28. FILE 28. ATOMIC RELAXATION DATA

28.1. General Comments on Atomic Relaxation

An atom can be ionized due to a variety of interactions. For example, due to photon or electron interactions the probability of ionizing a particular subshell of the atomic structure (K, L1, L2, *etc*.) is determined by using the subshell cross sections (MT=534-599). For example, if an incident photon of energy E ionizes the K subshell with binding energy EK, the atom will emit an electron with energy E-EK, and the atomic structure will be left ionized, with a "hole" in the K subshell. One way the atom can proceed to fill this hole is to bring down an electron from a higher energy level, for example L1, with the simultaneous emission of an X-ray of energy EK-EL1. This is a radiative transition. An alternative path is to bring down an electron from a higher level with the simultaneous emission of an electron from that level or a higher one. As an example, you might see an electron of energy EK-EL1-EM1, which fills the vacancy in the K shell and leaves new holes in the L1 and M1 shells. These are called non-radiative transitions. The process will then continue by filling the new holes from higher levels, *etc*., until all the ionization energy has been accounted for by the emission of X-rays and electrons.

The electrons produced by this atomic relaxation can be used as a source for a subsequent electron transport calculation, or their energy can just be added to the local heating. The X-rays can be transported elsewhere to cause additional photo-atomic reactions. In general, the use of File 28 is indicated when high-Z materials are present and photon energies of less than 1 MeV are of interest.

This file is provided to give the information necessary to compute the emission of X-rays and electrons associated with atomic relaxation cross section. It is based on EADL, the Evaluated Atomic Data Library developed by D. E. (Red) Cullen at the Lawrence Livermore National Laboratory (LLNL).

28.2. General Description

This file gives the subshell energies, emission energies, transition probabilities, and other quantities needed to compute the X-ray and electron spectra from ionized atoms. It always uses MT=533. It works together with the photoelectric subshell cross sections from MF=23, MT=534-599.

28.3. Formats

The following quantities are defined

ZA, AWR	Standard material charge and mass parameters
NSS	Number of subshells
SUBI	Subshell designator (see the table below)
SUBJ	Secondary subshell designator
SUBK	Tertiary subshell designator (if SUBK is zero for a particular transition, it is a radiative transition; otherwise, it is a non-radiative transition.)
EBI	Binding energy for subshell (eV)
ELN	Number of electrons in subshell when neutral (given as a floating-point value)
NTR	Number of transitions
FTR	Fractional probability of transition
ETR	Energy of transition (eV)

Table of Subshell Designators

Designator	Subshell	MT
1.	K (1s1/2)	534
2.	L1 (2s1/2)	535
3.	L2 (2p1/2)	536
4.	L3 (2p3/2)	537
5.	M1 (3s1/2)	538
6.	M2 (3p1/2)	539
etc.		

The structure of a section of File 28 is as follows:

```
[MAT,28,533/   ZA,     AWR,      0,     0, NSS,    0]HEAD
[MAT,28,533/SUBI1,    0.0,      0,     0,  NW, NTR/ NW=6*(1+NTR)
           EBI1 ,     ELN1,    0.0,  0.0, 0.0, 0.0,
           SUBJ1,    SUBK1,  ETR1, FTR1, 0.0, 0.0,
           ------------------------------------
           SUBJNTR,SUBKNTR,ETRNTR,FTRNTR,  0.0,  0.0]LIST
           ------------------------------------
           [repeat LIST for the rest of the NSS subshells]
[MAT,28,533/  0.0,     0.0,     0,     0,    0,    0] SEND
```

28.4 Procedures

Sections with MF=28,MT=533 are used together with either photo-atomic or electro-atomic data evaluations. The value of NSS must be consistent with the number of subshell ionization cross sections given in File 23 (MT=534,535, ...). Note that the subshell cross section MT value equals the subshell designator number SUBI plus 533. Subshell LIST records are given in order of increasing SUBI. Similarly, transitions are given in order of increasing SUBJ first, and increasing SUBK second. This means that radiative transitions appear before non-radiative ones for each subshell.

It is possible to have NTR=0 if there are no allowed transitions from higher subshells to a particular subshell.

Example 1: Atomic Relaxation Data

```
                                                                   1 0  0    0
 6.000000+3 11.9078164         -1          0          0          0 600 1451    1
 0.000000+0 0.000000+0          0          0          0          6 600 1451    2
 0.000000+0 0.000000+0          0          0          6          6 600 1451    3
 0.000000+0 0.000000+0          0          0          6          2 600 1451    4
 6-C -  0 LLNL        EVAL-DEC90 CULLEN                            600 1451    5
                      DIST-                                        600 1451    6
----ENDF/B-VI         MATERIAL  600                                600 1451    7
-----ATOMIC RELAXATION DATA                                        600 1451    8
------ENDF-6 FORMAT                                                600 1451    9
 converted from EADL                                               600 1451   10
                                1        451         12          0 600 1451   11
                               28        533         17          0 600 1451   12
                                                                   600 1  0   13
                                                                   600 0  0   14
 6.000000+3 11.9078164          0          0          4          0 60028533   15
 1.000000+0 0.000000+0          0          0         54          8 60028533   16
 2.910100+2 2.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 60028533   17
 5.000000+0 0.000000+0 2.820200+2 5.614880-4 0.000000+0 0.000000+0 60028533   18
 6.000000+0 0.000000+0 2.820300+2 1.120600-3 0.000000+0 0.000000+0 60028533   19
 3.000000+0 3.000000+0 2.558900+2 4.136090-1 0.000000+0 0.000000+0 60028533   20
 3.000000+0 5.000000+0 2.644600+2 1.361900-1 0.000000+0 0.000000+0 60028533   21
 3.000000+0 6.000000+0 2.644700+2 2.710990-1 0.000000+0 0.000000+0 60028533   22
 5.000000+0 5.000000+0 2.730300+2 4.207480-3 0.000000+0 0.000000+0 60028533   23
 5.000000+0 6.000000+0 2.730400+2 1.100120-1 0.000000+0 0.000000+0 60028533   24
 6.000000+0 6.000000+0 2.730500+2 6.320080-2 0.000000+0 0.000000+0 60028533   25
 3.000000+0 0.000000+0          0          0          6          0 60028533   26
 1.756000+1 2.000000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 60028533   27
 5.000000+0 0.000000+0          0          0          6          0 60028533   28
 8.990000+0 6.700000-1 0.000000+0 0.000000+0 0.000000+0 0.000000+0 60028533   29
 6.000000+0 0.000000+0          0          0          6          0 60028533   30
 8.980000+0 1.330000+0 0.000000+0 0.000000+0 0.000000+0 0.000000+0 60028533   31
                                                                   60028  0   32
                                                                   600 0  0   33
                                                                     0 0  0   34
                                                                    -1 0  0   35
```

Example 2: Electron Interaction Data

```
electron interaction data converted from EEDL                         1 0  0    0
 6.000000+3 11.9078164         -1          0          0          0 600 1451    1
 0.000000+0 0.000000+0          0          0          0          6 600 1451    2
 5.438673-4 1.00000+11          0          0        113          6 600 1451    3
 0.000000+0 0.000000+0          0          0          6         14 600 1451    4
 6-C -  0 LLNL        EVAL-DEC89 CULLEN                            600 1451    5
                      DIST-                                        600 1451    6
----ENDF/B-VI         MATERIAL  600                                600 1451    7
-----ELECTRO-ATOMIC DATA                                           600 1451    8
------ENDF-6 FORMAT                                                600 1451    9
 converted from EEDL                                               600 1451   10
                                1        451         24          0 600 1451   11
                               23        526         37          0 600 1451   12
                               23        527         31          0 600 1451   13
                               23        528         64          0 600 1451   14
                               23        534         12          0 600 1451   15
                               23        536         14          0 600 1451   16
                               23        538         15          0 600 1451   17
                               23        539         15          0 600 1451   18
                               26        526        353          0 600 1451   19
                               26        527        197          0 600 1451   20
                               26        534        120          0 600 1451   21
                               26        536        151          0 600 1451   22
                               26        538        155          0 600 1451   23
                               26        539        155          0 600 1451   24
                                                                   600 1  0   25
                                                                   600 0  0   26
 6.000000+3 11.9078164          0          0          0          0 60023526   27
 0.000000+0 0.000000+0          0          0          1        101 60023526   28
        101          2                                             60023526   29
 1.000000+1 3.063510+9 1.258930+1 2.498030+9 1.584890+1 2.036940+9 60023526   30
 1.995260+1 1.660950+9 2.511890+1 1.354370+9 3.162280+1 1.104370+9 60023526   31
 3.981070+1 9.008210+8 5.011870+1 7.347880+8 6.309570+1 5.993570+8 60023526   32
 7.943280+1 4.889770+8 1.000000+2 3.991460+8 1.258930+2 3.258180+8 60023526   33
 1.584890+2 2.659610+8 1.995260+2 2.171000+8 2.511890+2 1.772160+8 60023526   34
 3.162280+2 1.447630+8 3.981070+2 1.183030+8 5.011870+2 9.667950+7 60023526   35
 6.309570+2 7.900840+7 7.943280+2 6.458900+7 1.000000+3 5.282720+7
  …
 6.000000+3 11.9078164          0          0          1          0 60026526  223
 1.100000+1 5.438673-4          0          2          1          2 60026526  224
          2          2                                             60026526  225
 1.000000+1 1.000000+0 1.00000+11 1.000000+0                       60026526  226
 0.000000+0 0.000000+0          0          0          1         16 60026526  227
         16          2                                             60026526  228
 0.000000+0 1.000000+1         12          0          4          2 60026526  229
-1.000000+0 5.000000-1 9.999990-1 5.000000-1                       60026526  230
 0.000000+0 1.000000+3         12          0         54         27 60026526  231
-1.000000+0 7.349540-3-6.350000-1 1.014680-2-3.300000-1 1.408430-2 60026526  232
-7.500000-2 1.996880-2 1.350000-1 2.832790-2 3.000000-1 3.982680-2 60026526  233
 4.300000-1 5.580130-2 5.350000-1 7.828660-2 6.225000-1 1.108190-1 60026526  234
 6.925000-1 1.559570-1 7.500000-1 2.204030-1 7.950000-1 3.078220-1 60026526  235
 8.325000-1 4.339260-1 8.625000-1 6.085020-1 8.875000-1 8.591520-1 60026526  236
 9.080000-1 1.212620+0 9.250000-1 1.713720+0 9.390000-1 2.413930+0 60026526  237
 9.510000-1 3.432260+0 9.610000-1 4.874960+0 9.690000-1 6.802370+0 60026526  238
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```
 9.760000-1 9.598280+0 9.820000-1 1.360430+1 9.870000-1 1.914880+1 60026526  239
 9.915001-1 2.744700+1 9.956001-1 4.014720+1 9.999990-1 6.259920+1 60026526  240
 0.000000+0 2.000000+3         12          0         64         32 60026526  241
-1.000000+0 3.008670-3-9.000000-1 3.301630-3-5.350000-1 4.906250-3
 …
 6.000000+3 11.9078164          0          0          1          0 60026534  775
 1.100000+1 5.438673-4          0          1          1          2 60026534  776
          2          2                                             60026534  777
 2.910100+2 1.000000+0 1.00000+11 1.000000+0                       60026534  778
 0.000000+0 0.000000+0          1          2          1          7 60026534  779
          7          2                                             60026534  780
 0.000000+0 2.910100+2          0          0          4          2 60026534  781
 1.000000-2 1.111110+1 1.000000-1 1.111110+1                       60026534  782
 0.000000+0 2.973140+2          0          0          4          2 60026534  783
 3.152220-2 3.265060-1 3.152220+0 3.143760-1                       60026534  784
 0.000000+0 1.995260+3          0          0         28         14 60026534  785
 1.000000-1 7.771360-3 6.309570+0 7.133700-3 1.412540+1 6.229690-3 60026534  786
 3.162280+1 5.440240-3 6.309570+1 4.054250-3 8.912520+1 3.138130-3 60026534  787
 1.258930+2 2.429030-3 1.778280+2 1.605960-3 2.511890+2 1.061790-3 60026534  788
 3.162280+2 7.491710-4 3.758380+2 5.767510-4 4.869680+2 3.895820-4 60026534  789
 6.309570+2 2.631530-4 8.521260+2 2.098710-4                       60026534  790
 0.000000+0 3.981070+4          0          0         70         35 60026534  791
 1.000000-1 7.237010-3 6.309570+0 6.655140-3 1.412540+1 5.837310-3 60026534  792
 3.162280+1 5.119990-3 6.309570+1 3.846900-3 8.912520+1 2.990940-3 60026534  793
 1.258930+2 2.325440-3 1.496240+2 1.886340-3 1.938660+2 1.378130-3
 …
 2.06836+10 4.46563-21 2.51189+10 3.13693-21 3.16228+10 2.30613-21 60026539 1357
 3.98107+10 1.69536-21 5.00000+10 1.51523-21                       60026539 1358
                                                                   60026  0 1359
                                                                   600 0  0 1360
                                                                     0 0  0 1361
                                                                    -1 0  0 1362
```