# A Deterministic Method to Calculate the Radiation Spectra of Nuclides

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Recently, the computer program IMRDEC has been developed to determine the radiation spectra due to a single atomic-subshell ionisation of a stable atom by a particle, or due to the atomic deexcitation or decay of nuclides. The data needed to describe the deexcitation or decay scheme are obtained from the Evaluated Nuclear Structure Data File (ENSDF) maintained at Brookhaven National Laboratory; this results in the simplest possible input specification. The atomic data as well as the atomic relaxation probabilities are taken from the Evaluated Atomic Data Library (EADL) from Lawrence Livermore National Laboratory. The program IMRDEC calculates the radiation spectra (inclusively the atomic relaxation cascades) deterministically rather than by the Monte Carlo method; this results in much shorter calculational time per nuclide. Since many assumptions still have to be made in determining the atomic relaxation probabilities and in calculating the atomc relaxation, the deterministic method seems to be a small source of inaccuracy.

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A computer program IMRDEC has recently been developed to determine the radiation spectra due to a single atomic-subshell ionisation of a stable atom by a particle, or due to the atomic deexcitation or decay of nuclides.

In the case of a single atomic-subshell ionisation of a stable atom by a particle, IMRDEC calculates only the atomic relaxation cascades. They are calculated deterministically using the atomic binding energies and the atomic relaxation data from the Evaluated Atomic Data Library (EADL) (1) from Lawrence Livermore National Laboratory.

In the case of the atomic deexcitation or decay of nuclides, the following procedures are built into IMRDEC: (1). The data needed to describe the completer deexcitation or decay scheme are obtained from the Evaluated Nuclear Structure Data File (ENSDF) (2) maintained at Brookhaven National Laboratory. This results in the simplest possible input specification because only the mother and daughter nuclides and the related ENSDF-file record have to be specified (2). The internal consistency of data in the ENSDF-file is checked (3). Numerical treatment of $\beta^{\pm}$ emission (4). Numerical treatment of electron capture and position emission (5). Detailed treatment of the internal conversion process; The internal conversion factors for all atomic subshells, E0 to E6 and M1 to M6 multipolarities and a large range of the conversion photon energies are taken from the INCOCO library (INternal COnversion COefficients) generated by the author using his own computer program IMRATO. This program is based on solution of the relativistic Dirac equations and accomplished by the Raff and Pauli's formulation of the internal conversion factors (3). Additionally, the possibility of internal pair formation is considered (6). The radiation cascades as a result of the subshell electron vacancies due to the deexcitation or decay are calculated deterministically using the atomic binding energies and the transition probabilities from the EADL file (7). The internal Bremsstrahlung as a result of electron capture and $\beta^{\pm}$ emission is calculated (8). Emissions of $\alpha$-particles, protons or other heavy particles are included (9). Nuclear recoil is considered.

Two types of output files are generated: (1) The first file consists of radiative and non-radiative yields and energies due to ionisation of the K, $L_1$, $L_2$, $L_3$, and M, and N shells. It is used as the library needed in the IMR version of the Monte Carlo code GEANT (4, 5) to calculate the radiation emissions due to the particle ionisation process, and (2). The second file contains the detailed radiation spectra of decaying atoms. It is used to define the spectrum

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of the radionuclides for further particle tracking in the Monte Carlo code GEANT.

## SPECTRUM CALCULATION

Photon, $\beta^{\pm}$, $\alpha$-particle, proton or heavy particle spectra are calculated deterministically using the emission probabilities and other required data from ENSDF library. Also electron capture and internal conversion processes are described using the data from ENSDF library.

In the case of atomic relaxation, the calculation consists of two basic steps: 1) Determination of the initial vacancies, and 2) calculation of the radiative and non-radiative atomic transitions due to the subsequent filling of the vacancies and forming other vacancies in higher subshells. In the first option the initial vacancy is determined by the ionisation process during the particle tracking in the medium. In the second option there are many initial vacancy-fractions in different subshells. They are calculated considering a) the electron capture decay-mode, and b) the electromagnetic decay-mode (deexcitation followed by the internal conversion process).

In the both cases the EADL file is used. This file containes the atomic structure data (number of subshells, number of electrons in subshells, the binding energies and the atomic relaxation data).

The procedures used in IMRDEC to calculate the atomic relaxation spectra are partly similar to those used in the program RELAX (8) developed by D. E. Cullen. IMRDEC reads the EADL file which contains the data describing the daughter atom i.e. the number of the subshell, the number of electrons per subshell and the electron binding energies. Furthermore, it contains the transition probabilities. Based on these data, it calculates atom relaxation spectra of x-rays and electrons due to bound-bound transitions. The program also calculates the spectrum of free-bound transition assuming that the atom returns back to its neutral ground state by filling all remaining electron vacancies through transitions capturing electrons directly from the continuum, i.e. from outside the atom. The sum of the total energy of emitted x-rays and electrons and of free-bound energy is equal to the sum of primary subshell-vacancies times the binding energy of the sunshell in which the primary vacancy is located.

Similarly to RELAX, IMRDEC also uses a deterministic method to calculate the atomic radiative and non-radiative relaxation spectra. After the vacancy fractions are determined due to EC or IC processes, or due to a particle ionisation of atom, the program starts to fill the vacancy-fraction in the innermost subshell considering in parallel both radiative and non-radiative transitions into this subshell. In this way a new vacancy fractions in yet higher subshells are created. The program then moves to the next higher subshell and the procedure is repeated.

As pointed out below, the EADL transition probabilities were calculated under the assumption that the atomic subshells from which an electron has to be removed contain the full number of electrons. In reality, multiple vacancies may exist within the atomic subshells. Therefore, the transition probabilities have to be reduced. Like Charlton and Booz (9), Humm (10), Pomplum et al. (11) and Howell (7) IMRDEC also employs the method of Krause & Carlson (12), i.e. the probabilities that an electron will be removed from a subshell are multiplied by the ratio of the real to the full number of elctrons in this subshell. After the multiplications, all probabilities are renormalized.

In the case of condensed phase the whole process in returning the atom to neutrality by radiative and non-radiative transition proceeds in a very short time (about $10^{-14}$ to $10^{-16}$ seconds), so that it can be treated as immediately following a previous subshell ionisation. When the vacancies reach the outermost subshells, vacancy filling by capturing electrons from the continuum, i.e. from the surrounding area, takes about $10^{-12}$ s.

The above procedure of vacancy moving will in practice continue up to the second outer-most subshell and produce multiple vacancies in the valence shell. In our case the EADL presently do not contain all transition probabilities. Therefore, the procedure stops if no more transitions are available and can produce vacancies in outer sunshells (in $O_1$ to $O_3$ in case of $^{125}I$, for example). The above described Krause and Carlson's procedure is not applied to these subshells.

In case of an isolated atom, there exists no possibility to return to neutrality after the cascades are terminated. The atom will stay in a multiply-ionised state. In this case the Krause and Carlson method is applied to all subshells. It is not allowed to remove more electrons than the number in a fully occupied subshell. If there is an electron fraction which still could be removed, it will be done and the related probability will be reduced.

The EC-decay of atoms can be described in two stages: 1) electron capture to a metastable state of the daughter atom, and 2) internal conversion of the metastable state of the daughter atom to its ground state. The half-life of the internal conversion is typically much longer than the time needed for atomic relaxation and neutralisation (1.47 ns in case of EC-decay of $^{125}I$). We therefore assume, like other (7, 9 cite-humm. 11), that the vacancies generated after electron capture stage will be fully filled before the second stage of the internal conversion.

If the vacancy in the i-th subshell is filled due to fluorescence (radiative) transition of one electron from an higher j-th subshell, it will be followed by the emission of x-ray with energy which is equal to the binding energy of the electron in the i-th subshell minus the binding energy of the electron in the j-th subshell:

$$E_{i,j} = B_i^z - B_j^z, \quad [1]$$

where Z is the atomic number of singly ionised atom or of the daughter nuclide of the decaying 'mother' radionuclide.

In the case of a decaying atom the binding energies of both the daughter and mother atoms have to be considered. This is due to interaction effects of two electrons involved in the transition. These effects are taken into account approximately by the following formula:

$$E_k = B_i^z - (1 - \Delta Z)(B_j^Z + B_k^Z) + \Delta Z(B_j^{Z+1} + B_k^{Z+1}). \quad [2]$$

Setting $\Delta Z = 0.5$ leads to the broadly used $Z/(Z+1)$-rule (7, 9, 10, 13).

In the case of radiation cascade as result of electron capture to a metastable state, $\Delta Z$ is set to 0.5; for internal conversion or ionisation of an atom by a charged particle, $\Delta Z$ is set to 0.0.

The uncertainty in the binding energies can result in transitions in which electrons with calculated negative energy are involved. In this case the transition is allowed because the related creation of vacancies can be important but the negative energy is set to be zero.

Presently the most accurate method of calculating the electron Auger and Coster-Kronig energies is that of Pomplun et al. (11). In this method the electron binding energies for electron configuration of each particular event are calculated. Unfortunately, it requires extensive CPU time. Furthermore, it should be accompanied by calculation of transition probabilities for each electron configuration; this is beyond present-day computer capability.

## RELAXATION PROBABILITIES

The atomic probabilities were determined by Scofield and Chen (1) using the relativistic Dirac-Hartree-Slater DHS j-j coupling scheme for the non-radiative relaxation probabilities. Chen et al. (6) have shown that the DHS j-j coupling results are adequate for atoms with atomic number Z above $\approx 60$, but for atoms with Z less than 60 the relativistic intermediate coupling scheme with configuration interaction (DHS IC-CI) is necessary to describe the relative nonradiation relaxation probabilities. The main reason why the DHS IC-CI scheme was not applied was (1) its extremely large computer CPU requirements if the non-radiative transitions would have to be calculated for all elements of Z up to 100 and (2) the fact that the both schemes lead to adequate total non-radiative yield for all Z.

The authors of the EADL file claim that by comparing EADL binding energies with values from other sources, there is a discrepancy of about 1%. The accuracy of K- and L-shell radiative transitions is assumed to be $\sim 10\%$. It decreases for higher shells. It is assumed, that for the outer subshells, the accuracy of the radiative transitions may be only about 30%. The accuracy of the Auger transitions is assumed to be better than 15%. The inaccuracy of the Coster-Kronig or super Coster-Kronig transitions may be much larger.

There are four major, commonly-used assumptions which may further limit the accuracy of calculated spectra (see Ref. 8): (1). It is assumed that the binding energies of the atom in any ionised state are the same as these in the

**Table 1**

*$^{55}$Fe average radiation spectrum per decay; Condensed phase*

| Process | Present work | | R. W. Howell (7) | |
|---|---|---|---|---|
| | Average energy (eV) | Yield | Average energy (eV) | Yield |
| Auger KLL | $5.08 \cdot 10^3$ | $4.87 \cdot 10^{-1}$ | $5.13 \cdot 10^3$ | $4.87 \cdot 10^{-1}$ |
| Auger KLX | $5.73 \cdot 10^3$ | $1.19 \cdot 10^{-1}$ | $5.77 \cdot 10^{-3}$ | $1.20 \cdot 10^{-1}$ |
| Auger KXY | $6.37 \cdot 10^3$ | $7.30 \cdot 10^{-3}$ | $6.42 \cdot 10^3$ | $8.20 \cdot 10^{-3}$ |
| CK LLX | $3.14 \cdot 10^1$ | $2.63 \cdot 10^{-1}$ | $5.52 \cdot 10^1$ | $3.10 \cdot 10^{-1}$ |
| Auger LMM | $5.58 \cdot 10^2$ | $1.40 \cdot 10^{+0}$ | $5.61 \cdot 10^2$ | $1.41 \cdot 10^{+0}$ |
| Auger LMX | $6.05 \cdot 10^2$ | $2.35 \cdot 10^{-1}$ | $6.06 \cdot 10^2$ | $1.94 \cdot 10^{-2}$ |
| CK MMX | $3.54 \cdot 10^1$ | $2.60 \cdot 10^{+0}$ | $4.18 \cdot 10^1$ | $2.54 \cdot 10^{+0}$ |
| Auger MXY | $4.90 \cdot 10^1$ | $2.31 \cdot 10^{-1}$ | $4.89 \cdot 10^3$ | $2.23 \cdot 10^{-2}$ |
| $K_{\alpha 1}$ x-ray | $5.86 \cdot 10^3$ | $1.62 \cdot 10^{-1}$ | $5.90 \cdot 10^3$ | $1.57 \cdot 10^{-1}$ |
| $K_{\alpha 2}$ x-ray | $5.85 \cdot 10^3$ | $8.24 \cdot 10^{-1}$ | $5.89 \cdot 10^3$ | $8.74 \cdot 10^{-2}$ |
| $K_{\beta 1}$ x-ray | $6.45 \cdot 10^3$ | $1.93 \cdot 10^{-1}$ | $6.49 \cdot 10^3$ | $1.92 \cdot 10^{-2}$ |
| $K_{\beta 3}$ x-ray | $6.45 \cdot 10^3$ | $9.82 \cdot 10^{-3}$ | $6.49 \cdot 10^3$ | $1.05 \cdot 10^{-2}$ |
| L x-rays | $5.87 \cdot 10^2$ | $6.90 \cdot 10^{-3}$ | $6.35 \cdot 10^2$ | $3.30 \cdot 10^{-3}$ |
| Y: Auger and CK el. | 5.07 | | 5.10 | |
| Y: x-rays | 0.27 | | 0.28 | |
| E: Total | 5815.07 eV | | 5810.00 eV | |
| E: Auger and CK el. | 4156.09 eV | | 4177.00 eV | |
| E: x-rays | 1589.50 eV | | 1633.00 eV | |
| E: Free-bound x-rays | 68.30 eV | | | |

ground state, (2). The transition probabilities available in the EADL data base were calculated assuming that the subshells from which the electron will be removed contain the full number of electrons which corresponds to the atom in the ground state, (3). The entire EADL data base (1) presently does not allow the double-Auger transitions, i.e. the emission of two electrons in one non-radiative transition, and the shake-off transitions, and (4). Currently, the transitions for Z = 1 throughout 5 and between some O and all P and Q subshells are not included in the EADL file. The consequence is that there will remain vacancies which can not be filled. The related energy is included into the free-bound energy, i.e. it is considered that these vacancies will be filled by electrons directly from continuum under the emission of x-rays.

## TESTING

R. W. Howell recently calculated the radiation spectra for many Auger-electron emitting radionuclides (7). In contrast to our deterministic procedure he used the Monte Carlo technique. The comparison of our results with his can test both methods as well as the different sources of the binding energies and relaxation data. Howell used transition probabilities combined from different sources (14–18). All of them are based on DHS j-j coupling scheme. The binding energies were taken from Sevier (19).

The comparisons of our and Howell's results displayed in Tables I and II indicate only minor differences, The overall agreement between the yields results from the fact that both EADL and Howell's transition probabilities are

**Table 2**

*$^{125}I$ average radiation spectrum per decay; Condensed phase*

| Process | Present work | | R. W. Howell (7) | |
|---|---|---|---|---|
| | Average energy (eV) | Yield | Average energy (eV) | Yield |
| IC γ1 | $3.55 \cdot 10^{4}$ | $6.66 \cdot 10^{-2}$ | $3.55 \cdot 10^{4}$ | $6.47 \cdot 10^{-2}$ |
| IC 1 electron K | $3.69 \cdot 10^{3}$ | $8.04 \cdot 10^{-1}$ | $3.65 \cdot 10^{3}$ | $7.97 \cdot 10^{-1}$ |
| IC 1 electron L | $3.06 \cdot 10^{4}$ | $1.08 \cdot 10^{-1}$ | $3.06 \cdot 10^{4}$ | $1.10 \cdot 10^{-1}$ |
| IC 1 electron X | $3.45 \cdot 10^{4}$ | $2.15 \cdot 10^{-2}$ | $3.47 \cdot 10^{4}$ | $2.84 \cdot 10^{-2}$ |
| Auger KLL | $2.36 \cdot 10^{4}$ | $1.18 \cdot 10^{-1}$ | $2.24 \cdot 10^{4}$ | $1.38 \cdot 10^{-1}$ |
| Auger KLX | $2.76 \cdot 10^{4}$ | $5.37 \cdot 10^{-2}$ | $2.64 \cdot 10^{4}$ | $5.90 \cdot 10^{-2}$ |
| Auger KXY | $3.16 \cdot 10^{4}$ | $5.84 \cdot 10^{-3}$ | $3.02 \cdot 10^{4}$ | $6.50 \cdot 10^{-3}$ |
| CK LLX | $3.15 \cdot 10^{2}$ | $2.52 \cdot 10^{-1}$ | $2.19 \cdot 10^{2}$ | $2.64 \cdot 10^{-1}$ |
| Auger LMM | $3.22 \cdot 10^{3}$ | $1.18 \cdot 10^{+0}$ | $3.05 \cdot 10^{3}$ | $1.25 \cdot 10^{+0}$ |
| Auger LMX | $3.85 \cdot 10^{3}$ | $3.55 \cdot 10^{-1}$ | $3.67 \cdot 10^{3}$ | $3.40 \cdot 10^{-1}$ |
| Auger LXY | $4.51 \cdot 10^{3}$ | $2.64 \cdot 10^{-2}$ | $4.34 \cdot 10^{3}$ | $2.11 \cdot 10^{-2}$ |
| CK MMX | $1.20 \cdot 10^{2}$ | $1.36 \cdot 10^{+0}$ | $1.27 \cdot 10^{2}$ | $1.44 \cdot 10^{+0}$ |
| Auger MXY | $4.85 \cdot 10^{2}$ | $3.17 \cdot 10^{+0}$ | $4.61 \cdot 10^{2}$ | $3.28 \cdot 10^{+0}$ |
| CK NNX | $2.63 \cdot 10^{1}$ | $3.68 \cdot 10^{+0}$ | $2.99 \cdot 10^{1}$ | $3.51 \cdot 10^{+0}$ |
| Auger NXY | $2.94 \cdot 10^{1}$ | $1.08 \cdot 10^{+1}$ | $3.24 \cdot 10^{1}$ | $1.09 \cdot 10^{+1}$ |
| CK OOX | — | — | $6.00 \cdot 10^{+0}$ | $3.66 \cdot 10^{+0}$ |
| $K_{\alpha 1}$ x-ray | $2.86 \cdot 10^{4}$ | $7.59 \cdot 10^{-1}$ | $2.75 \cdot 10^{4}$ | $7.51 \cdot 10^{-1}$ |
| $K_{\alpha 2}$ x-ray | $2.83 \cdot 10^{4}$ | $4.07 \cdot 10^{-1}$ | $2.72 \cdot 10^{4}$ | $3.94 \cdot 10^{-1}$ |
| $K_{\beta 1}$ x-ray | $3.23 \cdot 10^{4}$ | $1.37 \cdot 10^{-1}$ | $3.10 \cdot 10^{4}$ | $1.38 \cdot 10^{-1}$ |
| $K_{\beta 2}$ x-ray | $3.30 \cdot 10^{4}$ | $4.35 \cdot 10^{-2}$ | $3.17 \cdot 10^{4}$ | $4.03 \cdot 10^{-2}$ |
| $K_{\beta 3}$ x-ray | $3.22 \cdot 10^{4}$ | $7.06 \cdot 10^{-2}$ | $1.09 \cdot 10^{4}$ | $6.85 \cdot 10^{-2}$ |
| $K_{\beta 4}$ x-ray | $3.31 \cdot 10^{4}$ | $2.79 \cdot 10^{-4}$ | — | — |
| $K_{\beta 5}$ x-ray | $3.25 \cdot 10^{4}$ | $1.57 \cdot 10^{-3}$ | $3.12 \cdot 10^{4}$ | $1.20 \cdot 10^{-3}$ |
| KMNO x-rays | $3.24 \cdot 10^{4}$ | $2.56 \cdot 10^{-3}$ | $3.17 \cdot 10^{4}$ | $3.00 \cdot 10^{-3}$ |
| L x-ray | $4.09 \cdot 10^{3}$ | $1.62 \cdot 10^{-1}$ | $3.93 \cdot 10^{3}$ | $1.32 \cdot 10^{-1}$ |
| M x-ray | $5.75 \cdot 10^{2}$ | $8.58 \cdot 10^{-3}$ | $5.42 \cdot 10^{2}$ | $4.00 \cdot 10^{-3}$ |
| N+ x-ray | $8.67 \cdot 10^{1}$ | $2.70 \cdot 10^{-4}$ | | |
| Y: Auger and CK el. | 20.98 | | 24.90 | |
| Y: IC electrons | 0.94 | | 0.94 | |
| Y: x-rays | 1.59 | | 1.53 | |
| Y: IC photons | 0.06 | | 0.07 | |
| E: Auger and CK el. | 11990.00 eV | | 12241.00 eV | |
| E: IC electrons | 6128.43 eV | | 7242.00 eV | |
| E: IC photons | 2162.70 eV | | 2294.00 eV | |
| E: x-rays | 42212.21 eV | | 39661.00 eV | |
| E: Internal Bremstrahlung | 4.19 eV | | | |
| E: Free-bound x-rays | 469.56 eV | | | |

**Table 3**

*$^{125}I$ average radiation spectrum per decay; Isolated atom*

| Process | Present work | | E. Pomplun (11) | |
|---|---|---|---|---|
| | Average energy (eV) | Yield | Average energy (eV) | Yield |
| IC $\gamma_1$ | $3.55 \cdot 10^{4}$ | $6.66 \cdot 10^{-2}$ | $3.55 \cdot 10^{4}$ | $6.80 \cdot 10^{-2}$ |
| IC 1 electron K | $3.69 \cdot 10^{3}$ | $8.04 \cdot 10^{-1}$ | $3.64 \cdot 10^{3}$ | $8.04 \cdot 10^{-2}$ |
| IC 1 electron L | $3.06 \cdot 10^{4}$ | $1.08 \cdot 10^{-1}$ | $3.07 \cdot 10^{4}$ | $1.02 \cdot 10^{-1}$ |
| IC 1 electron X | $3.45 \cdot 10^{4}$ | $2.15 \cdot 10^{-2}$ | $3.49 \cdot 10^{4}$ | $2.51 \cdot 10^{-2}$ |
| Auger KLL | $2.36 \cdot 10^{4}$ | $1.18 \cdot 10^{-1}$ | $2.25 \cdot 10^{1}$ | $1.34 \cdot 10^{-1}$ |
| Auger KLX | $2.76 \cdot 10^{4}$ | $5.38 \cdot 10^{-2}$ | $2.64 \cdot 10^{4}$ | $5.69 \cdot 10^{-2}$ |
| Auger KXY | $3.16 \cdot 10^{4}$ | $5.84 \cdot 10^{-3}$ | $3.03 \cdot 10^{4}$ | $4.80 \cdot 10^{-3}$ |
| CK LLX | $3.15 \cdot 10^{2}$ | $2.52 \cdot 10^{-1}$ | $2.83 \cdot 10^{2}$ | $2.60 \cdot 10^{-1}$ |
| Auger LMM | $3.22 \cdot 10^{3}$ | $1.18 \cdot 10^{+0}$ | $3.02 \cdot 10^{3}$ | $1.25 \cdot 10^{+0}$ |
| Auger LMX | $3.85 \cdot 10^{3}$ | $3.56 \cdot 10^{-1}$ | $3.66 \cdot 10^{3}$ | $3.46 \cdot 10^{-1}$ |
| Auger LXY | $4.51 \cdot 10^{3}$ | $2.64 \cdot 10^{-2}$ | $4.27 \cdot 10^{3}$ | $2.09 \cdot 10^{-2}$ |
| CK MMX | $1.20 \cdot 10^{2}$ | $1.36 \cdot 10^{+0}$ | $9.00 \cdot 10^{1}$ | $1.43 \cdot 10^{+0}$ |
| Auger MXY | $4.84 \cdot 10^{2}$ | $3.18 \cdot 10^{+0}$ | $3.77 \cdot 10^{2}$ | $3.31 \cdot 10^{+0}$ |
| CK NNX | $2.62 \cdot 10^{1}$ | $3.69 \cdot 10^{+0}$ | $2.70 \cdot 10^{1}$ | $1.80 \cdot 10^{+0}$ |
| Auger NXY | $3.42 \cdot 10^{1}$ | $5.63 \cdot 10^{+0}$ | $3.80 \cdot 10^{1}$ | $1.66 \cdot 10^{+0}$ |
| $K_{\alpha 1}$ x-ray | $2.86 \cdot 10^{4}$ | $7.60 \cdot 10^{-1}$ | $2.75 \cdot 10^{4}$ | $7.59 \cdot 10^{-1}$ |
| $K_{\alpha 2}$ x-ray | $2.83 \cdot 10^{4}$ | $4.08 \cdot 10^{-1}$ | $2.72 \cdot 10^{4}$ | $4.12 \cdot 10^{-1}$ |
| $K_{\beta 1}$ x-ray | $3.23 \cdot 10^{4}$ | $1.37 \cdot 10^{-1}$ | $3.10 \cdot 10^{4}$ | $1.32 \cdot 10^{-1}$ |
| $K_{\beta 2}$ x-rays | $3.30 \cdot 10^{4}$ | $4.36 \cdot 10^{-2}$ | $3.17 \cdot 10^{4}$ | $3.94 \cdot 10^{-2}$ |
| $K_{\beta 3}$ x-ray | $3.22 \cdot 10^{4}$ | $7.07 \cdot 10^{-2}$ | $3.09 \cdot 10^{4}$ | $6.80 \cdot 10^{-2}$ |
| $K_{\beta 4}$ x-rays | $3.31 \cdot 10^{4}$ | $2.79 \cdot 10^{-4}$ | — | — |
| $K_{\beta 5}$ x-rays | $3.25 \cdot 10^{4}$ | $1.57 \cdot 10^{-3}$ | $3.12 \cdot 10^{3}$ | $1.86 \cdot 10^{-3}$ |
| KMNO x-rays | $3.24 \cdot 10^{4}$ | $2.57 \cdot 10^{-3}$ | — | — |
| L x-rays | $4.09 \cdot 10^{3}$ | $1.62 \cdot 10^{-1}$ | $3.93 \cdot 10^{3}$ | $1.41 \cdot 10^{-1}$ |
| M x-rays | $5.75 \cdot 10^{2}$ | $8.61 \cdot 10^{-3}$ | — | — |
| N+ x-rays | $4.86 \cdot 10^{1}$ | $1.80 \cdot 10^{-0}$ | — | — |
| Y: Auger and CK el. | 15.85 | | 10.27 | |
| Y: IC electrons | 0.94 | | 0.90 | |
| Y: x-rays | 3.39 | | 1.55 | |
| Y: IC photons | 0.06 | | 0.07 | |
| E: Auger and CK el. | 11799.00 | | — | |
| E: IC electrons | 6128.43 eV | | 6933.95 eV | |
| E: IC photons | 2162.70 eV | | 2294.00 eV | |
| E: x-rays | 42362.00 eV | | — | |
| E: Internal Bremstrahlung | 1.69 eV | | — | |
| E: Free-bound x-rays | 405.00 eV | | — | |

based on the DHS j-j coupling scheme. The small differences are due to the older and combined sources used by Howell. The energies agree well for lower-shell Auger transitions. Differences in the energies of the Coster-Kronig and higher-shell Auger transitions lies in the use of the less accurate and older Sevier values. Howell included the OOX Coster-Kronig transitions for $^{125}I$ using the approximative method of Kassis et al. (20) to obtain the required transition probabilities. These are not included in the EADL file. The inclusion of these transitions is questionable because it requires accurate O-shell binding energies to obtain an energy of 6 eV, whereas the use of the EADL binding energies would give only about 1 eV. The total K, L and M Auger and CK (Coster-Kronig) yields are similar, namely 6.66 (present work) and 6.83 (Howell).

In Table 3, our results are compared with Pomplun's (11) both calculated for an isolated atom of $^{125}I$. Pomplun's results agree well with ours, with the exception of N-shell Auger and CK electron yields. The total K-, L- and M-shell Auger and CK electron yields are similar, namely 6.66 (present work) and 6.81 (Pomplun). The differences in N-shell Auger and CK electron yields may be explained by our use of zero-energy electrons, and by large inaccuracies in the transition probabilities between atomic shells of low electron binding energy. Comparing the total K-, L- and M-shell Auger and CK yields for isolated atom and condensed phase indicates that the differences between isolated atom and condensed phase is mainly due to differences in the N-and O-shell Auger and CK electron yields.

## CONCLUSIONS

Many assumptions still have to be made in calculating atomic relaxation. One limitation on the accuracy arises from the relaxation probabilities based on the DHS j-j coupling scheme if applied to elements with Z less than ~60. Additionally, Coster-Kronig transitions can not be accurately calculated for any Z. Here transition probabilities based on the DHS IC-CI scheme should be used to obtain reliable results.

Considering these limitations, together with that many assumptions still have to be made in calculating the atomic relaxation, the deterministic method seems to be a small source of inaccuracy. The advantage of the deterministic method over the Monte Carlo is its high speed; it requires only the CPU time needed for a few of Monte Carlo histories.

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