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

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March 1992

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

DE92 013751

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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.

MASTER

Comments from RELAX

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 TRANSITIONS	REL00340
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 SUBSHELL	REL00660

C TO FILL A HOLE IN ANOTHER SUBSHELL - IN THIS CASE REL00670
 C THE SET OF EQUATIONS DOES NOT HAVE A UNIQUE SOLUTION REL00680
 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 THEIR REL00770
 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 TRIANGULAR 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 SATISFIED 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 $E(X\text{-RAY}) = B.E.(K) - B.E.(I)$ 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 APPROXIMATELY REL01170
 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

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 ELECTRON	REL01410
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 CALCULATED 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

DEFINITIONS BELOW). NEXT THE USER SPECIFIES A RANGE OF ELEMENTS AND SUBSHELLS TO PROCESS.

THE SPECTRA FOR EACH REQUESTED ELEMENT/SUBSHELL ARE CALCULATED SEPARATELY AND ARE ONLY AVAILABLE IN CORE BEFORE THE SPECTRA FOR THE NEXT ELEMENT/SUBSHELL ARE CALCULATED. SUBSHELL AVERAGED PARAMETERS ARE ACCUMULATED FOR EACH ELEMENT SEPARATELY AND ARE ONLY AVAILABLE IN CORE BEFORE CALCULATIONS START ON THE NEXT ELEMENT.

ONCE THE ENTIRE USER SPECIFIED RANGE OF ELEMENTS AND SUBSHELLS HAVE BEEN PROCESSED THE PROGRAM WILL ATTEMPT TO READ THE NEXT USER SPECIFIED RANGE OF ELEMENTS AND SUBSHELLS. CALCULATIONS WILL CONTINUE UNTIL AN END OF FILE IS READ ON THE INPUT FILE.

OUTPUT OPTIONS

THIS PROGRAM CONTAINS INPUT OPTIONS TO PRODUCE THE FOLLOWING OUTPUT,

- 1) A LISTING - A SUMMARY OF EACH SUBSHELL AND THE SPECTRA
- 2) ENDL - CALCULATE SUBSHELL AVERAGED VALUES AND NORMALIZED TRANSITION DATA IN THE ENDL FORMAT
- 3) PLOTTAB - SPECTRA IN THE PLOTTAB FORMAT WHICH CAN BE USED WITH PROGRAM PLOTTAB TO OBTAIN PLOTS OF THE RESULTS.

USER INTERFACE

IF YOU WISH TO OBTAIN RESULTS IN ANY OTHER FORM YOU MAY DO SO BY INSERTING CODING INTO SUBROUTINE USER1 AND/OR USER2. USER1 IS CALLED AFTER THE SPECTRA HAVE BEEN CALCULATED FOR EACH SUBSHELL - IF YOU WANT THE SPECTRA THIS IS THE TIME AND PLACE TO GET THEM. USER2 IS CALLED AFTER ALL RESULTS HAVE BEEN CALCULATED FOR EACH ELEMENT - IF YOU WANT SUBSHELL AVERAGED RESULTS THIS IS THE TIME AND PLACE TO GET THEM.

ALL VARIABLES OF INTEREST TO THE USERS ARE DESCRIBED BELOW.

I/O FILES

INPUT FILES

UNIT	FILENAME	DESCRIPTION
5	RELAX.INP	INPUT PARAMETERS
10	ENDL.IN	ENDL FORMATTED DATA

OUTPUT FILES

UNIT	FILENAME	DESCRIPTION
6	RELAX.LST	OUTPUT LISTING
11	ENDL.OUT	ENDL FORMATTED DATA
12	PLOTTAB.CUR	NORMALIZED INTEGRAL OF SPECTRA FLUORESCENCE YIELD VS. Z BY SUBSHELL
14	PLOTTAB.PNT	SPECTRA POINT VALUES
15	PLOTTAB.INP	PLOTTAB INPUT PARAMETERS
17	PLOTTAB.FLU	FLUORESCENCE YIELD VS. Z BY SHELL

INPUT PARAMETERS

LINE	COLS.	FORMAT	DESCRIPTION
1	1- 5	I5	LISTING OPTION = 0 - NO OUTPUT LISTING = 1 - SUMMARY OF EACH SUBSHELL - NO SPECTRA

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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	ERMEV = 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 OR	REL04190
C	OFF USING PROGRAM CONVERT - CONTACT THE AUTHOR FOR A COPY OF THIS	REL04200
C	PROGRAM.	REL04210
C		REL04220
C	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

Non-radiative (electron) Emission Spectrum
due to a single vacancy in the K-shell of uranium

Free-bound (X-ray) Emission Spectrum
due to a single vacancy in the K-shell of uranium

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