PROGRAM RELAX
A Code Designed to Calculate Atomic Relaxation Spectra of X-Rays and Electrons

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Introduction

The code RELAX is designed to calculate atomic relaxation spectra of X-rays and electrons due to bound-bound transitions. This calculation is based on the atomic transition data contained in the Livermore Evaluated Atomic Data Library (EADL).

The results produced by this code for fluorescence yield vs. atomic number (Z) have been published in "Tables and Graphs of Atomic Subshell and Relaxation Data Derived from the LLNL Evaluated Atomic Data Library (EADL), Z = 1 - 100", UCRL-50400, Vol. 30, October 31, 1991, Lawrence Livermore National Laboratory.

Code Documentation

This code is designed to be self-documenting, in the sense that the latest documentation for the code is included as comment lines at the beginning of the code. Printed documentation, such as this report, are periodically published and consists mostly of a copy of the comment lines from the beginning of the code. The user should be aware that the comment lines within the code are continuously updated to reflect the most recent status of the code and these comment lines should always be considered to be the most recent documentation for the code and may supercede published documentation, such as this report. Therefore the user is advised to always read the documentation within the actual code.

The remainder of this report consists of a listing of the documentation which appears at the beginning of the RELAX code and example output. The example output is for the K-shell of uranium and includes the output report as well as graphs of the emission spectra.

Comments from RELAX

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C     PROGRAM RELAX(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE10,        REL00010
C    1 TAPE11,TAPE12,TAPE14,TAPE15)                                      REL00020
C                                                                        REL00030
C     PROGRAM RELAX                                                      REL00040
C     VERSION 90-1 (DECEMBER 1990)                                       REL00050
C     VERSION 91-1 (NOVEMBER 1991)*UPDATED TO PERFORM CALCULATIONS 2     REL00060
C                                  SEPARATE WAYS AND INSURE COMPLETE     REL00070
C                                  NUMBER OF PARTICLES AND ENERGY        REL00080
C                                  BALANCE.                              REL00090
C                                                                        REL00100
C     WRITTEN BY DERMOTT E. CULLEN                                       REL00110
C                LAWRENCE LIVERMORE NATIONAL LABORATORY                  REL00120
C                L-298                                                   REL00130
C                P.O. BOX 808                                            REL00140
C                LIVERMORE, CA 94550                                     REL00150
C                U.S.A.                                                  REL00160
C     TELEPHONE  415-423-7359                                            REL00170
C                                                                        REL00180
C     PURPOSE                                                            REL00190
C     ================================================================REL00200
C     THIS PROGRAM IS DESIGNED TO CALCULATE ATOM RELAXATION SPECTRA OF   REL00210
C     X-RAYS AND ELECTRONS DUE TO BOUND-BOUND TRANSITIONS. THIS          REL00220
C     CALCULATION IS BASED ON THE ATOM TRANSITION DATA CONTAINED IN      REL00230
C     THE LIVERMORE EVALUATED ATOMIC DATA LIBRARY (EADL).                REL00240
C                                                                        REL00250
C     THE PROGRAM WILL ALSO CALCULATE THE SPECTRUM OF FREE-BOUND         REL00260
C     TRANSITIONS ASSUMING THAT THE ATOM WILL RELAX BACK TO IT NEUTRAL   REL00270
C     GROUND STATE BY FILLING ALL REMAINING ELECTRON HOLES THROUGH       REL00280
C     TRANSITIONS CAPTURING ELECTRONS DIRECTLY FROM THE CONTINUUM.       REL00290
C                                                                        REL00300
C     THIS PROGRAM WILL ALSO CALCULATE SUBSHELL AVERAGED VALUES, SUCH    REL00310
C     AS TOTAL ENERGY TO X-RAYS, ELECTRONS AND FREE-BOUND, AVERAGE       REL00320
C     NUMBER OF EMITTED X-RAYS, ELECTRONS AND FREE-BOUND TRANSITIONS     REL00330
C     AND AVERAGE ENERGY OF X-RAYS, ELECTRONS AND FREE-BOUND TRANSITIONSREL00340
C                                                                        REL00350
C     THE SUM OF THE TOTAL ENERGY TO X-RAYS, ELECTRONS AND FREE-BOUND    REL00360
C     IS EQUAL TO THE BINDING ENERGY OF THE SUBSHELL IN WHICH THE        REL00370
C     INITIAL VACANCY (HOLE) IS LOCATED. THE DIVISION OF ENERGY BETWEEN  REL00380
C     X-RAYS, ELECTRONS AND FREE-BOUND IS COMPLETELY DEFINED BY THE      REL00390
C     DATA IN EADL. HOWEVER, THE SPECTRUM OF FREE-BOUND TRANSITIONS      REL00400
C     IS NOT COMPLETELY DEFINED AND THE ASSUMPTION THAT IS USED HERE     REL00410
C     WILL CONSERVE THE TOTAL ENERGY OF THE SUM OF ALL FREE-BOUND        REL00420
C     TRANSITIONS AND PRODUCE THE HARDEST POSSIBLE SPECTRUM WITH THE     REL00430
C     FEWEST POSSIBLE EMITTED X-RAYS.                                    REL00440
C                                                                        REL00450
C     DESCRIPTION OF FINAL ATOM                                          REL00460
C     ================================================================REL00470
C     THIS PROGRAM CAN CALCULATE RESULTS FOR A FINAL ATOM,               REL00480
C                                                                        REL00490
C     1) NEUTRAL  - AS ELECTRONS ARE EJECTED FROM THE ATOMS, HOLES CAN   REL00500
C                   BE FILLED BY ELECTRONS FROM THE CONTINUUM (OUTSIDE   REL00510
C                   THE ATOM). IN THIS CASE TRANSITIONS CAN ALWAYS       REL00520
C                   OCCUR, SINCE WE ASSUME THAT AS ELECTRONS LEAVE A     REL00530
C                   SUBSHELL THEY ARE REPLACED BY ELECTRONS UNDERGOING   REL00540
C                   TRANSITIONS FROM ANOTHER SUBSHELL OR THE CONTINUUM,  REL00550
C                   I.E., WE HAVE AN INFINITE SUPPLY OF ELECTRONS        REL00560
C                   AVAILABLE. IN THIS CASE THE SET OF EQUATIONS HAS A   REL00570
C                   UNIQUE SOLUTION.                                     REL00580
C                                                                        REL00590
C     2) ISOLATED - HOLES CANNOT BE FILLED BY ELECTRONS FROM THE         REL00600
C                   CONTINUUM. IN THIS CASE TRANSITIONS BETWEEN          REL00610
C                   SUBSHELLS CAN ONLY OCCUR IF THERE ARE REMAINING      REL00620
C                   ELECTRONS IN THE SUBSHELL FROM WHICH THE ELECTRON    REL00630
C                   IS UNDERGOING A TRANSITION TO FILL A HOLE. IN THIS   REL00640
C                   CASE THERE WILL BE COMPETITION BETWEEN THE VARIOUS   REL00650
C                   SUBSHELLS FOR ELECTRON TRANSITIONS FROM ONE SUBSHELLREL00660
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C                TO FILL A HOLE IN ANOTHER SUBSHELL - IN THIS CASE   REL00670
C                THE SET OF EQUATIONS DOES NOT HAVE A UNIQUE SOLUTIONREL00680
C                - THIS PROGRAM WILL CALCULATE THE SOLUTION THAT     REL00690
C                CORRESPONDS TO THE MAXIMUM ENERGY RADIATED FROM THE REL00700
C                ATOM BY THE MINIMUM NUMBER OF X-RAYS AND ELECTRON   REL00710
C                BY GIVING PRIORITY TO INNER SUBSHELL TRANSITIONS    REL00720
C                OVER OUTER SUBSHELLS TO DEFINE THE COMPETITION.     REL00730
C                                                                    REL00740
C     ASSUMPTIONS                                                    REL00750
C     ===========================================================    REL00760
C     1) WE ASSUME THAT THE BINDING ENERGY OF THE NEUTRAL ATOMS IN THEIRREL00770
C        GROUND STATE IS THE SAME AS THE BINDING ENERGY IN ANY IONIZED REL00780
C        STATE - THIS ASSUMPTION IS BASED ON THE FACT THAT AS YET OUR  REL00790
C        DATA BASE - EADL - ONLY CONTAINS A SINGLE BINDING ENERGY TO   REL00800
C        DESCRIBE EACH SUBSHELL - AT THE CURRENT TIME IT IS BEYOND OUR REL00810
C        CAPABILITIES TO PROVIDE MORE EXTENSIVE SETS OF BINDING ENERGY REL00820
C        TO DESCRIBE ALL COMBINATIONS OF IONIZED STATES OF EACH ATOM.  REL00830
C                                                                     REL00840
C     2) WE ASSUME AN INITIAL CONDITION OF ONE SUBSHELL OF ONE ELEMENT REL00850
C        TO BE SINGLY IONIZED AND THEN DESCRIBE THE RELAXATION DUE TO  REL00860
C        BOUND-BOUND TRANSITIONS. WE DO NOT CONSIDER EXCITED ATOMS AND REL00870
C        EADL DOES NOT UNIQUELY DEFINE FREE-BOUND TRANSITIONS.         REL00880
C                                                                     REL00890
C     3) WE ASSUME THAT THE RADIATIVE AND NON-RADIATIVE TRANSITION    REL00900
C        DATA IS IN UPPER TRIANGLAR FORM BASED ON ASCENDING SUBSHELL   REL00910
C        INDEX - I.E., NO TRANSITIONS BETWEEN SUBSHELL I AND SUBSHELL  REL00920
C        K IF I IS GREATER THAN OR EQUAL TO K. THIS CONDITION IS       REL00930
C        SATIFIED BY THE ENTIRE EADL DATA BASE AS OF DECEMBER 1990.    REL00940
C                                                                     REL00950
C     ENERGY OF EMITTED X-RAYS AND ELECTRONS                          REL00960
C     ===========================================================    REL00970
C     FOR A RADIATIVE TRANSITION BETWEEN SUBSHELLS I AND K THE ENERGY REL00980
C     OF THE EMITTED X-RAY IS DEFINED TO BE,                          REL00990
C                                                                     REL01000
C     E(X-RAY)     = B.E.(K) - B.E.(I)                                REL01010
C                                                                     REL01020
C     B.E.(K)      = BINDING ENERGY OF AN ELECTRON IN THE K-TH SUBSHELL REL01030
C     B.E.(I)      = BINDING ENERGY OF AN ELECTRON IN THE I-TH SUBSHELL REL01040
C                                                                     REL01050
C     FOR A NON-RADIATIVE TRANSITION BETWEEN SUBSHELLS I AND K IN WHICH REL01060
C     AN ELECTRON IS EMITTED FROM SUBSHELL J THE ENERGY OF THE EMITTED REL01070
C     ELECTRON IS DEFINED TO BE,                                      REL01080
C                                                                     REL01090
C     E(ELECTRON) = B.E.(K) - (B.E.(I) + B.E.(J))                     REL01100
C                                                                     REL01110
C     UNCERTAINTY IN RESULTS                                          REL01120
C     ===========================================================    REL01130
C     SINCE THERE IS A UNCERTAINTY ASSOCIATED WITH EACH BINDING ENERGY REL01140
C     (B.E.) THERE WILL ALSO BE AN UNCERTAINTY ASSOCIATED WITH THE    REL01150
C     ENERGY OF THE EMITTED X-RAYS AND ELECTRONS. THE UNCERTAINTY IN  REL01160
C     THE BINDING ENERGY FOR GROUND STATE NEUTRAL ATOMS IS APPROXIMATELYREL01170
C     1 PER-CENT AND IS MORE FOR IONIZED ATOMS. THIS MEANS THAT FOR   REL01180
C     TRANSITIONS WHERE THE BINDING ENERGIES ARE ALMOST EQUAL THERE   REL01190
C     WILL BE A RATHER LARGE UNCERTAINTY IN THE EMISSION ENERGY OF THE REL01200
C     X-RAYS AND ELECTRONS. GENERALLY THIS WILL OCCUR FOR RATHER LOW  REL01210
C     ENERGY X-RAYS AND ELECTRONS, WHERE THE EMISSION ENERGY IS MUCH  REL01220
C     LESS THAN ANY OF THE BINDING ENERGIES INVOLVED IN THE TRANSITION, REL01230
C     E.G., FOR RADIATIVE, B.E.(K) ALMOST EQUAL TO B.E.(I), FOR       REL01240
C     NON-RADIATIVE, B.E.(K) ALMOST EQUAL TO B.E.(I)+B.E.(J).         REL01250
C                                                                     REL01260
C     NEGATIVE ENERGY ELECTRONS AND ENERGY RE-BALANCE                 REL01270
C     ===========================================================    REL01280
C     THE UNCERTAINTY IN THE BINDING ENERGY CAN RESULT IN TRANSITIONS REL01290
C     IN WHICH THE CALCULATED ENERGY OF EMITTED ELECTRONS CAN BE      REL01300
C     NEGATIVE, I.E. B.E.(I)+B.E.(J) EXCEEDS B.E.(K). IN THIS CASE    REL01310
C     THE TRANSITION CANNOT BE SIMPLY IGNORED, SINCE THE CREATION OF  REL01320
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C     HOLES DUE TO THESE TRANSITIONS CAN BE VERY IMPORTANT IN DEFINING  REL01330
C     THE NUMBER OF EMITTED X-RAYS AND ELECTRONS.                       REL01340
C                                                                       REL01350
C     IN THIS CODE WHEN THE CALCULATED ENERGY OF AN EMITTED ELECTRON    REL01360
C     IS NEGATIVE THE TRANSITION IS ALLOWED TO PROCEED AND THE ELECTRON REL01370
C     IS ASSIGNED AN ENERGY OF EXACTLY ZERO. THIS PROCEDURE HAS BEEN    REL01380
C     FOUND TO IN ALL CASES BE CONSISTENT WITH THE ASSUMED UNCERTAINTY  REL01390
C     IN THE BINDING ENERGIES, I.E., A CALCULATED NEGATIVE ELECTRON     REL01400
C     ENERGY REALLY INDICATES THE EMISSION OF A VERY LOW ENERGY ELECTRONREL01410
C     WITH A LARGE UNCERTAINTY IN ITS ENERGY - WHICH WE HERE DEFINE TO  REL01420
C     BE A ZERO ENERGY ELECTRON.                                        REL01430
C                                                                       REL01440
C     THIS PROCEDURE CAN RESULT IN THE LOSS OF AN ENERGY BALANCE. THE   REL01450
C     TOTAL ENERGY TO X-RAYS, ELECTRONS CAN BE DEFINED BY SUMMING OVER  REL01460
C     ALL TRANSITIONS THE PRODUCT OF THE EMISSION ENERGY AND THE        REL01470
C     TRANSITION PROBABILITY. SIMILARLY THE TOTAL ENERGY TO LOCAL (FREE-REL01480
C     BOUND) CAN BE DEFINED BY SUMMING OVER ALL ELECTRON HOLES THAT     REL01490
C     REMAIN = THE PRODUCT OF THE BINDING ENERGY AND THE NUMBER OF      REL01500
C     HOLES IN EACH SUBSHELL. THIS PROCEDURE RESULTS IN AN EXACT ENERGY REL01510
C     BALANCE, EXCEPT IN THE CASE WHERE WE HAVE ASSIGNED ZERO ENERGY    REL01520
C     TO ELECTRONS WHOSE CALCULATED EMISSION ENERGY IS NEGATIVE.        REL01530
C                                                                       REL01540
C     IN THE CASE WHEN WE ASSIGN ZERO ENERGY TO ELECTRONS THE RESULT    REL01550
C     IS THAT THE CACULATED ENERGY BALANCE AS THE SUM OF THE TOTAL      REL01560
C     X-RAY, ELECTRON AND LOCAL ENERGIES EXCEEDS THE BINDING ENERGY,    REL01570
C     I.E., WE DO NOT HAVE AN ENERGY BALANCE.                           REL01580
C                                                                       REL01590
C     TO ACHIEVE AN ENERGY BALANCE WE CALCULATE THE TOTAL ENERGY TO     REL01600
C     X-RAYS AND ELECTRONS AND DEFINE THE LOCAL ENERGY TO BE THE        REL01610
C     DIFFERENCE BETWEEN THIS SUM AND THE BINDING ENERGY. IN ORDER      REL01620
C     TO HAVE THE CALCULATED LOCAL ENERGY BASED ON REMAINING HOLES      REL01630
C     AND BINDING ENERGIES BE EQUAL TO THE CALCULATED LOCAL ENERGY      REL01640
C     BASED ON THE BINDING ENERGY MINUS THE SUM OF THE TOTAL ENERGY     REL01650
C     TO X-RAYS AND ELECTRONS, WE DEFINE THE ENERGY OF FREE-BOUND       REL01660
C     TRANSITIONS TO BE SLIGHTLY LESS THAN THE BINDING ENERGY, BY       REL01670
C     AN AMOUNT CORRESPONDING TO THE RATIO OF THE LOCAL ENERGY          REL01680
C     CALCULATED BY THE TWO METHODS - THUS FORCING AN ENERGY BALANCE.   REL01690
C                                                                       REL01700
C     GENERALLY WHEN NEGATIVE ENERGY ELECTRONS OCCUR THE SUM OF         REL01710
C     THEIR ENERGIES IS ONLY A SMALL FRACTION OF 1 PER-CENT OF THE      REL01720
C     BINDING ENERGY, I.E., MUCH LESS THAN THE UNCERTAINTY IN THE       REL01730
C     BINDING ENERGIES. THEREFORE THIS RE-BALANCE PROCEDURE WILL        REL01740
C     GENERALLY SHIFT THE FREE-BOUND EMISSION ENERGIES BY ONLY A        REL01750
C     SMALL FRACTION OF 1 PER-CENT, MUCH LESS THAN THE UNCERTAINTY      REL01760
C     IN THE BINDING ENERGY AND AS SUCH OF NO PRACTICAL CONCERN.        REL01770
C                                                                       REL01780
C     NOTE - THIS RE-BALANCE SHOULD NEVER BE ACHIEVED BY CHANGING       REL01790
C     THE NUMBER OF REMAINING HOLES IN EACH SUBSHELL, BECAUSE THESE     REL01800
C     HOLES ARE REQUIRED TO EVENTUALLY RETURN THE ATOM TO EXACT         REL01810
C     NEUTRALITY.                                                       REL01820
C                                                                       REL01830
C     THIS ENERGY RE-BALANCE PROCEDURE, WHICH IS ONLY NECESSARY WHEN    REL01840
C     USING THE BINDING ENERGIES WOULD LEAD TO THE EMISSION OF A        REL01850
C     NON-PHYSICAL NEGATIVE ENERGY ELECTRON, IS CONSISTENT WITH THE     REL01860
C     KNOWN UNCERTAINTY IN THE BINDING ENERGIES.                        REL01870
C                                                                       REL01880
C     INPUT ENDL FORMAT                                                 REL01890
C     ================================================================REL01900
C     THIS PROGRAM ONLY USES THE ENDL CHARACTER OR CARD IMAGE FORMAT    REL01910
C     (AS OPPOSED TO THE BINARY FORMAT). THE SOURCE OF ALL EVALUATED    REL01920
C     DATA USED BY THIS PROGRAM IS THE LIVERMORE EVALUATED ATOMIC DATA  REL01930
C     LIBRARY (EADL).                                                   REL01940
C                                                                       REL01950
C     PROGRAM OPERATION                                                 REL01960
C     ================================================================REL01970
C     BY INPUT PARAMETERS THE USER FIRST SELECTS OUTPUT OPTIONS (SEE,   REL01980
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C     DEFINITIONS BELOW). NEXT THE USER SPECIFIES A RANGE OF ELEMENTS   REL01990
C     AND SUBSHELLS TO PROCESS.                                         REL02000
C                                                                       REL02010
C     THE SPECTRA FOR EACH REQUESTED ELEMENT/SUBSHELL ARE CALCULATED    REL02020
C     SEPARATELY AND ARE ONLY AVAILABLE IN CORE BEFORE THE SPECTRA FOR  REL02030
C     THE NEXT ELEMENT/SUBSHELL ARE CALCULATED. SUBSHELL AVERAGED       REL02040
C     PARAMETERS ARE ACCUMULATED FOR EACH ELEMENT SEPARATELY AND ARE    REL02050
C     ONLY AVAILABLE IN CORE BEFORE CALCULATIONS START ON THE NEXT      REL02060
C     ELEMENT.                                                          REL02070
C                                                                       REL02080
C     ONCE THE ENTIRE USER SPECIFIED RANGE OF ELEMENTS AND SUBSHELLS    REL02090
C     HAVE BEEN PROCESSD THE PROGRAM WILL ATTEMPT TO READ THE NEXT      REL02100
C     USER SPECIFIED RANGE OF ELEMENTS AND SUBSHELLS. CALCULATIONS      REL02110
C     WILL CONTINUE UNTIL AN END OF FILE IS READ ON THE INPUT FILE.     REL02120
C                                                                       REL02130
C     OUTPUT OPTIONS                                                    REL02140
C     ================================================================REL02150
C     THIS PROGRAM CONTAINS INPUT OPTIONS TO PRODUCE THE FOLLOWING      REL02160
C     OUTPUT,                                                           REL02170
C     1) A LISTING - A SUMMARY OF EACH SUBSHELL AND THE SPECTRA         REL02180
C     2) ENDL      - CALCULATE SUBSHELL AVERAGED VALUES AND NORMALIZED  REL02190
C                    TRANSITION DATA IN THE ENDL FORMAT                 REL02200
C     3) PLOTTAB   - SPECTRA IN THE PLOTTAB FORMAT WHICH CAN BE USED    REL02210
C                    WITH PROGRAM PLOTTAB TO OBTAIN PLOTS OF THE        REL02220
C                    RESULTS.                                           REL02230
C                                                                       REL02240
C     USER INTERFACE                                                    REL02250
C     ================================================================REL02260
C     IF YOU WISH TO OBTAIN RESULTS IN ANY OTHER FORM YOU MAY DO SO     REL02270
C     BY INSERTING CODING INTO SUBROUTINE USER1 AND/OR USER2. USER1     REL02280
C     IS CALLED AFTER THE SPECTRA HAVE BEEN CALCULATED FOR EACH         REL02290
C     SUBSHELL - IF YOU WANT THE SPECTRA THIS IS THE TIME AND PLACE     REL02300
C     TO GET THEM. USER2 IS CALLED AFTER ALL RESULTS HAVE BEEN          REL02310
C     CALCULATED FOR EACH ELEMENT - IF YOU WANT SUBSHELL AVERAGED       REL02320
C     RESULTS THIS IS THE TIME AND PLACE TO GET THEM.                   REL02330
C                                                                       REL02340
C     ALL VARIABLES OF INTEREST TO THE USERS ARE DESCRIBED BELOW.       REL02350
C                                                                       REL02360
C     I/O FILES                                                         REL02370
C     ================================================================REL02380
C     INPUT FILES                                                       REL02390
C     -----------                                                       REL02400
C     UNIT  FILENAME     DESCRIPTION                                    REL02410
C     ----  --------     -----------                                    REL02420
C       5   RELAX.INP    INPUT PARAMETERS                               REL02430
C      10   ENDL.IN      ENDL FORMATTED DATA                            REL02440
C                                                                       REL02450
C     OUTPUT FILES                                                      REL02460
C     -----------                                                       REL02470
C     UNIT  FILENAME     DESCRIPTION                                    REL02480
C     ----  --------     -----------                                    REL02490
C       6   RELAX.LST    OUTPUT LISTING                                 REL02500
C      11   ENDL.OUT     ENDL FORMATTED DATA                            REL02510
C      12   PLOTTAB.CUR  NORMALIZED INTEGRAL OF SPECTRA                 REL02520
C                        FLUORESCENCE YIELD VS. Z BY SUBSHELL           REL02530
C      14   PLOTTAB.PNT  SPECTRA POINT VALUES                           REL02540
C      15   PLOTTAB.INP  PLOTTAB INPUT PARAMETERS                       REL02550
C      17   PLOTTAB.FLU  FLUORESCENCE YIELD VS. Z BY SHELL              REL02560
C                                                                       REL02570
C     INPUT PARAMETERS                                                  REL02580
C     ================================================================REL02590
C     LINE  COLS.  FORMAT  DESCRIPTION                                  REL02600
C     ----  -----  ------  -----------                                  REL02610
C       1    1- 5    I5    LISTING OPTION                               REL02620
C                          = 0 - NO OUTPUT LISTING                      REL02630
C                          = 1 - SUMMARY OF EACH SUBSHELL - NO SPECTRA  REL02640
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C                                 = 2 - SUMMARY AND SPECTRA OF EACH SUBSHELL   REL02650
C            6-10     I5          ENDL OUTPUT OPTION                           REL02660
C                                 = 0 - NO ENDL OUTPUT                         REL02670
C                                 = 1 - ENDL OUTPUT                            REL02680
C           11-15     I5          SPECTRA AND INTEGRAL OPTION                  REL02690
C                                 = 0 - NO PLOTTAB OUTPUT                      REL02700
C                                 = 1 - PLOTTAB OUTPUT                         REL02710
C           16-20     I5          FLUORESCENCE VS. Z (BY SUBSHELL) OPTION      REL02720
C                                 = 0 - NO PLOTTAB OUTPUT                      REL02730
C                                 = 1 - PLOTTAB OUTPUT                         REL02740
C           21-25     I5          LISTING UNIT                                 REL02750
C                                 = 0 - TO FILE RELAX.LST                      REL02760
C                                 = 1 - ON-LINE - DO NOT OPEN RELAX.LST        REL02770
C     2-N    1- 5     I5          MINIMUM Z                                    REL02780
C            6-10     I5          MAXIMUM Z                                    REL02790
C           11-15     I5          MINIMUM SUBSHELL DESIGNATOR                  REL02800
C           16-20     I5          MAXIMUM SUBSHELL DESIGNATOR                  REL02810
C           21-25     I5          DESCRIPTION OF FINAL ATOM                    REL02820
C                                 = 0 - RETURN TO NEUTRALITY                   REL02830
C                                 = 1 - ISOLATED                               REL02840
C                                                                              REL02850
C     LINE 2 MAY BE REPEATED ANY NUMBER OF TIMES. EACH ELEMENT/SUBSHELL        REL02860
C     REQUEST WILL BE PROCESSED SEPARATELY AND PROCESSING WILL CONTINUE        REL02870
C     UNTIL AN END OF FILE IS READ ON THE INPUT FILE.                          REL02880
C                                                                              REL02890
C     THE MINIMUM AND MAXIMUM Z MUST BE BETWEEN 1 AND 100 AND THE              REL02900
C     MAXIMUM MUST BE EQUAL TO OR GREATER THAN THE MINIMUM. SIMILARLY          REL02910
C     THE MINIMUM AND MAXIMUM SUBSHELL DESIGNATORS MUST BE BETWEEN 1           REL02920
C     AND 61 AND THE MAXIMUM MUST BE EQUAL TO OR GREATER THAN THE              REL02930
C     MINIMUM. IF THE INPUT PARAMETERS DO NOT SATISFY THESE                    REL02940
C     CONDITIONS THE PROGRAM WILL TERMINATE EXECUTION.                         REL02950
C                                                                              REL02960
C     EXAMPLE INPUT NO. 1                                                      REL02970
C     -------------------                                                      REL02980
C     PROCESS THE ENTIRE EADL LIBRARY WITH ALL OUTPUT OPTIONS ON. THE          REL02990
C     FOLLOWING 2 INPUT LINES ARE REQUIRED,                                    REL03000
C                                                                              REL03010
C         2    1    1    1    0                                               REL03020
C         1  100    1   61    0                                               REL03030
C                                                                              REL03040
C     EXAMPLE INPUT NO. 2                                                      REL03050
C     -------------------                                                      REL03060
C     PROCESS THE MAGNESIUM (Z=12), K SHELL (SUBSHELL DESIGNATOR = 1)          REL03070
C     AND ONLY OUTPUT A FULL LISTING. THE FOLLOWING 2 INPUT LINES ARE          REL03080
C     REQUIRED,                                                                REL03090
C                                                                              REL03100
C         2    0    0    0    0                                               REL03110
C        12   12    1    1    0                                               REL03120
C                                                                              REL03130
C     EXAMPLE INPUT NO. 3                                                      REL03140
C     -------------------                                                      REL03150
C     PROCESS ALL SUBSHELLS OF Z = 6 THROUGH 10 AND 90 THROUGH 100.            REL03160
C     OUTPUT A SUMMARY OF EACH SUBSHELL AND PLOTTAB FORMATTED SPECTRA.         REL03170
C     THE FOLLOWING 3 INPUT LINES ARE REQUIRED,                                REL03180
C                                                                              REL03190
C         1    0    1    0    0                                               REL03200
C         6   10    1   61    0                                               REL03210
C        90  100    1   61    0                                               REL03220
C                                                                              REL03230
C      DEFINITION OF ENDL SUBSHELL DESIGNATORS                                 REL03240
C==============================================================================REL03250
C  1 = K (1s1/2)    17 = N23 (4p)     32 = O4 (5d3/2)   47 = P5 (6d5/2)       REL03260
C  2 = L (2)        18 = N2 (4p1/2)   33 = O5 (5d5/2)   48 = P67 (6f)         REL03270
C  3 = L1 (2s1/2)   19 = N3 (4p3/2)   34 = O67 (5f)     49 = P6 (6f5/2)      REL03280
C  4 = L23 (2p)     20 = N45 (4d)     35 = O6 (5f5/2)   50 = P7 (6f7/2)      REL03290
C  5 = L2 (2p1/2)   21 = N4 (4d3/2)   36 = O7 (5f7/2)   51 = P89 (6g)        REL03300
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C  6 = L3 (2p3/2)  22 = N5 (4d5/2)  37 = O89 (5g)    52 = P8 (6g7/2)    REL03310
C  7 = M (3)       23 = N67 (4f)    38 = O8 (5g7/2)  53 = P9 (6g9/2)    REL03320
C  8 = M1 (3s1/2)  24 = N6 (4f5/2)  39 = O9 (5g9/2)  54 = P1011 (6h)    REL03330
C  9 = M23 (3p)    25 = N7 (4f7/2)  40 = P (6)       55 = P10 (6h9/2)   REL03340
C 10 = M2 (3p1/2)  26 = O (5)       41 = P1 (6s1/2)  56 = P11 (6h11/2)  REL03350
C 11 = M3 (3p3/2)  27 = O1 (5s1/2)  42 = P23 (6p)    57 = Q (7)         REL03360
C 12 = M45 (3d)    28 = O23 (5p)    43 = P2 (6p1/2)  58 = Q1 (7s1/2)    REL03370
C 13 = M4 (3d3/2)  29 = O2 (5p1/2)  44 = P3 (6p3/2)  59 = Q23 (7p)      REL03380
C 14 = M5 (3d5/2)  30 = O3 (5p3/2)  45 = P45 (6d)    60 = Q2 (7p1/2)    REL03390
C 15 = N (4)       31 = O45 (5d)    46 = P4 (6d3/2)  61 = Q3 (7p3/2)    REL03400
C 16 = N1 (4s1/2)                                                       REL03410
C=======================================================================REL03420
C                                                                       REL03430
C     DEFINITION OF VARIABLES                                           REL03440
C     =======================================================================REL03450
C     BASIS DATA                                                        REL03460
C     -----------------------------------------------------------------REL03470
C     IZGET   = Z FOR ELEMENT (1 TO 100)                                REL03480
C     ISUBGT  = SUBSHELL INDEX (1 TO 61)                                REL03490
C     MAXSUB  = MAXIMUM SUBSHELL INDEX THAT MUST BE USED IN CALCULATION REL03500
C     MAXTRA  = MAXIMUM SUBSHELL INDEX THAT HAS TRANSITIONS TO IT       REL03510
C     ATWTGT  = ATOMIC WEIGHT OF ELEMENT IZGET                          REL03520
C     EBMEV   = SUBSHELL BINDING ENERGY (MEV)                           REL03530
C     EBEV    = SUBSHELL BINDING ENERGY (EV)                            REL03540
C     TR      = RADIATIVE TRANSITION PROBABILITIES                      REL03550
C     TNR     = NON-RADIATIVE TRANSITION PROBABILITIES                  REL03560
C     NSUBR   = RADIATIVE TRANSITIONS READ FLAG                         REL03570
C     NSUBN   = NON-RADIATIVE TRANSITIONS READ FLAG                     REL03580
C     -----------------------------------------------------------------REL03590
C     SPECTRA FOR ONE SUBSHELL - CALCULATED BY THIS CODE                REL03600
C     -----------------------------------------------------------------REL03610
C     ERO     = ENERGY OF RADIATIVE TRANSITION (EV)                     REL03620
C     PROBRO  = PROBABILITY OF RADIATIVE TRANSITION                     REL03630
C     NR      = NUMBER OF RADIATIVE TRANSITIONS                         REL03640
C     ENO     = ENERGY OF NON-RADIATIVE TRANSITION (EV)                 REL03650
C     PROBNO  = PROBABILITY OF NON-RADIATIVE TRANSITION                 REL03660
C     NN      = NUMBER OF NON-RADIATIVE TRANSITIONS                     REL03670
C     ELO     = ENERGY OF FREE-BOUND TRANSITION (EV)                    REL03680
C     PROBLO  = PROBABILITY OF FREE-BOUND TRANSITION                    REL03690
C     NL      = NUMBER OF FREE-BOUND TRANSITIONS                        REL03700
C     -----------------------------------------------------------------REL03710
C     AVERAGE VALUES FOR ALL SUBSHELLS - CALCULATED BY THIS CODE        REL03720
C     -----------------------------------------------------------------REL03730
C     OUTR    = AVERAGE NUMBER OF X-RAYS EMITTED                        REL03740
C     OUTN    = AVERAGE NUMBER OF ELECTRONS EMITTED                     REL03750
C     OUTL    = AVERAGE NUMBER OF FREE-BOUND TRANSITIONS                REL03760
C     OUTRE   = TOTAL EMITTED X-RAY ENERGY (EV)                         REL03770
C     OUTNE   = TOTAL EMITTED ELECTRON ENERGY (EV)                      REL03780
C     OUTLE   = TOTAL EMITTED FREE-BOUND ENERGY (EV)                    REL03790
C     OUTAVR  = AVERAGE EMITTED X-RAY ENERGY (EV)                       REL03800
C     OUTAVN  = AVERAGE EMITTED ELECTRON ENERGY (EV)                    REL03810
C     OUTAVL  = AVERAGE EMITTED FREE-BOUND ENERGY (EV)                  REL03820
C                                                                       REL03830
C     USING THE RESULTS                                                 REL03840
C     =======================================================================REL03850
C     AFTER RESULTS HAVE BEEN CALCULATED FOR EACH SUBSHELL SUBROUTINE   REL03860
C     USER1 IS CALLED - AT THIS POINT THE SPECTRA FOR THE SUBSHELL ARE  REL03870
C     AVAILABLE FOR USE.                                                REL03880
C                                                                       REL03890
C     AFTER RESULTS HAVE BEEN CALCULATED FOR ALL SUBSHELLS OF AN        REL03900
C     ELEMENT SUBROUTINE USER2 IS CALLED - AT THIS POINT THE AVERAGE    REL03910
C     VALUES FOR ALL SUBSHELLS OF THE ELEMENT ARE AVAILABLE FOR USE.    REL03920
C                                                                       REL03930
C***** COMPUTER DEPENDENT CODING ******                                 REL03940
C                                                                       REL03950
C     THE COMPUTER DEPENDENT CODING IN THIS PROGRAM INCLUDES,           REL03960
```

```
C                                                                       REL03970
C     (1) DOUBLE/SINGLE                                                 REL03980
C         TREAT ENERGY DEPENDENT VARIABLES IN SINGLE OR DOUBLE          REL03990
C         PRECISION. ON LONG WORD LENGTH COMPUTERS (E.G., CRAY)         REL04000
C         THIS PROGRAM CAN BE OPTIMIZED BY USING SINGLE PRECISION.      REL04010
C         ON SHORT WORD LENGTH COMPUTERS (E.G., IBM) DOUBLE             REL04020
C         PRECISION MUST - REPEAT MUST - BE USED IN ORDER TO OBTAIN     REL04030
C         ACCURATE RESULTS.                                             REL04040
C                                                                       REL04050
C     (2) CHARACTER/INTEGER                                             REL04060
C         ALL CHARACTER VARIABLES ARE TREATED AS CHARACTERS - THE OLDER REL04070
C         CONVENTION FOR COMPILERS WHICH DID NOT ALLOW CHARACTER TYPE   REL04080
C         VARIABLES - TREAT ALL AS INTEGERS - IS NOT SUPPORTED IN THIS  REL04090
C         PROGRAM.                                                      REL04100
C                                                                       REL04110
C     (3) STOP/EXIT                                                     REL04120
C         TERMINATE PROGRAM USING STOP OR CALL EXIT                     REL04130
C                                                                       REL04140
C     (4) SAVE                                                          REL04150
C         FORTRAN OPTION TO SAVE ALL VARIABLES BETWEEN SUBROUTINE       REL04160
C         CALLS - REQUIRED FOR SOME NEWER FORTRAN COMPILERS             REL04170
C                                                                       REL04180
C     ANY COMBINATION OF THESE OPTIONS CAN BE AUTOMATICALLY TURNED ON ORREL04190
C     OFF USING PROGRAM CONVERT - CONTACT THE AUTHOR FOR A COPY OF THIS REL04200
C     PROGRAM.                                                          REL04210
C                                                                       REL04220
C***** COMPUTER DEPENDENT CODING ******                               REL04230
```

Example RELAX Output Report

This example is for the K-shell of uranium

Only a portion of the listing is included here. The complete listing includes 154 radiative and 2772 non-radiative bound-bound transitions and 10 free-bound transitions. The results have been edited to present here one page of example results for the radiative and non-radiative transitions.

From the enclosed listing we can see that the binding energy of a K-shell electron in uranium is 116.11 keV. We can also see that 89.5 % of this energy will be re-radiated as x-rays and most of these x-rays will be re-radiated with energies in the range 95 to 116 keV - just below the uranium K-edge, where the photoelectric cross section has a minimum, making these x-rays very penetrating.

Calculation of X-Ray and Electron Relaxation Spectra (RELAX 91-1)

Output Listing.....Full
ENDL Output.....No
Spectra and Integral.....Yes
Fluorescence Yield vs. Z by Subshell.....No
Listing Unit.....RELAX.LST

Process Z..... 92 through 92
Subshell..... 1 through 1
Description of Final Atom..... Neutral

92-U -Nat K (1s1/2) Ensemble Averaged Values per Initial Vacancy

Total Bound-Bound X-Ray Energy.....	103930.96 eV	89.5108 %
Total Bound-Bound Electron Energy.....	11381.38 eV	9.8022 %
Total Free-Bound X-Ray Energy (Local)...	797.66 eV	0.6870 %
Binding Energy (Sum of Above Terms).....	116110.00 eV	100.0000 %

Average Bound-Bound X-Ray Energy.....	72260.29 eV/X-Ray
Average Bound-Bound Electron Energy.....	1189.41 eV/Electron
Average Free-Bound X-Ray Energy.....	75.47 eV/X-Ray

Average Number of Bound-Bound X-Rays....	1.438286
Average Number of Bound-Bound Electrons.	9.568942
Average Number of Free-Bound X-Rays.....	10.568942

Distributions - Initial and Final after All Bound-Bound Transitions

Subshell	Binding Energy (eV)	Initial Electrons	Initial Holes	Final Electrons	Final Holes
K	116110.00	1.000000	1.000000	2.000000	0.000000
L1	21768.00	2.000000	0.000000	2.000000	0.000000
L2	21044.00	2.000000	0.000000	2.000000	0.000000
L3	17182.00	4.000000	0.000000	4.000000	0.000000
M1	5521.30	2.000000	0.000000	2.000000	0.000000
M2	5181.50	2.000000	0.000000	2.000000	0.000000
M3	4289.60	4.000000	0.000000	4.000000	0.000000
M4	3736.80	4.000000	0.000000	4.000000	0.000000
M5	3555.20	6.000000	0.000000	6.000000	0.000000
N1	1419.90	2.000000	0.000000	2.000000	0.000000
N2	1264.20	2.000000	0.000000	2.000000	0.000000
N3	1030.50	4.000000	0.000000	4.000000	0.000000
N4	778.18	4.000000	0.000000	4.000000	0.000000
N5	735.14	6.000000	0.000000	6.000000	0.000000
N6	402.09	6.000000	0.000000	6.000000	0.000000
N7	390.75	8.000000	0.000000	8.000000	0.000000
O1	320.65	2.000000	0.000000	2.000000	0.000000
O2	259.38	2.000000	0.000000	2.000000	0.000000
O3	203.39	4.000000	0.000000	4.000000	0.000000
O4	112.35	4.000000	0.000000	1.527173	2.472827
O5	104.02	6.000000	0.000000	1.705910	4.294090
O6	8.91	1.290000	0.000000	0.283758	1.006242
O7	7.95	1.710000	0.000000	0.562892	1.147108
P1	52.23	2.000000	0.000000	1.507922	0.492078
P2	34.09	2.000000	0.000000	1.552342	0.447658
P3	24.57	4.000000	0.000000	3.384672	0.615328
P4	4.74	0.400000	0.000000	0.379126	0.020874
P5	4.13	0.600000	0.000000	0.574716	0.025284
Q1	5.78	2.000000	0.000000	1.952547	0.047453
	Sum	91.000000	1.000000	81.431058	10.568942

Bound-Bound X-Ray Spectrum

Index	Emitted Energy (eV)	Probability per Initial Vacancy	Per-cent of Binding Energy	Transition
1	61.27	0.00000062	0.0000	O1 O2
2	91.04	0.00000103	0.0000	O3 O4
3	99.37	0.00001224	0.0000	O3 O5
4	117.26	0.00000894	0.0000	O1 O3
5	147.03	0.00002959	0.0000	O2 O4
		.		
		.		
		.		
		.		
		.		
112	17174.05	0.00000601	0.0001	L3 O7
113	17176.22	0.00001745	0.0003	L3 Q1
114	17307.20	0.10968770	1.6350	L2 M4
115	17478.40	0.00105765	0.0159	L1 M3
116	18031.20	0.00005622	0.0009	L1 M4
117	18212.80	0.00008378	0.0013	L1 M5
118	19624.10	0.00083786	0.0142	L2 N1
119	20013.50	0.00004800	0.0008	L2 N3
120	20265.82	0.02484217	0.4336	L2 N4
121	20503.80	0.00032863	0.0058	L1 N2
122	20641.91	0.00015447	0.0027	L2 N6
123	20723.35	0.00021515	0.0038	L2 O1
124	20737.50	0.00032725	0.0058	L1 N3
125	20840.61	0.00001174	0.0002	L2 O3
126	20931.65	0.00481117	0.0867	L2 O4
127	20989.82	0.00000957	0.0002	L1 N4
128	20991.77	0.00004431	0.0008	L2 P1
129	21019.43	0.00000201	0.0000	L2 P3
130	21032.86	0.00001535	0.0003	L1 N5
131	21035.09	0.00000344	0.0001	L2 O6
132	21038.22	0.00000504	0.0001	L2 Q1
133	21508.62	0.00007965	0.0015	L1 O2
134	21564.61	0.00008041	0.0015	L1 O3
135	21655.65	0.00000173	0.0000	L1 O4
136	21663.98	0.00000280	0.0001	L1 O5
137	21733.91	0.00001440	0.0003	L1 P2
138	21743.43	0.00001396	0.0003	L1 P3
139	95066.00	0.28926099	23.6835	K L2
140	98928.00	0.46281099	39.4324	K L3
141	110928.50	0.05337110	5.0989	K M2
142	111820.40	0.10438000	10.0524	K M3
143	112373.20	0.00186730	0.1807	K M4
144	112554.80	0.00213010	0.2065	K M5
145	114845.80	0.01334800	1.3203	K N2
146	115079.50	0.02700010	2.6760	K N3
147	115331.82	0.00054954	0.0546	K N4
148	115374.86	0.00062878	0.0625	K N5
149	115850.62	0.00326591	0.3259	K O2
150	115906.61	0.00647761	0.6466	K O3
151	115997.65	0.00011236	0.0112	K O4
152	116005.98	0.00012758	0.0128	K O5
153	116075.91	0.00058230	0.0582	K P2
154	116085.43	0.00109740	0.1097	K P3
	Sum	1.43828591	89.5108	

Bound-Bound Electron Spectrum

Index	Emitted Energy (eV)	Probability per Initial Vacancy	Per-cent of Binding Energy	Transition		
1	0.00	0.00012626	0.0000	L1	L2	N5
2	0.00	0.02092736	0.0000	M3	M5	N5
3	0.00	0.26399983	0.0000	O3	O5	O5
4	0.00	0.00057823	0.0000	N1	N3	N6
5	0.00	0.00182561	0.0000	N1	N3	N7
		.				
		.				
		.				
		.				
		.				
2736	114525.15	0.00000488	0.0005	K	N2	O1
2737	114577.75	0.00000013	0.0000	K	N1	O4
2738	114586.08	0.00000006	0.0000	K	N1	O5
2739	114586.42	0.00000028	0.0000	K	N2	O2
2740	114596.68	0.00000020	0.0000	K	N4	N5
2741	114639.72	0.00000006	0.0000	K	N5	N5
2742	114642.41	0.00000260	0.0003	K	N2	O3
2743	114677.41	0.00000003	0.0000	K	N3	N6
2744	114688.75	0.00000003	0.0000	K	N3	N7
2745	114733.45	0.00000013	0.0000	K	N2	O4
2746	114741.78	0.00000025	0.0000	K	N2	O5
2747	114758.85	0.00000184	0.0002	K	N3	O1
2748	114820.12	0.00000263	0.0003	K	N3	O2
2749	114876.11	0.00000260	0.0003	K	N3	O3
2750	114967.15	0.00000035	0.0000	K	N3	O4
2751	114975.48	0.00000025	0.0000	K	N3	O5
2752	115011.17	0.00000017	0.0000	K	N4	O1
2753	115054.21	0.00000009	0.0000	K	N5	O1
2754	115072.44	0.00000017	0.0000	K	N4	O2
2755	115115.48	0.00000028	0.0000	K	N5	O2
2756	115128.43	0.00000043	0.0000	K	N4	O3
2757	115171.47	0.00000032	0.0000	K	N5	O3
2758	115227.80	0.00000003	0.0000	K	N4	O5
2759	115262.51	0.00000003	0.0000	K	N5	O4
2760	115270.84	0.00000003	0.0000	K	N5	O5
2761	115468.70	0.00000074	0.0001	K	O1	O1
2762	115529.97	0.00000114	0.0001	K	O1	O2
2763	115585.96	0.00000043	0.0000	K	O1	O3
2764	115591.24	0.00000003	0.0000	K	O2	O2
2765	115647.23	0.00000060	0.0001	K	O2	O3
2766	115677.00	0.00000003	0.0000	K	O1	O4
2767	115685.33	0.00000003	0.0000	K	O1	O5
2768	115703.22	0.00000030	0.0000	K	O3	O3
2769	115738.27	0.00000003	0.0000	K	O2	O4
2770	115746.60	0.00000006	0.0000	K	O2	O5
2771	115794.26	0.00000009	0.0000	K	O3	O4
2772	115802.59	0.00000006	0.0000	K	O3	O5
	Sum	9.56894169	9.8022			

Free-Bound X-Ray Spectrum

Index	Emitted Energy (eV)	Probability per Initial Vacancy	Per-cent of Binding Energy	Transition
1	4.12	0.02528359	0.0001	P5
2	4.73	0.02087392	0.0001	P4
3	5.77	0.04745336	0.0002	Q1
4	7.94	1.14710813	0.0078	O7
5	8.89	1.00624157	0.0077	O6
6	24.52	0.61532770	0.0130	P3
7	34.03	0.44765811	0.0131	P2
8	52.13	0.49207822	0.0221	P1
9	103.83	4.29409049	0.3840	O5
10	112.14	2.47282659	0.2388	O4
	Sum	10.56894169	0.6870	

Bound-Bound X-Ray and Electron Spectra are based on EADL Relaxation data.

Free-Bound X-Ray Spectrum assumes the atom will return to neutrality by electron transitions directly from the continuum to fill all remaining electron holes, resulting in the emission of X-Rays with energy equal to the binding energy of the electron holes.

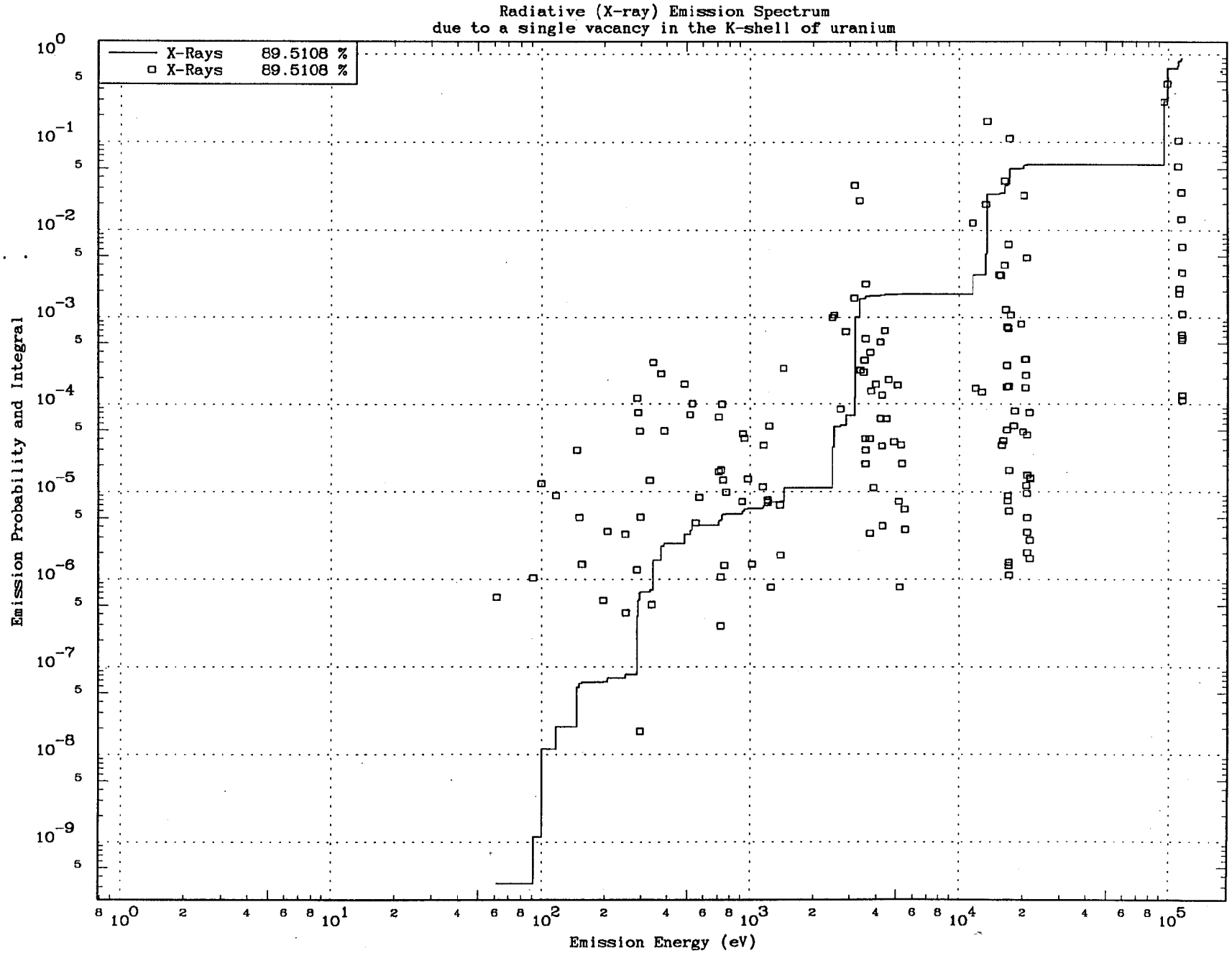
Example PLOTTAB graph of RELAX output results

This example is for the K-shell of uranium

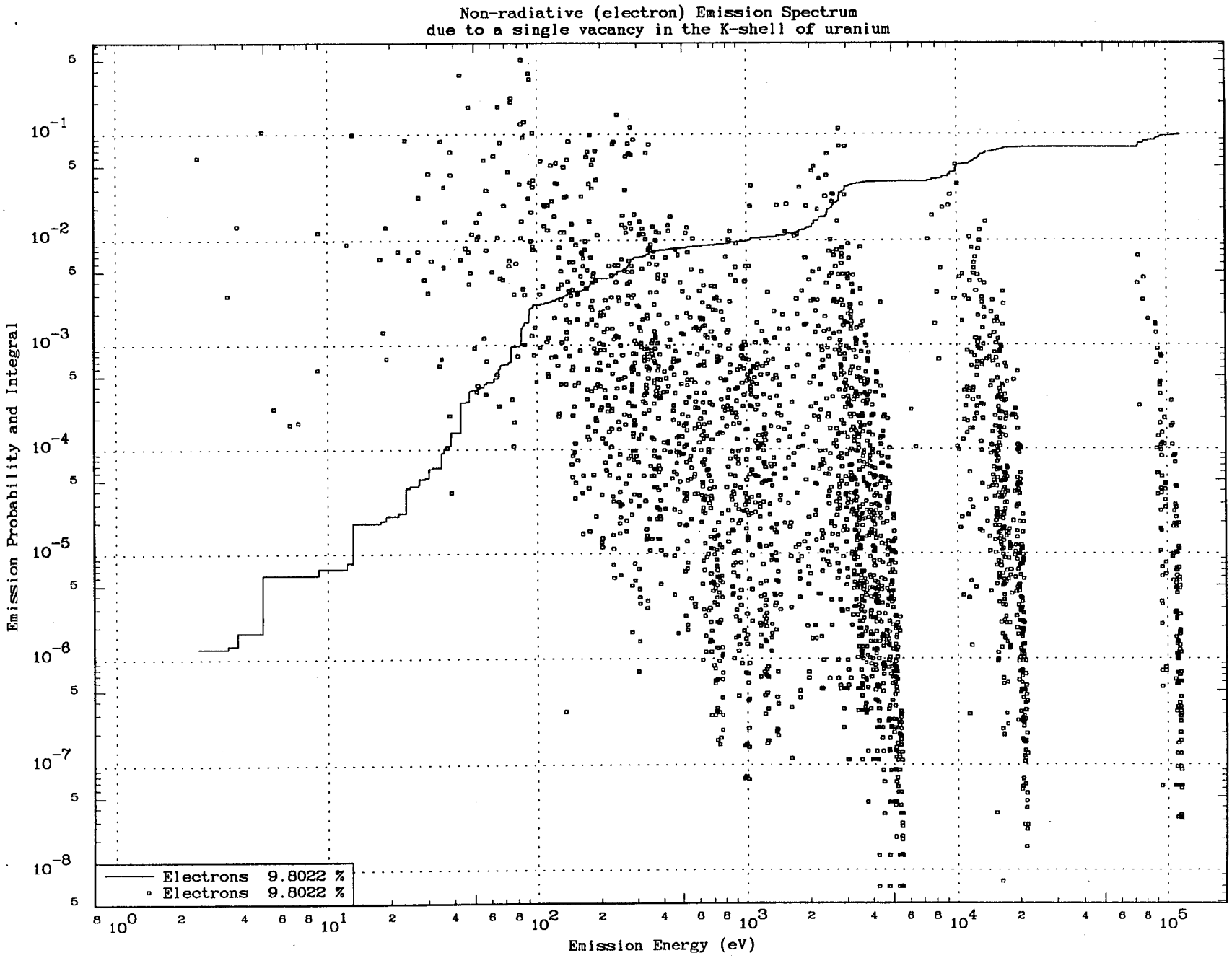
On these graphs the points represent the emission probability for individual x-rays or electrons. The curves represent the integral of the fraction of the binding energy of an electron in the K-shell of uranium.

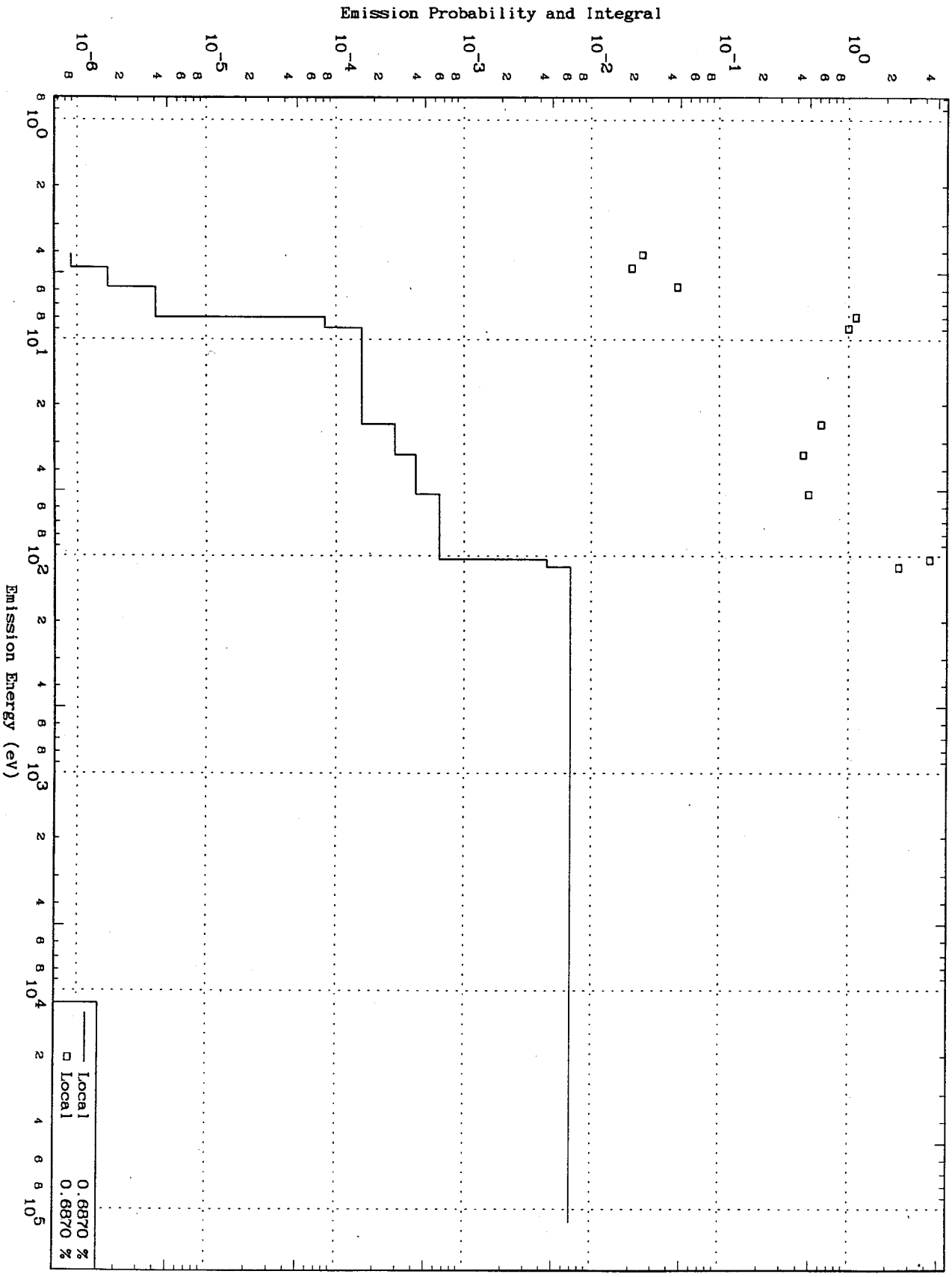
The legend box identifies the type of emission presented on each graph: x-ray, electron or local, respectively for the three graphs. In addition the legend box defines the fraction of the K-shell binding energy included in each spectrum: x-rays 89.5 %, electrons 9.8%, local 0.68%.

Consider a photon with an energy slightly higher than the binding energy of a K-shell electron in uranium. If this photon undergoes a photoelectric event with a uranium atom, the photon will disappear. An electron will be ejected from the K-shell with an energy equal to the difference between the energy of the photon and the binding energy of the electron. Then the atom will relax back to neutrality emitting x-rays and electrons with a combined energy equal to the binding energy of a K-shell electron. In this process most (89.5%) of the energy will be re-emitted as photons (x-rays). The result will be that rather than the initial photon and its energy disappearing (being deposited locally), most of the energy will be re-radiated and can transport a considerable distance.


Radiative (X-ray) Emission Spectrum
due to a single vacancy in the K-shell of uranium
X-Rays 89.5108 %
X-Rays 89.5108 %
Emission Probability and Integral
Emission Energy (eV)

12


Non-radiative (electron) Emission Spectrum
due to a single vacancy in the K-shell of uranium
Emission Probability and Integral
Emission Energy (eV)
Electrons 9.8022 %
Electrons 9.8022 %


Free-bound (X-ray) Emission Spectrum
due to a single vacancy in the K-shell of uranium
Emission Probability and Integral
Emission Energy (eV)
Local 0.6870 %
Local 0.6870 %

```
C     PROGRAM RELAX(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE10,
C    1 TAPE11,TAPE12,TAPE14,TAPE15,TAPE17,TAPE18)
C
C     PROGRAM RELAX
C     VERSION 90-1 (DECEMBER 1990)
C     VERSION 91-1 (NOVEMBER 1991)*UPDATED TO PERFORM CALCULATIONS 2
C                                  SEPARATE WAYS AND INSURE COMPLETE
C                                  NUMBER OF PARTICLES AND ENERGY
C                                  BALANCE.
C     VERSION 91-2 (MAY 1992)     *ADDED SUM OVER SUBSHELL TO DEFINE
C                                  EQUIVALENT SHELL RESULTS
C
C     WRITTEN BY DERMOTT E. CULLEN
C                LAWRENCE LIVERMORE NATIONAL LABORATORY
C                L-298
C                P.O. BOX 808
C                LIVERMORE, CA 94550
C                U.S.A.
C     TELEPHONE  415-423-7359
C
C     PURPOSE
C
C=====================================================================
C     THIS PROGRAM IS DESIGNED TO CALCULATE ATOM RELAXATION SPECTRA OF
C     X-RAYS AND ELECTRONS DUE TO BOUND-BOUND TRANSITIONS. THIS
C     CALCULATION IS BASED ON THE ATOM TRANSITION DATA CONTAINED IN
C     THE LIVERMORE EVALUATED ATOMIC DATA LIBRARY (EADL).
C
C     THE PROGRAM WILL ALSO CALCULATE THE SPECTRUM OF FREE-BOUND
C     TRANSITIONS ASSUMING THAT THE ATOM WILL RELAX BACK TO IT NEUTRAL
C     GROUND STATE BY FILLING ALL REMAINING ELECTRON HOLES THROUGH
C     TRANSITIONS CAPTURING ELECTRONS DIRECTLY FROM THE CONTINUUM.
C
C     THIS PROGRAM WILL ALSO CALCULATE SUBSHELL AVERAGED VALUES, SUCH
C     AS TOTAL ENERGY TO X-RAYS, ELECTRONS AND FREE-BOUND, AVERAGE
C     NUMBER OF EMITTED X-RAYS, ELECTRONS AND FREE-BOUND TRANSITIONS
C     AND AVERAGE ENERGY OF X-RAYS, ELECTRONS AND FREE-BOUND TRANSITIONS
C
C     THE SUM OF THE TOTAL ENERGY TO X-RAYS, ELECTRONS AND FREE-BOUND
C     IS EQUAL TO THE BINDING ENERGY OF THE SUBSHELL IN WHICH THE
C     INITIAL VACANCY (HOLE) IS LOCATED. THE DIVISION OF ENERGY BETWEEN
C     X-RAYS, ELECTRONS AND FREE-BOUND IS COMPLETELY DEFINED BY THE
C     DATA IN EADL. HOWEVER, THE SPECTRUM OF FREE-BOUND TRANSITIONS
C     IS NOT COMPLETELY DEFINED AND THE ASSUMPTION THAT IS USED HERE
C     WILL CONSERVE THE TOTAL ENERGY OF THE SUM OF ALL FREE-BOUND
C     TRANSITIONS AND PRODUCE THE HARDEST POSSIBLE SPECTRUM WITH THE
C     FEWEST POSSIBLE EMITTED X-RAYS.
C
C     DESCRIPTION OF FINAL ATOM
C
C=====================================================================
C     THIS PROGRAM CAN CALCULATE RESULTS FOR A FINAL ATOM,
```

```
C
C     1) NEUTRAL  - AS ELECTRONS ARE EJECTED FROM THE ATOMS, HOLES CAN
C                   BE FILLED BY ELECTRONS FROM THE CONTINUUM (OUTSIDE
C                   THE ATOM). IN THIS CASE TRANSITIONS CAN ALWAYS
C                   OCCUR, SINCE WE ASSUME THAT AS ELECTRONS LEAVE A
C                   SUBSHELL THEY ARE REPLACED BY ELECTRONS UNDERGOING
C                   TRANSITIONS FROM ANOTHER SUBSHELL OR THE CONTINUUM,
C                   I.E., WE HAVE AN INFINITE SUPPLY OF ELECTRONS
C                   AVAILABLE. IN THIS CASE THE SET OF EQUATIONS HAS A
C                   UNIQUE SOLUTION.
C
C     2) ISOLATED - HOLES CANNOT BE FILLED BY ELECTRONS FROM THE
C                   CONTINUUM. IN THIS CASE TRANSITIONS BETWEEN
C                   SUBSHELLS CAN ONLY OCCUR IF THERE ARE REMAINING
C                   ELECTRONS IN THE SUBSHELL FROM WHICH THE ELECTRON
C                   IS UNDERGOING A TRANSITION TO FILL A HOLE. IN THIS
C                   CASE THERE WILL BE COMPETITION BETWEEN THE VARIOUS
C                   SUBSHELLS FOR ELECTRON TRANSITIONS FROM ONE SUBSHELL
C                   TO FILL A HOLE IN ANOTHER SUBSHELL - IN THIS CASE
C                   THE SET OF EQUATIONS DOES NOT HAVE A UNIQUE SOLUTION
C                   - THIS PROGRAM WILL CALCULATE THE SOLUTION THAT
C                   CORRESPONDS TO THE MAXIMUM ENERGY RADIATED FROM THE
C                   ATOM BY THE MINIMUM NUMBER OF X-RAYS AND ELECTRON
C                   BY GIVING PRIORITY TO INNER SUBSHELL TRANSITIONS
C                   OVER OUTER SUBSHELLS TO DEFINE THE COMPETITION.
C
C     ASSUMPTIONS
C
C=====================================================================
C     1) WE ASSUME THAT THE BINDING ENERGY OF THE NEUTRAL ATOMS IN THEIR
C        GROUND STATE IS THE SAME AS THE BINDING ENERGY IN ANY IONIZED
C        STATE - THIS ASSUMPTION IS BASED ON THE FACT THAT AS YET OUR
C        DATA BASE - EADL - ONLY CONTAINS A SINGLE BINDING ENERGY TO
C        DESCRIBE EACH SUBSHELL - AT THE CURRENT TIME IT IS BEYOND OUR
C        CAPABILITIES TO PROVIDE MORE EXTENSIVE SETS OF BINDING ENERGY
C        TO DESCRIBE ALL COMBINATIONS OF IONIZED STATES OF EACH ATOM.
C
C     2) WE ASSUME AN INITIAL CONDITION OF ONE SUBSHELL OF ONE ELEMENT
C        TO BE SINGLY IONIZED AND THEN DESCRIBE THE RELAXATION DUE TO
C        BOUND-BOUND TRANSITIONS. WE DO NOT CONSIDER EXCITED ATOMS AND
C        EADL DOES NOT UNIQUELY DEFINE FREE-BOUND TRANSITIONS.
C
C     3) WE ASSUME THAT THE RADIATIVE AND NON-RADIATIVE TRANSITION
C        DATA IS IN UPPER TRIANGLAR FORM BASED ON ASCENDING SUBSHELL
C        INDEX - I.E., NO TRANSITIONS BETWEEN SUBSHELL I AND SUBSHELL
C        K IF I IS GREATER THAN OR EQUAL TO K. THIS CONDITION IS
C        SATIFIED BY THE ENTIRE EADL DATA BASE AS OF DECEMBER 1990.
C
C     ENERGY OF EMITTED X-RAYS AND ELECTRONS
C
C=====================================================================
C     FOR A RADIATIVE TRANSITION BETWEEN SUBSHELLS I AND J THE ENERGY
```

```
C     OF THE EMITTED X-RAY IS DEFINED TO BE,
C
C     E(X-RAY)    = B.E.(I) - B.E.(J)
C
C     FOR A NON-RADIATIVE TRANSITION BETWEEN SUBSHELLS I AND J IN WHICH
C     AN ELECTRON IS EMITTED FROM SUBSHELL K THE ENERGY OF THE EMITTED
C     ELECTRON IS DEFINED TO BE,
C
C     E(ELECTRON) = B.E.(I) - (B.E.(J) + B.E.(K))
C
C     TRANSITION PROBABILITIES
C
C=====================================================================
C     TRANSISTION PROBABILITIES ARE DEFINED BY 2 MATRICES
C
C     TR(I,J)    = RADIATIVE TRANSISTIONS    - AN ELECTRON TRANSITION
C                  J ---> I, ACCOMPANIED BY THE EMISSION OF A PHOTON,
C                  FILLING A VACANCY IN I, BUT CREATING A VACANCY IN J.
C     TNR(I,J,K) = NON-RADIATIVE TRANSITIONS - AN ELECTRON TRANSITION
C                  J ---> I, ACCOMPANIED BY THE EMISSION OF AN
C                  ELECTRON FROM K, FILLING A VACANCY IN I, BUT
C                  CREATING VACANCIES IN BOTH J AND K.
C
C     WHERE I, J, K REFER TO ATOM SUBSHELLS
C
C     THESE 2 MATRICES ARE DERIVED BY THIS CODE DIRECTLY FROM THE
C     EADL TRANSITION PROBABILITIES - INSURING EXACT NORMALIZATION
C     IN ORDER TO RETURN AN ATOM TO NEUTRALITY,
C
C     1 = SUM (OVER J) TR(I,J) + SUM (OVER J AND K) TNR(I,J,K)
C
C     I.E., ANY HOLE WILL ALWAYS BE EXACTLY FILLED.
C
C     THEREFORE THIS PROGRAM IS MERELY SOLVING A SET OF COUPLED MATRIX
C     EQUATIONS TO DEFINED THE EMITTED PHOTON AND ELECTRON SPECTRA.
C
C     FOR A SINGLE VACANCY IN SUBSHELL I, TR(I,J) AND TNR(I,J,K)
C     DEFINE BOTH WHAT IS EMITTED AS THE HOLE IN I IS FILLED - AND
C     WHAT HOLES WILL RESULT IN J AND K. THEREFORE STARTING FROM I
C     THIS CODE MUST SOLVE FOR ALL OF THE TRANSITIONS - BOTH DUE TO
C     PRIMARY EMISSION AS THE INITIAL VACANCY IS FILLED - AND ALL
C     SECONDARY HOLES (VACANCIES) THAT ARE CREATED DUE TO PRIMARY
C     TRANSITIONS. THIS IS ACCOMPLISHED BY STARTING WITH ONLY A SINGLE
C     VACANCY IN I, KEEPING TRACK OF ALL VACANCIES GENERATED IN OTHER
C     SUBSHELLS, AND WORKING FROM INNER (HIGHER ENERGY) SUBSHELL TO
C     THE OUTER MOST (LOWEST ENERGY) SUBSHELL, OF AN ATOM.
C
C     UNCERTAINTY IN RESULTS
C
C=====================================================================
C     SINCE THERE IS AN UNCERTAINTY ASSOCIATED WITH EACH BINDING ENERGY
C     (B.E.) THERE WILL ALSO BE AN UNCERTAINTY ASSOCIATED WITH THE
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C     ENERGY OF THE EMITTED X-RAYS AND ELECTRONS. THE BINDING ENERGIES
C     FOR GROUND STATE NEUTRAL ATOMS IS ABOUT 1 PER-CENT AND IS MORE
C     FOR IONIZED ATOMS. THIS IMPLIES THAT FOR TRANSITIONS WHERE THE
C     BINDING ENERGIES ARE ALMOST EQUAL THERE WILL BE A RATHER LARGE
C     UNCERTAINTY IN THE EMISSION ENERGY. GENERALLY THIS OCCURS FOR
C     LOW ENERGY X-RAYS AND ELECTRONS, WHERE THE EMISSION ENERGY IS
C     MUCH LESS THAN ANY OF THE BINDING ENERGIES INVOLVED IN THE
C     TRANSITION, E.G., FOR RADIATIVE, B.E.(K) ALMOST EQUAL TO B.E.(I),
C     FOR NON-RADIATIVE, B.E.(K) ALMOST EQUAL TO B.E.(I)+B.E.(J).
C
C     NEGATIVE ENERGY ELECTRONS AND ENERGY RE-BALANCE
C
================================================================
C     THE UNCERTAINTY IN THE BINDING ENERGY CAN RESULT IN TRANSITIONS
C     IN WHICH THE CALCULATED ENERGY OF EMITTED ELECTRONS CAN BE
C     NEGATIVE, I.E. B.E.(I)+B.E.(J) EXCEEDS B.E.(K). IN THIS CASE
C     THE TRANSITION CANNOT BE SIMPLY IGNORED, SINCE THE CREATION OF
C     HOLES DUE TO THESE TRANSITIONS CAN BE VERY IMPORTANT IN DEFINING
C     THE NUMBER OF EMITTED X-RAYS AND ELECTRONS.
C
C     IN THIS CODE WHEN THE CALCULATED ENERGY OF AN EMITTED ELECTRON
C     IS NEGATIVE THE TRANSITION IS ALLOWED TO PROCEED AND THE ELECTRON
C     IS ASSIGNED AN ENERGY OF EXACTLY ZERO. THIS PROCEDURE HAS BEEN
C     FOUND TO IN ALL CASES BE CONSISTENT WITH THE ASSUMED UNCERTAINTY
C     IN THE BINDING ENERGIES, I.E., A CALCULATED NEGATIVE ELECTRON
C     ENERGY REALLY INDICATES THE EMISSION OF A VERY LOW ENERGY ELECTRON
C     WITH A LARGE UNCERTAINTY IN ITS ENERGY - WHICH WE HERE DEFINE TO
C     BE A ZERO ENERGY ELECTRON.
C
C     THIS PROCEDURE CAN RESULT IN THE LOSS OF AN ENERGY BALANCE. THE
C     TOTAL ENERGY TO X-RAYS, ELECTRONS CAN BE DEFINED BY SUMMING OVER
C     ALL TRANSITIONS THE PRODUCT OF THE EMISSION ENERGY AND THE
C     TRANSITION PROBABILITY. SIMILARLY THE TOTAL ENERGY TO LOCAL (FREE-
C     BOUND) CAN BE DEFINED BY SUMMING OVER ALL ELECTRON HOLES THAT
C     REMAIN = THE PRODUCT OF THE BINDING ENERGY AND THE NUMBER OF
C     HOLES IN EACH SUBSHELL. THIS PROCEDURE RESULTS IN AN EXACT ENERGY
C     BALANCE, EXCEPT IN THE CASE WHERE WE HAVE ASSIGNED ZERO ENERGY
C     TO ELECTRONS WHOSE CALCULATED EMISSION ENERGY IS NEGATIVE.
C
C     IN THE CASE WHEN WE ASSIGN ZERO ENERGY TO ELECTRONS THE RESULT
C     IS THAT THE CACULATED ENERGY BALANCE AS THE SUM OF THE TOTAL
C     X-RAY, ELECTRON AND LOCAL ENERGIES EXCEEDS THE BINDING ENERGY,
C     I.E., WE DO NOT HAVE AN ENERGY BALANCE.
C
C     TO ACHIEVE AN ENERGY BALANCE WE CALCULATE THE TOTAL ENERGY TO
C     X-RAYS AND ELECTRONS AND DEFINE THE LOCAL ENERGY TO BE THE
C     DIFFERENCE BETWEEN THIS SUM AND THE BINDING ENERGY. IN ORDER
C     TO HAVE THE CALCULATED LOCAL ENERGY BASED ON REMAINING HOLES
C     AND BINDING ENERGIES BE EQUAL TO THE CALCULATED LOCAL ENERGY
C     BASED ON THE BINDING ENERGY MINUS THE SUM OF THE TOTAL ENERGY
C     TO X-RAYS AND ELECTRONS, WE DEFINE THE ENERGY OF FREE-BOUND
C     TRANSITIONS TO BE SLIGHTLY LESS THAN THE BINDING ENERGY, BY
```

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C     AN AMOUNT CORRESPONDING TO THE RATIO OF THE LOCAL ENERGY
C     CALCULATED BY THE TWO METHODS - THUS FORCING AN ENERGY BALANCE.
C
C     GENERALLY WHEN NEGATIVE ENERGY ELECTRONS OCCUR THE SUM OF
C     THEIR ENERGIES IS ONLY A SMALL FRACTION OF 1 PER-CENT OF THE
C     BINDING ENERGY, I.E., MUCH LESS THAN THE UNCERTAINTY IN THE
C     BINDING ENERGIES. THEREFORE THIS RE-BALANCE PROCEDURE WILL
C     GENERALLY SHIFT THE FREE-BOUND EMISSION ENERGIES BY ONLY A
C     SMALL FRACTION OF 1 PER-CENT, MUCH LESS THAN THE UNCERTAINTY
C     IN THE BINDING ENERGY AND AS SUCH OF NO PRACTICAL CONCERN.
C
C     NOTE - THIS RE-BALANCE SHOULD NEVER TO ACHIEVED BY CHANGING
C     THE NUMBER OF REMAINING HOLES IN EACH SUBSHELL BECAUSE THESE
C     HOLES ARE REQUIRED TO EVENTUALLY RETURN THE ATOM THE EXACT
C     NEUTRALITY.
C
C     THIS ENERGY RE-BALANCE PROCEDURE, WHICH IS ONLY NECESSARY WHEN
C     USING THE BINDING ENERGIES WOULD LEAD TO THE EMISSION OF A
C     NON-PHYSICAL NEGATIVE ENERGY ELECTRON, IS CONSISTENT WITH THE
C     KNOWN UNCERTAINTY IN THE BINDING ENERGIES.
C
C     INPUT ENDL FORMAT
C
C=====================================================================
C     THIS PROGRAM ONLY USES THE ENDL CHARACTER OR CARD IMAGE FORMAT
C     (AS OPPOSED TO THE BINARY FORMAT). THE SOURCE OF ALL EVALUATED
C     DATA USED BY THIS PROGRAM IS THE LIVERMORE EVALUATED ATOMIC DATA
C     LIBRARY (EADL).
C
C     PROGRAM OPERATION
C
C=====================================================================
C     BY INPUT PARAMETERS THE USER FIRST SELECTS OUTPUT OPTIONS (SEE,
C     DEFINITIONS BELOW). NEXT THE USER SPECIFIES A RANGE OF ELEMENTS
C     AND SUBSHELLS TO PROCESS.
C
C     THE SPECTRA FOR EACH REQUESTED ELEMENT/SUBSHELL ARE CALCULATED
C     SEPARATELY AND ARE ONLY AVAILABLE IN CORE BEFORE THE SPECTRA FOR
C     THE NEXT ELEMENT/SUBSHELL ARE CALCULATED. SUBSHELL AVERAGED
C     PARAMETERS ARE ACCUMULATED FOR EACH ELEMENT SEPARATELY AND ARE
C     ONLY AVAILABLE IN CORE BEFORE CALCULATIONS START ON THE NEXT
C     ELEMENT.
C
C     ONCE THE ENTIRE USER SPECIFIED RANGE OF ELEMENTS AND SUBSHELLS
C     HAVE BEEN PROCESSD THE PROGRAM WILL ATTEMPT TO READ THE NEXT
C     USER SPECIFIED RANGE OF ELEMENTS AND SUBSHELLS. CALCULATIONS
C     WILL CONTINUE UNTIL AN END OF FILE IS READ ON THE INPUT FILE.
C
C     OUTPUT OPTIONS
C
C=====================================================================
C     THIS PROGRAM CONTAINS INPUT OPTIONS TO PRODUCE THE FOLLOWING
```

```
C     OUTPUT,
C     1) A LISTING - A SUMMARY OF EACH SUBSHELL AND THE SPECTRA
C     2) ENDL      - CALCULATE SUBSHELL AVERAGED VALUES AND NORMALIZED
C                    TRANSITION DATA IN THE ENDL FORMAT
C     3) PLOTTAB   - SPECTRA IN THE PLOTTAB FORMAT WHICH CAN BE USED
C                    WITH PROGRAM PLOTTAB TO OBTAIN PLOTS OF THE
C                    RESULTS.
C
C     USER INTERFACE
C
=====================================================================
C     IF YOU WISH TO OBTAIN RESULTS IN ANY OTHER FORM YOU MAY DO SO
C     BY INSERTING CODING INTO SUBROUTINE USER1 AND/OR USER2. USER1
C     IS CALLED AFTER THE SPECTRA HAVE BEEN CALCULATED FOR EACH
C     SUBSHELL - IF YOU WANT THE SPECTRA THIS IS THE TIME AND PLACE
C     TO GET THEM. USER2 IS CALLED AFTER ALL RESULTS HAVE BEEN
C     CALCULATED FOR EACH ELEMENT - IF YOU WANT SUBSHELL AVERAGED
C     RESULTS THIS IS THE TIME AND PLACE TO GET THEM.
C
C     ALL VARIABLES OF INTEREST TO THE USERS ARE DESCRIBED BELOW.
C
C     I/O FILES
C
=====================================================================
C     INPUT FILES
C     -----------
C     UNIT  FILENAME     DESCRIPTION
C     ----  --------     -----------
C       5   RELAX.INP    INPUT PARAMETERS
C      10   ENDL.IN      ENDL FORMATTED DATA
C
C     OUTPUT FILES
C     -----------
C     UNIT  FILENAME          DESCRIPTION
C     ----  --------          -----------
C       6   RELAX.LST         OUTPUT LISTING
C      11   ENDL.OUT          ENDL FORMATTED DATA
C      12   PLOTTAB.CUR       NORMALIZED INTEGRAL OF SPECTRA
C                             FLUORESCENCE YIELD VS. Z BY SUBSHELL
C      14   PLOTTAB.PNT       SPECTRA POINT VALUES
C      15   PLOTTAB.INP       PLOTTAB INPUT PARAMETERS
C      17   PLOTTAB.CUR.SHELL PLOTTAB OUTPUT SUMMED OVER SHELLS
C      18   TRANS.TAB         TABLE OF INDIVIDUAL TRANSITIONS
C      19   SHELL.SUM         TABLE OF TRANSITIONS SUMMED OVER SHELLS
C
C     PLOTTAB FORMATTED OUTPUT
C
=====================================================================
C     PLOTTAB FORMATTED OUTPUT MAY BE DISPLAYED ON VIRTUALLY ANY
C     PLOTTING DEVICE - ON SCREEN OR HARDCOPY - SEE, UCRL-ID-110240
C     (MARCH 1992) - FOR A DESCRIPTION OF THE CODE - CONTACT THE
C     AUTHOR OF THIS CODE FOR A COPY OF PLOTTAB.
```

```
C
C     INPUT PARAMETERS
C
================================================================
C     LINE  COLS.  FORMAT  DESCRIPTION
C     ----  -----  ------  -----------
C       1    1- 5    I5    LISTING OPTION
C                          = 0 - NO OUTPUT LISTING
C                          = 1 - SUMMARY OF EACH SUBSHELL - NO SPECTRA
C                          = 2 - SUMMARY AND SPECTRA OF EACH SUBSHELL
C            6-10    I5    ENDL OUTPUT OPTION
C                          = 0 - NO ENDL OUTPUT
C                          = 1 - ENDL OUTPUT
C           11-15    I5    SPECTRA AND INTEGRAL OPTION
C                          = 0 - NO PLOTTAB OUTPUT
C                          = 1 - PLOTTAB OUTPUT
C           16-20    I5    FLUORESCENCE VS. Z (BY SUBSHELL) OPTION
C                          = 0 - NO PLOTTAB OUTPUT
C                          = 1 - PLOTTAB OUTPUT
C           21-25    I5    LISTING UNIT
C                          = 0 - TO FILE RELAX.LST
C                          = 1 - ON-LINE - DO NOT OPEN RELAX.LST
C           26-30    I5    RESULTS BY SHELL SUMMED OVER SUBSHELL
C                          = 0 - NO SHELL RESULTS
C                          = 1 - SHELL RESULTS
C     2-N    1- 5    I5    MINIMUM Z
C            6-10    I5    MAXIMUM Z
C           11-15    I5    MINIMUM SUBSHELL DESIGNATOR
C           16-20    I5    MAXIMUM SUBSHELL DESIGNATOR
C           21-25    I5    DESCRIPTION OF FINAL ATOM
C                          = 0 - RETURN TO NEUTRALITY
C                          = 1 - ISOLATED
C
C     LINE 2 MAY BE REPEATED ANY NUMBER OF TIMES. EACH ELEMENT/SUBSHELL
C     REQUEST WILL BE PROCESSED SEPARATELY AND PROCESSING WILL CONTINUE
C     UNTIL AN END OF FILE IS READ ON THE INPUT FILE.
C
C     THE MINIMUM AND MAXIMUM Z MUST BE BETWEEN 1 AND 100 AND THE
C     MAXIMUM MUST BE EQUAL TO OR GREATER THAN THE MINIMUM. SIMILARLY
C     THE MINIMUM AND MAXIMUM SUBSHELL DESIGNATORS MUST BE BETWEEN 1
C     AND 61 AND THE MAXIMUM MUST BE EQUAL TO OR GREATER THAN THE
C     MINIMUM. IF THE INPUT PARAMETERS DO NOT SATISFY THESE
C     CONDITIONS THE PROGRAMM WILL TERMINATE EXECUTION.
C
C     EXAMPLE INPUT NO. 1
C     -------------------
C     PROCESS THE ENTIRE EADL LIBRARY WITH ALL OUTPUT OPTIONS ON. THE
C     FOLLOWING 2 INPUT LINES ARE REQUIRED,
C
C         2    1    1    1    0
C         1  100    1   61    0
C
```

```
C     EXAMPLE INPUT NO. 2
C     -------------------
C     PROCESS THE MAGNESIUM (Z=12), K SHELL (SUBSHELL DESIGNATOR = 1)
C     AND ONLY OUTPUT A FULL LISTING. THE FOLLOWING 2 INPUT LINES ARE
C     REQUIRED,
C
C         2    0    0    0    0
C        12   12    1    1    0
C
C     EXAMPLE INPUT NO. 3
C     -------------------
C     PROCESS ALL SUBSHELLS OF Z = 6 THROUGH 10 AND 90 THROUGH 100.
C     OUTPUT A SUMMARY OF EACH SUBSHELL AND PLOTTAB FORMATTED SPECTRA.
C     THE FOLLOWING 3 INPUT LINES ARE REQUIRED,
C
C         1    0    1    0    0
C         6   10    1   61    0
C        90  100    1   61    0
C
C      DEFINITION OF ENDL SUBSHELL DESIGNATORS
C=====================================================================
==
C  1 = K (1s1/2)   17 = N23 (4p)    32 = O4 (5d3/2)  47 = P5 (6d5/2)
C  2 = L (2)       18 = N2 (4p1/2)  33 = O5 (5d5/2)  48 = P67 (6f)
C  3 = L1 (2s1/2)  19 = N3 (4p3/2)  34 = O67 (5f)    49 = P6 (6f5/2)
C  4 = L23 (2p)    20 = N45 (4d)    35 = O6 (5f5/2)  50 = P7 (6f7/2)
C  5 = L2 (2p1/2)  21 = N4 (4d3/2)  36 = O7 (5f7/2)  51 = P89 (6g)
C  6 = L3 (2p3/2)  22 = N5 (4d5/2)  37 = O89 (5g)    52 = P8 (6g7/2)
C  7 = M (3)       23 = N67 (4f)    38 = O8 (5g7/2)  53 = P9 (6g9/2)
C  8 = M1 (3s1/2)  24 = N6 (4f5/2)  39 = O9 (5g9/2)  54 = P1011 (6h)
C  9 = M23 (3p)    25 = N7 (4f7/2)  40 = P (6)       55 = P10 (6h9/2)
C 10 = M2 (3p1/2)  26 = O (5)       41 = P1 (6s1/2)  56 = P11 (6h11/2)
C 11 = M3 (3p3/2)  27 = O1 (5s1/2)  42 = P23 (6p)    57 = Q (7)
C 12 = M45 (3d)    28 = O23 (5p)    43 = P2 (6p1/2)  58 = Q1 (7s1/2)
C 13 = M4 (3d3/2)  29 = O2 (5p1/2)  44 = P3 (6p3/2)  59 = Q23 (7p)
C 14 = M5 (3d5/2)  30 = O3 (5p3/2)  45 = P45 (6d)    60 = Q2 (7p1/2)
C 15 = N (4)       31 = O45 (5d)    46 = P4 (6d3/2)  61 = Q3 (7p3/2)
C 16 = N1 (4s1/2)
C=====================================================================
==
C
C     DEFINITION OF VARIABLES
C
=====================================================================
C     BASIS DATA
C
---------------------------------------------------------------------
C     IZGET   = Z FOR ELEMENT (1 TO 100)
C     ISUBGT  = SUBSHELL INDEX (1 TO 61)
C     MAXSUB  = MAXIMUM SUBSHELL INDEX THAT MUST BE USED IN CALCULATION
C     MAXTRA  = MAXIMUM SUBSHELL INDEX THAT HAS TRANSITIONS TO IT
C     ATWTGT  = ATOMIC WEIGHT OF ELEMENT IZGET
```

```
C     EBMEV   = SUBSHELL BINDING ENERGY (MEV)
C     EBEV    = SUBSHELL BINDING ENERGY (EV)
C     TR      = RADIATIVE TRANSITION PROBABILITIES
C     TNR     = NON-RADIATIVE TRANSITION PROBABILITIES
C     NSUBR   = RADIATIVE TRANSITIONS READ FLAG
C     NSUBN   = NON-RADIATIVE TRANSITIONS READ FLAG
C
-----------------------------------------------------------------
C     SPECTRA FOR ONE SUBSHELL - CALCULATED BY THIS CODE
C
-----------------------------------------------------------------
C     ERO     = ENERGY OF RADIATIVE TRANSITION (EV)
C     PROBRO  = PROBABILITY OF RADIATIVE TRANSITION
C     NR      = NUMBER OF RADIATIVE TRANSITIONS
C     ENO     = ENERGY OF NON-RADIATIVE TRANSITION (EV)
C     PROBNO  = PROBABILITY OF NON-RADIATIVE TRANSITION
C     NN      = NUMBER OF NON-RADIATIVE TRANSITIONS
C     ELO     = ENERGY OF FREE-BOUND TRANSITION (EV)
C     PROBLO  = PROBABILITY FREE-BOUND TRANSITION
C     NL      = NUMBER OF FREE-BOUND TRANSITIONS
C
-----------------------------------------------------------------
C     AVERAGE VALUES FOR ALL SUBSHELLS - CALCULATED BY THIS CODE
C
-----------------------------------------------------------------
C     OUTR    = AVERAGE NUMBER OF X-RAYS EMITTED
C     OUTN    = AVERAGE NUMBER OF ELECTRONS EMITTED
C     OUTL    = AVERAGE NUMBER OF FREE-BOUND TRANSITIONS
C     OUTRE   = TOTAL EMITTED X-RAY ENERGY (EV)
C     OUTNE   = TOTAL EMITTED ELECTRON ENERGY (EV)
C     OUTLE   = TOTAL EMITTED FREE-BOUND ENERGY (EV)
C     OUTAVR  = AVERAGE EMITTED X-RAY ENERGY (EV)
C     OUTAVN  = AVERAGE EMITTED ELECTRON ENERGY (EV)
C     OUTAVL  = AVERAGE EMITTED FREE-BOUND ENERGY (EV)
C
C     USING THE RESULTS
C
=================================================================
C     AFTER RESULTS HAVE BEEN CALCULATED FOR EACH SUBSHELL SUBROUTINE
C     USER1 IS CALLED - AT THIS POINT THE SPECTRA FOR THE SUBSHELL ARE
C     AVAILABLE FOR USE.
C
C     AFTER RESULTS HAVE BEEN CALCULATED FOR ALL SUBSHELLS OF AN
C     ELEMENT SUBROUTINE USER2 IS CALLED - AT THIS POINT THE AVERAGE
C     VALUES FOR ALL SUBSHELLS OF THE ELEMENT ARE AVAILABLE FOR USE.
C
C***** COMPUTER DEPENDENT CODING ******
C
C     THE COMPUTER DEPENDENT CODING IN THIS PROGRAM INCLUDING,
C
C     (1) DOUBLE/SINGLE
C         TREAT ENERGY DEPENDENT VARIABLES IN SINGLE OR DOUBLE
```

```
C         PRECISION. ON LONG WORD LENGTH COMPUTERS (E.G., CDC)
C         THIS PROGRAM CAN BE OPTIMIZED BY USING SINGLE PRECISION.
C         ON SHORT WORD LENGTH COMPUTERS (E.G., IBM) DOUBLE
C         PRECISION MUST BE USED.
C
C     (2) SAVE
C         FORTRAN OPTION TO SAVE ALL VARIABLES BETWEEN SUBROUTINE
C         CALLS - REQUIRED FOR SOME NEWER FORTRAN COMPILERS
C
C     ANY COMBINATION OF THIS OPTIONS CAN BE AUTOMATICALLY TURNED ON OR
C     OFF USING PROGRAM CONVERT - CONTACT THE AUTHOR FOR A COPY OF THIS
C     PROGRAM.
C
C***** COMPUTER DEPENDENT CODING ******
C***** SAVE *****
C     SAVE
C***** SAVE *****
C***** DOUBLE *****
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 MEV2EV
C***** DOUBLE *****
C***** SINGLE *****
C     REAL*4 MEV2EV
C***** SINGLE *****
      CHARACTER*1 ZABCD,SHBCD
      CHARACTER*8 OPCODE
      INTEGER OUTP,OTAPE
      COMMON/UNITS/INP,OUTP,ITAPE,OTAPE,KTAPE,LTAPE,
     1 IPLOT1,IPLOT2,IPLOT3,IPLOT4
      COMMON/WHERE/ATWTGT,IZGET,ISUBGT,MAXSUB,MAXTRA
      COMMON/WHEREC/ZABCD(12),SHBCD(12)
      COMMON/SPECTR/ERO(5000),PROBRO(5000),NR
      COMMON/SPECTN/ENO(5000),PROBNO(5000),NN
      COMMON/SPECTL/ELO(39),PROBLO(39),NL
      COMMON/TRANS/TR(39,39),TNR(39,39,39),NSUBR(39),NSUBN(39)
      COMMON/EADL/EBMEV(39),EBEV(39),ELECT(39),HOLES(39)
      COMMON/OUTER/OUTR(39),OUTN(39),OUTL(39),OUTRE(39),OUTNE(39),
     1 OUTLE(39),OUTAVR(39),OUTAVN(39),OUTAVL(39)
      COMMON/FLUORS/FLUOR(100,39,6),MSHELL,MSUB1,MSUB2
      COMMON/OUTOPS/IMOUT(6)
      DIMENSION OPCODE(5),TNORM(39),SHELLP(7,7),SHELLE(7,7,7)
      DATA IZNEXT/0/
      DATA IZNOW/0/
      DATA OPCODE/
     1 'None    ',
     2 'Summary ',
     3 'Full    ',
     4 'No      ',
     5 'Yes     '/
C***** DOUBLE *****
      DATA ZERO/0.0D+00/
      DATA ONE/1.0D+00/
```

```
      DATA MEV2EV/1.0D+06/
C***** DOUBLE *****
C***** SINGLE *****
C     DATA ZERO/0.0E+00/
C     DATA ONE/1.0D+00/
C     DATA MEV2EV/1.0E+06/
C***** SINGLE *****
C-----DEFINE I/O UNITS.
      INP=5
      OUTP=6
      ITAPE=10
      OTAPE=11
      KTAPE=18
      LTAPE=19
      IPLOT1=12
      IPLOT2=14
      IPLOT3=15
      IPLOT4=17
      OPEN(INP,FILE='RELAX.INP')
      OPEN(ITAPE,FILE='ENDL.IN')
      OPEN(OTAPE,FILE='ENDL.OUT')
      OPEN(KTAPE,FILE='TRANS.TAB')
      OPEN(LTAPE,FILE='SHELL.SUM')
      OPEN(IPLOT1,FILE='PLOTTAB.CUR')
      OPEN(IPLOT2,FILE='PLOTTAB.PNT')
      OPEN(IPLOT3,FILE='PLOTTAB.INP')
      OPEN(IPLOT4,FILE='PLOTTAB.CUR.SHELL')
C
C     INITIALIZE FLUORESCENCE YIELD.
C
      DO 10 I=1,100
      DO 10 J=1,39
      DO 10 K=1,6
   10 FLUOR(I,J,K)=ZERO
C
C     READ AND LIST OUTPUT OPTIONS.
C
      READ(INP,5000,END=370,ERR=370) IMOUT
      IF(IMOUT(1).LT.0) IMOUT(1)=0
      IF(IMOUT(1).GT.2) IMOUT(1)=2
      IF(IMOUT(2).NE.0) IMOUT(2)=1
      IF(IMOUT(3).NE.0) IMOUT(3)=1
      IF(IMOUT(4).NE.0) IMOUT(4)=1
      IF(IMOUT(5).NE.0) IMOUT(5)=1
      IF(IMOUT(6).NE.0) IMOUT(6)=1
      I1=IMOUT(1)+1
      I2=IMOUT(2)+4
      I3=IMOUT(3)+4
      I4=IMOUT(4)+4
      I6=IMOUT(6)+4
C-----IF REQUESTED OPEN FILE FOR OUTPUT REPORT.
      IF(IMOUT(5).EQ.0) OPEN(OUTP,FILE='RELAX.LST')
```

```
C-----IDENTIFY PROGRAM.
      WRITE(OUTP,6000)
C-----LIST DESCRIPTION OF OPTIONS.
      WRITE(OUTP,6020) OPCODE(I1),OPCODE(I2),OPCODE(I3),OPCODE(I4)
      IF(IMOUT(5).EQ.0) WRITE(OUTP,6022)
      IF(IMOUT(5).NE.0) WRITE(OUTP,6024)
      WRITE(OUTP,6026) OPCODE(I6)
C
C     READ AND LIST NEXT REQUESTED Z AND SUBSHELL INDEX.
C
   20 READ(INP,5000,END=370,ERR=370) IZ1,IZ2,ISUB1,ISUB2,MYWAY
      WRITE(OUTP,6030) IZ1,IZ2,ISUB1,ISUB2
      IF(MYWAY.EQ.0) WRITE(OUTP,6032)
      IF(MYWAY.NE.0) WRITE(OUTP,6034)
C-----STOP ON ILLEGAL DATA.
      IF(IZ1.LT.1.OR.IZ1.GT.100) GO TO 360
      IF(IZ2.LT.1.OR.IZ2.GT.100) GO TO 360
      IF(IZ1.GT.IZ2) GO TO 360
      IF(ISUB1.LT.1.OR.ISUB2.LT.1) GO TO 360
      IF(ISUB1.GT.61.OR.ISUB2.GT.61) GO TO 360
      IF(ISUB1.GT.ISUB2) GO TO 360
C
C     LOOP OVER ELEMENTS.
C
      DO 350 IZGET=IZ1,IZ2
C-----DEFINE ELEMENT.
      CALL ZAHOL(1000*IZGET,ZABCD)
C-----INITIALIZE DATA FOUND FLAG.
      IGOTIT=0
C-----IF DATA IS ALREADY IN CORE USE IT.
      IF(IZGET.EQ.IZNOW) GO TO 290
C-----INITIALIZE BINDING ENERGIES, ELECTRONS PER SUBSHELL, SUBSHELL
C-----USED FLAGS AND AVERAGE VALUES.
      DO 30 I=1,39
      EBMEV(I)=ZERO
      ELECT(I)=ZERO
      TNORM(I)=ZERO
      NSUBR(I)=0
      NSUBN(I)=0
      OUTR(I)=ZERO
      OUTN(I)=ZERO
      OUTL(I)=ZERO
      OUTRE(I)=ZERO
      OUTNE(I)=ZERO
      OUTLE(I)=ZERO
      OUTAVR(I)=ZERO
      OUTAVN(I)=ZERO
   30 OUTAVL(I)=ZERO
      MAXSUB=1
      MAXTRA=0
C-----IF REQUESTED Z IS THE NEXT ONE THE FIRST LINE IS ALREADY
C-----IN CORE.
```

```
      IF(IZGET.EQ.IZNEXT) GO TO 50
C-----IF PAST REQUESTED Z REWIND BEFORE SEARCH.
      IF(IZGET.LT.IZNEXT) REWIND ITAPE
      IZNEXT=0
      IZNOW=0
C
C     LOCATE REQUESTED Z.
C
C-----READ ALL RADIATIVE AND NON-RADIATIVE TRANSITIONS.
   40 READ(ITAPE,1000,END=200,ERR=200) IZ,ATWT
C-----CHECK FOR REQUESTED Z.
      IF(IZ-IZGET) 60,50,210
C-----FIND RELAXATION DATA.
   50 READ(ITAPE,1010,END=200,ERR=200) IC,II,SUB1
C-----CHECK FOR BINDING ENERGIES.
      IF(IC.EQ.91.AND.II.EQ.913) GO TO 70
C-----CHECK FOR ELECTRONS PER SUBSHELL.
      IF(IC.EQ.91.AND.II.EQ.912) GO TO 100
C-----CHECK FOR RADIATIVE TRANSITIONS.
      IF(IC.EQ.92.AND.II.EQ.931) GO TO 120
C-----CHECK FOR NON-RADIATIVE TRANSITIONS.
      IF(IC.EQ.92.AND.II.EQ.932) GO TO 160
C-----SKIP SECTION.
   60 READ(ITAPE,1020,END=200,ERR=200) IFLAG
      IF(IFLAG) 60,60,40
C
C     READ BINDING ENERGIES.
C
C-----SAVE ATOMIC WEIGHT FOR OUTPUT.
   70 ATWTGT=ATWT
C-----INDICATE DATA HAS BEEN FOUND.
      IGOTIT=1
   80 READ(ITAPE,1035,END=200,ERR=200) SUB1,END1,IFLAG
      IF(IFLAG) 90,90,40
   90 KSUBX1=SUB1
      KSUB1=ISDOWN(KSUBX1)
      EBMEV(KSUB1)=END1
      EBEV(KSUB1)=MEV2EV*EBMEV(KSUB1)
      IF(KSUB1.GT.MAXSUB) MAXSUB=KSUB1
      GO TO 80
C
C     READ ELECTRONS PER SUBSHELL.
C
  100 READ(ITAPE,1035,END=200,ERR=200) SUB1,END1,IFLAG
      IF(IFLAG) 110,110,40
  110 KSUBX1=SUB1
      KSUB1=ISDOWN(KSUBX1)
      ELECT(KSUB1)=END1
      GO TO 100
C
C     READ RADIATIVE TRANSITIONS.
C
```

```
C-----INDICATE SUBSHELL USED AND INITIALIZE ARRAYS.
  120 KSUBX1=SUB1
      KSUB1=ISDOWN(KSUBX1)
      NSUBR(KSUB1)=1
      IF(KSUB1.GT.MAXTRA) MAXTRA=KSUB1
      DO 130 J=1,39
  130 TR(KSUB1,J)=ZERO
  140 READ(ITAPE,1030,END=200,ERR=200) SUB2,PROB1,IFLAG
      IF(IFLAG) 150,150,40
  150 KSUBX2=SUB2
      KSUB2=ISDOWN(KSUBX2)
      TR(KSUB1,KSUB2)=PROB1
      TNORM(KSUB1)=TNORM(KSUB1)+PROB1
      GO TO 140
C
C     READ NON-RADIATIVE TRANSITIONS.
C
C-----INDICATE SUBSHELL USED AND INITIALIZE ARRAYS.
  160 KSUBX1=SUB1
      KSUB1=ISDOWN(KSUBX1)
      NSUBN(KSUB1)=1
      IF(KSUB1.GT.MAXTRA) MAXTRA=KSUB1
      DO 170 J=1,39
      DO 170 K=1,39
  170 TNR(KSUB1,J,K)=ZERO
  180 READ(ITAPE,1040,END=200,ERR=200) SUB2,SUB3,PROB1,IFLAG
      IF(IFLAG) 190,190,40
  190 KSUBX2=SUB2
      KSUBX3=SUB3
      KSUB2=ISDOWN(KSUBX2)
      KSUB3=ISDOWN(KSUBX3)
      TNR(KSUB1,KSUB2,KSUB3)=PROB1
      TNORM(KSUB1)=TNORM(KSUB1)+PROB1
      GO TO 180
C
C     ALL DATA READ. PROCESS IT.
C
C-----END OF ENDL DATA.
  200 IZ=200
  210 IZNEXT=IZ
      IZNOW=IZGET
C
C     THERE IS NOTHING TO DO IF NO DATA WAS FOUND.
C
      IF(IGOTIT.LE.0) GO TO 350
C
C     RE-NORMALIZE TRANSITIONS. ONLY USE DATA IF NON-RADIATIVE DATA
C     ARE GIVEN.
C
      DO 250 ISUB=1,MAXSUB
      IF(NSUBN(ISUB).GT.0.AND.TNORM(ISUB).GT.ZERO) GO TO 220
      NSUBN(ISUB)=0
```

```
      NSUBR(ISUB)=0
      GO TO 250
  220 RNORMR=ONE/TNORM(ISUB)
      RNORMN=ONE/TNORM(ISUB)
      DO 240 I=ISUB,MAXSUB
      TR(ISUB,I)=TR(ISUB,I)*RNORMR
      DO 230 J=ISUB,MAXSUB
  230 TNR(ISUB,I,J)=TNR(ISUB,I,J)*RNORMN
  240 CONTINUE
  250 CONTINUE
C
C     DEFINE AND OUTPUT SHELL RESULTS.
C
C-----INITIALIZE.
      DO 260 I=1,7
      DO 260 J=1,7
      SHELLP(I,J)=0.0
      DO 260 K=1,7
  260 SHELLE(I,J,K)=0.0
C-----SUM OVER SUBSHELLS IN EACH SHELL.
      DO 280 I=1,MAXSUB
      IF(NSUBN(I).LE.0.OR.TNORM(I).LE.ZERO) GO TO 280
      IS=ISUP(I)
      CALL SHELL1(IS,ISH)
      DO 270 J=I,MAXSUB
      JS=ISUP(J)
      CALL SHELL1(JS,JSH)
      SHELLP(ISH,JSH)=SHELLP(ISH,JSH)+TR(I,J)
      DO 270 K=I,MAXSUB
      KS=ISUP(K)
      CALL SHELL1(KS,KSH)
  270 SHELLE(ISH,JSH,KSH)=SHELLE(ISH,JSH,KSH)+TNR(I,J,K)
  280 CONTINUE
C-----OUTPUT RESULTS.
      WRITE(LTAPE,2010) IZGET
      WRITE(LTAPE,2000) SHELLP
      WRITE(LTAPE,2000) SHELLE
C
C     LOOP OVER SUBSHELLS.
C
  290 DO 340 KSUBGT=ISUB1,ISUB2
      ISUBGT=ISDOWN(KSUBGT)
C-----IGNORE UNUSED SUBSHELLS.
      IF(ISUBGT.LE.0) GO TO 340
C-----IGNORE SUBSHELLS WITH NO BINDING ENERGY.
      IF(EBMEV(ISUBGT).LE.ZERO) GO TO 340
C-----DEFINE SUBSHELL.
      CALL SUBHOL(KSUBGT,SHBCD)
C-----INITIALIZE NUMBER OF EMISSIONS.
      NR=0
      NN=0
      NL=0
```

```
C-----CALCULATION NOT REQUIRED IF NO TRANSITION DATA.
      IF(NSUBN(ISUBGT).LE.0) GO TO 300
      IF(ISUBGT.LE.MAXTRA) GO TO 310
C-----NO TRANSITIONS. ASSIGN EVERYTHING TO LOCAL FOR OUTPUT.
  300 OUTL(ISUBGT)=ONE
      OUTLE(ISUBGT)=EBEV(ISUBGT)
      OUTAVL(ISUBGT)=EBEV(ISUBGT)
      GO TO 330
C-----DEFINE SHELL INDICES.
  310 CALL MYSHEL(KSUBGT,MSUB1,MSUB2)
      MSUB1=ISDOWN(MSUB1)
      MSUB2=ISDOWN(MSUB2)
C-----CALCULATE SPECTRA AND AVERAGE VALUES.
      IF(MYWAY.NE.0) GO TO 320
      CALL SPECTA
      GO TO 330
  320 CALL SPECTB
C-----LIST RESULTS.
  330 CALL LIST1
C
C     END OF SUBSHELL. USER INTERFACE ROUTINE.
C
      CALL USER1
  340 CONTINUE
C
C     END OF ELEMENT. USER INTERFACE ROUTINE.
C
      CALL USER2
C
C     END OF ELEMENT LOOP
C
  350 CONTINUE
      GO TO 20
C
C     ERROR IN INPUT.
C
  360 WRITE(OUTP,6040)
C
C     END OF RUN.
C
C     LIST FLUORESCENCE YIELD.
C
  370 CALL LIST2
      WRITE(OUTP,6010)
      STOP
 1000 FORMAT(I3,9X,D12.4)
 1010 FORMAT(I2,I3,15X,D12.4)
 1020 FORMAT(71X,I1)
 1030 FORMAT(2D11.4,49X,I1)
 1035 FORMAT(D11.4,D11.4,49X,I1)
 1040 FORMAT(3D11.4,38X,I1)
 2000 FORMAT(1PE11.4,1PE11.4,1PE11.4,1PE11.4,1PE11.4,1PE11.4,1PE11.4)
```

```
 2010 FORMAT(I11)
 5000 FORMAT(14I5)
 6000 FORMAT(' Calculation of X-Ray and Electron Relaxation',
     1 ' Spectra (RELAX 91-2)')
 6010 FORMAT(1X,72('=')/
     1 ' Bound-Bound X-Ray and Electron Spectra are based on EADL',
     2 ' Relaxation data.'//
     3 ' Free-Bound X-Ray Spectrum assumes the atom will return to',
     4 ' Neutrality by'/
     5 ' electron transitions directly from the continuum to fill all',
     6 ' remaining'/
     7 ' electron holes, resulting in the emission of X-Rays with',
     8 ' energy equal'/
     9 ' to the binding energy of the electron holes.')
 6020 FORMAT(1X,72('=')/
     1 ' Output Listing............................',A8/
     2 ' ENDL Output...............................',A8/
     3 ' Spectra and Integral......................',A8/
     4 ' Fluorescence Yield vs. Z by Subshell......',A8)
 6022 FORMAT(
     1 ' Listing Unit..............................RELAX.LST')
 6024 FORMAT(
     1 ' Listing Unit..............................ON-LINE')
 6026 FORMAT(
     1 ' Shell Results Summed Over Subshells.......',A8)
 6030 FORMAT(1X,72('=')/
     1 ' Process Z.................................',I4,' through',I4/
     2 '         Subshell..........................',I4,' through',I4)
 6032 FORMAT(
     1 ' Description of Final Atom................. Neutral')
 6034 FORMAT(
     1 ' Description of Final Atom................. Isolated')
 6040 FORMAT(1X,72('=')/
     1 ' Error in input ranges.'/
     2 ' Z range may be 1 to 100.'/
     3 ' Subshell range may be 1 to 61.'/
     4 ' Execution Terminated.')
      END
      SUBROUTINE MYSHEL(ISUB,ISUB1,ISUB2)
C
C     DEFINE SUBSHELL INDICES FOR SAME SHELL.
C
      DIMENSION MYSUB(2,7)
C-----SUBSHELL DESIGNATOR RANGES FOR EACH SHELL.
      DATA MYSUB/
     1    1,    1,
     2    3,    6,
     3    8,   14,
     4   16,   25,
     5   27,   39,
     6   41,   56,
     7   58,   61/
```

```
      DO 10 ISHELL=1,7
      IF(ISUB.GE.MYSUB(1,ISHELL).AND.
     1   ISUB.LE.MYSUB(2,ISHELL)) GO TO 20
   10 CONTINUE
      ISHELL=7
   20 ISUB1=MYSUB(1,ISHELL)
      ISUB2=MYSUB(2,ISHELL)
      RETURN
      END
      SUBROUTINE SHELL1(ISUB,ISHELL)
C
C     DEFINE SHELL CORRESPONDING TO SUBSHELL.
C
      DIMENSION MYSUB(2,7)
C-----SUBSHELL DESIGNATOR RANGES FOR EACH SHELL.
      DATA MYSUB/
     1    1,    1,
     2    3,    6,
     3    8,   14,
     4   16,   25,
     5   27,   39,
     6   41,   56,
     7   58,   61/
      DO 10 ISHELL=1,7
      IF(ISUB.GE.MYSUB(1,ISHELL).AND.
     1   ISUB.LE.MYSUB(2,ISHELL)) GO TO 20
   10 CONTINUE
      ISHELL=7
   20 RETURN
      END
      SUBROUTINE SHELL2(ISUB,ISHELL)
C
C     DEFINE SHELL CORRESPONDING TO SUBSHELL+L1,L2,L3
C
      DIMENSION MYSUB(2,9)
C-----SUBSHELL DESIGNATOR RANGES FOR EACH SHELL.
      DATA MYSUB/
     1    1,    1,
     2    3,    3,
     3    5,    5,
     4    6,    6,
     5    8,   14,
     6   16,   25,
     7   27,   39,
     8   41,   56,
     9   58,   61/
      DO 10 ISHELL=1,9
      IF(ISUB.GE.MYSUB(1,ISHELL).AND.
     1   ISUB.LE.MYSUB(2,ISHELL)) GO TO 20
   10 CONTINUE
      ISHELL=9
   20 RETURN
```

```
      END
      SUBROUTINE LIST1
C
C     LIST SUBSHELL RESULTS
C
C***** SAVE *****
C     SAVE
C***** SAVE *****
C***** DOUBLE *****
      IMPLICIT REAL*8 (A-H,O-Z)
C***** DOUBLE *****
      CHARACTER*1 ZABCD,SHBCD,SHBCD1,SHBCD2,SHBCD3,STARX,STAR1,BLANK,
     1 CROSSX,CROSS1
      INTEGER OUTP,OTAPE
      COMMON/UNITS/INP,OUTP,ITAPE,OTAPE,KTAPE,LTAPE,
     1 IPLOT1,IPLOT2,IPLOT3,IPLOT4
      COMMON/WHERE/ATWTGT,IZGET,ISUBGT,MAXSUB,MAXTRA
      COMMON/WHEREC/ZABCD(12),SHBCD(12)
      COMMON/SPECTR/ERO(5000),PROBRO(5000),NR
      COMMON/SPECTN/ENO(5000),PROBNO(5000),NN
      COMMON/SPECTL/ELO(39),PROBLO(39),NL
      COMMON/EADL/EBMEV(39),EBEV(39),ELECT(39),HOLES(39)
      COMMON/OUTER/OUTR(39),OUTN(39),OUTL(39),OUTRE(39),OUTNE(39),
     1 OUTLE(39),OUTAVR(39),OUTAVN(39),OUTAVL(39)
      COMMON/INDEXS/INDEXR(5000),INDEXN(5000),INDEXL(39)
      COMMON/OUTOPS/IMOUT(6)
      DIMENSION SHBCD1(12),SHBCD2(12),SHBCD3(12)
      DATA STARX/'*'/
      DATA CROSSX/'+'/
      DATA BLANK/' '/
      DATA IZLAST/0/
C***** DOUBLE *****
      DATA ZERO/0.0D+00/
      DATA ONE/1.0D+00/
      DATA HOLMIN/1.0D-10/
      QABS(Q)=DABS(Q)
C***** DOUBLE *****
C***** SINGLE *****
C     DATA ZERO/0.0E+00/
C     DATA ONE/1.0E+00/
C     DATA HOLMIN/1.0E-10/
C     QABS(Q)=ABS(Q)
C***** SINGLE *****
C
C     NOTHING TO DO IF LISTED OUTPUT NOT REQUESTED.
C
      IF(IMOUT(1).LE.0) GO TO 40
C-----NOTHING TO DO IF SUBSHELL ENERGY IS NOT DEFINED.
      IF(EBMEV(ISUBGT).LE.ZERO) RETURN
C
C     ONLY A SUMMARY OF REMAINING SUBSHELLS AFTER ALL SUBSHELLS WITH
C     TRANSITIONS HAVE BEEN PROCESSED.
```

```
C
      IF(ISUBGT.LE.MAXTRA) GO TO 10
      IF(IZGET.NE.IZLAST) WRITE(OUTP,6110) ZABCD
      IZLAST=IZGET
      II=ISUP(ISUBGT)
      CALL SUB4(II,SHBCD1)
      WRITE(OUTP,6070) (SHBCD1(K),K=1,4),EBEV(ISUBGT),ELECT(ISUBGT)
      RETURN
C-----FRACTION OF ENERGY TO RADIATIVE/NON-RADIATIVE/LOCAL/TOTAL.
   10 FRACTR=100.0*OUTRE(ISUBGT)/EBEV(ISUBGT)
      FRACTN=100.0*OUTNE(ISUBGT)/EBEV(ISUBGT)
      FRACTL=100.0*OUTLE(ISUBGT)/EBEV(ISUBGT)
      FRACT=100.0
C
C     PRINT SUBSHELL SUMMARY.
C
      WRITE(OUTP,6050) ZABCD,SHBCD,OUTRE(ISUBGT),FRACTR,
     1 OUTNE(ISUBGT),FRACTN,OUTLE(ISUBGT),FRACTL,EBEV(ISUBGT),
     2 FRACT,OUTAVR(ISUBGT),OUTAVN(ISUBGT),OUTAVL(ISUBGT),
     3 OUTR(ISUBGT),OUTN(ISUBGT),OUTL(ISUBGT)
C
C     INITIAL AND FINAL ELECTRONS AND HOLES.
C
      WRITE(OUTP,6060)
      SUM1=ZERO
      SUM2=ZERO
      SUM3=ZERO
      SUM4=ZERO
      HOLEX=ONE
      IF(ELECT(ISUBGT).LT.ONE) HOLEX=ELECT(ISUBGT)
      IMNEG=0
      ILIST=0
      DO 30 I=ISUBGT,MAXSUB
      IF(EBMEV(I).LE.ZERO) GO TO 30
      II=ISUP(I)
      CALL SUB4(II,SHBCD1)
      HOLE0=ZERO
      IF(I.EQ.ISUBGT) HOLE0=HOLEX
      ELECT0=ELECT(I)-HOLE0
      HOLE1=HOLES(I)
      IF(QABS(HOLEI).LE.HOLMIN) HOLEI=ZERO
      ELECT1=ELECT(I)-HOLE1
      CROSS1=BLANK
      IF(I.EQ.ISUBGT.AND.HOLEX.LT.ONE) CROSS1=CROSSX
      STAR1=BLANK
      IF(QABS(ELECT1).LE.HOLMIN) ELECT1=ZERO
      IF(ELECT1.GE.ZERO) GO TO 20
      STAR1=STARX
      IMNEG=1
   20 WRITE(OUTP,6070) (SHBCD1(K),K=1,4),EBEV(I),ELECT0,HOLE0,CROSS1,
     1 ELECT1,STAR1,HOLE1
      ILIST=ILIST+1
```

```
      SUM1=SUM1+ELECT0
      SUM2=SUM2+HOLE0
      SUM3=SUM3+ELECT1
      SUM4=SUM4+HOLES(I)
   30 CONTINUE
      IF(ILIST.GT.1) WRITE(OUTP,6080) SUM1,SUM2,SUM3,SUM4
      IF(IMNEG.NE.0) WRITE(OUTP,6090)
      IF(HOLEX.LT.ONE) WRITE(OUTP,6100) HOLEX
C
C     OUTPUT SHELL RESULTS SUMMED OVER SUBSHELLS.
C
   40 CALL SHELLO
C
C     NOTHING ELSE TO DO IF LISTED SPECTRA NOT REQUESTED.
C
      IF(IMOUT(1).LE.1) RETURN
C
C     LIST SPECTRA.
C
C-----X-RAYS
      IF(NR.GT.0) GO TO 50
      WRITE(OUTP,6020)
      GO TO 70
   50 WRITE(OUTP,6002)
      SUMFR=ZERO
      SUMHOL=ZERO
      DO 60 I=1,NR
      ERO(I)=ERO(I)
      FRACT=100.0*ERO(I)*PROBRO(I)/EBEV(ISUBGT)
      SUMFR=SUMFR+FRACT
      SUMHOL=SUMHOL+PROBRO(I)
      II1X=INDEXR(I)/100
      II2X=MOD(INDEXR(I),100)
      II1=ISUP(II1X)
      II2=ISUP(II2X)
      CALL SUB4(II1,SHBCD1)
      CALL SUB4(II2,SHBCD2)
   60 WRITE(OUTP,6040) I,ERO(I),PROBRO(I),FRACT,(SHBCD1(K),K=1,4),
     1 (SHBCD2(K),K=1,4)
      IF(NR.GT.1) WRITE(OUTP,6045) SUMHOL,SUMFR
C-----ELECTRONS
   70 IF(NN.GT.0) GO TO 80
      WRITE(OUTP,6030)
      GO TO 100
   80 WRITE(OUTP,6010)
      SUMFN=ZERO
      SUMHOL=ZERO
      DO 90 I=1,NN
      ENO(I)=ENO(I)
      FRACT=100.0*ENO(I)*PROBNO(I)/EBEV(ISUBGT)
      SUMFN=SUMFN+FRACT
      SUMHOL=SUMHOL+PROBNO(I)
```

```
      II1X=INDEXN(I)/10000
      II2X=MOD(INDEXN(I),10000)/100
      II3X=MOD(INDEXN(I),100)
      II1=ISUP(II1X)
      II2=ISUP(II2X)
      II3=ISUP(II3X)
      CALL SUB4(II1,SHBCD1)
      CALL SUB4(II2,SHBCD2)
      CALL SUB4(II3,SHBCD3)
   90 WRITE(OUTP,6040) I,ENO(I),PROBNO(I),FRACT,(SHBCD1(K),K=1,4),
     1 (SHBCD2(K),K=1,4),(SHBCD3(K),K=1,4)
      IF(NN.GT.1) WRITE(OUTP,6045) SUMHOL,SUMFN
C-----FREE-BOUND
  100 IF(NL.GT.0) GO TO 110
      WRITE(OUTP,6035)
      GO TO 130
  110 WRITE(OUTP,6015)
      SUMFL=ZERO
      SUMHOL=ZERO
      DO 120 I=1,NL
      ELO(I)=ELO(I)
      FRACT=100.0*ELO(I)*PROBLO(I)/EBEV(ISUBGT)
      SUMFL=SUMFL+FRACT
      SUMHOL=SUMHOL+PROBLO(I)
      II1=ISUP(INDEXL(I))
      CALL SUB4(II1,SHBCD1)
      WRITE(OUTP,6040) I,ELO(I),PROBLO(I),FRACT,(SHBCD1(K),K=1,4)
  120 CONTINUE
      IF(NL.GT.1) WRITE(OUTP,6045) SUMHOL,SUMFL
  130 RETURN
 6002 FORMAT(1X,72('=')/' Bound-Bound X-Ray Spectrum by Subshell'/
     1       1X,72('=')/
     2 ' Index   Emitted      Probability per    Per-cent of',
     3 '     Transition'/
     4 '         Energy (eV)  Initial Vacancy    Binding Energy'/
     5 1X,72('='))
 6010 FORMAT(1X,72('=')/' Bound-Bound Electron Spectrum'/1X,72('=')/
     1 ' Index   Emitted      Probability per    Per-cent of',
     2 '     Transition'/
     2 '         Energy (eV)  Initial Vacancy    Binding Energy'/
     3 1X,72('='))
 6015 FORMAT(1X,72('=')/' Free-Bound X-Ray Spectrum'/1x,72('=')/
     1 ' Index   Emitted      Probability per    Per-cent of',
     2 '     Transition'/
     2 '         Energy (eV)  Initial Vacancy    Binding Energy'/
     3 1X,72('='))
 6020 FORMAT(1X,72('=')/' No Bound-Bound X-Rays Emitted'/1X,72('='))
 6030 FORMAT(1X,72('=')/' No Bound-Bound Electrons Emitted'/1X,72('='))
 6035 FORMAT(1X,72('=')/' No Free-Bound X-Rays Emitted'/1X,72('='))
 6040 FORMAT(I6,2X,F11.2,2X,F11.8,6X,F11.4,8X,4A1,4A1,4A1)
 6045 FORMAT(16X,'Sum',2X,F11.8,6X,F11.4)
 6050 FORMAT(1X,72('=')/1X,12A1,1X,12A1,
```

```
     1 ' Ensemble Averaged Values per Initial Vacancy'/1X,72('=')/
     2 ' Total Bound-Bound X-Ray Energy.........',F11.2,' eV',F11.4,
     3 ' %'/
     4 ' Total Bound-Bound Electron Energy.......',F11.2,' eV',F11.4,
     5 ' %'/
     6 ' Total Free-Bound X-Ray Energy (Local)...',F11.2,' eV',F11.4,
     7 ' %'/
     5 ' Binding Energy (Sum of Above Terms).....',F11.2,' eV',F11.4,
     9 ' %'/
     6 1X,72('-')/
     6 ' Average Bound-Bound X-Ray Energy........',F11.2,' eV/X-Ray'/
     7 ' Average Bound-Bound Electron Energy.....',F11.2,' eV/Electron'/
     8 ' Average Free-Bound X-Ray Energy.........',F11.2,' eV/X-Ray'/
     6 1X,72('-')/
     9 ' Average Number of Bound-Bound X-Rays....',F11.6/
     A ' Average Number of Bound-Bound Electrons.',F11.6/
     B ' Average Number of Free-Bound X-Rays.....',F11.6)
 6060 FORMAT(1X,72('=')/' Distributions - Initial and Final',
     1 ' after All Bound-Bound Transitions'/1X,72('=')/
     2 ' Subshell  Binding              Initial      ',
     3 '            Final'/
     4 '           Energy (eV)   Electrons      Holes',
     5 '      Electrons      Holes'/1x,72('='))
 6070 FORMAT(1X,4A1,4X,F11.2,3X,F11.6,F11.6,A1,3X,F11.6,A1,F10.6)
 6080 FORMAT(17X,'Sum',3X,F11.6,F11.6,4X,F11.6,F11.6)
 6090 FORMAT(1X,72('=')/
     1 ' * - The Final Electrons can be negative since the effect of'/
     2 '     Free-Bound transitions filling holes is not included here')
 6100 FORMAT(1X,72('=')/
     1 ' + - Subshell initially contained only ',F8.6,' electrons.'/
     2 '     The above table is normalized to ',F8.6,' initial holes.'/
     3 '     All other results are per initial vacancy.')
 6110 FORMAT(1X,72('=')/12A1,
     1 ' No Transitions for the following Subshells'/1X,72('=')/
     2 ' Subshell  Binding       Electrons'/
     4 '           Energy (eV)'/1X,72('='))
      END
      SUBROUTINE SHELLO
C
C     OUTPUT SHELL RESULTS SUMMED OVER SUBSHELLS.
C
C***** SAVE *****
C     SAVE
C***** SAVE *****
C***** DOUBLE *****
      IMPLICIT REAL*8 (A-H,O-Z)
C***** DOUBLE *****
      CHARACTER*1 ZABCD,SHBCD,SHBCD1,SHBCD2,SHBCD3
      INTEGER OUTP,OTAPE
      COMMON/UNITS/INP,OUTP,ITAPE,OTAPE,KTAPE,LTAPE,
     1 IPLOT1,IPLOT2,IPLOT3,IPLOT4
      COMMON/WHERE/ATWTGT,IZGET,ISUBGT,MAXSUB,MAXTRA
```

```
      COMMON/WHEREC/ZABCD(12),SHBCD(12)
      COMMON/EADL/EBMEV(39),EBEV(39),ELECT(39),HOLES(39)
      COMMON/SPECTR/ERO(5000),PROBRO(5000),NR
      COMMON/INDEXS/INDEXR(5000),INDEXN(5000),INDEXL(39)
      COMMON/OUTOPS/IMOUT(6)
      DIMENSION SHBCD1(12),SHBCD2(12),SHBCD3(12),PSHELL(9,9),
     1 ESHELL(9,9),KSHELL(9,9),NSHELL(9)
C-----INDICES CORRESPONDING TO SUBSHELL INDICE ASSIGNED TO EACH SHELL.
      DATA NSHELL/1,3,5,6,7,15,26,40,57/
C***** DOUBLE *****
      DATA ZERO/0.0D+00/
C***** DOUBLE *****
C***** SINGLE *****
C     DATA ZERO/0.0E+00/
C***** SINGLE *****
C-----NOTHING TO DO IF OUTPUT NOT REQUESTED OR NO TRANSITIONS.
      IF(IMOUT(1).LE.0.AND.IMOUT(6).LE.0.OR.NR.LE.0) RETURN
      KSUB=ISUP(ISUBGT)
      CALL SUB4(KSUB,SHBCD3)
C-----INITIALIZE ARRAYS.
      DO 10 IS=1,9
      DO 10 KS=1,9
      KSHELL(IS,KS)=0
      PSHELL(IS,KS)=0.0
   10 ESHELL(IS,KS)=0.0
C-----SUM OVER INDIVIDUAL TRANSITIONS.
      DO 20 I=1,NR
      II1X=INDEXR(I)/100
      II2X=MOD(INDEXR(I),100)
      II1=ISUP(II1X)
      II2=ISUP(II2X)
      CALL SHELL2(II1,ISHEL1)
      CALL SHELL2(II2,ISHEL2)
      KSHELL(ISHEL1,ISHEL2)=KSHELL(ISHEL1,ISHEL2)+1
      PSHELL(ISHEL1,ISHEL2)=PSHELL(ISHEL1,ISHEL2)+PROBRO(I)
      ESHELL(ISHEL1,ISHEL2)=ESHELL(ISHEL1,ISHEL2)+
     1 ERO(I)*PROBRO(I)
   20 CONTINUE
C-----OUTPUT RESULTS SHELL RESULTS
      IF(IMOUT(1).GT.0) WRITE(OUTP,6000)
      SUMFR=ZERO
      SUMHOL=ZERO
      DO 40 IS=1,9
      CALL SUB4(NSHELL(IS),SHBCD1)
      DO 30 KS=1,9
      IF(PSHELL(IS,KS).LE.0.0) GO TO 30
      FRACT=100.0*ESHELL(IS,KS)/EBEV(ISUBGT)
      SUMFR=SUMFR+FRACT
      SUMHOL=SUMHOL+PSHELL(IS,KS)
      CALL SUB4(NSHELL(KS),SHBCD2)
      AVERE=ESHELL(IS,KS)/PSHELL(IS,KS)
      IF(IMOUT(1).GT.0)
```

```
     1 WRITE(OUTP,6042) AVERE,PSHELL(IS,KS),FRACT,(SHBCD1(K),K=1,4),
     2 (SHBCD2(K),K=1,4)
      IF(IMOUT(6).GT.0)
     1 WRITE(KTAPE,2000) ZABCD,(SHBCD3(K),K=1,2),SHBCD1(1),SHBCD1(2),
     2 SHBCD2(1),SHBCD2(1),PSHELL(IS,KS),AVERE,EBEV(ISUBGT),FRACT,
     3 KSHELL(IS,KS)
   30 CONTINUE
   40 CONTINUE
      IF(IMOUT(1).GT.0) WRITE(OUTP,6045) SUMHOL,SUMFR
C-----OUTPUT SUM OVER ALL TRANSITIONS.
      IF(IMOUT(1).GT.0) WRITE(OUTP,6010)
      SUMFR=ZERO
      SUMHOL=ZERO
      DO 60 IS=1,9
      CALL SUB4(NSHELL(IS),SHBCD1)
      ESUM=0.0
      PSUM=0.0
      DO 50 KS=1,9
      IF(PSHELL(IS,KS).LE.0.0) GO TO 50
      ESUM=ESUM+ESHELL(IS,KS)
      PSUM=PSUM+PSHELL(IS,KS)
   50 CONTINUE
      IF(PSUM.LE.0.0) GO TO 60
      FRACT=100.0*ESUM/EBEV(ISUBGT)
      SUMFR=SUMFR+FRACT
      SUMHOL=SUMHOL+PSUM
      AVERE=ESUM/PSUM
      IF(IMOUT(1).GT.0)
     1 WRITE(OUTP,6042) AVERE,PSUM,FRACT,(SHBCD1(K),K=1,4)
   60 CONTINUE
      IF(IMOUT(1).GT.0) WRITE(OUTP,6045) SUMHOL,SUMFR
      RETURN
 2000 FORMAT(12A1,1X,2A1,1X,2A1,1X,2A1,1PD12.5,1PD12.5,1PD12.5,
     1 0PF12.7,I6)
 6000 FORMAT(1X,72('=')/' Bound-Bound X-Ray Spectrum'
     1 ' For Each Shell Summed Over Subshells'/1X,72('=')/
     2 ' Average Emitted      Probability per    Per-cent of',
     3 '     Transition'/
     4 '         Energy (eV)  Initial Vacancy    Binding Energy'/
     5 1X,72('='))
 6010 FORMAT(1X,72('=')/' Bound-Bound X-Ray Spectrum'
     1 ' For Each Shell Summed Over All Transitions'/1X,72('=')/
     2 ' Average Emitted      Probability per    Per-cent of',
     3 '     Transition'/
     4 '         Energy (eV)  Initial Vacancy    Binding Energy'/
     5 1X,72('='))
 6042 FORMAT(6X,2X,F11.2,2X,F11.8,6X,F11.4,8X,4A1,4A1,4A1)
 6045 FORMAT(16X,'Sum',2X,F11.8,6X,F11.4)
      END
      SUBROUTINE LIST2
C
C     OUTPUT SHELL FLUORESCENCE YIELD
```

```
C
C***** DOUBLE *****
      IMPLICIT REAL*8 (A-H,O-Z)
C***** DOUBLE *****
      CHARACTER*1 SHBCD,MYNAME
      INTEGER OUTP,OTAPE
      COMMON/UNITS/INP,OUTP,ITAPE,OTAPE,KTAPE,LTAPE,
     1 IPLOT1,IPLOT2,IPLOT3,IPLOT4
      COMMON/FLUORS/FLUOR(100,39,6),MSHELL,MSUB1,MSUB2
      COMMON/OUTOPS/IMOUT(6)
      DIMENSION SHBCD(12),MYNAME(7),MYSUB(2,7),SHELL(100),FNORM(100)
      DATA MYNAME/'K','L','M','N','O','P','Q'/
C-----SUBSHELL DESIGNATOR RANGES FOR EACH SHELL.
      DATA MYSUB/
     1    1,    1,
     2    3,    6,
     3    8,   14,
     4   16,   25,
     5   27,   39,
     6   41,   56,
     7   58,   61/
C***** DOUBLE *****
      DATA ZERO/0.0D+00/
      DATA ONE/1.0D+00/
C***** DOUBLE *****
C***** SINGLE *****
C     DATA ZERO/0.0E+00/
C     DATA ONE/1.0E+00/
C***** SINGLE *****
C-----NOTHING TO DO IF OUTPUT NOT REQUESTED.
      IF(IMOUT(4).LE.0) RETURN
C
C     BY SHELL.
C
      DO 80 MSHELL=1,7
      KSUB1=ISDOWN(MYSUB(1,MSHELL))
      KSUB2=ISDOWN(MYSUB(2,MSHELL))
      DO 70 INDEX=1,6
C-----INITIALIZE.
      DO 10 IZ=1,100
      FNORM(IZ)=ZERO
   10 SHELL(IZ)=ZERO
C-----SUM SUBSHELLS IN SHELL.
      DO 50 KSUB=KSUB1,KSUB2
      DO 20 IZ=1,100
      IF(FLUOR(IZ,KSUB,INDEX).GT.ZERO) GO TO 30
   20 CONTINUE
      GO TO 50
   30 DO 40 KZ=IZ,100
      FNORM(KZ)=FNORM(KZ)+ONE
   40 SHELL(KZ)=SHELL(KZ)+FLUOR(KZ,KSUB,INDEX)
   50 CONTINUE
```

```
C-----START OUTPUT AT FIRST NON-ZERO VALUE.
      CALL RANGER(SHELL,IZ1,IZ2,100)
      IF(IZ2.LE.0) GO TO 70
      IF(INDEX.EQ.1) WRITE(IPLOT4,1130) MYNAME(MSHELL)
      IF(INDEX.EQ.2) WRITE(IPLOT4,1140) MYNAME(MSHELL)
      IF(INDEX.EQ.3) WRITE(IPLOT4,1150) MYNAME(MSHELL)
      IF(INDEX.EQ.4) WRITE(IPLOT4,1130) MYNAME(MSHELL)
      IF(INDEX.EQ.5) WRITE(IPLOT4,1140) MYNAME(MSHELL)
      IF(INDEX.EQ.6) WRITE(IPLOT4,1150) MYNAME(MSHELL)
      DO 60 KZ=IZ1,IZ2
      ZK=KZ
   60 CALL POINT1(IPLOT4,ZK,SHELL(KZ),DUM,DUM,1,1,0,0)
      WRITE(IPLOT4,1120)
   70 CONTINUE
   80 CONTINUE
C
C     BY SUBSHELL.
C
      DO 110 J=1,39
      DO 100 I=1,6
      CALL RANGER(FLUOR(1,J,I),IZ1,IZ2,100)
      IF(IZ2.LE.0) GO TO 100
      ISUB=ISUP(J)
      CALL SUBHOL(ISUB,SHBCD)
      IF(I.EQ.1) WRITE(IPLOT1,1100) SHBCD
      IF(I.EQ.2) WRITE(IPLOT1,1105) SHBCD
      IF(I.EQ.3) WRITE(IPLOT1,1108) SHBCD
      IF(I.EQ.4) WRITE(IPLOT1,1100) SHBCD
      IF(I.EQ.5) WRITE(IPLOT1,1105) SHBCD
      IF(I.EQ.6) WRITE(IPLOT1,1108) SHBCD
      DO 90 M=IZ1,IZ2
      ZM=M
   90 CALL POINT1(IPLOT1,ZM,FLUOR(M,J,I),DUM,DUM,1,1,0,0)
      WRITE(IPLOT1,1120)
  100 CONTINUE
  110 CONTINUE
      RETURN
 1100 FORMAT(1X,12A1,' Direct  ')
 1105 FORMAT(1X,12A1,' Enhanced')
 1108 FORMAT(1X,12A1,' Total   ')
 1120 FORMAT(30X,'(END OF CURVE)')
 1130 FORMAT(1X,A1,' Direct')
 1140 FORMAT(1X,A1,' Enhanced')
 1150 FORMAT(1X,A1,' Total')
      END
      SUBROUTINE USER1
C
C     USER INTERFACE ROUTINE. CALLED AFTER EACH SUBSHELL.
C
C***** SAVE *****
C     SAVE
C***** SAVE *****
```

```
C***** DOUBLE *****
      IMPLICIT REAL*8 (A-H,O-Z)
C***** DOUBLE *****
      CHARACTER*1 ZABCD,SHBCD,KSIGN1,KSIGN2
      INTEGER OUTP,OTAPE
      COMMON/UNITS/INP,OUTP,ITAPE,OTAPE,KTAPE,LTAPE,
     1 IPLOT1,IPLOT2,IPLOT3,IPLOT4
      COMMON/WHERE/ATWTGT,IZGET,ISUBGT,MAXSUB,MAXTRA
      COMMON/WHEREC/ZABCD(12),SHBCD(12)
      COMMON/SPECTR/ERO(5000),PROBRO(5000),NR
      COMMON/SPECTN/ENO(5000),PROBNO(5000),NN
      COMMON/SPECTL/ELO(39),PROBLO(39),NL
      COMMON/EADL/EBMEV(39),EBEV(39),ELECT(39),HOLES(39)
      COMMON/OUTER/OUTR(39),OUTN(39),OUTL(39),OUTRE(39),OUTNE(39),
     1 OUTLE(39),OUTAVR(39),OUTAVN(39),OUTAVL(39)
      COMMON/OUTOPS/IMOUT(6)
C***** DOUBLE *****
      DATA ZERO/0.0D+00/
      DATA ONE/1.0D+00/
      DATA XPLOT/1.35D+01/
      DATA YPLOT/1.0D+01/
C***** DOUBLE *****
C***** SINGLE *****
C     DATA ZERO/0.0E+00/
C     DATA ONE/1.0D+00/
C     DATA XPLOT/1.35E+01/
C     DATA YPLOT/1.0E+01/
C***** SINGLE *****
      DATA IPASS/0/
      DATA IZERO/0/
      DATA IONE/1/
      DATA ITHREE/3/
      DATA KSIGN2/'+'/
      DATA KEXP2/1/
C
C     SPECTRA AND INTEGRAL - PLOTTAB FORMATTED OUTPUT
C
C     NOTHING TO DO IF PLOTTAB OUTPUT NOT REQUESTED.
C
      IF(IMOUT(3).LE.0) RETURN
C
C     NO PLOTTAB OUTPUT UNLESS ALL ARE PRESENT.
C
      IF(NR.LE.0.OR.NN.LE.0.OR.NL.LE.0) RETURN
C
C     OUTPUT PLOT LAYOUT TO START.
C
      IF(IPASS.NE.0) GO TO 10
      IPASS=1
      WRITE(IPLOT3,8000) ZERO,XPLOT,ZERO,YPLOT,IONE,IONE
      WRITE(IPLOT3,8010) ITHREE,ITHREE,IZERO,IZERO,IZERO,IZERO
      WRITE(IPLOT3,8020)
```

```
C-----DESCRIPTION OF ELEMENT AND SUBSHELL...X RANGE 10 EV TO BINDING
C-----ENERGY...Y RANGE 1.0E-6 TO MAXIMUM.
   10 CALL NORMX(EBEV(ISUBGT),XNORM1,KSIGN1,KEXP1)
      WRITE(IPLOT3,8030) ZABCD,SHBCD,EBEV(ISUBGT),ONE,KSIGN2,KEXP2,
     1 XNORM1,KSIGN1,KEXP1,(IZERO,I=1,8)
C-----FRACTION OF ENERGY TO RADIATIVE/NON-RADIATIVE/LOCAL.
      FRACTR=100.0*OUTRE(ISUBGT)/EBEV(ISUBGT)
      FRACTN=100.0*OUTNE(ISUBGT)/EBEV(ISUBGT)
      FRACTL=100.0*OUTLE(ISUBGT)/EBEV(ISUBGT)
C
C     SPECTRA AND INTEGRAL OF SPECTRA.
C
C-----X-RAYS.
      WRITE(IPLOT1,7000) FRACTR
      WRITE(IPLOT2,7000) FRACTR
      SUMP=ZERO
      DO 20 I=1,NR
      IF(ERO(I).LE.ZERO) GO TO 20
      IF(SUMP.GT.ZERO)
     1 CALL POINT1(IPLOT1,ERO(I),SUMP,DUM,DUM,1,1,0,0)
      SUMP=SUMP+ERO(I)*PROBRO(I)/EBEV(ISUBGT)
      CALL POINT1(IPLOT1,ERO(I),SUMP,DUM,DUM,1,1,0,0)
      CALL POINT1(IPLOT2,ERO(I),DUM,DUM,PROBRO(I),1,0,0,1)
   20 CONTINUE
      CALL POINT1(IPLOT1,EBEV(ISUBGT),SUMP,DUM,DUM,1,1,0,0)
      WRITE(IPLOT1,7030)
      WRITE(IPLOT2,7030)
C-----ELECTRONS
      WRITE(IPLOT1,7010) FRACTN
      WRITE(IPLOT2,7010) FRACTN
      SUMP=ZERO
      DO 30 I=1,NN
      IF(ENO(I).LE.ZERO) GO TO 30
      IF(SUMP.GT.ZERO)
     1 CALL POINT1(IPLOT1,ENO(I),SUMP,DUM,DUM,1,1,0,0)
      SUMP=SUMP+ENO(I)*PROBNO(I)/EBEV(ISUBGT)
      CALL POINT1(IPLOT1,ENO(I),SUMP,DUM,DUM,1,1,0,0)
      CALL POINT1(IPLOT2,ENO(I),DUM,DUM,PROBNO(I),1,0,0,1)
   30 CONTINUE
      CALL POINT1(IPLOT1,EBEV(ISUBGT),SUMP,DUM,DUM,1,1,0,0)
      WRITE(IPLOT1,7030)
      WRITE(IPLOT2,7030)
C-----FREE-BOUND
      WRITE(IPLOT1,7015) FRACTL
      WRITE(IPLOT2,7015) FRACTL
      SUMP=ZERO
      DO 40 I=1,NL
      IF(ELO(I).LE.ZERO) GO TO 40
      IF(SUMP.GT.ZERO)
     1 CALL POINT1(IPLOT1,ELO(I),SUMP,DUM,DUM,1,1,0,0)
      SUMP=SUMP+ELO(I)*PROBLO(I)/EBEV(ISUBGT)
      CALL POINT1(IPLOT1,ELO(I),SUMP,DUM,DUM,1,1,0,0)
```

```
      CALL POINT1(IPLOT2,ELO(I),DUM,DUM,PROBLO(I),1,0,0,1)
   40 CONTINUE
      CALL POINT1(IPLOT1,EBEV(ISUBGT),SUMP,DUM,DUM,1,1,0,0)
      WRITE(IPLOT1,7030)
      WRITE(IPLOT2,7030)
      RETURN
 7000 FORMAT('X-Rays   ',F8.4,' %')
 7010 FORMAT('Electrons',F8.4,' %')
 7015 FORMAT('Local    ',F8.4,' %')
 7030 FORMAT('                              ')
 8000 FORMAT(4F11.5,2I11)
 8010 FORMAT(6I11)
 8020 FORMAT(' Emission Energy (eV)'/
     1 ' Spectra and Normalized Integrals')
 8030 FORMAT(12A1,12A1,F10.2,' eV Binding Energy'/
     1 ' Atom Relaxation Spectra and Normalized Integrals'/
     2 F8.5,A1,I2,F8.5,A1,I2,4I11/22X,4I11)
      END
      SUBROUTINE USER2
C
C     USER INTERFACE ROUTINE. CALLED AFTER EACH ELEMENT.
C
C***** SAVE *****
C     SAVE
C***** SAVE *****
C***** DOUBLE *****
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 MEV2EV
C***** DOUBLE *****
C***** SINGLE *****
C     REAL*4 MEV2EV
C***** SINGLE *****
      CHARACTER*1 KSIGN1,KSIGN2,KSIGN3
      INTEGER OUTP,OTAPE
      COMMON/UNITS/INP,OUTP,ITAPE,OTAPE,KTAPE,LTAPE,
     1 IPLOT1,IPLOT2,IPLOT3,IPLOT4
      COMMON/WHERE/ATWTGT,IZGET,ISUBGT,MAXSUB,MAXTRA
      COMMON/TRANS/TR(39,39),TNR(39,39,39),NSUBR(39),NSUBN(39)
      COMMON/EADL/EBMEV(39),EBEV(39),ELECT(39),HOLES(39)
      COMMON/OUTER/OUTR(39),OUTN(39),OUTL(39),OUTRE(39),OUTNE(39),
     1 OUTLE(39),OUTAVR(39),OUTAVN(39),OUTAVL(39)
      COMMON/OUTOPS/IMOUT(6)
C***** DOUBLE *****
      DATA ZERO/0.0D+00/
      DATA XNORM2/0.0D+00/
      DATA MEV2EV/1.0D+06/
C***** DOUBLE *****
C***** SINGLE *****
C     DATA ZERO/0.0E+00/
C     DATA XNORM2/0.0E+00/
C     DATA MEV2EV/1.0E+06/
C***** SINGLE *****
```

```
      DATA KSIGN2/'+'/
      DATA KEXP2/0/
      DATA IDATE/901205/
C
C     ENDL FORMATTED OUTPUT.
C
C     NOTHING TO DO IF ENDL FORMATTED OUTPUT NOT REQUESTED.
C
      IF(IMOUT(2).LE.0) RETURN
      IZA=1000*IZGET
      CALL NORMX(ATWTGT,XNORM1,KSIGN1,KEXP1)
C
C     ELECTRONS PER SUBSHELL.
C
      WRITE(OTAPE,1000) IZA,XNORM1,KSIGN1,KEXP1,IDATE,
     1 (XNORM2,KSIGN2,KEXP2,K=1,3)
      WRITE(OTAPE,1020) (XNORM2,KSIGN2,KEXP2,K=1,5)
      DO 10 I=1,MAXSUB
      IF(ELECT(I).LE.ZERO) GO TO 10
      SUB=ISUP(I)
      CALL POINT1(OTAPE,SUB,ELECT(I),DUM,DUM,1,1,0,0)
   10 CONTINUE
      WRITE(OTAPE,1060)
C
C     BINDING ENERGY.
C
      WRITE(OTAPE,1000) IZA,XNORM1,KSIGN1,KEXP1,IDATE,
     1 (XNORM2,KSIGN2,KEXP2,K=1,3)
      WRITE(OTAPE,1022) (XNORM2,KSIGN2,KEXP2,K=1,5)
      DO 20 I=1,MAXSUB
      IF(EBMEV(I).LE.ZERO) GO TO 20
      SUB=ISUP(I)
      CALL POINT1(OTAPE,SUB,EBMEV(I),DUM,DUM,1,1,0,0)
   20 CONTINUE
      WRITE(OTAPE,1060)
C
C     LOCAL ENERGY. SKIP IF ALL ARE ZERO.
C
      CALL RANGER(OUTLE,IZ1,IZ2,39)
      IF(IZ2.LE.0) GO TO 40
      WRITE(OTAPE,1000) IZA,XNORM1,KSIGN1,KEXP1,IDATE,
     1 (XNORM2,KSIGN2,KEXP2,K=1,3)
      WRITE(OTAPE,1024) (XNORM2,KSIGN2,KEXP2,K=1,5)
      DO 30 I=IZ1,IZ2
      IF(EBMEV(I).LE.ZERO) GO TO 30
      IF(OUTLE(I).LE.ZERO) GO TO 30
      SUB=ISUP(I)
      XX=OUTLE(I)/MEV2EV
      CALL POINT1(OTAPE,SUB,XX,DUM,DUM,1,1,0,0)
   30 CONTINUE
      WRITE(OTAPE,1060)
C
```

```
C     X-RAYS
C
C-----NUMBER OF X-RAYS. SKIP IF ALL ARE ZERO.
   40 CALL RANGER(OUTR,IZ1,IZ2,39)
      IF(IZ2.LE.0) GO TO 70
      WRITE(OTAPE,1012) IZA,XNORM1,KSIGN1,KEXP1,IDATE,
     1 (XNORM2,KSIGN2,KEXP2,K=1,3)
      WRITE(OTAPE,1030) (XNORM2,KSIGN2,KEXP2,K=1,5)
      DO 50 I=IZ1,IZ2
      IF(EBMEV(I).LE.ZERO) GO TO 50
      IF(OUTR(I).LE.ZERO) GO TO 50
      SUB=ISUP(I)
      CALL POINT1(OTAPE,SUB,OUTR(I),DUM,DUM,1,1,0,0)
   50 CONTINUE
      WRITE(OTAPE,1060)
C-----ENERGY.
      WRITE(OTAPE,1012) IZA,XNORM1,KSIGN1,KEXP1,IDATE,
     1 (XNORM2,KSIGN2,KEXP2,K=1,3)
      WRITE(OTAPE,1035) (XNORM2,KSIGN2,KEXP2,K=1,5)
      DO 60 I=IZ1,IZ2
      IF(EBMEV(I).LE.ZERO) GO TO 60
      IF(OUTRE(I).LE.ZERO) GO TO 60
      SUB=ISUP(I)
      XX=OUTRE(I)/MEV2EV
      CALL POINT1(OTAPE,SUB,XX,DUM,DUM,1,1,0,0)
   60 CONTINUE
      WRITE(OTAPE,1060)
C
C     ELECTRONS
C
C-----NUMBER OF ELECTRONS. SKIP IF ALL ARE ZERO.
   70 CALL RANGER(OUTN,IZ1,IZ2,39)
      IF(IZ2.LE.0) GO TO 100
      WRITE(OTAPE,1016) IZA,XNORM1,KSIGN1,KEXP1,IDATE,
     1 (XNORM2,KSIGN2,KEXP2,K=1,3)
      WRITE(OTAPE,1030) (XNORM2,KSIGN2,KEXP2,K=1,5)
      DO 80 I=IZ1,IZ2
      IF(EBMEV(I).LE.ZERO) GO TO 80
      IF(OUTN(I).LE.ZERO) GO TO 80
      SUB=ISUP(I)
      CALL POINT1(OTAPE,SUB,OUTN(I),DUM,DUM,1,1,0,0)
   80 CONTINUE
      WRITE(OTAPE,1060)
C-----ENERGY.
      WRITE(OTAPE,1016) IZA,XNORM1,KSIGN1,KEXP1,IDATE,
     1 (XNORM2,KSIGN2,KEXP2,K=1,3)
      WRITE(OTAPE,1035) (XNORM2,KSIGN2,KEXP2,K=1,5)
      DO 90 I=IZ1,IZ2
      IF(EBMEV(I).LE.ZERO) GO TO 90
      IF(OUTNE(I).LE.ZERO) GO TO 90
      SUB=ISUP(I)
      XX=OUTNE(I)/MEV2EV
```

```
      CALL POINT1(OTAPE,SUB,XX,DUM,DUM,1,1,0,0)
   90 CONTINUE
      WRITE(OTAPE,1060)
C
C     PRIMARY TRANSITIONS AND ENERGY.
C
  100 DO 180 ISUB=1,MAXSUB
      IF(EBMEV(ISUB).LE.ZERO) GO TO 180
      SUBI=ISUP(ISUB)
      CALL NORMX(SUBI,XNORM3,KSIGN3,KEXP3)
C-----RADIATIVE. SKIP IF ALL ARE ZERO.
      IF(NSUBR(ISUB).LE.0) GO TO 140
      DO 110 KSUB=1,MAXSUB
      IF(TR(ISUB,KSUB).GT.ZERO) GO TO 120
  110 CONTINUE
      GO TO 140
  120 WRITE(OTAPE,1012) IZA,XNORM1,KSIGN1,KEXP1,IDATE,
     1 (XNORM2,KSIGN2,KEXP2,K=1,3)
      WRITE(OTAPE,1036) XNORM2,KSIGN2,KEXP2,XNORM3,KSIGN3,KEXP3,
     1 (XNORM2,KSIGN2,KEXP2,K=3,5)
      DO 130 KSUB=1,MAXSUB
      IF(TR(ISUB,KSUB).LE.ZERO) GO TO 130
      SUBK=ISUP(KSUB)
      ET=EBMEV(ISUB)-EBMEV(KSUB)
      IF(ET.LT.ZERO) ET=ZERO
      CALL POINT1(OTAPE,SUBK,TR(ISUB,KSUB),ET,DUM,1,1,1,0)
  130 CONTINUE
      WRITE(OTAPE,1060)
C-----NON-RADIATIVE. SKIP IF ALL ARE ZERO.
  140 IF(NSUBN(ISUB).LE.0) GO TO 180
      DO 150 KSUB=1,MAXSUB
      DO 150 LSUB=1,MAXSUB
      IF(TNR(ISUB,KSUB,LSUB).GT.ZERO) GO TO 160
  150 CONTINUE
      GO TO 180
  160 WRITE(OTAPE,1016) IZA,XNORM1,KSIGN1,KEXP1,IDATE,
     1 (XNORM2,KSIGN2,KEXP2,K=1,3)
      WRITE(OTAPE,1037) XNORM2,KSIGN2,KEXP2,XNORM3,KSIGN3,KEXP3,
     1 (XNORM2,KSIGN2,KEXP2,K=3,5)
      DO 170 KSUB=1,MAXSUB
      DO 170 LSUB=1,MAXSUB
      IF(TNR(ISUB,KSUB,LSUB).LE.ZERO) GO TO 170
      SUBK=ISUP(KSUB)
      SUBL=ISUP(LSUB)
      ET=EBMEV(ISUB)-(EBMEV(KSUB)+EBMEV(LSUB))
      IF(ET.LT.ZERO) ET=ZERO
      CALL POINT1(OTAPE,SUBK,SUBL,TNR(ISUB,KSUB,LSUB),ET,1,1,1,1)
  170 CONTINUE
      WRITE(OTAPE,1060)
  180 CONTINUE
      RETURN
 1000 FORMAT(I6,'  0  0',F9.5,A1,I2,I7,'  2',3(F9.5,A1,I2))
```

```
 1012 FORMAT(I6,'  0  7',F9.5,A1,I2,I7,'  2',3(F9.5,A1,I2))
 1016 FORMAT(I6,'  0  9',F9.5,A1,I2,I7,'  2',3(F9.5,A1,I2))
 1020 FORMAT('91912  0',5(F9.5,A1,I2))
 1022 FORMAT('91913  0',5(F9.5,A1,I2))
 1024 FORMAT('92935  0',5(F9.5,A1,I2))
 1030 FORMAT('92933  0',5(F9.5,A1,I2))
 1035 FORMAT('92934  0',5(F9.5,A1,I2))
 1036 FORMAT('92931 91',5(F9.5,A1,I2))
 1037 FORMAT('92932 91',5(F9.5,A1,I2))
 1060 FORMAT(71X,'1')
      END
      SUBROUTINE POINT1(IUNIT,Z1,Z2,Z3,Z4,I1,I2,I3,I4)
C
C     OUTPUT ONE POINT (A LINE) WITH UP TO 4 FIELD
C
C     TYPES OF LAYOUT CONSIDERED INCLUDE,
C     1 2
C     1 2 3
C     1 2 3 4
C     1     4
C
C***** SAVE *****
C     SAVE
C***** SAVE *****
C***** DOUBLE *****
      IMPLICIT REAL*8 (A-H,O-Z)
C***** DOUBLE *****
      CHARACTER*1 KSIGN1,KSIGN2,KSIGN3,KSIGN4
C-----ERROR IF FIELD 1 IS NOT SELECTED.
      IF(I1.LE.0) RETURN
C-----ALWAYS USE FIELD 1
      CALL NORMX(Z1,XNORM1,KSIGN1,KEXP1)
C-----SELECT FORMAT
      IF(I2.EQ.0) GO TO 30
      CALL NORMX(Z2,XNORM2,KSIGN2,KEXP2)
      IF(I3.NE.0) GO TO 10
C----- 1 2
      WRITE(IUNIT,1000) XNORM1,KSIGN1,KEXP1,XNORM2,KSIGN2,KEXP2
      GO TO 40
   10 CALL NORMX(Z3,XNORM3,KSIGN3,KEXP3)
      IF(I4.NE.0) GO TO 20
C----- 1 2 3
      WRITE(IUNIT,1000) XNORM1,KSIGN1,KEXP1,XNORM2,KSIGN2,KEXP2,
     1 XNORM3,KSIGN3,KEXP3
      GO TO 40
C----- 1 2 3 4
   20 CALL NORMX(Z4,XNORM4,KSIGN4,KEXP4)
      WRITE(IUNIT,1000) XNORM1,KSIGN1,KEXP1,XNORM2,KSIGN2,KEXP2,
     1 XNORM3,KSIGN3,KEXP3,XNORM4,KSIGN4,KEXP4
      GO TO 40
C----- 1     4
   30 CALL NORMX(Z4,XNORM4,KSIGN4,KEXP4)
```

```
      WRITE(IUNIT,1010) XNORM1,KSIGN1,KEXP1,XNORM4,KSIGN4,KEXP4
   40 RETURN
 1000 FORMAT(4(F8.5,A1,I2))
 1010 FORMAT(F8.5,A1,I2,22X,F8.5,A1,I2)
      END
      SUBROUTINE SPECTA
C
C     DEFINE SPECTRUM OF EMITTED X-RAYS AND ELECTRONS.
C
C     RETURN ATOM TO NEUTRALITY
C
C***** SAVE *****
C     SAVE
C***** SAVE *****
C***** DOUBLE *****
      IMPLICIT REAL*8 (A-H,O-Z)
C***** DOUBLE *****
      COMMON/WHERE/ATWTGT,IZGET,ISUBGT,MAXSUB,MAXTRA
      COMMON/TRANS/TR(39,39),TNR(39,39,39),NSUBR(39),NSUBN(39)
      COMMON/SPECTR/ERO(5000),PROBRO(5000),NR
      COMMON/SPECTN/ENO(5000),PROBNO(5000),NN
      COMMON/SPECTL/ELO(39),PROBLO(39),NL
      COMMON/EADL/EBMEV(39),EBEV(39),ELECT(39),HOLES(39)
      COMMON/OUTER/OUTR(39),OUTN(39),OUTL(39),OUTRE(39),OUTNE(39),
     1 OUTLE(39),OUTAVR(39),OUTAVN(39),OUTAVL(39)
      COMMON/INDEXS/INDEXR(5000),INDEXN(5000),INDEXL(39)
      COMMON/FLUORS/FLUOR(100,39,6),MSHELL,MSUB1,MSUB2
C***** DOUBLE *****
      DATA ZERO/0.0D+00/
      DATA ONE/1.0D+00/
      DATA HOLMIN/1.0D-10/
C***** DOUBLE *****
C***** SINGLE *****
C     DATA ZERO/0.0E+00/
C     DATA ONE/1.0E+00/
C     DATA HOLMIN/1.0E-10/
C***** SINGLE *****
C-----NOTHING TO DO IF SUBSHELL ENERGY IS NOT DEFINED.
      IF(EBMEV(ISUBGT).LE.ZERO) RETURN
C-----INITIALIZE NUMBER OF HOLES.
      DO 10 I=ISUBGT,MAXSUB
   10 HOLES(I)=ZERO
      HOLES(ISUBGT)=ONE
      HOLEX=ONE
      IF(ELECT(ISUBGT).LT.ONE) HOLEX=ELECT(ISUBGT)
      HOLES(ISUBGT)=HOLEX
      HNORM=ONE/HOLEX
C
C     LOOP OVER SUBSHELLS.
C
      DO 60 ISUB=ISUBGT,MAXSUB
C-----ONLY CONSIDER SUBSHELLS FOR WHICH HOLES EXIST AND DATA HAS
```

```
C-----BEEN READ.
      IF(HOLES(ISUB).EQ.ZERO) GO TO 60
C
C     FILL INITIAL HOLE AND GENERATE X-RAYS AND ELECTRONS.
C
C     RADIATIVE.
C
C-----DEFINE INITIAL NUMBER OF HOLES.
      HOLEK=HOLES(ISUB)
      IF(NSUBR(ISUB).LE.0) GO TO 40
C-----LOOP OVER TRANSITIONS.
      DO 30 I=ISUB,MAXSUB
      IF(TR(ISUB,I).LE.ZERO) GO TO 30
C-----FILL AND CREATE HOLE.
      HOLEI=HOLEK*TR(ISUB,I)
      HOLE1=HNORM*HOLEI
      HOLES(ISUB)=HOLES(ISUB)-HOLEI
      HOLES(I)=HOLES(I)+HOLEI
C-----FLUORESCENCE YIELD - TRANSITIONS.
      FLUOR(IZGET,ISUBGT,3)=FLUOR(IZGET,ISUBGT,3)+HOLEI
      IF(ISUB.GT.MSUB2) GO TO 20
      FLUOR(IZGET,ISUBGT,2)=FLUOR(IZGET,ISUBGT,2)+HOLEI
      IF(ISUB.NE.ISUBGT) GO TO 20
      FLUOR(IZGET,ISUBGT,1)=FLUOR(IZGET,ISUBGT,1)+HOLEI
C-----EMIT X-RAY.
   20 NR=NR+1
      IF(NR.GT.5000) GO TO 150
      ERO(NR)=EBEV(ISUB)-EBEV(I)
      PROBRO(NR)=HOLE1
      INDEXR(NR)=100*ISUB+I
      IF(ERO(NR).LT.ZERO) ERO(NR)=ZERO
C-----FLUORESCENCE YIELD - ENERGY.
      EHOLEI=ERO(NR)*HOLEI
      FLUOR(IZGET,ISUBGT,6)=FLUOR(IZGET,ISUBGT,6)+EHOLEI
      IF(ISUB.GT.MSUB2) GO TO 30
      FLUOR(IZGET,ISUBGT,5)=FLUOR(IZGET,ISUBGT,5)+EHOLEI
      IF(ISUB.NE.ISUBGT) GO TO 30
      FLUOR(IZGET,ISUBGT,4)=FLUOR(IZGET,ISUBGT,4)+EHOLEI
C-----EMIT X-RAY.
   30 CONTINUE
C
C     NON-RADIATIVE.
C
   40 IF(NSUBN(ISUB).LE.0) GO TO 60
C-----LOOP OVER TRANSITIONS.
      DO 50 I=ISUB,MAXSUB
      DO 50 J=ISUB,MAXSUB
      IF(TNR(ISUB,I,J).LE.ZERO) GO TO 50
C-----FILL AND CREATE 2 HOLES.
      HOLEIJ=HOLEK*TNR(ISUB,I,J)
      HOLE1=HNORM*HOLEIJ
      HOLES(ISUB)=HOLES(ISUB)-HOLEIJ
```

```
      HOLES(I)=HOLES(I)+HOLEIJ
      HOLES(J)=HOLES(J)+HOLEIJ
C-----EMIT ELECTRON.
      NN=NN+1
      IF(NN.GT.5000) GO TO 160
      ENO(NN)=EBEV(ISUB)-(EBEV(I)+EBEV(J))
      PROBNO(NN)=HOLE1
      INDEXN(NN)=10000*ISUB+100*I+J
      IF(ENO(NN).LT.ZERO) ENO(NN)=ZERO
   50 CONTINUE
C
C     NEXT SUBSHELL.
C
   60 CONTINUE
C
C     LOCAL = FREE-BOUND TRANSITIONS...BASED ON REMAINING HOLES
C     AND SUBSHELL BINDING ENERGIES.
C
      DO 70 ISUB=MAXSUB,ISUBGT,-1
      IF(HOLES(ISUB).LE.HOLMIN) GO TO 70
      NL=NL+1
      ELO(NL)=EBEV(ISUB)
      PROBLO(NL)=HNORM*HOLES(ISUB)
      INDEXL(NL)=ISUB
   70 CONTINUE
C
C     SORT SPECTRA INTO ASCENDING ENERGY ORDER.
C
      CALL SORTS(ERO,PROBRO,INDEXR,NR)
      CALL SORTS(ENO,PROBNO,INDEXN,NN)
      CALL SORTS(ELO,PROBLO,INDEXL,NL)
C
C     DEFINE NUMBER OF PARTICLES AND ENERGY EMITTED.
C
C-----X-RAYS.
      SUMR=ZERO
      ERAD=ZERO
      IF(NR.LE.0) GO TO 90
      DO 80 I=1,NR
      SUMR=SUMR+PROBRO(I)
   80 ERAD=ERAD+PROBRO(I)*ERO(I)
C-----ELECTRONS.
   90 SUMN=ZERO
      ENORAD=ZERO
      IF(NN.LE.0) GO TO 110
      DO 100 I=1,NN
      SUMN=SUMN+PROBNO(I)
  100 ENORAD=ENORAD+PROBNO(I)*ENO(I)
C-----LOCAL.
  110 SUML=ZERO
      ELOC1=ZERO
      ELOCAL=ZERO
```

```
      IF(NL.LE.0) GO TO 140
      DO 120 I=1,NL
      SUML=SUML+PROBLO(I)
  120 ELOC1=ELOC1+PROBLO(I)*ELO(I)
C
C     RE-BALANCE TO OBTAIN EXACT ENERGY BALANCE (ENERGY WILL NOT
C     BALANCE ONLY IN THE CASE WHERE THE TRANSITIONS INDICATE A
C     NEGATIVE ENERGY ELECTRON EMITTED AND ITS ENERGY HAS BEEN
C     SET TO ZERO, ABOVE...THIS WILL RESULT IN TOO MUCH ENERGY
C     REMAINING IN THE ATOM...BASED ON REMAINING HOLES AND THE
C     BINDING ENERGY OF THE SUBSHELLS IN WHICH HOLES REMAIN.
C     THE NUMBER OF HOLES CANNOT BE CHANGED IF THE ATOM IS TO
C     RETURN TO NEUTRALITY AND ELECTRONS CONSERVED. RE-BALANCE
C     IS ACHIEVED BY SLIGHTLY CHANGING THE ENERGY OF FREE-BOUND
C     TRANSITIONS.
C
      ELOCAL=EBEV(ISUBGT)-(ERAD+ENORAD)
      RATLOC=ELOCAL/ELOC1
      DO 130 I=1,NL
  130 ELO(I)=RATLOC*ELO(I)
C
C     SAVE AVERAGE VALUES.
C
C-----SAVE NUMBER OF X-RAYS, ELECTRONS AND FREE-BOUND EMISSIONS.
  140 OUTR(ISUBGT)=SUMR
      OUTN(ISUBGT)=SUMN
      OUTL(ISUBGT)=SUML
C-----SAVE ENERGY.
      OUTRE(ISUBGT)=ERAD
      OUTNE(ISUBGT)=ENORAD
      OUTLE(ISUBGT)=ELOCAL
C-----SAVE AVERAGE EMISSION ENERGIES.
      OUTAVR(ISUBGT)=ZERO
      OUTAVN(ISUBGT)=ZERO
      OUTAVL(ISUBGT)=ZERO
      IF(SUMR.GT.ZERO) OUTAVR(ISUBGT)=ERAD/SUMR
      IF(SUMN.GT.ZERO) OUTAVN(ISUBGT)=ENORAD/SUMN
      IF(SUML.GT.ZERO) OUTAVL(ISUBGT)=ELOCAL/SUML
      RETURN
C
C     SPECTRA CORE EXCEEDED.
C
  150 WRITE(6,6000)
      STOP
  160 WRITE(6,6010)
      STOP
 6000 FORMAT(' RADIATIVE SPECTRUM CORE EXCEEDED')
 6010 FORMAT(' NON-RADIATIVE SPECTRUM CORE EXCEEDED')
      END
      SUBROUTINE SPECTB
C
C     DEFINE SPECTRUM OF EMITTED X-RAYS AND ELECTRONS.
```

```
C
C     ISOLATED ATOM
C
C***** SAVE *****
C     SAVE
C***** SAVE *****
C***** DOUBLE *****
      IMPLICIT REAL*8 (A-H,O-Z)
C***** DOUBLE *****
      COMMON/WHERE/ATWTGT,IZGET,ISUBGT,MAXSUB,MAXTRA
      COMMON/TRANS/TR(39,39),TNR(39,39,39),NSUBR(39),NSUBN(39)
      COMMON/SPECTR/ERO(5000),PROBRO(5000),NR
      COMMON/SPECTN/ENO(5000),PROBNO(5000),NN
      COMMON/SPECTL/ELO(39),PROBLO(39),NL
      COMMON/EADL/EBMEV(39),EBEV(39),ELECT(39),HOLES(39)
      COMMON/OUTER/OUTR(39),OUTN(39),OUTL(39),OUTRE(39),OUTNE(39),
     1 OUTLE(39),OUTAVR(39),OUTAVN(39),OUTAVL(39)
      COMMON/INDEXS/INDEXR(5000),INDEXN(5000),INDEXL(39)
      COMMON/FLUORS/FLUOR(100,39,6),MSHELL,MSUB1,MSUB2
      DIMENSION ENOW(39)
C***** DOUBLE *****
      DATA ZERO/0.0D+00/
      DATA ONE/1.0D+00/
      DATA HOLMIN/1.0D-10/
C***** DOUBLE *****
C***** SINGLE *****
C     DATA ZERO/0.0E+00/
C     DATA ONE/1.0E+00/
C     DATA HOLMIN/1.0E-10/
C***** SINGLE *****
C-----NOTHING TO DO IF SUBSHELL ENERGY IS NOT DEFINED.
      IF(EBMEV(ISUBGT).LE.ZERO) RETURN
C-----INITIALIZE NUMBER OF HOLES.
      DO 10 I=ISUBGT,MAXSUB
      ENOW(I)=ELECT(I)
   10 HOLES(I)=ZERO
      HOLES(ISUBGT)=ONE
      HOLEX=ONE
      IF(ELECT(ISUBGT).LT.ONE) HOLEX=ELECT(ISUBGT)
      ENOW(ISUBGT)=ENOW(ISUBGT)-HOLEX
      HOLES(ISUBGT)=HOLEX
      HNORM=ONE/HOLEX
C
C     LOOP OVER SUBSHELLS.
C
      DO 60 ISUB=ISUBGT,MAXSUB
C-----ONLY CONSIDER SUBSHELLS FOR WHICH HOLES EXIST AND DATA HAS
C-----BEEN READ.
      IF(HOLES(ISUB).EQ.ZERO) GO TO 60
C
C     FILL INITIAL HOLE AND GENERATE X-RAYS AND ELECTRONS.
C
```

```
C     RADIATIVE.
C
C-----DEFINE INITIAL NUMBER OF HOLES.
      HOLEK=HOLES(ISUB)
      IF(NSUBR(ISUB).LE.0) GO TO 40
C-----LOOP OVER TRANSITIONS.
      DO 30 I=ISUB,MAXSUB
      IF(TR(ISUB,I).LE.ZERO) GO TO 30
C-----FILL AND CREATE HOLE UP TO THE NUMBER OF ELECTRONS AVAILABLE.
      HOLEI=HOLEK*TR(ISUB,I)
      IF(HOLEI.GT.ENOW(I)) HOLEI=ENOW(I)
      HOLE1=HNORM*HOLEI
      HOLES(ISUB)=HOLES(ISUB)-HOLEI
      HOLES(I)=HOLES(I)+HOLEI
      ENOW(ISUB)=ENOW(ISUB)+HOLEI
      ENOW(I)=ENOW(I)-HOLEI
C-----FLUORESCENCE YIELD - TRANSITIONS.
      FLUOR(IZGET,ISUBGT,3)=FLUOR(IZGET,ISUBGT,3)+HOLEI
      IF(ISUB.GT.MSUB2) GO TO 20
      FLUOR(IZGET,ISUBGT,2)=FLUOR(IZGET,ISUBGT,2)+HOLEI
      IF(ISUB.NE.ISUBGT) GO TO 20
      FLUOR(IZGET,ISUBGT,1)=FLUOR(IZGET,ISUBGT,1)+HOLEI
C-----EMIT X-RAY.
   20 NR=NR+1
      IF(NR.GT.5000) GO TO 150
      ERO(NR)=EBEV(ISUB)-EBEV(I)
      PROBRO(NR)=HOLE1
      INDEXR(NR)=100*ISUB+I
      IF(ERO(NR).LT.ZERO) ERO(NR)=ZERO
C-----FLUORESCENCE YIELD - ENERGY.
      EHOLEI=ERO(NR)*HOLEI
      FLUOR(IZGET,ISUBGT,6)=FLUOR(IZGET,ISUBGT,6)+EHOLEI
      IF(ISUB.GT.MSUB2) GO TO 30
      FLUOR(IZGET,ISUBGT,5)=FLUOR(IZGET,ISUBGT,5)+EHOLEI
      IF(ISUB.NE.ISUBGT) GO TO 30
      FLUOR(IZGET,ISUBGT,4)=FLUOR(IZGET,ISUBGT,4)+EHOLEI
C-----EMIT X-RAY.
   30 CONTINUE
C
C     NON-RADIATIVE.
C
   40 IF(NSUBN(ISUB).LE.0) GO TO 60
C-----LOOP OVER TRANSITIONS.
      DO 50 I=ISUB,MAXSUB
      DO 50 J=ISUB,MAXSUB
      IF(TNR(ISUB,I,J).LE.ZERO) GO TO 50
C-----FILL AND CREATE HOLE UP TO THE NUMBER OF ELECTRONS AVAILABLE.
      HOLEIJ=HOLEK*TNR(ISUB,I,J)
      IF(HOLEIJ.GT.ENOW(I)) HOLEIJ=ENOW(I)
      IF(HOLEIJ.GT.ENOW(J)) HOLEIJ=ENOW(J)
      IF(I.EQ.J.AND.HOLEIJ.GT.0.5*ENOW(I)) HOLEIJ=0.5*ENOW(I)
      HOLE1=HNORM*HOLEIJ
```

```
      HOLES(ISUB)=HOLES(ISUB)-HOLEIJ
      HOLES(I)=HOLES(I)+HOLEIJ
      HOLES(J)=HOLES(J)+HOLEIJ
      ENOW(ISUB)=ENOW(ISUB)+HOLEIJ
      ENOW(I)=ENOW(I)-HOLEIJ
      ENOW(J)=ENOW(J)-HOLEIJ
C-----EMIT ELECTRON.
      NN=NN+1
      IF(NN.GT.5000) GO TO 160
      ENO(NN)=EBEV(ISUB)-(EBEV(I)+EBEV(J))
      PROBNO(NN)=HOLE1
      INDEXN(NN)=10000*ISUB+100*I+J
      IF(ENO(NN).LT.ZERO) ENO(NN)=ZERO
   50 CONTINUE
C
C     NEXT SUBSHELL.
C
   60 CONTINUE
C
C     LOCAL = FREE-BOUND TRANSITIONS...BASED ON REMAINING HOLES
C     AND SUBSHELL BINDING ENERGIES.
C
      DO 70 ISUB=MAXSUB,ISUBGT,-1
      IF(HOLES(ISUB).LE.HOLMIN) GO TO 70
      NL=NL+1
      ELO(NL)=EBEV(ISUB)
      PROBLO(NL)=HNORM*HOLES(ISUB)
      INDEXL(NL)=ISUB
   70 CONTINUE
C
C     SORT SPECTRA INTO ASCENDING ENERGY ORDER.
C
      CALL SORTS(ERO,PROBRO,INDEXR,NR)
      CALL SORTS(ENO,PROBNO,INDEXN,NN)
      CALL SORTS(ELO,PROBLO,INDEXL,NL)
C
C     DEFINE NUMBER OF PARTICLES AND ENERGY EMITTED.
C
C-----X-RAYS.
      SUMR=ZERO
      ERAD=ZERO
      IF(NR.LE.0) GO TO 90
      DO 80 I=1,NR
      SUMR=SUMR+PROBRO(I)
   80 ERAD=ERAD+PROBRO(I)*ERO(I)
C-----ELECTRONS.
   90 SUMN=ZERO
      ENORAD=ZERO
      IF(NN.LE.0) GO TO 110
      DO 100 I=1,NN
      SUMN=SUMN+PROBNO(I)
  100 ENORAD=ENORAD+PROBNO(I)*ENO(I)
```

```
C-----LOCAL.
  110 SUML=ZERO
      ELOC1=ZERO
      ELOCAL=ZERO
      IF(NL.LE.0) GO TO 140
      DO 120 I=1,NL
      SUML=SUML+PROBLO(I)
  120 ELOC1=ELOC1+PROBLO(I)*ELO(I)
C
C     RE-BALANCE TO OBTAIN EXACT ENERGY BALANCE (ENERGY WILL NOT
C     BALANCE ONLY IN THE CASE WHERE THE TRANSITIONS INDICATE A
C     NEGATIVE ENERGY ELECTRON EMITTED AND ITS ENERGY HAS BEEN
C     SET TO ZERO, ABOVE...THIS WILL RESULT IN TOO MUCH ENERGY
C     REMAINING IN THE ATOM...BASED ON REMAINING HOLES AND THE
C     BINDING ENERGY OF THE SUBSHELLS IN WHICH HOLES REMAIN.
C     THE NUMBER OF HOLES CANNOT BE CHANGED IF THE ATOM IS TO
C     RETURN TO NEUTRALITY AND ELECTRONS CONSERVED. RE-BALANCE
C     IS ACHIEVED BY SLIGHTLY CHANGING THE ENERGY OF FREE-BOUND
C     TRANSITIONS.
C
      ELOCAL=EBEV(ISUBGT)-(ERAD+ENORAD)
      RATLOC=ELOCAL/ELOC1
      DO 130 I=1,NL
  130 ELO(I)=RATLOC*ELO(I)
C
C     SAVE AVERAGE VALUES.
C
C-----SAVE NUMBER OF X-RAYS, ELECTRONS AND FREE-BOUND EMISSIONS.
  140 OUTR(ISUBGT)=SUMR
      OUTN(ISUBGT)=SUMN
      OUTL(ISUBGT)=SUML
C-----SAVE ENERGY.
      OUTRE(ISUBGT)=ERAD
      OUTNE(ISUBGT)=ENORAD
      OUTLE(ISUBGT)=ELOCAL
C-----SAVE AVERAGE EMISSION ENERGIES.
      OUTAVR(ISUBGT)=ZERO
      OUTAVN(ISUBGT)=ZERO
      OUTAVL(ISUBGT)=ZERO
      IF(SUMR.GT.ZERO) OUTAVR(ISUBGT)=ERAD/SUMR
      IF(SUMN.GT.ZERO) OUTAVN(ISUBGT)=ENORAD/SUMN
      IF(SUML.GT.ZERO) OUTAVL(ISUBGT)=ELOCAL/SUML
      RETURN
C
C     SPECTRA CORE EXCEEDED.
C
  150 WRITE(6,6000)
      STOP
  160 WRITE(6,6010)
      STOP
 6000 FORMAT(' RADIATIVE SPECTRUM CORE EXCEEDED')
 6010 FORMAT(' NON-RADIATIVE SPECTRUM CORE EXCEEDED')
```

```
      END
      SUBROUTINE SORTS(X,Y,INDEX,NXY)
C
C     SORT AN ARRAY INTO ASCENDING FLOATING POINT ORDER.
C
C     ARGUMENTS
C     ---------
C     X      = ARRAY TO SORT (DIMENSION NXY)
C     Y      = COMPANION ARRAY (DIMENSION NXY)
C     INDEX  = COMPANION ARRAY (DIMENSION NXY)
C     NXY    = NUMBER OF ELEMENTS TO SORT
C
C***** SAVE *****
C     SAVE
C***** SAVE *****
C***** DOUBLE *****
      IMPLICIT REAL*8 (A-H,O-Z)
C***** DOUBLE *****
      INTEGER SWITCH
      DIMENSION X(NXY),Y(NXY),INDEX(NXY)
C-----IF LESS THAN TWO (2) ELEMENTS NO SORT IS REQUIRED.
      IF(NXY.LT.2) RETURN
C-----SET INNER LOOP INDICES
      LTOP=NXY+1
C-----SET UP OUTER LOOP
      DO 30 IN=2,NXY
C-----INITIALIZE EXCHANGE SWITCH OFF.
      SWITCH=0
C-----SET UPPER INDEX TO INNER LOOP
      LTOP=LTOP-1
C-----SET LARGEST ELEMENT INDICATOR TO FIRST ELEMENT
      LBIG=1
C-----SET UP INNER LOOP
      DO 20 J=2,LTOP
C-----COMPARE ELEMENTS
      IF(X(LBIG).GT.X(J)) GO TO 10
C-----ELEMENTS ARE IN NUMERICAL ORDER. RESET INDEX TO LARGER ELEMENT.
      LBIG=J
      GO TO 20
C-----ELEMENTS ARE NOT IN NUMERICAL ORDER. SET INTERCHANGE SWITCH.
   10 SWITCH=1
C-----END OF INNER LOOP
   20 CONTINUE
C-----ARE ALL ELEMENTS ALREADY IN ORDER......
      IF(SWITCH.LE.0) RETURN
C-----NO. MOVE LARGEST ELEMENT TO TOP OF REMAINING TABLE
      DUMMY=X(LBIG)
      X(LBIG)=X(LTOP)
      X(LTOP)=DUMMY
      DUMMY=Y(LBIG)
      Y(LBIG)=Y(LTOP)
      Y(LTOP)=DUMMY
```

```
      IDUM=INDEX(LBIG)
      INDEX(LBIG)=INDEX(LTOP)
      INDEX(LTOP)=IDUM
   30 CONTINUE
      RETURN
      END
      SUBROUTINE ZAHOL(ZA,ZABCD)
C
C     GIVEN ANY ZA (1000*Z+A) THIS ROUTINE WILL DEFINE A 12 CHARACTER
C     EQUIVALENT IN ONE OF THE FOLLOWING 2 FORMS,
C
C     (1) Z GREATER THAN 0
C         ZZZ-SS-AAA  - ZZZ = Z
C                        SS = CHEMICCAL SYMBOL
C                       AAA = A
C
C     FOR EXAMPLE ZA = 92238 IS RETURNED AS 92-U -238
C
C     (2) Z EQUAL TO 0
C         12 CHARACTERS FOR ENDF/B SPECIAL MATERIALS
C
C     FOR EXAMPLE ZA = 302 IS RETURNED AS ZIRCALLOY-2
C
C***** SAVE ******
C     SAVE
C***** SAVE ******
      INTEGER ZA,Z,A
      CHARACTER*1 DUM1,DUM2,ZABCD,ZATAB,GOOF,MINUS,NATURE,BLANK,DIGITS
      DIMENSION ZATAB(2,103),DUM1(2,54),DUM2(2,49),ZABCD(12),GOOF(12),
     1 NATURE(4),DIGITS(10)
      EQUIVALENCE (ZATAB(1,1),DUM1(1,1)),(ZATAB(1,55),DUM2(1,1))
      DATA GOOF/'Z','A',' ','U','n','k','n','o','w','n',' ',' '/
      DATA MINUS/'-'/
      DATA NATURE/'N','a','t',' '/
      DATA BLANK/' '/
      DATA DIGITS/'0','1','2','3','4','5','6','7','8','9'/
      DATA DUM1/
     1 'H',' ','H','e','L','i','B','e','B',' ','C',' ',
     1 'N',' ','O',' ','F',' ','N','e','N','a','M','g',
     1 'A','l','S','i','P',' ','S',' ','C','l','A','r',
     1 'K',' ','C','a','S','c','T','i','V',' ','C','r',
     1 'M','n','F','e','C','o','N','i','C','u','Z','n',
     1 'G','a','G','e','A','s','S','e','B','r','K','r',
     1 'R','b','S','r','Y',' ','Z','r','N','b','M','o',
     1 'T','c','R','u','R','h','P','d','A','g','C','d',
     1 'I','n','S','n','S','b','T','e','I',' ','X','e'/
      DATA DUM2/
     1 'C','s','B','a','L','a','C','e','P','r','N','d',
     1 'P','m','S','m','E','u','G','d','T','b','D','y',
     1 'H','o','E','r','T','m','Y','b','L','u','H','f',
     1 'T','a','W',' ','R','e','O','s','I','r','P','t',
     1 'A','u','H','g','T','l','P','b','B','i','P','o',
```

```
     1 'A','t','R','n','F','r','R','a','A','c','T','h',
     1 'P','a','U',' ','N','p','P','u','A','m','C','m',
     1 'B','k','C','f','E','s','F','m','M','d','N','o',
     1 'L','r'/
C-----BLANK OUT ZABCD TO START.
      DO 10 I=1,12
   10 ZABCD(I)=BLANK
C-----DEFINE Z AND A SEPARATELY.
      Z=ZA/1000
      A=ZA-1000*Z
C-----INSURE Z IS IN LEGAL RANGE.
      IF(Z.GE.0.AND.Z.LE.103) GO TO 30
      DO 20 I=1,12
   20 ZABCD(I)=GOOF(I)
      RETURN
C-----DEFINE SYMBOL FOR ELEMENT.
   30 ZABCD(5)=MINUS
      ZABCD(6)=ZATAB(1,Z)
      ZABCD(7)=ZATAB(2,Z)
      ZABCD(8)=MINUS
C-----DEFINE Z FIRST DIGIT TO LAST.
      IDIV=100
      IMON=0
      II=2
      DO 50 I=1,3
      IZ=Z/IDIV
      IF(IZ.EQ.0.AND.IMON.EQ.0) GO TO 40
      IMON=1
      ZABCD(II)=DIGITS(IZ+1)
   40 II=II+1
      Z=Z-IDIV*IZ
   50 IDIV=IDIV/10
      IF(A.GT.0) GO TO 60
C-----NATURAL ISOTOPIC MIXTURE.
      ZABCD(9)=NATURE(1)
      ZABCD(10)=NATURE(2)
      ZABCD(11)=NATURE(3)
      ZABCD(12)=NATURE(4)
      GO TO 90
C-----DEFINE A FIRST DIGIT TO LAST.
   60 IDIV=100
      IMON=0
      II=8
      DO 80 I=1,3
      IA=A/IDIV
      IF(IA.EQ.0.AND.IMON.EQ.0) GO TO 70
      IMON=1
      II=II+1
      ZABCD(II)=DIGITS(IA+1)
   70 A=A-IDIV*IA
   80 IDIV=IDIV/10
   90 RETURN
```

```
      END
      SUBROUTINE SUB4(ISHELL,SHBCD)
C
C     SHORT FORM OF SUBSHELL I.D.
C
C***** SAVE ******
C     SAVE
C***** SAVE ******
      CHARACTER*1 SHBCD,BLANK
      DIMENSION SHBCD(12)
      DATA BLANK/' '/
      CALL SUBHOL(ISHELL,SHBCD)
      DO 10 I=1,12
      IF(SHBCD(I).EQ.BLANK) GO TO 20
   10 CONTINUE
      RETURN
   20 DO 30 K=I,12
   30 SHBCD(K)=BLANK
      RETURN
      END
      SUBROUTINE SUBHOL(ISHELL,SHBCD)
C
C     USE ENDL SUBSHELL DESIGNATOR TO DEFINE SUBSHELL
C
C     ARGUMENTS
C     =========
C     ISHELL  = ENDL SUBSHELL DESIGNATOR
C     SHBCD   = HOLLERITH EQUIVALENT RETURNED IN 3A4 FORMAT
C
C     FOR EXAMPLE, FOR ISHELL=1, SHBCD IS RETURNED AS 'K (1S1/2)   '
C     WITHOUT THE ENCLOSING QUOTES.
C
C***** SAVE ******
C     SAVE
C***** SAVE ******
      CHARACTER*4 SHTAB,SHTAB1,SHTAB2,SHTAB3,SHBCD,TOTAL
      DIMENSION SHTAB(3,62),SHTAB1(3,27),SHTAB2(3,27),SHTAB3(3,8),
     1 SHBCD(3),TOTAL(3)
      EQUIVALENCE (SHTAB(1,1),SHTAB1(1,1)),(SHTAB(1,28),SHTAB2(1,1)),
     1 (SHTAB(1,55),SHTAB3(1,1))
      DATA SHTAB1/
     1 'K (1','s1/2',')   ','L (2',')   ','    ','L1 (','2s1/','2)  ',
     2 'L23 ','(2p)','    ','L2 (','2p1/','2)  ','L3 (','2p3/','2)  ',
     3 'M (3',')   ','    ','M1 (','3s1/','2)  ','M23 ','(3p)','    ',
     4 'M2 (','3p1/','2)  ','M3 (','3p3/','2)  ','M45 ','(3d)','    ',
     5 'M4 (','3d3/','2)  ','M5 (','3d5/','2)  ','N (4',')   ','    ',
     6 'N1 (','4s1/','2)  ','N23 ','(4p)','    ','N2 (','4p1/','2)  ',
     7 'N3 (','4p3/','2)  ','N45 ','(4d)','    ','N4 (','4d3/','2)  ',
     8 'N5 (','4d5/','2)  ','N67 ','(4f)','    ','N6 (','4f5/','2)  ',
     9 'N7 (','4f7/','2)  ','O (5',')   ','    ','O1 (','5s1/','2)  '/
      DATA SHTAB2/
     1 'O23 ','(5p)','    ','O2 (','5p1/','2)  ','O3 (','5p3/','2)  ',
```

```
     2 'O45 ','(5d)','    ','O4 (','5d3/','2)  ','O5 (','5d5/','2)  ',
     3 'O67 ','(5f)','    ','O6 (','5f5/','2)  ','O7 (','5f7/','2)  ',
     4 'O89 ','(5g)','    ','O8 (','5g7/','2)  ','O9 (','5g9/','2)  ',
     5 'P (6',')   ','    ','P1 (','6s1/','2)  ','P23 ','(6p)','    ',
     6 'P2 (','6p1/','2)  ','P3 (','6p3/','2)  ','P45 ','(6d)','    ',
     7 'P4 (','6d3/','2)  ','P5 (','6d5/','2)  ','P67 ','(6f)','    ',
     8 'P6 (','6f5/','2)  ','P7 (','6f7/','2)  ','P89 ','(6g)','    ',
     9 'P8 (','6g7/','2)  ','P9 (','6g9/','2)  ','P101','1 (6','h)  '/
      DATA SHTAB3/
     1 'P10 ','(6h9','/2) ','P11 ','(6h1','1/2)','Q (7',')   ','    ',
     2 'Q1 (','7s1/','2)  ','Q23 ','(7p)','    ','Q2 (','7p1/','2)  ',
     3 'Q3 (','7p3/','2)  ','ERRO','R   ','    '/
      DATA TOTAL/'Tota','l   ','   '/
C-----INSURE SUBSHELL INDEX IS IN LEGAL RANGE (1 TO 61).
      KSHELL=ISHELL
      IF(KSHELL.NE.0) GO TO 20
      DO 10 I=1,3
   10 SHBCD(I)=TOTAL(I)
      RETURN
   20 IF(KSHELL.LT.1.OR.KSHELL.GT.61) KSHELL=62
C-----DEFINE SUBSHELL.
      DO 30 I=1,3
   30 SHBCD(I)=SHTAB(I,KSHELL)
      RETURN
      END
      SUBROUTINE NORMX(X,XNORM,KSIGN,KEXP)
C
C     CONVERT FLOATING POINT NUMBER TO NORMAL FORM FOR OUTPUT.
C     OUTPUT WILL BE IN THE FORM X.XXXXX+/-NN, WHICH GIVES
C     AN ADDITIONAL DIGIT OF ACCURACY WHEN COMPARED TO E11.4
C     FORTRAN OUTPUT. IN ADDITION THE OUTPUT WILL BE COMPUTER
C     INDEPENDENT (I.E. SAME ON IBM, CDC, UNIVAC ETC.)
C
C***** DOUBLE *****
      IMPLICIT REAL*8 (A-H,O-Z)
C***** DOUBLE *****
      CHARACTER*1 KSIGN,PLUS,MINUS
C-----DEFINE TWO POSSIBLE SIGNS FOR EXPONENT.
      DATA PLUS/'+'/
      DATA MINUS/'-'/
C***** DOUBLE *****
      DATA ZERO/0.0D+00/
      DATA ONE/1.0D+00/
      DATA TEN/1.0D+01/
      DATA XLOW/1.0D+00/
      DATA XHIGH/9.999995D+00/
      QABS(Q)=DABS(Q)
      QLOG10(Q)=DLOG10(Q)
C***** DOUBLE *****
C***** SINGLE *****
C     DATA ZERO/0.0E+00/
C     DATA ONE/1.0E+00/
```

```
C     DATA TEN/1.0E+01/
C     DATA XLOW/1.0E+00/
C     DATA XHIGH/9.999995E+00/
C     QABS(Q)=ABS(Q)
C     QLOG10(Q)=ALOG10(Q)
C***** SINGLE *****
C-----COMPUTE SIGNED EXPONENT FROM ABSOLUTE VALUE.
      XABS=QABS(X)
C-----IF NUMBER IS 0.0 DEFINE 0.00000+ 0
      IF(XABS) 50,50,10
C-----DEFINE EXPONENT TO NORMALIZE MANTISSA.
   10 KEXP=QLOG10(XABS)
      IF(XABS.LT.ONE) KEXP=KEXP-1
      SHIFT=TEN**KEXP
      XNORM=XABS/SHIFT
C-----ADJUST MANTISSA TO EXACT POWERS OF 10 DUE TO OUTPUT ROUNDING.
      IF(XNORM.GE.XLOW) GO TO 20
      XNORM=ONE
      GO TO 30
   20 IF(XNORM.LT.XHIGH) GO TO 30
      KEXP=KEXP+1
      XNORM=ONE
C-----COMPUTE SIGNED MANTISSA.
   30 IF(X.LT.ZERO) XNORM=-XNORM
C-----DEFINE SIGN OF EXPONENT AND INSURE EXPONENT IS POSITIVE.
      IF(KEXP) 40,60,70
   40 KSIGN=MINUS
      KEXP=-KEXP
      RETURN
C-----X IS 0.0. DEFINE AS 0.00000+ 0
   50 XNORM=ZERO
   60 KEXP=0
C-----EXPONENT IS ZERO OR POSITIVE. THEREFORE SIGN IS POSITIVE.
   70 KSIGN=PLUS
      RETURN
      END
      FUNCTION ISDOWN(I)
C
C     COLLAPSE SUBSHELL INDICES TO MINIMUM SIZE.
C
      DIMENSION ISTAB(61)
      DATA ISTAB/
     1  1, 0, 2, 0, 3,
     2  4, 0, 5, 0, 6,
     3  7, 0, 8, 9, 0,
     4 10, 0,11,12, 0,
     5 13,14, 0,15,16,
     6  0,17, 0,18,19,
     7  0,20,21, 0,22,
     8 23, 0,24,25, 0,
     9 26, 0,27,28, 0,
     A 29,30, 0,31,32,
```

```
     B  0,33,34, 0,35,
     C 36, 0,37, 0,38,
     D 39/
      ISDOWN=ISTAB(I)
      RETURN
      END
      FUNCTION ISUP(I)
C
C     EXPAND SUBSHELL INDICE TO ORIGINAL SIZE.
C
      DIMENSION ISTAB(39)
      DATA ISTAB/
     1  1, 3, 5, 6, 8,
     2 10,11,13,14,16,
     3 18,19,21,22,24,
     4 25,27,29,30,32,
     5 33,35,36,38,39,
     6 41,43,44,46,47,
     7 49,50,52,53,55,
     8 56,58,60,61/
      ISUP=ISTAB(I)
      RETURN
      END
      SUBROUTINE RANGER(Z,IZ1,IZ2,IZMAX)
C
C     DEFINE NON-ZERO RANGE OF VS. Z DATA
C
C***** DOUBLE *****
      IMPLICIT REAL*8 (A-H,O-Z)
C***** DOUBLE *****
      DIMENSION Z(IZMAX)
C***** DOUBLE *****
      DATA ZERO/0.0D+00/
C***** DOUBLE *****
C***** SINGLE *****
C     DATA ZERO/0.0E+00/
C***** SINGLE *****
      DO 10 IZ1=1,IZMAX
      IF(Z(IZ1).NE.ZERO) GO TO 20
   10 CONTINUE
      IZ1=0
      IZ2=0
      RETURN
   20 DO 30 IZ2=IZMAX,IZ1,-1
      IF(Z(IZ2).NE.ZERO) GO TO 40
   30 CONTINUE
      IZ1=0
      IZ2=0
   40 RETURN
      END
```