+1
LAUG>5
yes
EAUGER(NAUGER)=EL2AUG(6,IZ)*1.0E-3
no
BRLA
.LE.
DFL2AUG(LAUG,IZ)
yes
no
EAUGER(NAUGER)=EL2AUG(LAUG,IZ)*1.0E-3
:L3-AUGER:
DFL3AUG(5,IZ)
.EQ.
0.0
"No L3-Auger"
yes
no
NAUGER=NAUGER+1
LAUG=1
LAUG=LAUG+1
LAUG>5
yes
EAUGER(NAUGER)=EL3AUG(6,IZ)*1.0E-3
no
BRLA
.LE.
DFL3AUG(LAUG,IZ)
yes
no
EAUGER(NAUGER)=EL3AUG(LAUG,IZ)*1.0E-3
RETURN TO
LSHELL