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Calculated K, L and M-shell X-ray line intensities for light ion impact on selected targets from Z=6 to 100.

by

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Abstract

A computer code to calculate the K, L, and M α, β and γ X-ray line intensities, ***KLMabgRatios***, is described together with the input tables used to calculate these intensities for light ion bombardment of targets with atomic numbers from Z=6 to 100. The ***KLMabgRatios*** program was written with the main aim of updating the 1980's data files used up till now (Clayton AAEC M113/1986), with more recent experimental and theoretical datasets published in the last 2 years or so. Preferred recommended K, L and M X-ray line intensities for light ion impact on selected targets for atomic numbers between Z=6 and 100 are given for 8 K lines, 17 L lines and 22 M lines as well as their corresponding ω_K, ω_L and ω_M total shell fluorescence yields.

In addition a program, ***wexplore***, has been written to carry out Gaussian fits to experimental K, L and M X-ray spectra to better determine L and M X-ray production subshell cross sections for light ion bombardment. A section on the use of this ***wexplore*** program is also included in this report.

Keywords: PIXE, K, L, M X-ray line intensities, X-ray cross sections

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1 Introduction

Proton induced X-ray emission (PIXE) analysis has been used for many years for the determination of elemental composition of materials using X-rays (e.g. PIXAN; Clayton 1986). One of the steps in the analysis is to fit the measured X-ray spectrum given the relative yield intensities for the material characteristic X-ray energies. The PIXAN program has been used since its development in the 1980s and continues to be used at ANSTO. The data tables used by PIXAN were published in 1986 (Cohen and Harrigan, 1986). Since that time a number of new datasets have been published (e.g. Campbell; 2003, 2009). The program, ***KLMabgRatios***, described in this report has been written to update the tables used by PIXAN, to include the latest K, L and M subshell data for selected elements with atomic numbers Z between 6 and 100.

The program ***KLMabgRatios*** has been written to calculate the X-ray line intensities for the K, L and M shells for proton, deuterium and helium bombardment of selected elements in the periodic table. The data needed for the calculation are stored into a number of files which are read by the program based on the user specified options. Two of the dataset files required by PIXAN, ***dset2*** and ***dset4***, are then generated based on the selected options and the updated datasets. The file ***dset2*** is used for the Gaussian peak fitting routines by the least squares fitting program BATTY (Clayton, 1986) to determine X-ray line peak areas and the ***dset4*** file is required by THIN and THIK (Clayton, 1986) programs to convert these peak areas to elemental concentrations for thin and thick targets.

In addition a program, ***wexplore***, has been written to carry out Gaussian fits to experimental spectra, particularly for M subshell analysis where more than a dozen Gaussian X-ray lines can be resolved by modern detectors. A section describing ***wexplore*** and its use is also included in this report.

2 K, L and M shell X-ray Line Intensities

For thin targets, the line intensity for a peak p is proportional to the X-ray production cross section, σ_p^x. The constant of proportionality is not needed if, for each shell, the intensities of each line are calculated relative to the primary K, L or M $\alpha = (\alpha_1+\alpha_2) = 100$ line, as such quantities as solid angle, beam curent etc. which are needed for yield calculations, cancel out when these ratios are used. In the following three sections the equations and data files used in the calculation of the production cross sections are given. For each of the K, L and M shells the relative X-ray line intensities are then generated by the ratio between the calculated production cross section for the given line to the sum of the α_1 and α_2 production cross section.

The ionization cross sections, $\sigma_{K,L}^I$, are calculated in the ECPSSR theory (Cohen and Harrigan, 1985), which uses the plane-wave Born approximation (PWBA) with corrections for energy loss (E), Coulomb deflection (C), perturbed-stationary-state (PSS), and relativistic (R) effects. The M-shell ionization cross sections are calculated using the Coulomb corrected Plane-Wave Borne-Approximation (CPWBA) according to Johnson et al. (1979) with corrections for Coulomb deflection according to the Brandt and Lapicki formalism (Brandt and Lapicki 1979).

The different theories for ionisation cross sections do differ slightly; however the different parameter sets used to convert ionisation cross sections to X-ray productions cross sections generally produce significantly larger variations than those between ECPSSR, CPWBA and ECUSAR theories. Generally to minimise these differences between theories we normalise the K, L and M subshell α, β and γ lines to their corresponding $\alpha = (\alpha_1+\alpha_2)$ lines.

Tables 1 and 2 show the typical differences between theories for L and M subshell ionisation cross sections by 2 MeV protons on W (Z=74) and U (Z=92).

Table 1: L subshell ionisation cross sections for 2 MeV protons on W and U.

2MeV protons	L shell ionisation cross sections (b) W (Z=74)		L shell ionisation cross sections (b) U (Z=90)	
	PWBA	ECPSSR	PWBA	ECPSSR
L_1	13.84	13.65	0.8621	0.7506
L_2	43.17	38.45	2.762	2.729
L_3	148.43	131.80	16.898	15.660
L_{tot}	205.44	183.90	20.522	19.140

Table 2: M subshell ionisation cross sections for 2 MeV protons on W and U.

2MeV protons	M shell ionisation cross sections (b) W (Z=74)				M shell ionisation cross sections (b) U (Z=90)			
	PWBA	CPWBA	ECPSSR	ECUSAR	PWBA	CPWBA	ECPSSR	ECUSAR
M_1	7,063	6,895	6,366	6,362	668	639	566	618
M_2	7,930	7,725	7,194	7,686	873	837	759	835
M_3	21,109	20,652	19,297	20,558	3,305	3,183	2,934	3,163
M_4	30,587	30,086	27,689	29,649	4,372	4,233	3,902	4,062
M_5	49,517	48,587	44,904	48,145	7,512	7,296	6,724	7,009
M_{tot}	116,206	113,945	105,450	112,400	16,729	16,187	14,886	15,687

2.1 K Shell X-ray production cross sections

The X-ray production cross sections for the K-shell are related to the ionization cross section by, (Cohen and Harrigan, 1986):

$$\sigma^{x}_{K_\alpha} = \left(\frac{\Gamma_{K_\alpha}}{\Gamma_K}\right)\omega_K \sigma^{I}_{K} \qquad (1)$$

and

$$\sigma^{x}_{K\beta} = \left(\frac{\Gamma_{K\beta}}{\Gamma_K}\right)\omega_K \sigma^{I}_{K} \qquad (2)$$

Where ω_K is the K-shell fluorescence yield, σ^{I}_{K} is the K-shell ionization cross section, $\Gamma_{K_\alpha}, \Gamma_{K_\beta}, \Gamma_K$ are the α, β and total K-shell emission rates, respectively.

The K-shell fluorescence yield (ω_K) can be selected from one of four tables:

- Bambynek et al. (1972), experimental values
- Krause (1979), experimental values
- Walters and Bhalla (1971)
- Chen and Craseman (1980).

The emission rate can be either Scofield (1974a) DF theory or Salem (1974), experimental.

2.2 L Shell X-ray production cross sections and total fluorescence yield

The L-shell X-ray production cross sections for the three L-subshells are related to the L-subshell ionization cross sections σ^{I}_{Li} (i= 1, 2, 3) as follows (Cohen and Harrigan, 1986):

$$ {}^{1}\sigma_{Lp}^{x} = \sigma_{L1}^{I}\omega_{L1}\left(\frac{\Gamma_{Lp}}{\Gamma_{L1}}\right), p = \beta_3, \beta_4, \gamma_2, \gamma_3, \gamma_{44}, p_{23} \quad (3) $$

$$ {}^{2}\sigma_{Lp}^{x} = \left(\sigma_{L1}^{I} f_{L1,2} + \sigma_{L2}^{I}\right)\omega_{L2}\left(\frac{\Gamma_{Lp}}{\Gamma_{L2}}\right), p = \beta_1, \eta, \gamma_1, \gamma_5, \gamma_6 \quad (4) $$

$$ {}^{3}\sigma_{Lp}^{x} = \begin{pmatrix} \sigma_{L1}^{I}\left(f_{L1,2} f_{L2,3} + f_{L1,3} + f_{L1,3}^{'}\right) + \\ \sigma_{L2}^{I} f_{L2,3} + \sigma_{L3}^{I} \end{pmatrix}\omega_{L3}\left(\frac{\Gamma_{Lp}}{\Gamma_{L3}}\right), p = \alpha_1, \alpha_2, \beta_5, \beta_6, \beta_{215}, l \quad (5) $$

The ECPSSR L-subshell ionization cross sections (σ_{Li}^{I}, i = 1, 2, 3) are calculated using the codes of Cohen and Harrigan (1985). The L-subshell fluorescence yield (ω_{Li}, i=1, 2, 3) can be optionally selected from Krause (1979) or Campbell (2003, 2009). The $f_{Li,j}$ are the L-shell Coster-Kronig probabilities and these can optionally be selected from Krause (1979) or Campbell (2003, 2009). Γ_{Lp} is the L-subshell emission rate for line p and Γ_{Li}, i = 1, 2, 3, is the total emission rate for the L-subshell *i*.e. L-subshell emission rates can be selected from the theoretical values of Scofield (1974b) or the experiment dataset of Salem et al. (1974)

The program also calculates the L-subshell effective fluorescence yield as follows:

$$ v_{L1} = \omega_{L1} + f_{L1,2}\omega_{L2} + \left(f_{L1,3} + f_{L1,2} f_{L2,3}\right)\omega_{L3} \quad (6) $$

$$ v_{L2} = \omega_{L2} + f_{L2,3}\omega_{L3} \quad (7) $$

$$ v_{L3} = \omega_{L3} \quad (8) $$

$$ \omega_{L} = \frac{\sum_{i=1}^{3} v_{Li}\sigma_{Li}^{I}}{\sum_{i=1}^{3} \sigma_{Li}^{I}} \quad (9) $$

2.3 M Shell X-ray production cross sections and total fluorescence yield

The M-shell production cross sections for the five M-subshells are related to the M-subshell ionization cross sections σ_{Mi}^{I} (i= 1, 2, 3, 4, 5) as follows:

$$ {}^{1}\sigma_{Mp}^{x} = \sigma_{M1}^{I}\omega_{ML1}\left(\frac{\Gamma_{Mp}}{\Gamma_{M1}}\right), p = M1-N23, M1-O23 \quad (10) $$

$$ {}^{2}\sigma_{Mp}^{x} = \left(\sigma_{M1}^{I} f_{M1,2} + \sigma_{M2}^{I}\right)\omega_{M2}\left(\frac{\Gamma_{Mp}}{\Gamma_{M2}}\right), p = M2-N1, M2-O1, M2-O4, M2-N4 \quad (11) $$

$$ {}^{3}\sigma_{Mp}^{x} = \left(\sigma_{M1}^{I}\left(f_{M1,2} f_{M2,3} + f_{M1,3}\right) + \sigma_{M2}^{I} f_{LM2\_3} + \sigma_{M3}^{I}\right)\omega_{M3}\left(\frac{\Gamma_{Mp}}{\Gamma_{M3}}\right), $$

$$ p = M3-N1, M3-N2, M3-O1, M3-O45, M3-N5, M3-N4, M3-N67 \quad (12) $$

$$ {}^{4}\sigma_{Mp}^{x} = \begin{pmatrix} \sigma_{M1}^{I}\left(f_{M1,4} + f_{M1,2} f_{M2,4} + f_{M1,3} f_{M3,4} + f_{M1,2} f_{M2,3} f_{M3,4}\right) + \\ \sigma_{M2}^{I}\left(f_{M2,4} + f_{M2,3} f_{M3,4}\right) + \sigma_{M3}^{I} f_{M3,4} + \sigma_{M4}^{I} \end{pmatrix}\omega_{M4}\left(\frac{\Gamma_{Mp}}{\Gamma_{M4}}\right), \quad (13) $$

$$ p = M4-N2, M4-N3, M4-N6, M4-O3, M4-O2 $$

$$
{}^{5}\sigma^{x}_{Mp} = \left(\begin{array}{l} \sigma^{I}_{M1}\left(\begin{array}{l} f_{M1,5} + f_{M1,2} f_{M2,5} + f_{M1,3} f_{M3,5} + f_{M1,4} f_{M4,5} + \\ f_{M1,2} f_{M2,3} f_{M3,5} + f_{M1,2} f_{M2,4} f_{M4,5} + f_{M1,3} f_{M3,4} f_{M4,5} + \\ f_{M1,2} f_{M2,3} f_{M3,4} f_{M4,5} \end{array} \right) + \\ \sigma^{I}_{M2}\left(f_{M2,5} + f_{M2,4} f_{M4,5} + f_{M2,3} f_{M3,5} + f_{M2,3} f_{M3,4} f_{M4,5} \right) \\ \sigma^{I}_{M3}\left(f_{M3,5} + f_{M3,4} f_{M4,5} \right) + \sigma^{I}_{M4} f_{M4,5} + \sigma^{I}_{M5} \end{array} \right) \omega_{M5} \left(\frac{\Gamma_{Mp}}{\Gamma_{M5}} \right), \qquad (14)
$$

$$
p = M5 - N3, M5 - N7, M5 - N6, M5 - O3
$$

The available M subshell data (fij, Sij, wi Γ_{Mp} etc) are highly variable and generally unreliable to better than ±50% or more in some cases. So it is difficult to select a consistent set which we could recommend across an atomic number range from Z=60 to 96. For this reason we have allowed several different data sets to be selected for the M line X-ray intensity ratio calculations.

The M-subshell fluorescence yield (ω_{Mi}, i=1, 2, 3, 4, 5) can be optionally selected from the theoretical Dirac-Hartree-Slater (DHS) model or Dirac-Flock (DF) model (Chauhan and Puri, 2008) or the experimental values of Durak et al (2001). The $f_{Mi,j}$ are the M-shell Coster-Kronig probabilities and these can optionally be selected from Bambynek et al (1972) or Chauhan and Puri (2008). Γ_{Mp} is the M-subshell emission rate for line p and Γ_{Mi}, i = 1, 2, 3, 4, 5 is the total emission rate for the M-subshell i. M-subshell emission rates can be selected from DF or DHS calculations (Puri 2007).

The program also calculates the M-subshell effective fluorescence yield as follows:

$$
\begin{array}{l} \nu_{M1} = \omega_{M1} + f_{M1,2}\omega_{L2} + \left(f_{M1,3} + f_{M1,2} f_{M2,3} \right)\omega_{M3} + \\ \left(f_{M1,4} + f_{M1,3} f_{M3,4} + f_{M1,2} f_{M2,4} + f_{M1,2} f_{M2,3} f_{M3,4} \right)\omega_{M4} + \\ \left(\begin{array}{l} f_{M1,5} + f_{M1,4} f_{M4,5} + f_{M1,3} f_{M3,5} + f_{M1,2} f_{M2,5} + f_{M1,3} f_{M3,4} f_{M4,5} + \\ f_{M1,2} f_{M2,4} f_{M4,5} + f_{M1,2} f_{M2,3} f_{M3,5} + f_{M1,3} f_{M3,4} f_{M4,5} \end{array} \right)\omega_{M5} \end{array} \qquad (15)
$$

$$
\begin{array}{l} \nu_{M2} = \omega_{M2} + f_{M2,3}\omega_{M3} + \left(f_{m2,4} + f_{M2,3} f_{M3,4} \right)\omega_{M4} + \\ \left(f_{m2,5} + f_{M2,4} f_{M4,5} + f_{M2,3} f_{M3,5} + f_{M2,3} f_{M3,4} f_{M4,5} \right)\omega_{M5} \end{array} \qquad (16)
$$

$$
\nu_{L3} = \omega_{M3} + f_{L3,4}\omega_{L4} + \left(f_{M3,5} + f_{M3,4} f_{M4,5} \right)\omega_{L5} \qquad (17)
$$

$$
\nu_{M4} = \omega_{M4} + f_{M4,5}\omega_{M5} \qquad (18)
$$

$$
\nu_{M5} = \omega_{M5} \qquad (19)
$$

$$
\omega_{M} = \frac{\sum_{i=1}^{5} \nu_{Mi}\sigma^{I}_{Mi}}{\sum_{i=1}^{5} \sigma^{I}_{Mi}} \qquad (20)
$$

3 Using program *KLMabgRatios*

The data files required by the program KLMabgRatios are specified and reproduced in Appendix 1 to 4. When running the program, where more than one table exists for the same data, the user is asked to select from the available options. The user is additionally requested to enter if a proton, deuteron or a helium ions are to be used and their energies in MeV and also the start and end atomic numbers Z of elements for which the X-ray intensities will be calculated. Once all the options have

been entered, the program selects the appropriate data files and calculates the production cross sections for each of the K, L and M subshells. For each line within each subshell the relative intensities are then calculated, relative to the main $(\alpha_1+\alpha_2) = 100$ line. The intensities are then printed to the screen as well as to a file called "***results.txt***". In addition the ionisation cross sections, the X-ray production cross sections and the effiective fluorescence yields are generated in file "***wbar.cs"*** and the cross sections for each line are presented in file "***xsectionresults.csv***".

3.1 Files for PIXAN

Two files are also generated for input to PIXAN thin and thick target yield programs THIN and THIK, namely:

- ***dset2-info-ddmmyy*** – for each element this file contains the table of energies and their relative intensities, normalised to $(\alpha_1+\alpha_2) = 1.00$ in the same format as the original ***dset2*** PIXAN file.
- ***dset4-info-ddmmyy*** – contains the same information in the same format as ***dset4*** used by PIXAN (described in Appendix 4). The old input file ***dset4*** is read following which the new file is generated containing the same information aside from two entries; ALFAK is replaced by the newly calculated ratio of the intensity of the reference line to the sum of all lines for each of the K and L shells, and WK is replaced by the selected fluorescence yield for the K-shell (i.e. one of Bambynek et al. 1972, Krause 1979, Walters and Bhalla 1971, Chen and Craseman 1980). For the L-shell the total fluorescence yield (ϖL) is replaced by one of Puri et al. 1993, Clayton 1986, or Bambynek et al. 1972). On start-up of the program the user is asked to select which table to be used for ϖL.

The string "***ddmmyy***" is the day, month and year on which the file was generated and "***info***" contains information on the data tables used. "***info***" has the following content "***KwxxExx-LwxxExxwTxx-MwxxExxCKxx***", where:

- ***KwxxExx*** is the information for the K shell, with the ***xx*** in "***wxx***" being the two characters to represent the choice of the K shell fluorescence yield table:
  - "***Ba***" for Bambynek et al. (1972), Experimental values
  - "***Kr***" for Krause (1979) Experimental values
  - "***WB***" for Walters and Bhalla (1971), and
  - "***Ch***" for Chen and Craseman (1980), theory values.

  The xx in "***Exx***" are the two characters to represent the choice of the K shell emission rate:
  - "***Sc***" for Scofield (1974a), DF theory and
  - "***Sa***" for Salem (1974) Experimental values.

- ***LwxxExxwTxx*** is the information for the L shell, with ***xx*** in "***wxx***" being the two characters to represent the choice of the L shell fluorescence yield table and Coster-Kronig probabilities:
  - "***Ca***" for Campbell (2003), Experimental and DF theory and
  - "***Kr***" for Krause (1979) Experimental values.

  The xx in "***Exx***" are the two characters to represent the choice of the L shell emission rate:
  - "***Sc***" for Scofield (1974b), DF theory and
  - "***Sa***" for Salem (1974) Experimental values.

The xx in "***wTxx***" are the two characters to represent the choice of the L shell total fluorescence yield:

- "***Pu***" for Puri et al. 1993 based on RDHS theory from Chen et al., 1981,
- "***EJ***" for PIXAN Clayton et al., (1986), and
- "***Ba***" for Bambynek et al. (1972) Experimental values.

- ***MwxxExxCKxx*** is the information for the M shell, with ***xx*** in "***wxx***" being the two characters to represent the choice of the M shell fluorescence yield table:
  - "***DH***" for DHS theory (Chauhan and Puri, 2008), and
  - "***DF***" for DF theory (Chauhan and Puri, 2008).

  The xx in "***Exx***" are the two characters to represent the choice of the M shell emission rate:
  - "***DH***" for DHS theory (Puri, 2007), and
  - "***DF***" for DF theory (Puri, 2007).

  The xx in "***CKxx***" are the two characters to represent the choice of the M shell Coster-Kronig probabilities:
  - "***Ba***" for the super Coster_Kronign probabilities (Bambynek et al., 1972), experimental values and
  - "***Ch***" for Chauhan and Puri (2008) DF and DHS theory values.

3.2 L and M shell Spectra

Theoretical L and M shell spectra, for a user selected atomic number Z, can also be optionally produced in the files ***Lshell_Spectrum.csv*** and ***Mshell_Spectrum.csv*** and the efficiency corrected total spectra for each sub-shell is produced in files ***Lsubshell.csv*** and ***Msubshell.csv***.

For each characteristic energy a Gaussian peak is calculated where the full width half maximum FWHM in keV is calculated as: $\sqrt{(a+b*E_x)}$ giving a standard deviation of FWHM/2.35482. Note $2\sqrt{}(2\ln 2)=2.35482$ and E_x is the X-ray energy in keV. Currently the value of a is 0.016037 and b is 0.00287895 for our Vortex X-ray detector and E_x in keV. The height of the peak is given by the relative line intensity.

4 Program *wexplore* - fitting Gaussians

The program ***wexplore*** reads two files and is normally run by redirecting standard output to a further file. For example, the command would read:

```
wexplore spectrum.txt control.txt > output.txt
```

The first two lines of the *spectrum.txt* file are header lines, which are read by the program and ignored. The spectra are typically in the GUPIX standard export format. Each subsequent line contains variables labelled, respectively:

```
Channel, Energy, Data, Fit, Residual, Data-Fit
```

`Channel` is an integer, the others are fixed point, which are read and processed as double precision reals. Each of the variables except the last on each line is followed by a comma, so that the fields are comma delineated. The input file can be read and displayed easily by EXCEL.

The program is exploratory and has a number of options specified in the ***control.txt*** file. As currently run, the program uses the Energy, Data, and Fit variables, which we will label e_k, d_k, and f_k

respectively. The program reads and stores the data for all the channels, and uses in the fitting procedure only those channels which have been selected in the ***control.txt*** file.

The basic problem solved by the program is to fit a number m of Gaussians + a background term to the spectrum variables d_j. The centreline energy E_i of each peak is an input in the ***control.txt*** file. Each Gaussian peak takes the form,

$$p_i(e) = \beta_i \exp\left(-\frac{(e - E_i)^2}{2\sigma_i^2} \right) \tag{21}$$

where the width (standard deviation), σ_i, is determined from the relation

$$\sigma_i = \frac{\sqrt{(\nu_1 + \nu_2 E_i)}}{2.35482} \tag{22}$$

and the parameters ν_1 and ν_2 are read from ***control.txt***.

The fit is achieved by minimising the weighted sum of squares

$$R(\beta) = \sum_{k=1}^{n} w_k \left(\sum_{i=1}^{m} \beta_i p_i(e_k) + \beta_{n+1} f_k - d_k \right)^2 \tag{23}$$

with respect to the coefficients β.

Determination of the background variables f_k are discussed later below.

The weights are given by

$$w_j = \frac{1}{d_j} \tag{24}$$

which assumes that the uncertainty in each d_j is proportional to $\sqrt{d_j}$.

The minimisation problem is a linear least squares problem, which can be solved by a variety of methods. We have chosen to use Cholesky decomposition to solve the symmetric matrix equation,

$$A\beta = c \tag{25}$$

Where

$$a_{i,j} = \sum_{k=1}^{m} w_k p_i(e_k) p_j(e_k) \qquad i, j = 1 \ldots n \tag{26}$$

$$a_{i,n+1} = \sum_{k=1}^{m} w_k p_i(e_k) f_k \qquad i = 1 \ldots n \tag{27}$$

and,

$$c_i = \sum_{k=1}^{m} w_k p_i(e_k) d_k \qquad i = 1 \ldots n \tag{28}$$

Having computed the peak height coefficients β, the program computes the fitted values,

$$g_k = \sum_{i=1}^{m} \beta_i p_i(e_k) + \beta_{n+1} f_k \qquad k = 1 \ldots m \tag{29}$$

and outputs them, along with the input data values, in comma delineated format suitable for display by EXCEL, and then computes the unweighted sum of squares,

$$S = \sum_{k=1}^{n} \left(\sum_{i=1}^{m} \beta_i p_i(e_k) + \beta_{n+1} f_k - d_k \right)^2 = \sum_{k=1}^{m} (g_k - d_k)^2 \tag{30}$$

Finally, as an additional check, the program computes the areas associated with each peak by two methods, firstly using,

$$b_i = \beta_i \sum_{k=1}^{m} c_k p_i(e_k) \tag{31}$$

and secondly by integrating the Gaussians analytically,

$$b_i = \beta_i \left(erf\left(\frac{E_i - e_1}{\sigma_i} \right) + erf\left(\frac{e_m - E_i}{\sigma_i} \right) \right) \tag{32}$$

and prints both.

The approximation for erf(x) is taken from Hastings (1955) Pg187 Sheet 63.

The background for the Gaussian fits was determined by performing a linear fit to the log of efficiency corrected spectrum. The first 5 channels to the right of the low energy marker and the last five channels to the left of the high energy marker were used to determine this background fit. The background was then corrected for detector efficiency again and the calculated Gaussians added to this.

Figure 1 below shows the results of such a background calculations for 2 MeV protons on a thin gold Micromatter foil.

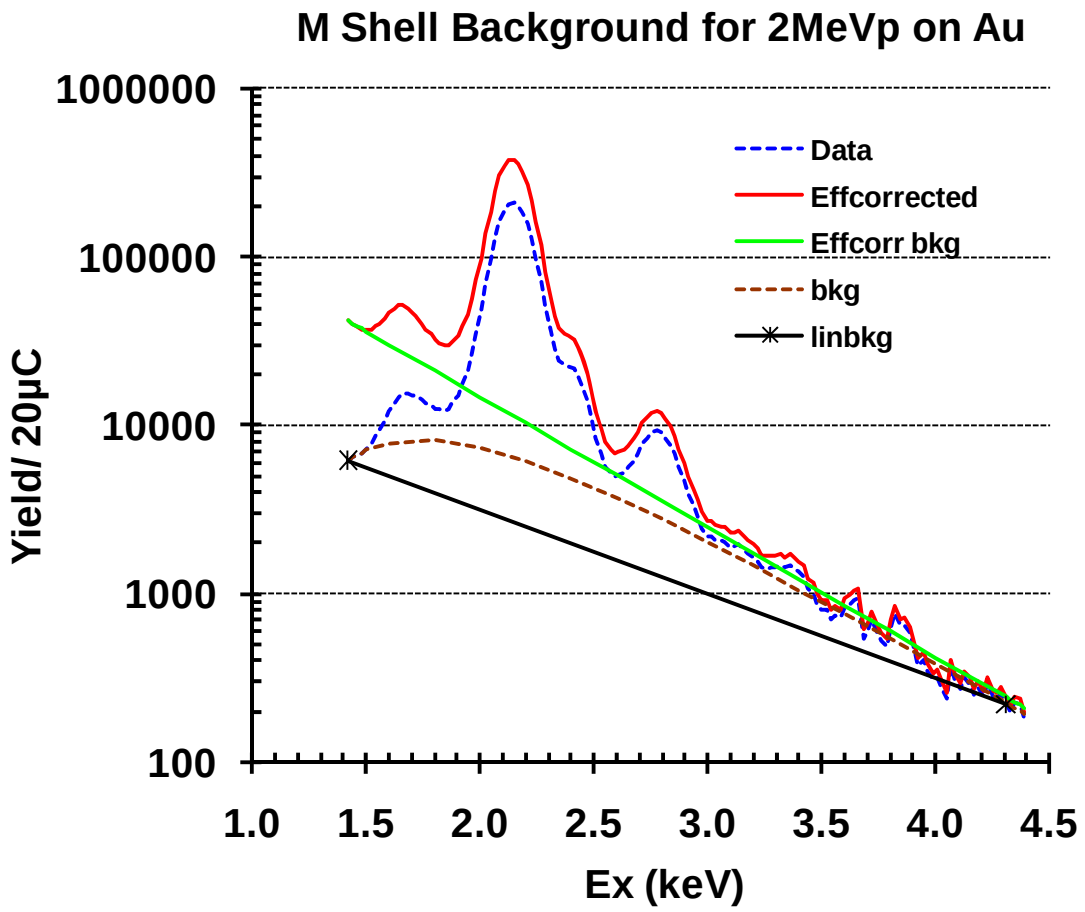

Fig. 1: **Determination of background for M shell lines from 2 MeV protons on gold.**

The solid background line shows how a straight line fit on a log plot differs from the detector efficiency corrected background used here (the dashed background line). This approach gives significantly smaller peak areas for the minor M subshell line intensities than the straight linear background approach. But we feel this is more realistic as it better approximates the secondary electron bremsstrahlung background in this low energy X-ray region.

5 *KLMabgRatios* Examples

5.1 Sample Run

Here we present a sample run of the program ***KLMabgRatios***. A screen dump of the options and the resulting selection (in bold) follows. The resulting line intensities are presented in Appendix 5. This sample run is for our preferred option of K, L and M subshell X-ray line intensities for 3 MeV protons on selected targets between Z=6 and 100.

```
Select from
       1: Proton
       2: Deuterium
       3: Helium
Your Selection: 1
 Enter proton energy start, then the energy increment and
 how many times to increment (e.g. 4 0.5 3): 3.0 0 0

  Enter z-start and z-end (e.g. 50 70): 1 100
```

```
 K shell options

 Select option for wK
      1: Bambynek
      2: Krause
      3: WB
      4: Chen
Select wK option: 2

 Select option for K shell emission rates
      1: Scofield
      2: Salem
Select emission rate option: 2

 L shell options

 Select option for wL
      1: Campbell
      2: Krause
Select wL option: 1

 Select option for L shell emissions rates
      1: Scofield
      2: Salem
Select emission rate option: 1

 Select option for wL bar
      1: Puri
      2: EJC
      3: Bambynek
Select wL bar option: 3

 M shell options

 Select option for M shell emission rates
      1: DHS
      2: DF
Select emission rate option: 2

 Select option for M shell fluorescence yield
      1: DHS
      2: DF
Select fluorescence yield option: 2

 Select option for M shell wbar
      1: DHS
      2: DF
      3: Exp
Select wM_bar option: 3

 Select option for M shell C-K transitions
      1: Bambynek
      2: Chauhan and Puri
Select C-K transitions option: 1

 Write to dset2 energies as
      1: supplied by GEOPIXE
      2: Calculated from above
         Select dset2 option: 2

Do you want to produce an L-shell spectrum: y
Which Z: 79
```

```
Do you want to produce an M-shell spectrum: y
Which Z: 79
```

5.2 Uranium

Here we present the output of the ***KLMabgRatios*** program for uranium. The theoretical L-shell energies and their intensities are presented in Table 3 and the corresponding spectrum is shown in Figure 2. Information (such as the shell total ionisation cross section, and the total fluorescence yield) on the L-shell and M-shell is presented in Table 4. The theoretical M-shell energies and their intensities are presented in Table 5 and the corresponding spectrum is shown in Figure 3.

Table 3: Uranium Line energies and intensities for 3 MeV protons – ECPSSR

Line	Energy	Ratio
	keV	Lα=1.00
Lα1	13.612	0.89767
Lα2	13.437	0.10233
Ll	11.616	0.06204
Lη	15.397	0.00632
Lβ6	15.723	0.01601
Lβ215	16.425	0.21840
Lβ4	16.573	0.01051
Lβ5	17.067	0.04663
Lβ1	17.217	0.22106
Lβ3	17.452	0.00919
Lγ5	19.504	0.00174
Lγ1	20.164	0.05233
Lγ2	20.481	0.00290
Lγ3	20.709	0.00294
Lγ6	20.839	0.01094
Lγ44	21.559	0.00142

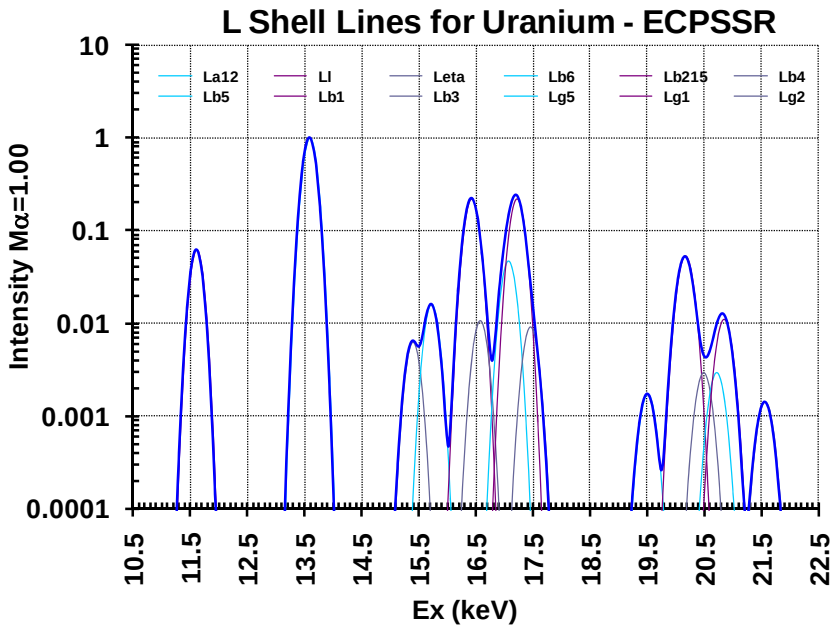

Table 3: Uranium Line energies and intensities for 3 MeV protons – ECPSSR

Fig. 2: Theoretical L shell spectrum for 3 MeV protons on uranium.

Table 4: Information for 3 MeV protons for the L and M shells.

Lα/Ltot=	0.60143	
ωLbar=	0.54117	
LαEff=	0.73672	
σLtot=	49.6427	barns ECPSSR
Mα/Mtot=	0.57862	
ωMbar=	0.05221	
σMtot=	24.8575	kbarns CPWBA

Table 5: Uranium M line energies and intensities for 3 MeV protons – CPWBA.

Line	Energy	Detector	Ratio
	keV	Efficiency	Mα=1.00
M5-N7	3.1746	0.7539	0.95147
M5-N6	3.1638	0.7518	0.04853
M4-N2	2.4570	0.5506	0.02293
M5-N3	2.5090	0.5705	0.03121
M4-N3	2.6850	0.6309	0.00210
M3-N1	2.8640	0.6829	0.01940
M3-N2	3.0320	0.7240	0.00007
M4-N6	3.3398	0.7838	0.51192
M5-O3	3.3600	0.7871	0.00637
M4-O2	3.4710	0.8043	0.00471
M3-N4	3.5247	0.8121	0.00909
M4-O3	3.5360	0.8136	0.00041
M3-N5	3.5668	0.8178	0.06831
M2-N1	3.7430	0.8397	0.00265
M3-N67	3.9202	0.8584	0.00115
M3-O1	3.9820	0.8642	0.00456
M3-O45	4.2045	0.8829	0.01581
M1-N23	4.3910	0.8960	0.00886
M2-N4	4.4037	0.8968	0.01280
M2-O1	4.8610	0.9215	0.00065
M2-O4	5.0792	0.9305	0.00290
M1-O23	5.3235	0.9391	0.00236

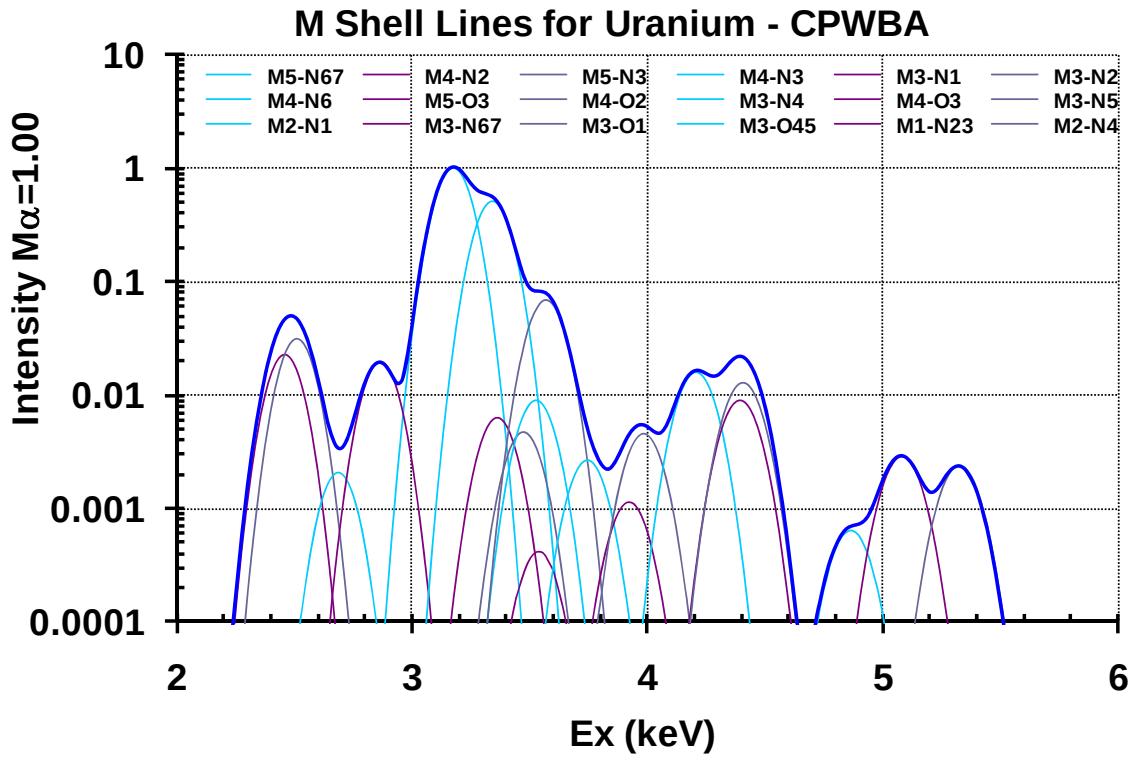

Fig. 3: **Theoretical M shell spectrum for 3 MeV protons on uranium.**

Figure 4 shows the experimental M shell spectrum for 2 MeV protons on Uranium. The 13 Gaussians and the background were fitted with the ***wexplore*** program described above. The Prefit

spectrum was obtained beforehand by fitting the full spectrum in GUPIX (Campbell et al 2010) without M lines and then exporting the resultant data-fitted spectrum through to ***wexplore*** for the Gaussian fitting.

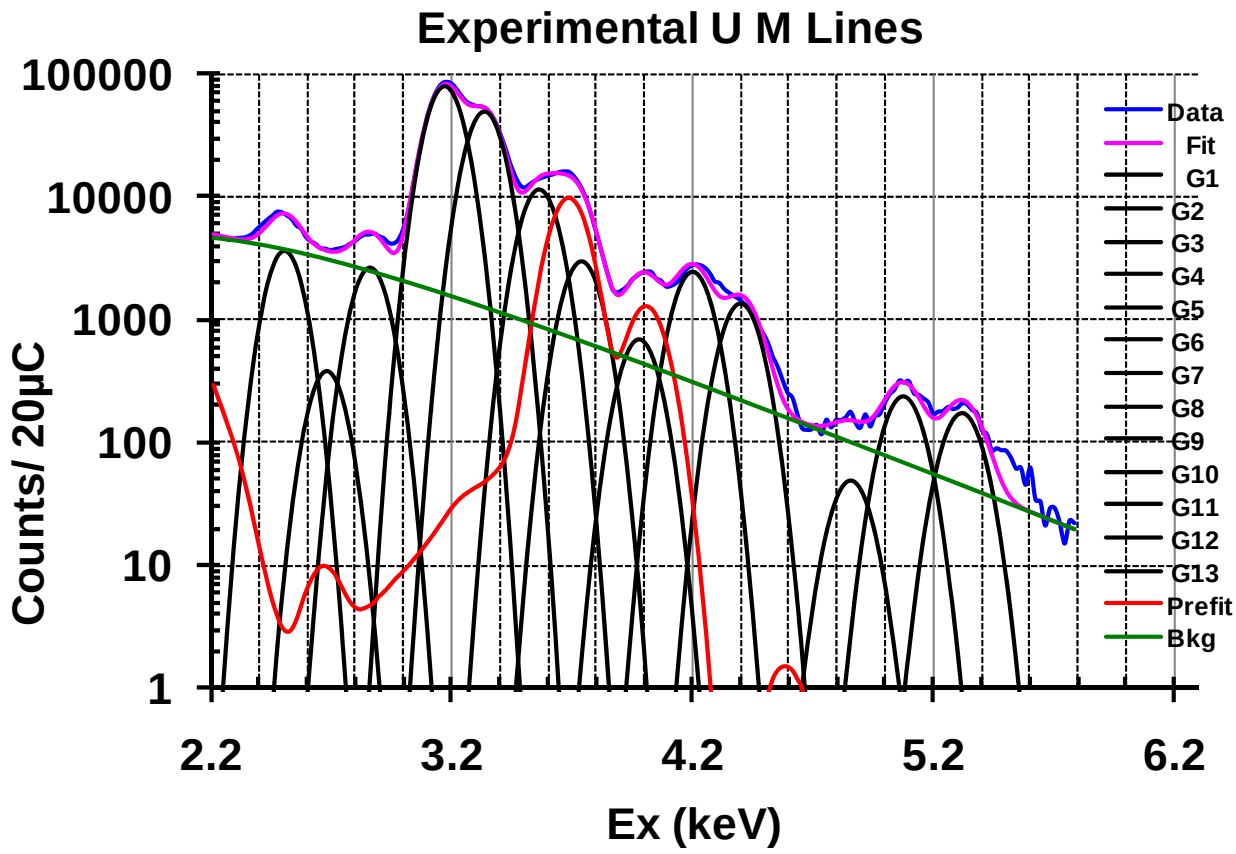

Fig. 4: Experimental M shell spectrum for 2 MeV protons on uranium.

The extra non-M subshell peaks in the Prefit spectrum are contamination peaks from Ca Kα and Kβ lines and are also fitted in the Prefit spectrum by ***wexplore*** as an independent Gaussian line.

6 Summary

In the 1980's we developed the PIXAN analysis package basically for K and L analysis of X-ray spectra and to determine elemental concentrations using mainly Kα X-ray lines parameters. Our preferred dataset parameters used then were ECPSSR K and L subshell ionisation cross section, experimental fluorescence yields and Coster-Kronig transitions from Krause 1979 and individual experimental X-ray line emission rates published by Salem et al in 1974.

The program described here, ***KLMabgRatios***, has been written to calculate these K, L and M subshell using the latest X-ray parameter datsets as well as the older original datasets from the 1970s and 1980s. Our preferred recommended K, L and M X-ray line intensities for 3 MeV proton impact on selected targets for atomic numbers between Z=6 and 100 are given in Tables 30 to 33 inclusive for 8 K lines, 17 L lines and 22 M lines as well as their corresponding ω_K, ω_L and ω_M total shell fluorescence yields. Note that although the line intensities are given for 3 MeV protons the program will calculate these line intensity ratios for any input ion energy as it has direct assess to the ECPSSR ionisation cross sections for K and L subshells and CPWBA ionisation cros sections for M subshells for protons, helium ions and deuterons.

7 References

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8 Appendix 1: Files for K shell calculations

For the K-shell relative intensity calculations the data tables, stored in the following files, are needed:

- ***upxk.input*** – atomic mass and edges for ionisation cross section calculations.
- ***KshellEmissionRatesScofield-Salem13Feb11.txt*** – K-shell emission rates for the two options (Scofield 1974a, Salem 1974).
- ***wK-Bambynek-Krause-WB-Chen13Feb11.txt*** – K-shell fluorescence yield for the four options (Bambynek et al. 1972, Krause 1979, Walters and Bhalla 1971, Chen and Craseman 1980).
- ***kshellenergiesa1-3b1-5at13Feb11.txt*** – K-shell characteristic X-ray energies.

8.1 K shell atomic mass and edges

The K shell edges are stored in file "***upxk.input***". The information in this file is used for the K shell ionisation cross sections calculations.

Table 6: Inputs for K shell ECPSSR cross sections.

```
*   ROOTS
0.095012509837637440185D0
0.281603550779258913230D0
0.458016777657227386342D0
0.617876244402643748447D0
0.755404408355003033895D0
0.865631202387831743880D0
0.944575023073232576078D0
0.989400934991649932596D0
*   WEIGHTS
0.189450610455068496285D0
0.182603415044923588867D0
0.169156519395002538189D0
0.149595988816576732081D0
0.124628971255533872052D0
0.095158511682492784810D0
0.062253523938647892863D0
0.027152459411754094852D0
*  SEND=1.0D-2  RNQW=10.0D0  RNQQ=10.0D0
  1.0d-3    20.0d0   20.0d0
  Proton Energy 3.0 -1
*  6.0(0.25)10.0 10.5(0.5)20.0  -1
* 0.1(0.02)0.5 1.0(0.5)6.0    -1
*  ENERGY HVY 0.5(0.1)2 2.2(.2)4.8 5(0.5)15 16(1)50   -1
*  ENEGRY P  0.5(.1)10   -1
* D 0.2(0.05)1.0 1.2(0.2)10.0 10.5(0.5)20.0     -1
*  ENERGY HE 0.2(0.1)2 2.2(.2)4.2 4.5(0.5)15    -1
*  LI 0.5 0.6(.2)4 4.5(.5)10 11(1)50 52(2)70 75(5)100  -1
*  ENERGY BE 0.5 0.6(0.2)4 4.5(0.5)10 11(1)50 52(2)90  -1
  ENERGIES FOR PLOT 20 50 PLOTMIN=1.0D-3 PLOTMAX=1.0D10
  ADIAB=0 ZERO=CORRECT NOT IN ONE=IN
  CPSSR=1 ZERO=CPSSR, ONE=ECPSSR, TWO=COHENECPSSR
 TEST POINTS FOR ADIABATIC FN 0.1(0.1)1 1.5 2(1)10

 *         INSERT     ION       ZS
         PROTON          1   1.00783
 *       DEUTERIUM       1   2.01410
```

*	HELIUM	2	4.00260
*	LI	3	7.01601
*	BE	4	9.01219
*	B	5	11.00930
*	C	6	12.00000
*	N	7	14.00310
*	O	8	15.99490
*	F	9	18.99840
*	NE	10	19.99240
*	SI	14	27.97690
*	S	16	31.97210

*	**INSERT**	**TARGET**	**ZS**	**Kedge**
	C	6	12.000	0.283
	N	7	14.000	0.399
	O	8	16.000	0.531
	F	9	19.000	0.687
	NE	10	20.179	0.867
	NA	11	22.989	1.072
	MG	12	24.300	1.305
	AL	13	26.980	1.559
	SI	14	28.090	1.838
	P	15	30.970	2.142
	S	16	32.060	2.472
	CL	17	35.453	2.822
	AR	18	39.948	3.202
	K	19	39.098	3.607
	CA	20	40.080	4.038
	SC	21	44.960	4.496
	TI	22	47.900	4.965
	V	23	50.940	5.465
	CR	24	51.996	5.989
	MN	25	54.938	6.540
	FE	26	55.847	7.112
	CO	27	58.930	7.709
	NI	28	58.700	8.333
	CU	29	63.546	8.979
	ZN	30	65.380	9.659
	GA	31	69.720	10.368
	GE	32	72.590	11.104
	AS	33	74.920	11.868
	SE	34	78.960	12.658
	BR	35	79.900	13.474
	KR	36	83.800	14.322
	RB	37	85.470	15.201
	SR	38	87.620	16.105
	Y	39	89.910	17.037
	ZR	40	91.220	17.998
	NB	41	92.910	18.986
	MO	42	95.940	20.002
	TC	43	97.000	21.054
	RU	44	101.070	22.118
	RH	45	102.910	23.224

PD	46	106.400	24.350
AG	47	107.868	25.514
CD	48	112.400	26.711
IN	49	114.820	27.940
SN	50	118.690	29.200
SB	51	121.750	30.491
TE	52	127.600	31.813
I	53	126.905	33.169
XE	54	131.300	34.582
CS	55	132.905	35.959
BA	56	137.340	37.441
LA	57	138.905	38.925
CE	58	140.120	40.449
PR	59	141.000	41.998
ND	60	144.240	43.571
PM	61	147.000	45.184
SM	62	150.350	46.834
EU	63	151.960	48.519
GD	64	157.250	50.240
Tb	65	158.942	51.996
DY	66	162.500	53.789
HO	67	164.930	55.615
ER	68	167.260	57.483
TM	69	168.934	59.930
YB	70	173.040	61.332
LU	71	174.970	63.304
HF	72	178.910	65.351
TA	73	180.950	67.414
W	74	183.850	69.524
RE	75	186.200	71.676
OS	76	190.200	73.871
IR	77	192.200	76.111
PT	78	195.090	78.395
AU	79	196.970	80.723
HG	80	200.590	83.102
TL	81	204.370	85.530
PB	82	207.200	88.006
BI	83	208.980	90.527
PO	84	210.000	93.105
AT	85	210.000	95.730
RN	86	222.000	98.404
FR	87	223.000	101.137
RA	88	226.000	103.922
AC	89	227.000	106.755
TH	90	232.000	109.649
PA	91	231.000	112.601
U	92	238.000	115.603
NP	93	237.000	118.678
PU	94	242.000	121.818
AM	95	243.000	124.876
CM	96	247.000	128.220
BK	97	247.000	131.590
CF	98	251.000	135.960
ES	99	254.000	139.490
FM	100	253.000	143.090

8.2 K shell emission rates

The K-shell emission rates for the two options (Scofield 1974a, Salem 1974) are stored in the file

KshellEmissionRatesScofield-Salem13Feb11.txt.

8.3 K shell fluorescence yield

The K shell fluorescence yields for the four options (Bambynek et al., 1972, Krause 1979, Walters and Bhalla 1971, Chen and Craseman 1980) are stored in file

wK-Bambynek-Krause-WB-Chen13Feb11.txt:

Table 7: K shell fluorescence yield.

***Bambynek et al wKs from Rev Mod Phys 44(1972)716-814**					
***Walters and Bhalla PhysRevA3(1971)1919**					
***Chen and Craseman Phys Rev A21(1980)436-441 DHS**					
***fit to (wk/(1-wK))^0.25 =oddPoly(Z^3)**					
*Coeffs					
*a0=	1.51E-02				
*a1	3.27E-02				
*a3	-6.40E-07				
***Elt**	**Z**	**Bambynek**	**Krause**	**WB**	**Chen**
C	6	0.00198	0.00280	0.00240	-9
N	7	0.00352	0.00520	0.00470	-9
O	8	0.00580	0.00830	0.00770	-9
F	9	0.00903	0.01300	0.01150	-9
NE	10	0.01341	0.01800	0.01640	-9
NA	11	0.01918	0.02300	0.02240	-9
MG	12	0.02655	0.03000	0.03010	-9
AL	13	0.03575	0.03900	0.03980	-9
SI	14	0.04696	0.05000	0.05140	-9
P	15	0.06036	0.06300	0.06530	-9
S	16	0.07608	0.07800	0.08180	-9
CL	17	0.09419	0.09700	0.10040	-9
AR	18	0.11471	0.11800	0.12150	0.1220
K	19	0.13760	0.14000	0.14480	0.1460
CA	20	0.16274	0.16300	0.17080	0.1700
SC	21	0.18995	0.18800	0.19910	0.2006
TI	22	0.21899	0.21400	0.22730	0.2312
V	23	0.24958	0.24300	0.26080	0.2618
CR	24	0.28139	0.27500	0.29390	0.2924
MN	25	0.31407	0.30800	0.32760	0.3230
FE	26	0.34727	0.34000	0.36240	0.3560
CO	27	0.38064	0.37300	0.39770	0.3890
NI	28	0.41384	0.40600	0.43290	0.4220
CU	29	0.44658	0.44000	0.46780	0.4550
ZN	30	0.47861	0.47400	0.50140	0.4880
GA	31	0.50969	0.50700	0.53380	0.5158
GE	32	0.53965	0.53500	0.56500	0.5436
AS	33	0.56835	0.56200	0.59470	0.5714
SE	34	0.59570	0.58900	0.62300	0.5992

BR	35	0.62164	0.61800	0.64980	0.6270
KR	36	0.64613	0.64250	0.67540	0.6510
RB	37	0.66918	0.66700	0.69870	0.6713
SR	38	0.69080	0.69000	0.72110	0.6915
Y	39	0.71102	0.71000	0.74200	0.7118
ZR	40	0.72990	0.73000	0.76110	0.7320
NB	41	0.74749	0.74700	0.77880	0.7485
MO	42	0.76385	0.76500	0.79510	0.7650
TC	43	0.77905	0.77950	0.80930	0.7793
RU	44	0.79317	0.79400	0.82360	0.7937
RH	45	0.80626	0.80800	0.83670	0.8080
PD	46	0.81840	0.82000	0.84910	0.8190
AG	47	0.82965	0.83100	0.86050	0.8300
CD	48	0.84008	0.84300	0.87070	0.8393
IN	49	0.84974	0.85300	0.88030	0.8487
SN	50	0.85870	0.86200	0.88890	0.8580
SB	51	0.86701	0.87000	0.89710	0.8660
TE	52	0.87471	0.87700	0.90460	0.8740
I	53	0.88186	0.88400	0.91120	0.8805
XE	54	0.88850	0.89100	0.91760	0.8870
CS	55	0.89466	0.89700	-9	0.8880
BA	56	0.90038	0.90200	-9	0.8890
LA	57	0.90571	0.90700	-9	0.8963
CE	58	0.91066	0.91200	-9	0.9035
PR	59	0.91528	0.91700	-9	0.9108
ND	60	0.91957	0.92100	-9	0.9180
PM	61	0.92358	0.92500	-9	0.9217
SM	62	0.92732	0.92900	-9	0.9253
EU	63	0.93081	0.93200	-9	0.9290
GD	64	0.93407	0.93500	-9	0.9318
TB	65	0.93712	0.93800	-9	0.9345
DY	66	0.93998	0.94100	-9	0.9373
HO	67	0.94265	0.94400	-9	0.9400
ER	68	0.94515	0.94700	-9	0.9423
TM	69	0.94750	0.94900	-9	0.9447
YB	70	0.94971	0.95100	-9	0.9470
LU	71	0.95178	0.95300	-9	0.9488
HF	72	0.95372	0.95500	-9	0.9505
TA	73	0.95555	0.95700	-9	0.9523
W	74	0.95727	0.95800	-9	0.9540
RE	75	0.95889	0.95900	-9	0.9553
OS	76	0.96041	0.96100	-9	0.9567
IN	77	0.96185	0.96200	-9	0.9580
PT	78	0.96321	0.96300	-9	0.9593
AU	79	0.96449	0.96400	-9	0.9607
HG	80	0.96570	0.96500	-9	0.9620
TL	81	0.96684	0.96600	-9	0.9627
PB	82	0.96792	0.96700	-9	0.9633
BI	83	0.96894	0.96800	-9	0.9640
PO	84	0.96990	0.96800	-9	0.9648
AT	85	0.97081	0.96900	-9	0.9656
HN	86	0.97168	0.96900	-9	0.9664
FR	87	0.97250	0.97000	-9	0.9672
BA	88	0.97327	0.97000	-9	0.9680

AC	89	0.97401	0.97100	-9	0.9685
TH	90	0.97471	0.97100	-9	0.9690
PA	91	0.97537	0.97200	-9	0.9695
U	92	0.97599	0.97200	-9	0.9700
NP	93	0.97659	0.97300	-9	0.9703
PU	94	0.97715	0.97300	-9	0.9705
AM	95	0.97769	0.97400	-9	0.9708
CM	96	0.97820	0.97400	-9	0.9710
BK	97	0.97868	0.97500	-9	0.9713
CP	98	0.97914	0.97500	-9	0.9715
ES	99	0.97957	0.97500	-9	0.9718
FM	100	0.97998	0.97600	-9	0.9720
HD	101	0.98037	0.97600	-9	-9
NO	102	0.98074	0.97600	-9	-9
LR	103	0.98109	0.97700	-9	-9

K shell Energies

The K shell energies, sourced from GEOPIXE (Ryan et al., 1990) and Kaye&Laby (http://www.kayelaby.npl.co.uk/atomic_and_nuclear_physics/4_2/4_2_1.html) are stored in file,

kshellenergiesa1-3b1-5at13Feb11.txt:

All energies are in keV.

Table 8: K shell characteristic X-ray energies.

* 23 November 2010										
* Energies obtained from GEOPIXE and Kaye&Laby										
* http://www.kayelaby.npl.co.uk/atomic_and_nuclear_physics/4_2/4_2_1.html										
*Elt	Z	Kα1	Kα2	Kα3	Kβ1	Kβ2	Kβ3	Kβ4	Kβ5	Kα	Kβ
C	6	0.2770	0.2770	0.2790	0.2770	0.2770	0.2770	0.2770	0.2770	0.2770	0.2770
N	7	0.3930	0.3930	0.3950	0.3924	0.3924	0.3924	0.3924	0.3924	0.3924	0.3924
O	8	0.5250	0.5250	0.5270	0.5249	0.5249	0.5249	0.5249	0.5249	0.5249	0.5249
F	9	0.6770	0.6770	0.6790	0.6768	0.6768	0.6768	0.6768	0.6768	0.6768	0.6768
Ne	10	0.8480	0.8480	0.8500	0.8580	0.8590	0.8580	0.8590	0.8580	0.8486	0.8486
Na	11	1.0410	1.0410	1.0430	1.0710	1.0710	1.0710	1.0710	1.0710	1.0410	1.0710
Mg	12	1.2530	1.2530	1.2550	1.3020	1.3020	1.3020	1.3020	1.3020	1.2536	1.3020
Al	13	1.4870	1.4860	1.4890	1.5570	1.5570	1.5570	1.5570	1.5570	1.4866	1.5570
Si	14	1.7400	1.7390	1.7420	1.8360	1.8360	1.8360	1.8360	1.8360	1.7398	1.8360
P	15	2.0140	2.0130	2.0160	2.1390	2.1390	2.1390	2.1390	2.1390	2.0134	2.1390
S	16	2.3080	2.3070	2.3100	2.4640	2.4640	2.4640	2.4640	2.4640	2.3074	2.4680
Cl	17	2.6220	2.6200	2.6240	2.8160	2.8160	2.8160	2.8160	2.8160	2.6219	2.8150
Ar	18	2.9580	2.9560	2.9600	3.1900	3.1910	3.1900	3.1910	3.1900	2.9570	3.1900
K	19	3.3140	3.3110	3.3160	3.5900	3.6030	3.5900	3.6030	3.6030	3.3129	3.5890
Ca	20	3.6920	3.6880	3.6940	4.0120	4.0130	4.0120	4.0130	4.0320	3.6905	4.0125
Sc	21	4.0900	4.0860	4.0920	4.4600	4.4870	4.4600	4.4870	4.4860	4.0891	4.4735
Ti	22	4.5110	4.5050	4.5130	4.9310	4.9620	4.9310	4.9620	4.9610	4.5088	4.9465
V	23	4.9520	4.9440	4.9540	5.4260	5.4630	5.4260	5.4630	5.4620	4.9497	5.4445

Cr	24	5.4150	5.4050	5.4170	5.9460	5.9870	5.9460	5.9870	5.9860	5.4116	5.9665
Mn	25	5.8990	5.8880	5.9010	6.4890	6.5350	6.4890	6.5350	6.5350	5.8951	6.5120
Fe	26	6.4040	6.3910	6.4060	7.0570	7.1080	7.0570	7.1080	7.1070	6.3995	7.0825
Co	27	6.9300	6.9150	6.9320	7.6480	7.7060	7.6480	7.7060	7.7050	6.9253	7.6770
Ni	28	7.4770	7.4600	7.4790	8.2630	8.3290	8.2630	8.3290	8.3270	7.4724	8.2960
Cu	29	8.0460	8.0260	8.0480	8.9040	8.9030	8.9030	8.9030	8.9760	8.0411	8.9035
Zn	30	8.6370	8.6140	8.6390	9.5700	9.6560	9.5670	9.6560	9.6480	8.6312	9.6130
Ga	31	9.2500	9.2230	9.2520	10.2630	10.3650	10.2590	10.3650	10.3460	9.2428	10.3140
Ge	32	9.8850	9.8540	9.8870	10.9800	11.0990	10.9760	11.0990	11.0730	9.8761	11.0395
As	33	10.5420	10.5060	10.5440	11.7240	11.8620	11.7180	11.8620	11.8190	10.5318	11.7930
Se	34	11.2200	11.1790	11.2220	12.4940	12.6500	12.4870	12.6500	12.5940	11.2087	12.5720
Br	35	11.9220	11.8760	11.9240	13.2890	13.4670	13.2820	13.4670	13.4020	11.9087	13.3780
Kr	36	12.6480	12.5960	12.6500	14.1100	14.3120	14.1020	14.3280	14.2350	12.6320	14.2110
Rb	37	13.3930	13.3330	13.3950	14.9590	15.1830	14.9490	15.2050	15.0820	13.3755	15.0710
Sr	38	14.1630	14.0950	14.1650	15.8330	16.0820	15.8220	16.1040	15.9660	14.1426	15.9575
Y	39	14.9560	14.8800	14.9580	16.7350	17.0130	16.7230	17.0360	16.8770	14.9332	16.8740
Zr	40	15.7720	15.6880	15.7740	17.6650	17.9670	17.6510	17.9940	17.8130	15.7470	17.8160
Nb	41	16.6120	16.5180	16.6140	18.6190	18.9530	18.6030	18.9950	18.9810	16.5837	18.7860
Mo	42	17.4760	17.3710	17.4780	19.6050	19.9620	19.5870	19.9960	19.7730	17.4443	19.7835
Tc	43	18.3640	18.2480	18.3660	20.6150	21.0020	20.5950	21.0500	20.6190	18.3283	20.8085
Ru	44	19.2760	19.1740	19.2780	21.6530	22.0700	21.6310	22.1040	21.8240	19.2363	21.8615
Rh	45	20.2130	20.0700	20.2150	22.7200	23.1690	22.6950	23.2170	22.9130	20.1686	22.9445
Pd	46	21.1740	21.0170	21.1760	23.8150	24.2950	23.7870	24.3460	23.9910	21.1248	24.0550
Ag	47	22.1590	21.9870	22.1610	24.9380	25.4520	24.9070	25.5120	25.1410	22.1054	25.1950
Cd	48	23.1700	22.9800	23.1720	26.0910	26.6390	26.0570	26.7200	26.0960	23.1104	26.3650
In	49	24.2060	23.9980	24.2080	27.2710	27.8560	27.2330	27.9280	27.4940	24.1405	27.5635
Sn	50	25.2670	25.0400	25.2690	28.4810	29.1040	28.4390	29.1750	28.7110	25.1955	28.7925
Sb	51	26.3550	26.1060	26.3570	29.7210	30.3880	29.6740	30.4604	29.9580	26.2763	30.0545
Te	52	27.4680	27.1970	27.4700	30.9900	31.6980	30.9390	31.8302	31.2982	27.3821	31.3440
I	53	28.6070	28.3120	28.6090	32.2890	33.0360	32.2340	33.2004	32.6384	28.5137	32.6625
Xe	54	29.7740	29.4530	29.7760	33.6190	34.4080	33.5560	34.5706	33.9786	29.6720	34.0135
Cs	55	30.9680	30.6200	30.9700	34.9810	35.8150	34.9130	35.9408	35.3188	30.8569	35.3980
Ba	56	32.1880	31.8120	32.1900	36.3720	37.2510	36.2980	37.3110	36.6590	32.0681	36.8115
La	57	33.4360	33.0280	33.4380	37.7950	38.7230	37.7140	38.8240	38.0880	33.3059	38.2590
Ce	58	34.7140	34.2730	34.7160	39.2510	40.2260	39.1630	40.3370	39.5510	34.5728	39.7385
Pr	59	36.0200	35.5440	36.0220	40.7410	41.7670	40.6460	42.1275	41.0960	35.8676	41.2540

Nd	60	37.3550	36.8410	37.3570	42.2640	43.3270	42.1590	43.9179	42.6410	37.1898	42.7955
Pm	61	38.7180	38.1650	38.7200	43.8180	44.9290	43.7050	45.7084	44.1860	38.5402	44.3735
Sm	62	40.1110	39.5160	40.1130	45.4130	46.5840	45.2890	47.4989	45.7310	39.9195	45.9985
Eu	63	41.5350	40.8950	41.5370	47.0360	48.2560	46.9020	49.2893	47.3915	41.3288	47.6460
Gd	64	42.9890	42.3020	42.9910	48.6960	49.9640	48.5540	51.0798	49.0520	42.7671	49.3300
Tb	65	44.4740	43.7370	44.4760	50.3820	51.7090	50.2280	52.8703	50.7730	44.2358	51.0455
Dy	66	45.9990	45.2080	46.0010	52.1190	53.4910	51.9560	54.6607	52.4940	45.7349	52.8050
Ho	67	47.5470	46.6990	47.5490	53.8780	55.3080	53.7070	56.4512	54.2460	47.2644	54.5930
Er	68	49.1280	48.2210	49.1300	55.6810	57.1640	55.4910	58.2417	56.0400	48.8255	56.4225
Tm	69	50.7420	49.7730	50.7440	57.5130	59.0590	57.3030	60.0321	57.9230	50.4186	58.2860
Yb	70	52.3890	51.3540	52.3910	59.3740	60.9910	59.1570	61.8226	59.7820	52.0439	60.1825
Lu	71	54.0700	52.9650	54.0720	61.2860	62.9600	61.0490	63.6131	61.7490	53.7015	62.1230
Hf	72	55.7900	54.6110	55.7920	63.2360	64.9730	62.9790	65.4035	63.7160	55.3973	64.1045
Ta	73	57.5330	56.2770	57.5350	65.2210	67.0110	64.9460	67.1940	65.6830	57.1137	66.1160
W	74	59.3180	57.9820	59.3200	67.2440	69.1000	66.9510	69.2940	67.7150	58.8727	68.1720
Re	75	61.1400	59.7180	61.1420	69.3090	71.2300	68.9940	71.4100	69.7860	60.6662	70.2695
Os	76	63.0010	61.4870	63.0030	71.4160	73.4040	71.0770	73.6150	71.8950	62.4959	72.4100
Ir	77	64.8960	63.2870	64.8980	73.5600	75.6200	73.2030	75.8210	74.0750	64.3593	74.5900
Pt	78	66.8320	65.1230	66.8340	75.7510	77.8830	75.3640	78.0690	76.2700	66.2587	76.8170
Au	79	68.8040	66.9900	68.8060	77.9850	80.1820	77.5800	80.3910	78.5100	68.1990	79.0835
Hg	80	70.8190	68.8940	70.8210	80.2610	82.5320	79.8220	82.7800	80.7500	70.1777	81.3965
Tl	81	72.8720	70.8320	72.8740	82.5750	84.9240	82.3840	85.1900	83.3046	72.1916	83.7495
Pb	82	74.9690	72.8040	74.9710	84.9360	87.3670	84.4500	87.5900	85.8592	74.2477	86.1515
Bi	83	77.1180	74.8150	77.1200	87.3540	89.8660	86.8310	90.1100	88.4138	76.3435	88.6100
Po	84	79.3010	76.8630	79.3030	89.8010	92.4030	89.2500	92.8200	90.9684	78.4807	91.1020
At	85	81.5230	78.9430	81.5250	92.3020	94.9830	91.7220	95.5300	93.5230	80.6633	93.6425
Rn	86	83.7930	81.0650	83.7950	94.8660	97.6170	94.2460	98.2400	96.0776	82.8767	96.2415
Fr	87	86.1140	83.2310	86.1160	97.4770	100.3060	96.8070	100.9500	98.6322	85.1433	98.8915
Ra	88	88.4760	85.4340	88.4780	100.1300	103.0390	99.4320	103.6600	101.1868	87.4567	101.5845
Ac	89	90.8840	87.6750	90.8860	102.6110	105.8370	102.1010	106.3700	103.7414	89.8127	104.2240
Th	90	93.3580	89.9520	93.3600	105.6110	108.6900	104.8310	109.0800	106.2960	92.2177	107.1505
Pa	91	95.8830	92.2870	95.8850	108.4350	111.6060	107.6060	112.0450	109.1530	94.6743	110.0205
U	92	98.4400	94.6590	98.4420	111.3030	114.5610	110.4240	115.0100	112.0100	97.1810	112.9320
NP	93	101.0680	97.0770	101.0700	114.2430	117.5910	113.3120	117.9750	114.8670	99.7377	115.9170
PU	94	103.7610	99.5520	103.7630	117.2610	120.7030	116.2770	120.9400	117.7240	102.3580	118.9820
AM	95	106.5230	102.0830	106.5250	120.3600	123.8910	119.3170	123.9050	120.5810	105.0430	122.1255

CM	96	109.2900	104.4410	109.2920	123.4230	127.0660	122.3250	126.8700	123.4380	107.6737	125.2445
BK	97	112.1380	107.2050	112.1400	126.6630	130.3550	125.4430	129.8350	126.2950	110.4937	128.5090
CR	98	116.0300	110.7100	116.0320	130.8510	134.6810	129.6010	132.8000	129.1520	114.2567	132.7660
ES	99	119.0800	113.4700	119.0820	134.2380	138.1690	132.9160	135.7650	132.0090	117.2100	136.2035
FM	100	122.1900	116.2800	122.1920	137.6930	141.7240	136.3470	138.7300	134.8660	120.2200	139.7085

9 Appendix 2: Files for L shell calculations

For the L-subshell relative intensity calculations the data tables, stored in the following files, are needed:

- ***upxl.input*** - atomic mass and edges for ECPSSR ionisation cross section calculations
- ***LsubshellEmissionRatesScofieldDHF-15Feb11.txt*** – emission rates for the Scofield option (Scofield 1974b).
- ***LsubshellEmissionRatesSalemExpt-15Feb11.txt*** – emission rates for the Salem option (Salem et al;. 1974).
- ***LsubshellwLfijCampbelKrauseat15Feb11.txt*** – fluorescence yield and Coster-Kronig probabilities for the two options (Krause 1979, Campbell 2003, 2009).
- ***krause_kd13.txt*** – the Krause k'$_{1,3}$ Coster-Kronig probability.
- ***LtotalwLbarPuriEJCBambynekat23Feb11.txt*** – L shell total fluorescence yield from Puri et al. (1993), Clayton (1986) and Bambynek et al. (1972).
- ***Lshellenergiesa1-2b1-6g1-6at13Feb11.txt*** - L-shell characteristic X-ray energies.

9.1 L shell atomic mass and edges

The L shell atomic mass and edges for ionisation cross section calculations are stored in file ***upxl.input***:

Table 9: L shell edges.

```
*  ROOTS
0.095012509837637440185D0
0.281603550779258913230D0
0.458016777657227386342D0
0.617876244402643748447D0
0.755404408355003033895D0
0.865631202387831743880D0
0.944575023073232576078D0
0.989400934991649932596D0
*   WEIGHTS
0.189450610455068496285D0
0.182603415044923588867D0
0.169156519395002538189D0
0.149595988816576732081D0
0.124628971255533872052D0
0.095158511682492784810D0
0.062253523938647892863D0
0.027152459411754094852D0
*  SEND=1.0D-2  RNQW=10.0D0  RNQQ=10.0D0
  1.0d-3   20.0d0    20.0d0
* 6.0(0.25)10.0 10.5(0.5)20.0   -1
* 0.1(0.02)0.5 1.0(0.5)6.0   -1
 ENEGRY P 0.1(.02)0.5 0.6(0.1)4 4.2(.2)10  -1
* ENERGY D 0.2(0.05)1 1.2(.2)10 10.5(.5)20    -1
*  ENERGY HE 0.2(0.1)2 2.2(.2)4.2 4.5(0.5)15  -1
*  ENERGY ALL 0.5(0.1)2 2.2(0.2)5 5.5(0.5)15 16(1)50   -1
* ENERGY LI 0.5 0.6(.2)4 4.5(.5)10 11(1)50 52(2)80  -1
* ENERGY SI S 5(1)48 50(2)100 105(5)150 160(20)300    -1
  ADIAB=0 ZERO=NONADIABATIC CORRECT OUT, ONE=IN
  CPSSR=1 ZERO=CPSSR, ONE=ECPSSR, TWO=ECPSSR-COHEN
  PROTON 1.0 1.007825
*  DEUTERIUM 1.0 2.01410
* HELIUM  2.0  4.0026
* LI 3.0 7.01601
```

```
*  BE 4.0  9.01219
*  B  5.0  11.00931
*  C  6.0  12.00
*  N  7.0  14.00307
*  O  8.0  15.99491
*  F  9.0  18.9984
*  NE  10.0  19.99244
*  SI  14.0  27.97693
*  S   16.0  31.97207
* TARGET Z MASS EDGES
* TARGET Z MASS EDGES
```

*	Z	Mass	L1	L2	L3
*AR	18	39.948	0.320	0.247	0.245
TI	22	47.9	0.564	0.462	0.456
CR	24	51.996	0.695	0.584	0.575
MN	25	54.93805	0.769	0.651	0.640
FE	26	55.847	0.846	0.721	0.708
NI	28	58.71	1.012	0.871	0.855
CU	29	63.54	1.100	0.951	0.932
ZN	30	65.37	1.196	1.043	1.021
GE	32	72.59	1.414	1.248	1.217
AS	33	74.9216	1.530	1.359	1.325
SE	34	78.96	1.654	1.476	1.436
BR	35	79.909	1.794	1.596	1.550
KR	36	83.8	1.921	1.727	1.675
RB	37	85.47	2.067	1.866	1.806
SR	38	87.62	2.216	2.007	1.94
Y	39	88.905	2.369	2.145	2.079
ZR	40	91.22	2.547	2.307	2.223
NB	41	92.906	2.698	2.465	2.371
MO	42	95.94	2.866	2.625	2.520
TC	43	99	3.054	2.795	2.677
RU	44	101.07	3.236	2.966	2.837
RH	45	102.905	3.419	3.146	3.003
PD	46	106.4	3.617	3.330	3.173
AG	47	107.87	3.806	3.524	3.351
CD	48	112.4	4.019	3.727	3.537
IN	49	114.82	4.237	3.938	3.730
SN	50	118.69	4.465	4.156	3.929
SB	51	121.75	4.698	4.381	4.132
TE	52	127.6	4.939	4.612	4.341
I	53	126.9044	5.188	4.852	4.557
XE	54	131.3	5.452	5.100	4.781
CS	55	132.905	5.720	5.358	5.011
BA	56	137.34	5.995	5.624	5.247
LA	57	138.91	6.267	5.891	5.483
CE	58	140.12	6.549	6.165	5.724
PR	59	140.907	6.846	6.443	5.968
ND	60	144.24	7.126	6.722	6.208
PM	61	145	7.427	7.012	6.459
SM	62	150.35	7.737	7.312	6.717
EU	63	151.96	8.069	7.624	6.983
GD	64	157.25	8.376	7.931	7.243
TB	65	158.924	8.708	8.252	7.515
DY	66	162.5	9.083	8.621	7.850
HO	67	164.93	9.395	8.919	8.071
ER	68	167.26	9.776	9.263	8.364
TM	69	168.934	10.116	9.618	8.648

```
 YB          70    173.04  10.486   9.978   8.943
 LU          71    174.97  10.867  10.345   9.241
 HF          72    178.49  11.264  10.739   9.561
 TA          73   180.948  11.680  11.139   9.881
 W           74    183.85  12.098  11.542  10.204
 Re          75     186.2  12.522  11.955  10.531
 OS          76     190.2  12.965  12.383  10.869
 IR          77     192.2  13.424  12.824  11.215
 PT          78    195.09  13.892  13.273  11.564
 AU          79   196.967  14.353  13.733  11.918
 HG          80    200.59  14.846  14.209  12.284
 TL          81    204.37  15.344  14.698  12.657
 PB          82    207.19  15.860  15.198  13.035
 BI          83    208.98  16.385  15.708  13.418
 PO          84       210  16.935  16.244  13.817
 AT          85       210  17.493  16.784  14.213
 RN          86       222  18.058  17.337  14.618
 FR          87       223  18.639  17.906  15.031
 RA          88       226  19.233  19.078  15.442
 AC          89       227  19.842  19.078  15.865
 TH          90   232.038  20.470  19.692  16.300
 PA          91  231.0359  21.104  20.313  16.733
 U           92    238.03  21.756  20.947  17.167
 NP          93       237  22.426  21.600  17.610
 PU          94       239  23.095  22.263  18.053
 AM          95       242  23.793  22.944  18.526
 CM          96       245  24.503  23.640  18.990

END -1 1 1 1 1
 END ALL -1 1
 1 2 3  -1
 ION Z MASS 2.0 4.0026
* TARGET Z MASS EDGES
AU 79.0 196.967 14.353 13.733 11.918
 END -1 1 1 1 1
 END ALL -1 1
```

9.2 L shell emission rates

The emission rates for the Scofield (Scofield 1974b) option are stored in file

LsubshellEmissionRatesScofieldDHF-15Feb11.txt

and the emission rates for the Salem option (Salem et al;.1974) are stored in file

LsubshellEmissionRatesSalemExpt-15Feb11.txt.

9.2.1 File LsubshellEmissionRatesScofieldDHF-15Feb11.txt

The three tables that follow are stored site by side in the file. Please note that the element name and Z are included in the second tables only in this appendix and not in the original file.

Table 10: L shell emission rates, L1 Subshell, (Scofield, 1974).

*Scofield L subshell emission rates									
*Scofield Phys Rev A10(1974)1507-1510 with erratum A12(1975)345									
*Lβ3=1.000									
*Elt	Z	Lβ3	Lβ4	Lγ2	Lγ3	Lγ44'	L1P23	Total	Sum
MN	25	1.000	0.5321	0	0	0	0	1.6000	1.5321
FE	26	1.000	0.5340	0	0	0	0	1.5817	1.5340
CO	27	1.000	0.5370	0	0	0	0	1.5802	1.5370
NI	28	1.000	0.5400	0	0	0	0	1.5787	1.5400
CU	29	1.000	0.5428	0	0	0	0	1.5889	1.5428
ZN	30	1.000	0.5455	0	0	0	0	1.5991	1.5455
GA	31	1.000	0.5483	0.00139	0.00295	0	0	1.6093	1.5526
GE	32	1.000	0.5510	0.0135	0.0246	0	0	1.6195	1.5891
AS	33	1.000	0.5538	0.0256	0.0463	0	0	1.6558	1.6256
SE	34	1.000	0.5565	0.0377	0.0679	0	0	1.6922	1.6621
BR	35	1.000	0.5593	0.0498	0.0896	0	0	1.7285	1.6986
KR	36	1.000	0.5620	0.0619	0.1112	0	0	1.7648	1.7351
RB	37	1.000	0.5653	0.0686	0.1226	0	0	1.7860	1.7564
SR	38	1.000	0.5685	0.0752	0.1340	0	0	1.8073	1.7777
Y	39	1.000	0.5718	0.0819	0.1454	0	0	1.8285	1.7990
ZR	40	1.000	0.5750	0.0885	0.1568	0	0	1.8497	1.8203
NB	41	1.000	0.5788	0.0919	0.1618	0	0	1.8624	1.8324
MO	42	1.000	0.5825	0.0953	0.1667	0	0	1.8750	1.8445
TC	43	1.000	0.5863	0.0987	0.1717	0	0	1.8877	1.8566
RU	44	1.000	0.5900	0.1021	0.1766	0	0	1.9003	1.8687
RH	45	1.000	0.5945	0.1056	0.1814	0	0	1.9141	1.8814
PD	46	1.000	0.5990	0.1090	0.1862	0	0	1.9279	1.8942
AG	47	1.000	0.6035	0.1125	0.1909	0	0	1.9416	1.9069
CD	48	1.000	0.6080	0.1159	0.1957	0	0	1.9554	1.9196
IN	49	1.000	0.6100	0.1203	0.2020	0	0	1.9750	1.9322
SN	50	1.000	0.6120	0.1246	0.2082	0.0104	0	1.9945	1.9552
SB	51	1.000	0.6170	0.1285	0.2134	0.0201	0	2.0197	1.9790
TE	52	1.000	0.6220	0.1324	0.2187	0.0298	0	2.0448	2.0028
I	53	1.000	0.6270	0.1362	0.2239	0.0394	0	2.0700	2.0265
XE	54	1.000	0.6320	0.1401	0.2291	0.0491	0	2.0951	2.0503
CS	55	1.000	0.6375	0.1443	0.2344	0.0569	0	2.1207	2.0731
BA	56	1.000	0.6430	0.1485	0.2396	0.0647	0	2.1463	2.0958
LA	57	1.000	0.6493	0.1511	0.2416	0.0643	0	2.1585	2.1062
CE	58	1.000	0.6555	0.1536	0.2436	0.0638	0	2.1707	2.1165
PR	59	1.000	0.6618	0.1562	0.2456	0.0634	0	2.1828	2.1269
ND	60	1.000	0.6680	0.1587	0.2476	0.0629	0	2.1950	2.1372
PM	61	1.000	0.6750	0.1612	0.2491	0.0624	0	2.2090	2.1476
SM	62	1.000	0.6820	0.1636	0.2505	0.0619	0	2.2229	2.1580
EU	63	1.000	0.6897	0.1661	0.2517	0.0614	0	2.2373	2.1689
GD	64	1.000	0.6973	0.1685	0.2529	0.0610	0	2.2516	2.1797
TB	65	1.000	0.7050	0.1710	0.2541	0.0605	0	2.2660	2.1906
DY	66	1.000	0.7140	0.1737	0.2551	0.0602	0	2.2821	2.2029
HO	67	1.000	0.7230	0.1763	0.2561	0.0598	0	2.2982	2.2152
ER	68	1.000	0.7320	0.1790	0.2571	0.0595	0	2.3143	2.2276

TM	69	1.000	0.7410	0.1816	0.2581	0.0591	0	2.3304	2.2399
YB	70	1.000	0.7500	0.1843	0.2591	0.0588	0	2.3465	2.2522
LU	71	1.000	0.7610	0.1881	0.2614	0.0623	0	2.3728	2.2728
HF	72	1.000	0.7720	0.1920	0.2636	0.0659	0	2.3991	2.2935
TA	73	1.000	0.7830	0.1958	0.2659	0.0694	0	2.4254	2.3141
W	74	1.000	0.7955	0.2004	0.2686	0.0725	0	2.4543	2.3369
RE	75	1.000	0.8080	0.2049	0.2712	0.0756	0	2.4831	2.3597
OS	76	1.000	0.8205	0.2095	0.2739	0.0787	0	2.5120	2.3825
IN	77	1.000	0.8330	0.2140	0.2765	0.0818	0	2.5408	2.4053
PT	78	1.000	0.8486	0.2192	0.2794	0.0863	0	2.5791	2.4335
AU	79	1.000	0.8642	0.2244	0.2823	0.0909	0	2.6175	2.4618
HG	80	1.000	0.8798	0.2296	0.2852	0.0954	0	2.6558	2.4900
TL	81	1.000	0.8954	0.2348	0.2881	0.1000	0	2.6942	2.5183
PB	82	1.000	0.9110	0.2400	0.2910	0.1045	0.00368	2.7325	2.5502
BI	83	1.000	0.9305	0.2464	0.2938	0.1093	0.00732	2.7818	2.5873
PO	84	1.000	0.9500	0.2529	0.2965	0.1141	0.01097	2.8311	2.6244
AT	85	1.000	0.9695	0.2593	0.2993	0.1188	0.01462	2.8803	2.6615
HN	86	1.000	0.9890	0.2657	0.3020	0.1236	0.01826	2.9296	2.6986
FR	87	1.000	1.0148	0.2741	0.3050	0.1288	0.02000	2.9919	2.7427
BA	88	1.000	1.0407	0.2825	0.3080	0.1339	0.02174	3.0542	2.7868
AC	89	1.000	1.0665	0.2909	0.3110	0.1391	0.02348	3.1166	2.8309
TH	90	1.000	1.0923	0.2992	0.3140	0.1442	0.02522	3.1789	2.8750
PA	91	1.000	1.1182	0.3076	0.3170	0.1494	0.02696	3.2412	2.9191
U	92	1.000	1.1440	0.3160	0.3200	0.1545	0.02870	3.3035	2.9632
NP	93	1.000	1.1765	0.3260	0.3235	0.1598	0.02960	3.3824	3.0154
PU	94	1.000	1.2090	0.3360	0.3270	0.1650	0.03050	3.4612	3.0675
AM	95	1.000	1.2415	0.3460	0.3305	0.1703	0.03140	3.5401	3.1197
CM	96	1.000	1.2740	0.3560	0.3340	0.1755	0.03230	3.6189	3.1718

Table 11: L shell emission rates, L2 SubShell, (Scofield, 1974).

		Scofield L subshell emission rates						
		Scofield Phys Rev A10(1974)1507-1510 with erratum A12(1975)345						
		Lβ1=1.000		**Added Lγ6+Lγ8**				
***Elt**	**Z**	**Lβ1**	**Lη**	**Lγ1**	**Lγ5**	**Lγ6**	**Total**	**Sum**
MN	25	1.000	0.10390	0	0.00933	0	1.1129	1.1132
FE	26	1.000	0.09050	0	0.00791	0	1.0985	1.0984
CO	27	1.000	0.07710	0	0.00649	0	1.0841	1.0836
NI	28	1.000	0.06370	0	0.00507	0	1.0697	1.0688
CU	29	1.000	0.05833	0	0.00484	0	1.0639	1.0632
ZN	30	1.000	0.05295	0	0.00461	0	1.0581	1.0576
GA	31	1.000	0.04758	0	0.00438	0	1.0523	1.0520
GE	32	1.000	0.04220	0	0.00415	0	1.0465	1.0464
AS	33	1.000	0.04063	0	0.00428	0	1.0451	1.0449
SE	34	1.000	0.03905	0	0.00441	0	1.0437	1.0435
BR	35	1.000	0.03748	0	0.00454	0	1.0422	1.0420
KR	36	1.000	0.03590	0	0.00467	0	1.0408	1.0406
RB	37	1.000	0.03503	0	0.00481	0	1.0444	1.0398

SR	38	1.000	0.03415	0	0.00495	0	1.0479	1.0391
Y	39	1.000	0.03327	0.00336	0.00510	0	1.0515	1.0417
ZR	40	1.000	0.03240	0.01585	0.00524	0.000722	1.0550	1.0542
NB	41	1.000	0.03190	0.02834	0.00532	0.000611	1.0669	1.0662
MO	42	1.000	0.03140	0.04083	0.00541	0.000501	1.0789	1.0781
TC	43	1.000	0.03090	0.05331	0.00549	0.000390	1.0908	1.0901
RU	44	1.000	0.03040	0.06580	0.00558	0.000279	1.1027	1.1021
RH	45	1.000	0.03019	0.07845	0.00563	0.000356	1.1151	1.1146
PD	46	1.000	0.02998	0.09110	0.00569	0.000433	1.1275	1.1272
AG	47	1.000	0.02978	0.10375	0.00575	0.000510	1.1399	1.1398
CD	48	1.000	0.02957	0.11640	0.00580	0.000587	1.1523	1.1524
IN	49	1.000	0.02935	0.12520	0.00589	0.000671	1.1615	1.1611
SN	50	1.000	0.02912	0.13400	0.00598	0.000754	1.1706	1.1699
SB	51	1.000	0.02894	0.14103	0.00607	0.000818	1.1776	1.1769
TE	52	1.000	0.02876	0.14805	0.00616	0.000883	1.1846	1.1839
I	53	1.000	0.02859	0.15507	0.00625	0.000947	1.1915	1.1909
XE	54	1.000	0.02841	0.16210	0.00634	0.001010	1.1985	1.1979
CS	55	1.000	0.02828	0.16810	0.00641	0.001090	1.2038	1.2039
BA	56	1.000	0.02814	0.17410	0.00648	0.001170	1.2090	1.2099
LA	57	1.000	0.02803	0.17573	0.00650	0.001160	1.2112	1.2114
CE	58	1.000	0.02792	0.17735	0.00652	0.001160	1.2134	1.2130
PR	59	1.000	0.02782	0.17898	0.00653	0.001150	1.2156	1.2145
ND	60	1.000	0.02771	0.18060	0.00655	0.001140	1.2178	1.2160
PM	61	1.000	0.02763	0.18175	0.00656	0.001130	1.2179	1.2171
SM	62	1.000	0.02755	0.18290	0.00657	0.001120	1.2180	1.2181
EU	63	1.000	0.02749	0.18373	0.00658	0.001110	1.2192	1.2189
GD	64	1.000	0.02744	0.18457	0.00659	0.001100	1.2203	1.2197
TB	65	1.000	0.02738	0.18540	0.00660	0.001090	1.2215	1.2205
DY	66	1.000	0.02735	0.18612	0.00661	0.001080	1.2223	1.2212
HO	67	1.000	0.02733	0.18684	0.00662	0.001080	1.2231	1.2219
ER	68	1.000	0.02730	0.18756	0.00664	0.001070	1.2238	1.2226
TM	69	1.000	0.02728	0.18828	0.00665	0.001060	1.2246	1.2233
YB	70	1.000	0.02725	0.18900	0.00666	0.001050	1.2254	1.2240
LU	71	1.000	0.02725	0.19120	0.00670	0.001090	1.2291	1.2262
HF	72	1.000	0.02726	0.19340	0.00673	0.002480	1.2328	1.2299
TA	73	1.000	0.02726	0.19560	0.00677	0.005560	1.2365	1.2352
W	74	1.000	0.02729	0.19800	0.00682	0.008640	1.2423	1.2408
RE	75	1.000	0.02733	0.20040	0.00687	0.011710	1.2481	1.2463
OS	76	1.000	0.02736	0.20280	0.00692	0.014790	1.2539	1.2519
IN	77	1.000	0.02739	0.20520	0.00697	0.017880	1.2597	1.2574
PT	78	1.000	0.02744	0.20710	0.00702	0.020410	1.2643	1.2620
AU	79	1.000	0.02749	0.20900	0.00707	0.022950	1.2689	1.2665
HG	80	1.000	0.02754	0.21090	0.00713	0.025480	1.2736	1.2711
TL	81	1.000	0.02759	0.21280	0.00718	0.028020	1.2782	1.2756
PB	82	1.000	0.02764	0.21470	0.00723	0.030550	1.2828	1.2801
BI	83	1.000	0.02772	0.21693	0.00729	0.032720	1.2875	1.2847
PO	84	1.000	0.02780	0.21915	0.00735	0.034900	1.2921	1.2892
AT	85	1.000	0.02787	0.22137	0.00741	0.037070	1.2968	1.2937
HN	86	1.000	0.02795	0.22360	0.00747	0.039240	1.3014	1.2983
FR	87	1.000	0.02806	0.22578	0.00754	0.040950	1.3057	1.3023

BA	88	1.000	0.02816	0.22797	0.00760	0.042650	1.3100	1.3064
AC	89	1.000	0.02827	0.23015	0.00766	0.044360	1.3143	1.3104
TH	90	1.000	0.02838	0.23233	0.00773	0.046080	1.3186	1.3145
PA	91	1.000	0.02848	0.23452	0.00780	0.047780	1.3229	1.3186
U	92	1.000	0.02859	0.23670	0.00786	0.049490	1.3272	1.3226
NP	93	1.000	0.02872	0.23880	0.00793	0.050630	1.3305	1.3261
PU	94	1.000	0.02885	0.24090	0.00800	0.051770	1.3338	1.3295
AM	95	1.000	0.02898	0.24300	0.00807	0.052910	1.3371	1.3330
CM	96	1.000	0.02911	0.24510	0.00814	0.054050	1.3404	1.3364

Table 12: L shell emission rates, L3 SubShell, (Scofield, 1974).

		Scofield L subshell emission rates							
		Scofield Phys Rev A10(1974)1507-1510 with erratum A12(1975)345							
		Lα(1+2)=1.000		Added Lβ5+Lβ7					
*Elt	Z	Lα1	Lα2	Ll	Lβ2,15	Lβ5	Lβ6	Total	Sum
MN	25	0.89738	0.10262	0.10804	0	0	0.00965	1.1187	1.1177
FE	26	0.89734	0.10266	0.09452	0	0	0.00821	1.1027	1.1027
CO	27	0.89730	0.10270	0.08099	0	0	0.00677	1.0868	1.0878
NI	28	0.89726	0.10274	0.06747	0	0	0.00534	1.0709	1.0728
CU	29	0.89734	0.10266	0.06213	0	0	0.00512	1.0658	1.0673
ZN	30	0.89742	0.10258	0.05679	0	0	0.00491	1.0606	1.0617
GA	31	0.89750	0.10250	0.05144	0	0	0.00468	1.0555	1.0561
GE	32	0.89759	0.10241	0.04610	0	0	0.00447	1.0504	1.0506
AS	33	0.89767	0.10233	0.04469	0	0	0.00466	1.0493	1.0493
SE	34	0.89775	0.10225	0.04327	0	0	0.00486	1.0482	1.0481
BR	35	0.89783	0.10217	0.04185	0	0	0.00505	1.0471	1.0469
KR	36	0.89791	0.10209	0.04043	0	0	0.00523	1.0460	1.0457
RB	37	0.89795	0.10205	0.03978	0	0	0.00544	1.0494	1.0452
SR	38	0.89799	0.10201	0.03913	0	0	0.00566	1.0528	1.0448
Y	39	0.89803	0.10197	0.03849	0.00351	0	0.00586	1.0563	1.0479
ZR	40	0.89807	0.10193	0.03784	0.01585	0.000834	0.00607	1.0597	1.0606
NB	41	0.89809	0.10191	0.03759	0.02819	0.000709	0.00623	1.0719	1.0727
MO	42	0.89811	0.10189	0.03735	0.04052	0.000584	0.00639	1.0841	1.0848
TC	43	0.89813	0.10187	0.03711	0.05286	0.000458	0.00654	1.0963	1.0970
RU	44	0.89815	0.10185	0.03687	0.06521	0.000333	0.00670	1.1085	1.1091
RH	45	0.89815	0.10185	0.03698	0.07760	0.000432	0.00683	1.1215	1.1218
PD	46	0.89815	0.10185	0.03708	0.08999	0.000531	0.00697	1.1345	1.1346
AG	47	0.89815	0.10185	0.03718	0.10239	0.000630	0.00710	1.1476	1.1473
CD	48	0.89815	0.10185	0.03728	0.11478	0.000729	0.00724	1.1606	1.1600

IN	49	0.89823	0.10177	0.03668	0.12337	0.000839	0.00742	1.1695	1.1683
SN	50	0.89831	0.10169	0.03609	0.13196	0.000952	0.00761	1.1785	1.1766
SB	51	0.89831	0.10169	0.03660	0.13877	0.00104	0.00781	1.1857	1.1842
TE	52	0.89831	0.10169	0.03712	0.14557	0.00114	0.00799	1.1930	1.1918
I	53	0.89831	0.10169	0.03764	0.15238	0.00124	0.00819	1.2002	1.1995
XE	54	0.89831	0.10169	0.03815	0.15918	0.00133	0.00839	1.2074	1.2071
CS	55	0.89827	0.10173	0.03840	0.16497	0.00146	0.00857	1.2134	1.2134
BA	56	0.89823	0.10177	0.03864	0.17075	0.00158	0.00876	1.2193	1.2197
LA	57	0.89823	0.10177	0.03895	0.17206	0.00158	0.00888	1.2211	1.2215
CE	58	0.89823	0.10177	0.03926	0.17336	0.00159	0.00900	1.2229	1.2232
PR	59	0.89823	0.10177	0.03957	0.17466	0.00160	0.00913	1.2246	1.2250
ND	60	0.89823	0.10177	0.03987	0.17596	0.00160	0.00925	1.2264	1.2267
PM	61	0.89823	0.10177	0.04024	0.17677	0.00161	0.00938	1.2284	1.2280
SM	62	0.89823	0.10177	0.04062	0.17758	0.00161	0.00949	1.2305	1.2293
EU	63	0.89821	0.10179	0.04104	0.17809	0.00161	0.00962	1.2317	1.2304
GD	64	0.89817	0.10183	0.04147	0.17858	0.00162	0.00974	1.2329	1.2314
TB	65	0.89815	0.10185	0.04189	0.17909	0.00163	0.00986	1.2341	1.2325
DY	66	0.89813	0.10187	0.04240	0.17943	0.00163	0.01000	1.2351	1.2335
HO	67	0.89812	0.10188	0.04291	0.17977	0.00163	0.01013	1.2362	1.2344
ER	68	0.89810	0.10190	0.04342	0.18011	0.00164	0.01027	1.2372	1.2354
TM	69	0.89809	0.10191	0.04393	0.18044	0.00165	0.01041	1.2383	1.2364
YB	70	0.89807	0.10193	0.04445	0.18078	0.00166	0.01054	1.2393	1.2374
LU	71	0.89804	0.10196	0.04505	0.18264	0.00174	0.01073	1.2434	1.2402
HF	72	0.89801	0.10199	0.04565	0.18448	0.00315	0.01093	1.2475	1.2442
TA	73	0.89799	0.10201	0.04626	0.18633	0.00594	0.01112	1.2515	1.2496
W	74	0.89796	0.10204	0.04694	0.18832	0.00874	0.01134	1.2572	1.2553
RE	75	0.89795	0.10205	0.04762	0.19032	0.01154	0.01157	1.2628	1.2610
OS	76	0.89792	0.10208	0.04829	0.19232	0.01434	0.01179	1.2685	1.2667
IN	77	0.89791	0.10209	0.04897	0.19431	0.01713	0.01201	1.2741	1.2724
PT	78	0.89789	0.10211	0.04973	0.19583	0.01954	0.01226	1.2792	1.2774
AU	79	0.89788	0.10212	0.05050	0.19735	0.02194	0.01249	1.2843	1.2823
HG	80	0.89786	0.10214	0.05125	0.19888	0.02433	0.01273	1.2894	1.2872
TL	81	0.89784	0.10216	0.05201	0.20040	0.02674	0.01296	1.2944	1.2921

PB	82	0.89783	0.10217	0.05277	0.20192	0.02913	0.01321	1.2995	1.2970
BI	83	0.89780	0.10220	0.05364	0.20365	0.03120	0.01348	1.3046	1.3020
PO	84	0.89779	0.10221	0.05450	0.20537	0.03327	0.01375	1.3098	1.3069
AT	85	0.89776	0.10224	0.05537	0.20709	0.03533	0.01401	1.3149	1.3118
HN	86	0.89775	0.10225	0.05624	0.20882	0.03740	0.01428	1.3200	1.3167
FR	87	0.89773	0.10227	0.05721	0.21041	0.03893	0.01457	1.3247	1.3211
BA	88	0.89772	0.10228	0.05817	0.21202	0.04048	0.01486	1.3294	1.3255
AC	89	0.89771	0.10229	0.05914	0.21361	0.04201	0.01515	1.3341	1.3299
TH	90	0.89769	0.10231	0.06011	0.21520	0.04356	0.01544	1.3388	1.3343
PA	91	0.89768	0.10232	0.06107	0.21681	0.04510	0.01573	1.3435	1.3387
U	92	0.89767	0.10233	0.06204	0.21840	0.04663	0.01601	1.3482	1.3431
NP	93	0.89763	0.10237	0.06309	0.21987	0.04761	0.01633	1.3520	1.3469
PU	94	0.89759	0.10241	0.06414	0.22134	0.04859	0.01663	1.3558	1.3507
AM	95	0.89755	0.10245	0.06519	0.22282	0.04956	0.01695	1.3596	1.3545
CM	96	0.89750	0.10250	0.06624	0.22429	0.05054	0.01725	1.3634	1.3583

9.2.2 File LsubshellEmissionRatesSalemExpt-15Feb11.txt

The following two tables are stored side by side in the file. Please note that the element name and Z are included in the second tables only in this appendix and not in the original file.

Table 13: L shell emission rates, L1 and L2 SubShells, (Salem 1974).

***Salem et al Expt L1 subshell emission rates 1979**									**Salem et al Expt L2 subshell emission rates 1979**					
***Lβ3=1.00**									**Lβ1=1.000**					
***Elt**	**Z**	**Lβ3**	**Lβ4**	**Lγ2**	**Lγ3**	**Lγ44'**	**Lβ910**	**Sum**	**Lβ1**	**Lη**	**Lγ1**	**Lγ5**	**Lγ6**	**Sum**
MN	25	1.000	0.5310	0	0.1575	0	0.00075	1.6893	1.000	0.08800	0	0.003	0	1.0910
FE	26	1.000	0.5340	0	0.1600	0	0.00150	1.6955	1.000	0.08400	0	0.003	0	1.0870
CO	27	1.000	0.5370	0	0.1625	0	0.00225	1.7018	1.000	0.08000	0	0.003	0	1.0830
NI	28	1.000	0.5400	0	0.1650	0	0.00300	1.7080	1.000	0.07600	0	0.003	0	1.0790
CU	29	1.000	0.5430	0	0.1675	0	0.00375	1.7143	1.000	0.07200	0	0.003	0	1.0750
ZN	30	1.000	0.5460	0	0.1700	0	0.00450	1.7205	1.000	0.06800	0	0.003	0	1.0710
GA	31	1.000	0.5485	0.0050	0.1715	0	0.00525	1.7303	1.000	0.06540	0	0.003	0	1.0684

GE	32	1.000	0.5510	0.0100	0.1730	0	0.00600	1.7400	1.000	0.06280	0	0.003	0	1.0658
AS	33	1.000	0.5535	0.0190	0.1765	0	0.00650	1.7555	1.000	0.06040	0	0.003	0	1.0634
SE	34	1.000	0.5560	0.0280	0.1800	0	0.00700	1.7710	1.000	0.05800	0	0.003	0	1.0610
BR	35	1.000	0.5590	0.0405	0.1810	0	0.00750	1.7880	1.000	0.05575	0	0.003	0	1.0588
KR	36	1.000	0.5620	0.0530	0.1820	0	0.00800	1.8050	1.000	0.05350	0	0.003	0	1.0565
RB	37	1.000	0.5650	0.0625	0.1850	0	0.00900	1.8215	1.000	0.05140	0	0.004	0	1.0554
SR	38	1.000	0.5680	0.0720	0.1880	0	0.01000	1.8380	1.000	0.04930	0	0.005	0	1.0543
Y	39	1.000	0.5710	0.0775	0.1890	0	0.01050	1.8480	1.000	0.04765	0.01650	0.005	0	1.0692
ZR	40	1.000	0.5740	0.0830	0.1900	0	0.01100	1.8580	1.000	0.04600	0.03300	0.005	0	1.0840
NB	41	1.000	0.6400	0.0870	0.1930	0	0.01150	1.9315	1.000	0.04450	0.04400	0.005	0	1.0935
MO	42	1.000	0.7060	0.0910	0.1960	0	0.01200	2.0050	1.000	0.04300	0.05500	0.005	0	1.1030
TC	43	1.000	0.6920	0.0965	0.1990	0	0.01300	2.0005	1.000	0.04150	0.06415	0.005	0	1.1107
RU	44	1.000	0.6780	0.1020	0.2020	0	0.01400	1.9960	1.000	0.04000	0.07330	0.005	0	1.1183
RH	45	1.000	0.6665	0.1055	0.2040	0	0.01500	1.9910	1.000	0.03875	0.09000	0.005	0	1.1338
PD	46	1.000	0.6550	0.1090	0.2060	0	0.01600	1.9860	1.000	0.03750	0.10670	0.005	0	1.1492
AG	47	1.000	0.6450	0.1125	0.2095	0	0.01675	1.9838	1.000	0.03650	0.10635	0.005	0	1.1479
CD	48	1.000	0.6350	0.1160	0.2130	0	0.01750	1.9815	1.000	0.03550	0.10600	0.005	0	1.1465
IN	49	1.000	0.6280	0.1205	0.2165	0.0035	0.01825	1.9868	1.000	0.03450	0.11200	0.0055	0	1.1520
SN	50	1.000	0.6210	0.1250	0.2200	0.0070	0.01900	1.9920	1.000	0.03350	0.11800	0.0060	0	1.1575
SB	51	1.000	0.6140	0.1290	0.2230	0.0140	0.02000	2.0000	1.000	0.03275	0.12250	0.0060	0	1.1613
TE	52	1.000	0.6070	0.1330	0.2260	0.0210	0.02100	2.0080	1.000	0.03200	0.12700	0.0060	0	1.1650
I	53	1.000	0.6025	0.1365	0.2295	0.0305	0.02250	2.0215	1.000	0.03100	0.13350	0.0060	0	1.1705
XE	54	1.000	0.5980	0.1400	0.2330	0.0400	0.02400	2.0350	1.000	0.03000	0.14000	0.0060	0	1.1760
CS	55	1.000	0.5965	0.1445	0.2365	0.0475	0.02500	2.0500	1.000	0.02925	0.14250	0.0060	0	1.1778
BA	56	1.000	0.5950	0.1490	0.2400	0.0550	0.02600	2.0650	1.000	0.02850	0.14500	0.0060	0	1.1795
LA	57	1.000	0.5935	0.1515	0.2430	0.0555	0.02725	2.0708	1.000	0.02775	0.14900	0.0060	0	1.1828
CE	58	1.000	0.5920	0.1540	0.2460	0.0560	0.02850	2.0765	1.000	0.02700	0.15300	0.0060	0	1.1860
PR	59	1.000	0.5930	0.1565	0.2500	0.0560	0.02975	2.0853	1.000	0.02650	0.15650	0.0060	0	1.1890
ND	60	1.000	0.5940	0.1590	0.2540	0.0560	0.03100	2.0940	1.000	0.02600	0.16000	0.0060	0	1.1920
PM	61	1.000	0.5970	0.1615	0.2585	0.0560	0.03250	2.1055	1.000	0.02525	0.16250	0.0060	0	1.1938
SM	62	1.000	0.6000	0.1640	0.2630	0.0560	0.03400	2.1170	1.000	0.02450	0.16500	0.0060	0	1.1955
EU	63	1.000	0.6040	0.1780	0.2665	0.0580	0.03550	2.1420	1.000	0.02400	0.16750	0.0060	0	1.1975
GD	64	1.000	0.6080	0.1920	0.2700	0.0600	0.03700	2.1670	1.000	0.02350	0.17000	0.0060	0	1.1995
TB	65	1.000	0.6130	0.1935	0.2750	0.0578	0.03900	2.1783	1.000	0.02300	0.17200	0.0060	0	1.2010
DY	66	1.000	0.6180	0.1950	0.2800	0.0556	0.04100	2.1896	1.000	0.02250	0.17400	0.0060	0	1.2025
HO	67	1.000	0.6265	0.1965	0.2850	0.0553	0.04300	2.2063	1.000	0.02205	0.17600	0.0060	0	1.2041

ER	68	1.000	0.6350	0.1980	0.2900	0.0550	0.04500	2.2230	1.000	0.02160	0.17800	0.0060	0	1.2056
TM	69	1.000	0.6450	0.2025	0.2940	0.0550	0.04700	2.2435	1.000	0.02130	0.17985	0.0060	0	1.2072
YB	70	1.000	0.6550	0.2070	0.2980	0.0550	0.04900	2.2640	1.000	0.02100	0.18170	0.0060	0	1.2087
LU	71	1.000	0.6665	0.2095	0.3025	0.0585	0.05100	2.2880	1.000	0.02090	0.18300	0.0060	0.00100	1.2109
HF	72	1.000	0.6780	0.2120	0.3070	0.0620	0.05300	2.3120	1.000	0.02080	0.18430	0.0060	0.00200	1.2131
TA	73	1.000	0.6915	0.2150	0.3125	0.0655	0.05550	2.3400	1.000	0.02090	0.18615	0.0065	0.00460	1.2182
W	74	1.000	0.7050	0.2180	0.3180	0.0690	0.05800	2.3680	1.000	0.02100	0.18800	0.0070	0.00720	1.2232
RE	75	1.000	0.7185	0.2240	0.3230	0.0730	0.06050	2.3990	1.000	0.02110	0.19070	0.0070	0.01185	1.2307
OS	76	1.000	0.7320	0.2300	0.3280	0.0770	0.06300	2.4300	1.000	0.02120	0.19340	0.0070	0.01650	1.2381
IN	77	1.000	0.7485	0.2375	0.3330	0.0800	0.06600	2.4650	1.000	0.02150	0.19535	0.0070	0.02025	1.2441
PT	78	1.000	0.7650	0.2450	0.3380	0.0830	0.06900	2.5000	1.000	0.02180	0.19730	0.0070	0.02400	1.2501
AU	79	1.000	0.7840	0.2540	0.3440	0.0870	0.07250	2.5415	1.000	0.02215	0.20040	0.0070	0.02750	1.2571
HG	80	1.000	0.8030	0.2630	0.3500	0.0910	0.07600	2.5830	1.000	0.02250	0.20350	0.0070	0.03100	1.2640
TL	81	1.000	0.8225	0.2745	0.3550	0.0955	0.07950	2.6270	1.000	0.02275	0.20640	0.0070	0.03375	1.2699
PB	82	1.000	0.8420	0.2860	0.3600	0.1000	0.08300	2.6710	1.000	0.02300	0.20930	0.0070	0.03650	1.2758
BI	83	1.000	0.8635	0.2995	0.3660	0.1050	0.08700	2.7210	1.000	0.02350	0.21235	0.0070	0.03900	1.2819
PO	84	1.000	0.8850	0.3130	0.3720	0.1100	0.09100	2.7710	1.000	0.02400	0.21540	0.0070	0.04150	1.2879
AT	85	1.000	0.9095	0.3275	0.3770	0.1150	0.09500	2.8240	1.000	0.02430	0.21870	0.0070	0.04350	1.2935
HN	86	1.000	0.9340	0.3420	0.3820	0.1200	0.09900	2.8770	1.000	0.02460	0.22200	0.0070	0.04550	1.2991
FR	87	1.000	0.9615	0.3585	0.3890	0.1255	0.10400	2.9385	1.000	0.02480	0.22535	0.0070	0.04710	1.3043
BA	88	1.000	0.9890	0.3750	0.3960	0.1310	0.10900	3.0000	1.000	0.02500	0.22870	0.0070	0.04870	1.3094
AC	89	1.000	1.0170	0.3935	0.4030	0.1365	0.11450	3.0645	1.000	0.02550	0.23150	0.0075	0.04945	1.3140
TH	90	1.000	1.0450	0.4120	0.4100	0.1420	0.12000	3.1290	1.000	0.02600	0.23430	0.0080	0.05020	1.3185
PA	91	1.000	1.0735	0.4310	0.4180	0.1470	0.12600	3.1955	1.000	0.02625	0.23765	0.0080	0.05070	1.3226
U	92	1.000	1.1020	0.4500	0.4260	0.1520	0.13200	3.2620	1.000	0.02650	0.24100	0.0080	0.05120	1.3267
NP	93	1.000	1.1320	0.4725	0.4330	0.1570	0.13950	3.3340	1.000	0.02675	0.24250	0.0080	0.05140	1.3287
PU	94	1.000	1.1620	0.4950	0.4400	0.1620	0.14700	3.4060	1.000	0.02700	0.24400	0.0080	0.05160	1.3306
AM	95	1.000	1.1960	0.5260	0.4485	0.1680	0.15600	3.4945	1.000	0.02725	0.24735	0.0080	0.05180	1.3344
CM	96	1.000	1.2300	0.5570	0.4570	0.1740	0.16500	3.5830	1.000	0.02750	0.25070	0.0080	0.05200	1.3382

Table 14: L shell emission rates, L3 SubShell, (Salem 1974).

		Salem et al Expt L3 subshell emission rates 1979						
		Lα(1+2)=1.000						
*Elt	Z	Lα1	Lα2	Ll	Lβ215	Lβ5	Lβ6	Sum
MN	25	0.9001	0.0999	0.10225	0	0	0.00360	1.1059
FE	26	0.9001	0.0999	0.09500	0	0	0.00360	1.0986
CO	27	0.9001	0.0999	0.08775	0	0	0.00360	1.0914
NI	28	0.9001	0.0999	0.08050	0	0	0.00360	1.0841
CU	29	0.9001	0.0999	0.07325	0	0	0.00360	1.0769
ZN	30	0.9001	0.0999	0.06600	0	0	0.00360	1.0696
GA	31	0.9001	0.0999	0.06200	0	0	0.00360	1.0656
GE	32	0.9001	0.0999	0.05800	0	0	0.00360	1.0616
AS	33	0.9001	0.0999	0.05490	0	0	0.00360	1.0585
SE	34	0.9001	0.0999	0.05180	0	0	0.00360	1.0554
BR	35	0.9001	0.0999	0.04965	0	0	0.00360	1.0533
KR	36	0.9001	0.0999	0.04750	0	0	0.00360	1.0511
RB	37	0.9001	0.0999	0.04590	0	0	0.00360	1.0495
SR	38	0.9001	0.0999	0.04430	0	0	0.00360	1.0479
Y	39	0.9001	0.0999	0.04315	0.00315	0	0.00495	1.0513
ZR	40	0.9001	0.0999	0.04200	0.00630	0	0.00630	1.0546
NB	41	0.9001	0.0999	0.04100	0.02642	0	0.00630	1.0737
MO	42	0.9001	0.0999	0.04000	0.04653	0	0.00630	1.0928
TC	43	0.9000	0.1000	0.03925	0.06511	0	0.00630	1.1107
RU	44	0.8999	0.1001	0.03850	0.08369	0	0.00630	1.1285
RH	45	0.8999	0.1001	0.03775	0.09494	0	0.00630	1.1390
PD	46	0.8999	0.1001	0.03700	0.1062	0	0.00630	1.1495
AG	47	0.8999	0.1001	0.03680	0.1176	0	0.00630	1.1607
CD	48	0.8999	0.1001	0.03660	0.1290	0	0.00630	1.1719
IN	49	0.8999	0.1001	0.03630	0.1365	0	0.00675	1.1795
SN	50	0.8999	0.1002	0.03600	0.1440	0	0.00720	1.1872
SB	51	0.8999	0.1002	0.03600	0.1530	0	0.00720	1.1962
TE	52	0.8999	0.1002	0.03600	0.1620	0	0.00720	1.2052
I	53	0.8999	0.1002	0.03600	0.1683	0	0.00720	1.2115
XE	54	0.8999	0.1002	0.03600	0.1746	0	0.00720	1.2178
CS	55	0.8999	0.1002	0.03610	0.1803	0	0.00720	1.2236
BA	56	0.8999	0.1002	0.03620	0.1860	0	0.00720	1.2294
LA	57	0.8998	0.1002	0.03650	0.1875	0	0.00720	1.2312
CE	58	0.8998	0.1002	0.03680	0.1890	0	0.00720	1.2330
PR	59	0.8998	0.1002	0.03700	0.1904	0	0.00754	1.2350
ND	60	0.8998	0.1002	0.03720	0.1919	0	0.00787	1.2370
PM	61	0.8998	0.1002	0.03730	0.1908	0	0.00810	1.2362
SM	62	0.8998	0.1002	0.03740	0.1896	0	0.00832	1.2353
EU	63	0.8998	0.1002	0.03760	0.1885	0	0.00862	1.2347
GD	64	0.8998	0.1002	0.03780	0.1874	0	0.00891	1.2341
TB	65	0.8998	0.1002	0.03805	0.1859	0	0.00918	1.2332
DY	66	0.8998	0.1002	0.03830	0.1845	0	0.00945	1.2322
HO	67	0.8997	0.1003	0.03865	0.1824	0	0.00976	1.2308
ER	68	0.8997	0.1003	0.03900	0.1803	0	0.01008	1.2294
TM	69	0.8997	0.1003	0.03960	0.1774	0	0.01030	1.2273

YB	70	0.8997	0.1003	0.04020	0.1745	0	0.01053	1.2253
LU	71	0.8997	0.1003	0.04075	0.1832	0.00135	0.01071	1.2360
HF	72	0.8997	0.1003	0.04130	0.1919	0.00270	0.01089	1.2468
TA	73	0.8996	0.1004	0.04205	0.1982	0.00360	0.01107	1.2550
W	74	0.8996	0.1004	0.04280	0.2046	0.00450	0.01125	1.2631
RE	75	0.8996	0.1004	0.04365	0.2075	0.00819	0.01178	1.2712
OS	76	0.8996	0.1004	0.04450	0.2105	0.01187	0.01232	1.2792
IN	77	0.8996	0.1004	0.04535	0.2132	0.01484	0.01259	1.2860
PT	78	0.8995	0.1005	0.04620	0.2159	0.01781	0.01286	1.2928
AU	79	0.8995	0.1005	0.04725	0.2181	0.02069	0.01318	1.2993
HG	80	0.8995	0.1005	0.04830	0.2204	0.02357	0.01349	1.3057
TL	81	0.8995	0.1005	0.04925	0.2219	0.02622	0.01376	1.3111
PB	82	0.8995	0.1005	0.05020	0.2234	0.02887	0.01403	1.3165
BI	83	0.8995	0.1005	0.05120	0.2247	0.03121	0.01430	1.3214
PO	84	0.8995	0.1005	0.05220	0.2261	0.03355	0.01457	1.3264
AT	85	0.8995	0.1005	0.05310	0.2282	0.03589	0.01484	1.3320
HN	86	0.8994	0.1006	0.05400	0.2303	0.03823	0.01511	1.3376
FR	87	0.8994	0.1006	0.05515	0.2317	0.04038	0.01547	1.3427
BA	88	0.8994	0.1006	0.05630	0.2331	0.04254	0.01583	1.3478
AC	89	0.8994	0.1006	0.05755	0.2343	0.04457	0.01610	1.3525
TH	90	0.8994	0.1006	0.05880	0.2354	0.04659	0.01637	1.3571
PA	91	0.8994	0.1006	0.05995	0.2364	0.04839	0.01668	1.3614
U	92	0.8994	0.1006	0.06110	0.2375	0.05019	0.01700	1.3657
NP	93	0.8994	0.1006	0.06205	0.2387	0.05172	0.01727	1.3697
PU	94	0.8994	0.1006	0.06300	0.2399	0.05325	0.01754	1.3737
AM	95	0.8994	0.1006	0.06450	0.2411	0.05478	0.01781	1.3781
CM	96	0.8994	0.1006	0.06600	0.2422	0.05631	0.01808	1.3826

9.3 L shell fluorescence yield and Coster-Kronig probabilities

The L shell fluorescence yield and Coster-Kronig probabilities for the two options (Krause 1979, Campbell 2003, 2009) are stored in file

LsubshellwLfijCampbelKrauseat15Feb11.txt

and the Krause $k'_{1,3}$ Coster-Kronig probabilities are stored in file

Krause_kd13.txt.

Table 15: L shell fluorescence yield and Coster-Kronig probabilities.

*L Shell Campbell Recommended values from 2003 and 2009 references								L Shell Krause 1979 Expt values					
*Elt	Z	ω1Rec	ω2Rec	ω3Rec	f12Rec	f13Rec	f23Rec	ω1 Krause	ω2 Krause	ω3 Krause	f12 Krause	f13 Krause	f23 Krause
MN	25	0.000410	0.0034	0.0039	0.2265	0.5180	0	0.00084	0.0050	0.0050	0.300	0.580	0
FE	26	0.000472	0.0048	0.0054	0.2299	0.5150	0	0.00100	0.0063	0.0063	0.300	0.570	0
CO	27	0.000546	0.0063	0.0071	0.2324	0.5127	0	0.00120	0.0077	0.0077	0.300	0.560	0
NI	28	0.000608	0.0079	0.0088	0.2358	0.5089	0	0.00140	0.0086	0.0093	0.300	0.550	0.02800
CU	29	0.000658	0.0096	0.0106	0.2383	0.5059	0	0.00160	0.0100	0.0110	0.300	0.540	0.02800
ZN	30	0.000707	0.0104	0.0101	0.2400	0.5014	0.0237	0.00180	0.0110	0.0120	0.290	0.540	0.02600
GA	31	0.001105	0.0122	0.0118	0.1732	0.5466	0.0220	0.00210	0.0120	0.0130	0.290	0.530	0.03200
GE	32	0.001303	0.0142	0.0136	0.1682	0.5473	0.0212	0.00240	0.0130	0.0150	0.280	0.530	0.05000
AS	33	0.001527	0.0162	0.0155	0.1640	0.5481	0.0203	0.00280	0.0140	0.0160	0.280	0.530	0.06300
SE	34	0.001800	0.0184	0.0175	0.1597	0.5488	0.0203	0.00320	0.0160	0.0180	0.280	0.520	0.07600
BR	35	0.002048	0.0206	0.0194	0.1597	0.5458	0.0195	0.00360	0.0180	0.0200	0.280	0.520	0.08800
KR	36	0.002619	0.0199	0.0202	0.1673	0.5300	0.0730	0.00410	0.0200	0.0220	0.270	0.520	0.10000
RB	37	0.004220	0.0223	0.0226	0.1166	0.5421	0.0800	0.00460	0.0220	0.0240	0.270	0.520	0.10900
SR	38	0.005089	0.0248	0.0251	0.0955	0.5549	0.0870	0.00510	0.0240	0.0260	0.270	0.520	0.11700
Y	39	0.005834	0.0276	0.0279	0.0811	0.5200	0.0940	0.00590	0.0260	0.0280	0.260	0.520	0.12600
ZR	40	0.006578	0.0292	0.0304	0.0744	0.5200	0.1000	0.00680	0.0280	0.0310	0.260	0.520	0.13200
NB	41	0.007571	0.0325	0.0339	0.0465	0.6100	0.1060	0.00940	0.0310	0.0340	0.100	0.610	0.13700
MO	42	0.008440	0.0360	0.0375	0.0473	0.6100	0.1120	0.01000	0.0340	0.0370	0.100	0.610	0.14100

TC	43	0.009433	0.0396	0.0410	0.0482	0.6100	0.1180	0.01100	0.0370	0.0400	0.100	0.610	0.14400
RU	44	0.01030	0.0430	0.0450	0.0482	0.6100	0.1240	0.01200	0.0400	0.0430	0.100	0.610	0.14800
RH	45	0.01105	0.0450	0.0470	0.0524	0.6000	0.1300	0.01300	0.0430	0.0460	0.100	0.600	0.15000
PD	46	0.01229	0.0500	0.0520	0.0549	0.6000	0.1380	0.01400	0.0470	0.0490	0.100	0.600	0.15100
AG	47	0.01378	0.0540	0.0560	0.0575	0.5900	0.1410	0.01600	0.0510	0.0520	0.100	0.590	0.15300
CD	48	0.01514	0.0590	0.0600	0.0600	0.5900	0.1430	0.01800	0.0560	0.0560	0.100	0.590	0.15500
IN	49	0.01663	0.0640	0.0650	0.0625	0.5900	0.1460	0.02000	0.0610	0.0600	0.100	0.590	0.15700
SN	50	0.04419	0.0680	0.0700	0.1589	0.2700	0.1480	0.03700	0.0650	0.0640	0.170	0.270	0.15700
SB	51	0.04741	0.0730	0.0750	0.1606	0.2800	0.1510	0.03900	0.0690	0.0690	0.170	0.280	0.15600
TE	52	0.05089	0.0780	0.0810	0.1631	0.2800	0.1530	0.04100	0.0740	0.0740	0.180	0.280	0.15500
I	53	0.05337	0.0840	0.0860	0.1648	0.2800	0.1560	0.04400	0.0790	0.0790	0.180	0.280	0.15400
XE	54	0.05710	0.0900	0.0920	0.1665	0.2800	0.1590	0.04600	0.0830	0.0850	0.190	0.280	0.15400
CS	55	0.06082	0.0970	0.0980	0.1682	0.2800	0.1590	0.04900	0.0900	0.0910	0.190	0.280	0.15400
BA	56	0.06578	0.1030	0.1040	0.1699	0.2800	0.1590	0.05200	0.0960	0.0970	0.190	0.280	0.15300
LA	57	0.07075	0.1110	0.1120	0.1699	0.2900	0.1590	0.05500	0.1030	0.1040	0.190	0.290	0.15300
CE	58	0.07571	0.1190	0.1190	0.1699	0.2900	0.1580	0.05800	0.1100	0.1110	0.190	0.290	0.15300
PR	59	0.08068	0.1280	0.1260	0.1699	0.2900	0.1580	0.06100	0.1170	0.1180	0.190	0.290	0.15300
ND	60	0.08316	0.1360	0.1340	0.1775	0.2500	0.1580	0.06400	0.1240	0.1250	0.190	0.300	0.15200
PM	61	0.08813	0.1450	0.1420	0.1783	0.2500	0.1560	0.06600	0.1320	0.1320	0.190	0.300	0.15100
SM	62	0.09309	0.1550	0.1500	0.1792	0.2500	0.1540	0.07100	0.1400	0.1390	0.190	0.300	0.15000
EU	63	0.09681	0.1640	0.1580	0.1817	0.2500	0.1520	0.07500	0.1490	0.1470	0.190	0.300	0.14900
GD	64	0.10200	0.1750	0.1670	0.1900	0.2790	0.1500	0.07900	0.1580	0.1550	0.190	0.300	0.14700
TB	65	0.10700	0.1860	0.1750	0.1820	0.2850	0.1480	0.08300	0.1860	0.1640	0.190	0.300	0.14500
DY	66	0.11100	0.1970	0.1840	0.1740	0.2900	0.1460	0.08900	0.1780	0.1740	0.190	0.300	0.14300
HO	67	0.11600	0.2080	0.1930	0.1660	0.2960	0.1440	0.09400	0.1890	0.1820	0.190	0.300	0.14200
ER	68	0.12100	0.2190	0.2030	0.1580	0.3010	0.1430	0.10000	0.2000	0.1920	0.190	0.300	0.14000
TM	69	0.13100	0.2310	0.2120	0.1500	0.3060	0.1410	0.10600	0.2110	0.2010	0.190	0.290	0.13900
YB	70	0.13400	0.2430	0.2220	0.1420	0.3120	0.1400	0.11200	0.2220	0.2100	0.190	0.290	0.13800
LU	71	0.13800	0.2560	0.2310	0.1340	0.3170	0.1380	0.12000	0.2340	0.2200	0.190	0.280	0.13600
HF	72	0.14100	0.2680	0.2410	0.1260	0.3220	0.1360	0.12800	0.2460	0.2310	0.180	0.280	0.13500
TA	73	0.14400	0.2800	0.2510	0.1180	0.3280	0.1340	0.13700	0.2580	0.2430	0.180	0.280	0.13400
W	74	0.14800	0.2910	0.2610	0.1100	0.3330	0.1320	0.14700	0.2700	0.2550	0.170	0.280	0.13300
RE	75	0.14700	0.3040	0.2710	0.0760	0.4820	0.1310	0.14400	0.2830	0.2680	0.160	0.330	0.13000
OS	76	0.14600	0.3180	0.2820	0.0760	0.4820	0.1300	0.13000	0.2950	0.2810	0.160	0.390	0.12800
IN	77	0.14500	0.3310	0.2920	0.0760	0.4820	0.1280	0.12000	0.3080	0.2940	0.150	0.450	0.12600
PT	78	0.11400	0.3440	0.3030	0.0750	0.5450	0.1260	0.11400	0.3210	0.3060	0.140	0.500	0.12400

AU	79	0.11700	0.3580	0.3130	0.0740	0.6150	0.1250	0.10700	0.3340	0.3200	0.140	0.530	0.12200
HG	80	0.12100	0.3700	0.3220	0.0720	0.6150	0.1230	0.10700	0.3470	0.3330	0.130	0.560	0.12000
TL	81	0.12400	0.3840	0.3320	0.0690	0.6150	0.1210	0.10700	0.3600	0.3470	0.130	0.570	0.11800
PB	82	0.12800	0.3970	0.3430	0.0660	0.6200	0.1190	0.11200	0.3730	0.3600	0.120	0.580	0.11600
BI	83	0.13200	0.4110	0.3530	0.0630	0.6200	0.1170	0.11700	0.3870	0.3730	0.110	0.580	0.11300
PO	84	0.13500	0.4240	0.3630	0.0600	0.6200	0.1150	0.12200	0.4010	0.3860	0.110	0.580	0.11100
AT	85	0.13800	0.4380	0.3740	0.0570	0.6200	0.1130	0.12800	0.4150	0.3990	0.100	0.590	0.11100
HN	86	0.14200	0.4510	0.3840	0.0530	0.6200	0.1110	0.13400	0.4290	0.4110	0.100	0.580	0.11000
FR	87	0.14600	0.4640	0.3940	0.0500	0.6200	0.1090	0.13900	0.4430	0.4240	0.100	0.580	0.10900
BA	88	0.15000	0.4760	0.4040	0.0470	0.6200	0.1070	0.14600	0.4560	0.4370	0.090	0.580	0.10800
AC	89	0.15400	0.4900	0.4140	0.0440	0.6200	0.1050	0.15300	0.4680	0.4500	0.090	0.580	0.10800
TH	90	0.15900	0.5030	0.4240	0.0400	0.6200	0.1030	0.16100	0.4790	0.4630	0.090	0.570	0.10800
PA	91	0.16400	0.4950	0.4340	0.0380	0.6200	0.1410	0.16200	0.4720	0.4760	0.080	0.580	0.13900
U	92	0.16800	0.5060	0.4440	0.0350	0.6200	0.1400	0.17600	0.4670	0.4890	0.080	0.570	0.16700
NP	93	0.20000	0.5190	0.4540	0.0300	0.6700	0.1360	0.18700	0.4660	0.5020	0.070	0.570	0.19200
PU	94	0.21000	0.4730	0.4630	0.0300	0.6800	0.2300	0.20500	0.4640	0.5140	0.050	0.560	0.19800
AM	95	0.22000	0.4870	0.4730	0.0300	0.6800	0.2220	0.21800	0.4710	0.5260	0.050	0.550	0.20300
CM	96	0.23000	0.5010	0.4820	0.0300	0.6800	0.2140	0.22800	0.4790	0.5390	0.040	0.550	0.20000

Table 16: L shell Krause f'$_{1,3}$ Coster-Kronig probabilities.

Element		Krause f'13
MG	12	2.00E-05
AL	13	1.60E-05
SI	14	1.40E-05
P	15	1.20E-05
SI	16	1.40E-05
CL	17	1.40E-05
AR	18	1.30E-05
K	19	1.20E-05
CA	20	1.40E-05
SC	21	1.40E-05
TI	22	1.50E-05
V	23	1.60E-05
CR	24	1.80E-05
MN	25	1.90E-05
FE	26	2.10E-05
CO	27	2.30E-05
NI	28	2.40E-05
CU	29	2.60E-05
ZN	30	2.80E-05
GA	31	3.00E-05
GE	32	3.20E-05
AS	33	3.40E-05
SE	34	3.60E-05
BR	35	3.80E-05
KR	36	4.10E-05
RB	37	4.40E-05
SR	38	4.70E-05
Y	39	5.20E-05
ZR	40	5.80E-05
NB	41	7.80E-05
MO	42	8.10E-05
TC	43	8.80E-05
RU	44	9.60E-05
RH	45	1.00E-04
PD	46	1.10E-04
AG	47	1.20E-04
CD	48	1.40E-04
IN	49	1.60E-04
SN	50	3.00E-04
SR	51	3.20E-04
TE	52	3.40E-04
I	53	3.70E-04
XE	54	4.00E-04
CS	55	4.30E-04
BA	56	4.70E-04
LA	57	5.10E-04
CE	58	5.50E-04
PR	59	6.00E-04
ND	60	6.60E-04
PM	61	7.20E-04
SM	62	7.90E-04
EU	63	8.70E-04
GD	64	9.60E-04
TB	65	1.10E-03
DY	66	1.20E-03
HO	67	1.30E-03
ER	68	1.40E-03
TM	69	1.60E-03
YB	70	1.80E-03
LU	71	2.00E-03
HF	72	2.30E-03
TA	73	2.60E-03
W	74	2.80E-03
RE	75	3.00E-03
OS	76	2.90E-03
IN	77	2.80E-03
PT	78	2.80E-03
AU	79	2.80E-03
HG	80	3.00E-03
TL	81	3.20E-03
PB	82	3.50E-03
BI	83	3.80E-03
PO	84	4.20E-03
AT	85	4.70E-03
RN	86	5.20E-03
FR	87	5.80E-03
RA	88	6.40E-03
AC	89	7.10E-03
TH	90	7.80E-03
PA	91	8.40E-03
U	92	9.70E-03
NP	93	1.10E-02
PU	94	1.30E-02
AM	95	1.40E-02
CM	96	1.60E-02
BK	97	1.70E-02
CP	98	1.90E-02
ES	99	2.10E-02
FM	100	2.30E-02
MD	101	2.60E-02
NO	102	2.80E-02
LR	103	3.00E-02

9.4 L shell total fluorescence yield

The L shell total fluorescence yield from Puri et al. (1993), Clayton (1986) and Bambynek et al. (1972) are stored in file

LtotalwLbarPuriEJCBambynekat23Feb11.txt.

Table 17: L shell total fluorescence yield.

*"ωLbar data from Puri et al. 1993, EJC DSET4 and Bambynek Expt 1972"			
*Z	ωLPuri93	ωLEJC	BambynekωL
25	0.00372	0.00703	0.00369
26	0.00531	0.00786	0.00476
27	0.00690	0.00876	0.00602
28	0.00848	0.00975	0.00748
29	0.01007	0.01082	0.00913
30	0.01025	0.01199	0.01099
31	0.01218	0.01326	0.01306
32	0.01410	0.01464	0.01535
33	0.01603	0.01614	0.01785
34	0.01795	0.01775	0.02056
35	0.01988	0.01950	0.02349
36	0.02088	0.02138	0.02663
37	0.02339	0.02341	0.02999
38	0.02605	0.02559	0.03355
39	0.02887	0.02794	0.03732
40	0.03186	0.03095	0.04129
41	0.03504	0.03354	0.04546
42	0.03843	0.03633	0.04983
43	0.04203	0.03931	0.05438
44	0.04587	0.04249	0.05912
45	0.04994	0.04589	0.06405
46	0.05427	0.04952	0.06916
47	0.05886	0.05338	0.07444
48	0.06372	0.05748	0.07991
49	0.06886	0.06184	0.08554
50	0.07428	0.06646	0.09136
51	0.07998	0.07135	0.09734
52	0.08598	0.07653	0.10350
53	0.09228	0.08199	0.10984
54	0.09887	0.08775	0.11635
55	0.10577	0.09381	0.12305
56	0.11296	0.10018	0.12992
57	0.12045	0.10687	0.13698
58	0.12823	0.11388	0.14424
59	0.13631	0.12121	0.15169
60	0.14468	0.12886	0.15934
61	0.15334	0.13684	0.16719
62	0.16228	0.14516	0.17526
63	0.17149	0.15379	0.18355
64	0.18096	0.16276	0.19207
65	0.19069	0.17204	0.20082
66	0.20067	0.18164	0.20982
67	0.21088	0.19155	0.21907
68	0.22131	0.20176	0.22857
69	0.23196	0.21227	0.23834
70	0.24281	0.22306	0.24839
71	0.25383	0.23412	0.25871
72	0.26503	0.24545	0.26932
73	0.27637	0.25701	0.28023
74	0.28785	0.26881	0.29143
75	0.29944	0.28082	0.30293
76	0.31112	0.29302	0.31474
77	0.32288	0.30541	0.32685
78	0.33468	0.31795	0.33927
79	0.34652	0.33063	0.35200
80	0.35836	0.34343	0.36504
81	0.37018	0.35633	0.37837
82	0.38195	0.36931	0.39199
83	0.39365	0.38235	0.40589
84	0.40525	0.39542	0.42007
85	0.41672	0.40851	0.43451
86	0.42804	0.42160	0.44919
87	0.43916	0.43467	0.46409
88	0.45006	0.44769	0.47920
89	0.46070	0.46066	0.49449
90	0.47106	0.47354	0.50993
91	0.48109	0.48633	0.52550
92	0.49076	0.49901	0.54117
93	0.50004	0.51376	0.55690
94	0.50888	0.52661	0.57267
95	0.51725	0.53934	0.58844
96	0.52511	0.55193	0.60418

9.5 L shell Energies

The L shell characteristic X-ray energies, sourced from Kaye&Laby (http://www.kayelaby.npl.co.uk/atomic_and_nuclear_physics/4_2/4_2_1.html) are stored in file

Lshellenergiesa1-2b1-6g1-6at13Feb11.txt.

A value of -9 implies that the energy is not available.

Table 18: L shell characteristic X-ray Energies.

*** 23 November 2010**																	
*** Energies obtained from GEOPIXE and * Kaye&Laby**																	
*** http://www.kayelaby.npl.co.uk/atomic_and_nuclear_physics/4_2/4_2_1.html**																	
*** Where enetries were missing for a certain z and an energy was available on**																	
*** either side and interpolation was carried out**																	
*** El**	**Z**	**Lα1**	**Lα2**	**Lβ1**	**Lβ2**	**Lβ3**	**Lβ4**	**Lβ5**	**Lβ6**	**Lγ1**	**Lγ2**	**Lγ3**	**Lγ4**	**Lγ5**	**Lγ6**	**Ll**	**Lη**
K	19	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9
Ca	20	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9
Sc	21	0.3950	0.3950	0.4000	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	0.3480	-9
Ti	22	0.4520	0.4520	0.4580	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9	0.3950	-9
V	23	0.5110	0.5110	0.5190	-9	0.5850	0.5850	-9	-9	-9	-9	-9	-9	-9	-9	0.4460	-9
Cr	24	0.5730	0.5730	0.5830	-9	0.6540	0.6540	-9	-9	-9	-9	-9	-9	-9	-9	0.5000	-9
Mn	25	0.6370	0.6370	0.6490	-9	0.7210	0.7210	-9	-9	-9	-9	-9	-9	-9	-9	0.5560	-9
Fe	26	0.7050	0.7050	0.7190	-9	0.7920	0.7920	-9	-9	-9	-9	-9	-9	-9	-9	0.6150	-9
Co	27	0.7760	0.7760	0.7910	-9	0.8700	0.8700	-9	-9	-9	-9	-9	-9	-9	-9	0.6780	-9
Ni	28	0.8520	0.8520	0.8690	-9	0.9410	0.9410	-9	-9	-9	-9	-9	-9	-9	-9	0.7430	-9
Cu	29	0.9300	0.9300	0.9500	-9	1.0230	1.0190	-9	-9	-9	-9	-9	-9	-9	-9	0.8110	-9
Zn	30	1.0120	1.0120	1.0340	-9	1.1070	1.1020	-9	-9	-9	-9	-9	-9	-9	-9	0.8840	-9
Ga	31	1.0980	1.0980	1.1250	-9	1.1970	1.1910	-9	-9	-9	-9	-9	-9	-9	-9	0.9570	-9
Ge	32	1.1880	1.1880	1.2180	-9	1.2940	1.2860	-9	-9	-9	-9	-9	-9	-9	-9	1.0360	1.0680
As	33	1.2820	1.2820	1.3170	-9	1.3880	1.3800	-9	-9	-9	-9	-9	-9	-9	-9	1.1200	1.1550
Se	34	1.3790	1.3790	1.4190	-9	1.4900	1.4850	-9	-9	-9	-9	-9	-9	-9	-9	1.2040	1.2440
Br	35	1.4800	1.4800	1.5260	-9	1.5960	1.5930	-9	-9	-9	-9	-9	-9	-9	-9	1.2930	1.3390
Kr	36	1.5860	1.5860	1.6360	-9	1.7060	1.6970	-9	1.6510	-9	-9	-9	-9	1.7030	-9	1.3860	1.4405

Rb	37	1.6940	1.6920	1.7520	-9	1.8260	1.8170	-9	1.7750	-9	2.0500	-9	-9	1.8353	-9	1.4820	1.5420
Sr	38	1.8060	1.8040	1.8710	-9	1.9470	1.9360	-9	1.9010	-9	2.1960	-9	-9	1.9692	-9	1.5820	1.6490
Y	39	1.9230	1.9200	1.9950	-9	2.0720	2.0600	-9	2.0340	-9	2.3460	-9	-9	2.1100	-9	1.6850	1.7610
Zr	40	2.0430	2.0399	2.1244	2.2150	2.2010	2.1873	-9	2.1712	2.3027	2.5020	-9	-9	2.2551	-9	1.7920	1.8765
Nb	41	2.1660	2.1630	2.2570	2.3570	2.3340	2.3190	-9	2.3120	2.4610	2.6630	-9	-9	2.4060	-9	1.9020	1.9960
Mo	42	2.2950	2.2910	2.3940	2.5080	2.4730	2.4550	-9	2.4550	2.6230	2.8300	-9	-9	2.5630	-9	2.0150	2.1200
Tc	43	2.4240	2.4210	2.5360	2.6640	2.6180	2.5980	-9	2.6090	2.7935	3.0050	-9	-9	2.7270	-9	2.1310	2.2510
Ru	44	2.5560	2.5540	2.6830	2.8250	2.7630	2.7410	-9	2.7630	2.9640	3.1800	-9	-9	2.8910	-9	2.2520	2.3820
Rh	45	2.6980	2.6920	2.8340	2.9920	2.9150	2.8900	-9	2.9220	3.1430	3.3630	-9	-9	3.0640	-9	2.3760	2.5190
Pd	46	2.8380	2.8330	2.9900	3.1710	3.0720	3.0450	-9	3.0870	3.3280	3.5530	-9	-9	3.2430	-9	2.5030	2.6600
Ag	47	2.9850	2.9790	3.1500	3.3470	3.2340	3.2030	-9	3.2550	3.5190	3.7432	3.7490	-9	3.4280	-9	2.6330	2.8060
Cd	48	3.1340	3.1310	3.3160	3.5280	3.4010	3.3670	-9	3.4290	3.7160	3.9513	3.9570	-9	3.6190	-9	2.7670	2.9560
In	49	3.2880	3.2800	3.4870	3.7130	3.5720	3.5350	-9	3.6080	3.9200	4.1650	4.1651	4.2367	3.8150	-9	2.9040	3.1120
Sn	50	3.4420	3.4330	3.6620	3.9040	3.7500	3.7080	-9	3.7920	4.1300	4.3760	4.3768	4.4638	4.0180	-9	3.0440	3.2720
Sb	51	3.6040	3.5940	3.8430	4.1000	3.9320	3.8860	-9	3.9790	4.3470	4.5990	4.5999	4.6967	4.2280	-9	3.1880	3.4360
Te	52	3.7700	3.7590	4.0290	4.3010	4.1200	4.0690	-9	4.1730	4.5700	4.8280	4.8280	4.9369	4.4430	-9	3.3350	3.6050
I	53	3.9370	3.9250	4.2200	4.5070	4.3130	4.2570	-9	4.3700	4.8000	5.0650	5.0650	5.1840	4.6650	-9	3.4840	3.7800
Xe	54	4.1100	4.0950	4.4150	4.7720	4.5160	4.4530	-9	4.5750	5.0395	5.3030	5.3085	5.4430	4.8965	-9	3.6250	3.9605
Cs	55	4.2860	4.2720	4.6190	4.9350	4.7160	4.6490	-9	4.7800	5.2790	5.5410	5.5520	5.7020	5.1280	-9	3.7940	4.1410
Ba	56	4.4650	4.4500	4.8270	5.1560	4.9260	4.8510	-9	4.9930	5.5300	5.7960	5.8080	5.9720	5.3700	-9	3.9530	4.3300
La	57	4.6470	4.6330	5.0410	5.3830	5.1430	5.0610	-9	5.2110	5.7880	6.0590	6.0600	6.2510	5.6200	-9	4.1240	4.5240
Ce	58	4.8390	4.8220	5.2610	5.6120	5.3640	5.2760	-9	5.4330	6.0510	6.3240	6.3400	6.5270	5.8740	-9	4.2870	4.7310
Pr	59	5.0330	5.0130	5.4880	5.8490	5.5910	5.4970	-9	5.6590	6.3210	6.5970	6.6150	6.8140	6.1350	-9	4.4520	4.9350
Nd	60	5.2290	5.2070	5.7210	6.0880	5.8280	5.7210	-9	5.8920	6.6010	6.8820	6.9000	7.1060	6.4050	-9	4.6320	5.1450
Pm	61	5.4320	5.4070	5.9600	6.3380	6.0700	5.9590	-9	6.1305	6.8910	7.1735	7.1925	7.4090	6.6860	-9	4.7850	5.3665
Sm	62	5.6350	5.6070	6.2040	6.5860	6.3170	6.1950	6.7126	6.3690	7.1770	7.4650	7.4850	7.7120	6.9670	7.3060	4.9940	5.5880
Eu	63	5.8450	5.8160	6.4550	6.8420	6.5700	6.4380	6.9735	6.6160	7.4790	7.7660	7.7950	8.0290	7.2550	7.6130	5.1760	5.8160
Gd	64	6.0560	6.0240	6.7120	7.1020	6.8300	6.6860	7.2374	6.8660	7.7840	8.0860	8.1040	8.3540	7.5530	7.9240	5.3610	6.0490
Tb	65	6.2720	6.2370	6.9770	7.3650	7.0950	6.9390	7.5094	7.1150	8.1000	8.3960	8.4220	8.6830	7.8520	8.2450	5.5460	6.2830
Dy	66	6.4940	6.4570	7.2460	7.6340	7.3690	7.2030	7.8055	7.3690	8.4170	8.7130	8.7520	9.0180	8.1650	8.5740	5.7420	6.5330
Ho	67	6.7190	6.6790	7.5240	7.9100	7.6500	7.4700	8.0610	7.6340	8.7460	9.0490	9.0860	9.3730	8.4800	8.9030	5.9420	6.7870
Er	68	6.9470	6.9040	7.8090	8.1880	7.9380	7.7440	8.3490	7.9080	9.0870	9.3840	9.4290	9.7210	8.8120	9.2530	6.1520	7.0570
Tm	69	7.1790	7.1320	8.1000	8.4670	8.2290	8.0240	8.6390	8.1760	9.4240	9.7280	9.7780	10.0830	9.1430	9.6060	6.3410	7.3080
Yb	70	7.4140	7.3660	8.4000	8.7570	8.5350	8.3120	8.9380	8.4550	9.7780	10.0880	10.1410	10.4580	9.4890	9.9750	6.5440	7.5790
Lu	71	7.6540	7.6040	8.7080	9.0470	8.8450	8.6050	9.2380	8.7360	10.1420	10.4580	10.5090	10.8400	9.8410	10.3410	6.7520	7.8560
Hf	72	7.8980	7.8430	9.0210	9.3460	9.1620	8.9040	9.5530	9.0210	10.5140	10.8320	10.8890	11.2380	10.1990	10.7310	6.9580	8.1380

Ta	73	8.1450	8.0860	9.3420	9.6500	9.4860	9.2110	9.8730	9.3140	10.8930	11.2150	11.2760	11.6430	10.5690	11.1290	7.1720	8.4270
W	74	8.3960	8.3340	9.6710	9.9600	9.8170	9.5240	10.1990	9.6100	11.2840	11.6060	11.6720	12.0610	10.9470	11.5370	7.3860	8.7230
Re	75	8.6510	8.5850	10.0080	10.2740	10.1580	9.8450	10.5300	9.9090	11.6830	12.0080	12.0800	12.4900	11.3320	11.9540	7.6020	9.0260
Os	76	8.9100	8.8400	10.3540	10.5970	10.5090	10.1740	10.8690	10.2150	12.0930	12.4200	12.4980	12.9210	11.7280	12.3830	7.8210	9.3350
Ir	77	9.1740	9.0980	10.7060	10.9190	10.8660	10.5090	11.2090	10.5230	12.5100	12.8400	12.9220	13.3660	12.1320	12.8180	8.0400	9.6490
Pt	78	9.4410	9.3600	11.0690	11.2490	11.2330	10.8520	11.5590	10.8400	12.9400	13.2680	13.3590	13.8260	12.5500	13.2690	8.2670	9.9730
Au	79	9.7120	9.6260	11.4400	11.5830	11.6080	11.2030	11.9140	11.1580	13.3790	13.7070	13.8070	14.2970	12.9720	13.7280	8.4930	10.3070
Hg	80	9.9870	9.8960	11.8210	11.9220	11.9930	11.5610	12.2750	11.4800	13.8280	14.1600	14.2620	14.7760	13.4080	14.1960	8.7200	10.6490
Tl	81	10.2670	10.1710	12.2110	12.2700	12.3880	11.9290	12.6410	11.8100	14.2890	14.6230	14.7340	15.2690	13.8500	14.6840	8.9520	10.9920
Pb	82	10.5500	10.4480	12.6120	12.6210	12.7910	12.3040	13.0130	12.1410	14.7620	15.0990	15.2150	15.7750	14.3050	15.1760	9.1830	11.3470
Bi	83	10.8370	10.7290	13.0210	12.9780	13.2080	12.6890	13.3930	12.4790	15.2450	15.5800	15.7080	16.2920	14.7710	15.6830	9.4190	11.7200
Po	84	11.1290	11.0140	13.4450	13.3380	13.6350	13.0830	13.7790	12.8160	15.7410	16.0570	16.2368	16.8502	15.2710	16.2150	9.6620	12.1078
At	85	11.4250	11.3030	13.8740	13.7080	14.0650	13.4870	14.1780	13.1705	16.2490	16.5868	16.7660	17.4080	15.7710	16.7640	9.8580	12.4960
Rn	86	11.7250	11.5960	14.3130	14.0790	14.5090	13.8910	14.5770	13.5250	16.7680	17.1165	17.2952	17.9658	16.2710	17.3130	10.0850	12.8842
Fr	87	12.0290	11.8930	14.7680	14.4480	14.9730	14.3060	14.9760	13.8795	17.3000	17.6463	17.8244	18.5236	16.7710	17.8620	10.3400	13.2724
Ra	88	12.3380	12.1940	15.2330	14.8390	15.4420	14.7450	15.3750	14.2340	17.8450	18.1760	18.3540	19.0810	17.2710	18.4110	10.6200	13.6610
Ac	89	12.6500	12.4990	15.7100	15.2270	15.9290	15.1860	15.7930	14.6035	18.4050	18.7390	18.9285	19.6850	17.8160	19.0035	10.8360	14.0840
Th	90	12.9670	12.8070	16.1990	15.6210	16.4230	15.6400	16.2110	14.9730	18.9790	19.3020	19.5030	20.2890	18.3610	19.5960	11.1170	14.5070
Pa	91	13.2880	13.1200	16.6990	16.0220	16.9270	16.1010	16.6340	15.3430	19.5650	19.8690	20.0940	20.8790	18.9250	20.2120	11.3640	14.9440
U	92	13.6120	13.4370	17.2170	16.4250	17.4520	16.5730	17.0670	15.7230	20.1640	20.4810	20.7090	21.5590	19.5040	20.8390	11.6160	15.3970
NP	93	13.9440	13.7600	17.7510	16.8400	17.9920	17.0610	17.5081	16.1300	20.7848	21.1100	21.3400	22.2000	20.1200	21.4880	11.8900	15.8760
PU	94	14.2790	14.0840	18.2930	17.2560	18.5400	17.5560	17.9506	16.4983	21.4173	21.7251	21.9824	22.8910	20.7040	22.1502	12.1240	16.3330
AM	95	14.6170	14.4120	18.8520	17.6760	19.1060	18.0630	18.3996	16.8870	22.0652	22.3610	-9	-9	-9	22.8282	12.3840	-9
CM	96	14.9590	14.7030	19.9520	-9	19.6630	18.5650	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9
BK	97	15.3200	15.0860	20.0190	-9	20.3480	19.1280	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9
CR	98	15.6770	15.4430	20.7630	-9	21.0010	19.7510	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9
ES	99	16.0360	15.7800	21.3900	-9	21.6480	20.3260	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9
FM	100	16.4020	16.1340	22.0440	-9	22.3030	20.9570	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9
MD	101	16.7680	16.4870	22.7070	-9	22.9840	21.5110	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9
NO	102	17.1390	16.8430	23.4030	-9	23.6920	22.1350	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9
LW	103	17.5000	17.2100	24.1300	-9	24.5300	22.7800	-9	-9	-9	-9	-9	-9	-9	-9	-9	-9

10 Appendix 3: Files for M shell calculations

For the M-shell relative intensity calculations the data tables, stored in the following files, are needed:

- ***table1.txt, table2.txt, table3.txt*** – tables from Johnson et al. (1979) for the M-shell ionization cross sections calculation.
- ***Mshell_edges.txt*** – M-shell edge energies (Weast 1970).
- ***MsubshellDHSEmissionRatesat28Feb11.txt*** – DHS emission rates (Puri, 2007).
- ***MsubshellDFEmissionRatesat28Feb11.txt*** – DF emission rates (Puri, 2007).
- ***MsubshellFluorescenceyldswisat31Mar11.txt*** – fluorescence yield (Chauhan and Puri, 2008).
- ***MsubshellSuperSijBambynekat4Mar11.txt*** – super Coster-Kronig probabilities (Bambynek at al. 1972).
- ***MsubshellCKfijsat28Feb11.txt*** – Coster-Kronig probabilities (Chauhan and Puri, 2008).
- ***MLineEnergies_Calculated.txt*** – M-shell characteristic X-ray energies.

10.1 M shell edge energies

The M-shell edge energies in keV are taken from (Weast 1970).

Table 19: M subshell edge energies (keV).

*Element	Z	Mass	M1	M2	M3	M4	M5
SN	50	118.690	0.8847	0.7565	0.7146	0.4932	0.4849
SB	51	121.750	0.9460	0.8127	0.7664	0.5375	0.5282
TE	52	127.600	1.0060	0.8708	0.8200	0.5834	0.5730
I	53	126.904	1.0720	0.9310	0.8750	0.6308	0.6193
XE	54	131.300	1.1487	1.0021	0.9406	0.6890	0.6764
CS	55	132.905	1.2110	1.0710	1.0030	0.7405	0.7266
BA	56	137.340	1.2930	1.1370	1.0630	0.7957	0.7805
LA	57	138.910	1.3620	1.2090	1.1280	0.8530	0.8360
CE	58	140.120	1.4360	1.2740	1.1870	0.9024	0.8838
PR	59	140.907	1.5110	1.3370	1.2420	0.9483	0.9288
ND	60	144.240	1.5750	1.4030	1.2970	1.0033	0.9804
PM	61	145.000	1.6490	1.4710	1.3570	1.0520	1.0270
SM	62	150.350	1.7230	1.5410	1.4200	1.1109	1.0834
EU	63	151.960	1.8000	1.6140	1.4810	1.1586	1.1275
GD	64	157.250	1.8810	1.6880	1.5440	1.2219	1.1896
TB	65	158.924	1.9680	1.7680	1.6110	1.2769	1.2411
DY	66	162.500	2.0470	1.8420	1.6760	1.3330	1.2926
HO	67	164.930	2.1280	1.9230	1.7410	1.3920	1.3510
ER	68	167.260	2.2070	2.0060	1.8120	1.4530	1.4090
TM	69	168.934	2.3070	2.0900	1.8850	1.5150	1.4680
YB	70	173.040	2.3980	2.1730	1.9500	1.5760	1.5280
LU	71	174.970	2.4910	2.2640	2.0240	1.6390	1.5890
HF	72	178.490	2.6010	2.3650	2.1080	1.7160	1.6620
TA	73	180.948	2.7080	2.4690	2.1940	1.7930	1.7350
W	74	183.850	2.8200	2.5750	2.2810	1.8720	1.8090

Re	75	186.200	2.9320	2.6820	2.3670	1.9490	1.8830
OS	76	190.200	3.0490	2.7920	2.4570	2.0310	1.9600
IR	77	192.200	3.1740	2.9090	2.5510	2.1160	2.0400
PT	78	195.090	3.2960	3.0270	2.6450	2.2020	2.1220
AU	79	196.967	3.4250	3.1480	2.7430	2.2910	2.2060
HG	80	200.590	3.5620	3.2790	2.8470	2.3850	2.2950
TL	81	204.370	3.7040	3.4160	2.9570	2.4850	2.3890
PB	82	207.190	3.8510	3.5540	3.0660	2.5860	2.4840
BI	83	208.980	3.9990	3.6960	3.1770	2.6880	2.5800
PO	84	210.000	4.1490	3.8540	3.3020	2.7980	2.6830
At	85	210.000	4.3170	4.0080	3.4260	2.9090	2.7870
RN	86	222.000	4.4820	4.1590	3.5380	3.0220	2.8920
FR	87	223.000	4.6520	4.3270	3.6630	3.1360	3.0000
RA	88	226.000	4.8220	4.4900	3.7920	3.2480	3.1050
AC	89	227.000	5.0020	4.6560	3.9090	3.3700	3.2190
TH	90	232.038	5.1820	4.8300	4.0460	3.4910	3.3320
PA	91	231.036	5.3670	5.0010	4.1740	3.6110	3.4420
U	92	238.030	5.5480	5.1820	4.3030	3.7280	3.5520
NP	93	237.000	5.7232	5.3662	4.4347	3.8503	3.6658
PU	94	239.000	5.9329	5.5412	4.5566	3.9726	3.7781
AM	95	242.000	6.1205	5.7102	4.6670	4.0921	3.8869
CM	96	245.000	6.2880	5.8950	4.7970	4.2270	3.9710

10.2 M shell emission rates

Two options are available for the M shell emission rates; DHS and DF (Puri, 2007).

10.2.1 DHS emission rates

The following two tables for the DHS emission rates are stored side by side in file

MsubshellDHSEmissionRatesat28Feb11.txt.

Please note that Z is included in the second tables only in this Appendix and not in the original file.

Table 20: M shell DHS emission rates (part I).

***Origin interpolated values**									
***DHS Theory**									
***Z**	**(M5-N3)**	**(M5-N7)**	**(M5-N6)**	**(M5-O3)**	**(M4-N2)**	**(M4-N3)**	**(M4-N6)**	**(M4-O3)**	**(M4-O2)**
65	5.920	100	5.130	0.780	6.120	0.840	100	0.110	0.830
66	5.845	100	5.140	0.755	6.105	0.825	100	0.105	0.815
67	5.770	100	5.150	0.730	6.090	0.810	100	0.100	0.800
68	5.700	100	5.155	0.705	6.080	0.795	100	0.095	0.785
69	5.630	100	5.160	0.680	6.070	0.780	100	0.090	0.770
70	5.485	100	5.165	0.665	5.985	0.755	100	0.090	0.765
71	5.340	100	5.170	0.650	5.900	0.730	100	0.090	0.760
72	5.135	100	5.165	0.650	5.745	0.700	100	0.090	0.765
73	4.930	100	5.160	0.650	5.590	0.670	100	0.090	0.770
74	4.745	100	5.155	0.645	5.445	0.645	100	0.090	0.775
75	4.560	100	5.150	0.640	5.300	0.620	100	0.090	0.780

76	4.395	100	5.140	0.640	5.170	0.595	100	0.090	0.785
77	4.230	100	5.130	0.640	5.040	0.570	100	0.090	0.790
78	4.080	100	5.125	0.635	4.920	0.545	100	0.090	0.795
79	3.930	100	5.120	0.630	4.800	0.520	100	0.090	0.800
80	3.835	100	5.120	0.635	4.735	0.505	100	0.090	0.810
81	3.740	100	5.120	0.640	4.670	0.490	100	0.090	0.820
82	3.690	100	5.120	0.645	4.655	0.485	100	0.090	0.835
83	3.640	100	5.120	0.650	4.640	0.480	100	0.090	0.850
84	3.590	100	5.120	0.660	4.630	0.470	100	0.090	0.870
85	3.540	100	5.120	0.670	4.620	0.460	100	0.090	0.890
86	3.495	100	5.120	0.675	4.610	0.450	100	0.090	0.905
87	3.450	100	5.120	0.680	4.600	0.440	100	0.090	0.920
88	3.410	100	5.120	0.690	4.590	0.435	100	0.090	0.935
89	3.370	100	5.120	0.700	4.580	0.430	100	0.090	0.950
90	3.325	100	5.120	0.705	4.570	0.420	100	0.090	0.970
91	3.280	100	5.120	0.710	4.560	0.410	100	0.090	0.990
92	3.240	100	5.120	0.710	4.550	0.400	100	0.090	1.000

Table 21: M shell DHS emission rates (part II).

*Z	(M3-N1)	(M3-N2)	(M3-O1)	(M3-O4,5)	(M3-N5)	(M3-N4)	(M3-N6,7)	(M2-N1)	(M2-O1)	(M2-O4)	(M2-N4)	(M1-N2,3)	(M1-O2,3)
65	26.34	0.040	4.520	0.000	100	12.36	0.510	20.17	3.520	0	100	100	15.81
66	26.35	0.045	4.460	0.000	100	12.41	0.530	20.04	3.450	0	100	100	15.48
67	26.36	0.050	4.400	0.000	100	12.45	0.550	19.90	3.380	0	100	100	15.14
68	26.37	0.050	4.340	0.000	100	12.49	0.570	19.77	3.315	0	100	100	14.84
69	26.37	0.050	4.280	0.000	100	12.53	0.590	19.64	3.250	0	100	100	14.53
70	26.38	0.050	4.310	0.000	100	12.57	0.615	19.54	3.255	0	100	100	14.67
71	26.38	0.050	4.340	0.000	100	12.60	0.640	19.44	3.260	0	100	100	14.80
72	26.39	0.055	4.450	2.755	100	12.64	0.680	19.36	3.335	9.22	100	100	15.39
73	26.39	0.060	4.560	2.860	100	12.67	0.720	19.28	3.410	9.56	100	100	15.97
74	26.39	0.060	4.670	2.965	100	12.70	0.765	19.21	3.480	9.91	100	100	16.58
75	26.39	0.060	4.780	3.070	100	12.73	0.810	19.13	3.550	10.25	100	100	17.19
76	26.39	0.060	4.900	3.175	100	12.77	0.860	19.06	3.625	10.60	100	100	17.83
77	26.39	0.060	5.020	3.280	100	12.80	0.910	18.99	3.700	10.94	100	100	18.46
78	26.40	0.065	5.135	3.395	100	12.83	0.960	18.92	3.775	11.30	100	100	19.13
79	26.40	0.070	5.250	3.510	100	12.86	1.010	18.85	3.850	11.65	100	100	19.79
80	26.49	0.070	5.375	9.480	100	12.90	1.060	18.89	3.940	12.20	100	100	20.42
81	26.57	0.070	5.500	15.450	100	12.93	1.110	18.92	4.030	12.74	100	100	21.05
82	26.75	0.075	5.630	16.365	100	12.97	1.150	19.06	4.140	13.51	100	100	21.63
83	26.92	0.080	5.760	17.280	100	13.00	1.190	19.19	4.250	14.28	100	100	22.21
84	27.10	0.080	5.890	18.280	100	13.04	1.235	19.33	4.355	15.12	100	100	22.80
85	27.27	0.080	6.020	19.280	100	13.07	1.280	19.46	4.460	15.96	100	100	23.39
86	27.44	0.080	6.155	20.365	100	13.11	1.325	19.59	4.570	16.88	100	100	23.99
87	27.61	0.080	6.290	21.450	100	13.14	1.370	19.72	4.680	17.80	100	100	24.59
88	27.78	0.085	6.430	22.625	100	13.17	1.415	19.85	4.795	18.80	100	100	25.21
89	27.94	0.090	6.570	23.800	100	13.20	1.460	19.98	4.910	19.80	100	100	25.82
90	28.11	0.090	6.710	25.075	100	13.24	1.510	20.12	5.030	20.89	100	100	26.44
91	28.28	0.090	6.850	26.350	100	13.27	1.560	20.25	5.150	21.97	100	100	27.06
92	28.44	0.090	6.990	27.710	100	13.30	1.610	20.37	5.260	23.12	100	100	27.69

10.2.2 DF emission rates

The following two tables for the DF emission rates are stored side by side in file

MsubshellDFEmissionRatesat28Feb11.txt.

Please note that Z is included in the second tables only in this Appendix and not in the original file.

Table 22: M shell DF emission rates (part I).

*Origin interpolated values									
*DF Theory									
*Z	(M5-N3)	(M5-N7)	(M5-N6)	(M5-O3)	(M4-N2)	(M4-N3)	(M4-N6)	(M4-O3)	(M4-O2)
65	10.460	100	5.500	0.600	9.880	1.490	100	0.070	0.560
66	9.605	100	5.735	0.545	8.805	1.310	100	0.065	0.505
67	8.750	100	5.970	0.490	7.730	1.130	100	0.060	0.450
68	8.050	100	5.845	0.460	7.300	1.050	100	0.055	0.430
69	7.350	100	5.720	0.430	6.870	0.970	100	0.050	0.410
70	6.780	100	5.600	0.405	6.500	0.905	100	0.045	0.390
71	6.210	100	5.480	0.380	6.130	0.840	100	0.040	0.370
72	5.735	100	5.370	0.355	5.810	0.785	100	0.040	0.350
73	5.260	100	5.260	0.330	5.490	0.730	100	0.040	0.330
74	4.990	100	5.205	0.340	5.300	0.695	100	0.040	0.350
75	4.720	100	5.150	0.350	5.110	0.660	100	0.040	0.370
76	4.595	100	5.150	0.405	5.035	0.640	100	0.050	0.430
77	4.470	100	5.150	0.460	4.960	0.620	100	0.060	0.490
78	4.355	100	5.145	0.520	4.885	0.600	100	0.070	0.575
79	4.240	100	5.140	0.580	4.810	0.580	100	0.080	0.660
80	4.155	100	5.130	0.600	4.770	0.565	100	0.085	0.680
81	4.070	100	5.120	0.620	4.730	0.550	100	0.090	0.700
82	3.995	100	5.115	0.630	4.695	0.540	100	0.090	0.725
83	3.920	100	5.110	0.640	4.660	0.530	100	0.090	0.750
84	3.860	100	5.115	0.655	4.630	0.520	100	0.090	0.770
85	3.800	100	5.120	0.670	4.600	0.510	100	0.090	0.790
86	3.750	100	5.120	0.680	4.585	0.500	100	0.090	0.810
87	3.700	100	5.120	0.690	4.570	0.490	100	0.090	0.830
88	3.625	100	5.120	0.695	4.560	0.475	100	0.090	0.845
89	3.550	100	5.120	0.700	4.550	0.460	100	0.090	0.860
90	3.460	100	5.115	0.690	4.525	0.445	100	0.090	0.880
91	3.370	100	5.110	0.680	4.500	0.430	100	0.090	0.900
92	3.280	100	5.100	0.670	4.480	0.410	100	0.080	0.920

Table 23: M shell DF emission rates (part II).

*Z	(M3-N1)	(M3-N2)	(M3-O1)	(M3-O4,5)	(M3-N5)	(M3-N4)	(M3-N6,7)	(M2-N1)	(M2-O1)	(M2-O4)	(M2-N4)	(M1-N2,3)	(M1-O2,3)
65	25.880	0.040	3.920	0	100	12.00	0.330	20.88	3.33	0	100	100	15.68
66	25.900	0.045	3.870	0	100	12.09	0.385	20.66	3.28	0	100	100	15.49
67	25.920	0.050	3.820	0	100	12.18	0.440	20.43	3.22	0	100	100	15.30
68	25.940	0.050	3.880	0	100	12.25	0.485	20.29	3.25	0	100	100	15.59
69	25.950	0.050	3.940	0	100	12.32	0.530	20.14	3.28	0	100	100	15.87
70	25.970	0.050	4.000	0	100	12.39	0.585	20.00	3.31	0	100	100	16.16
71	25.980	0.050	4.060	0	100	12.45	0.640	19.86	3.34	0	100	100	16.45
72	26.000	0.055	4.120	0.550	100	12.52	0.705	19.73	3.37	0.565	100	100	16.74
73	26.010	0.060	4.180	2.050	100	12.59	0.770	19.59	3.40	2.060	100	100	17.03
74	26.020	0.060	4.255	3.550	100	12.63	0.825	19.50	3.45	3.555	100	100	17.43
75	26.030	0.060	4.330	5.050	100	12.67	0.880	19.40	3.49	5.050	100	100	17.83
76	26.040	0.060	4.420	6.550	100	12.69	0.925	19.34	3.55	6.545	100	100	18.35
77	26.040	0.060	4.510	8.050	100	12.71	0.970	19.28	3.61	8.040	100	100	18.87
78	26.050	0.065	4.600	10.360	100	12.73	1.015	19.23	3.67	10.355	100	100	19.41
79	26.050	0.070	4.690	12.670	100	12.74	1.060	19.17	3.73	12.670	100	100	19.94
80	26.100	0.070	4.825	13.785	100	12.80	1.105	19.18	3.83	13.525	100	100	20.53
81	26.150	0.070	4.960	14.900	100	12.85	1.150	19.18	3.93	14.380	100	100	21.11
82	26.230	0.070	5.095	15.930	100	12.89	1.190	19.21	4.03	15.300	100	100	21.73
83	26.300	0.070	5.230	16.960	100	12.92	1.230	19.24	4.13	16.220	100	100	22.34
84	26.400	0.075	5.365	17.825	100	12.94	1.275	19.30	4.23	17.195	100	100	23.00
85	26.500	0.080	5.500	18.690	100	12.95	1.320	19.36	4.33	18.170	100	100	23.65
86	26.650	0.080	5.635	19.605	100	12.98	1.365	19.45	4.45	19.140	100	100	24.25
87	26.790	0.080	5.770	20.520	100	13.01	1.410	19.54	4.56	20.110	100	100	24.85
88	27.060	0.085	5.935	21.195	100	13.07	1.460	19.74	4.67	20.775	100	100	25.28
89	27.330	0.090	6.100	21.870	100	13.12	1.510	19.93	4.78	21.440	100	100	25.71
90	27.690	0.090	6.285	22.290	100	13.18	1.570	20.19	4.88	21.840	100	100	26.03
91	28.050	0.090	6.470	22.710	100	13.24	1.630	20.45	4.98	22.240	100	100	26.34
92	28.400	0.100	6.670	23.140	100	13.30	1.690	20.71	5.08	22.650	100	100	26.65

10.3 M shell Fluorescence Yield

The M shell fluorescence yields were obtained from Chauhan and Puri (2008) and are stored in file

MsubshellFluorescenceyldswisat31Mar11.txt.

Table 24: M shell fluorescence yield.

*Y Chauhan, S. Puri, Atomic Data and Nuclear data Tables 94-2008 38-49.													
*M subshell fluorescence yields wi													
*Z	ω1(DF)	ω2(DF)	ω3(DF)	ω4(DF)	ω5(DF)	ωMbar (DF)	ω1(DHS)	ω2(DHS)	ω3(DHS)	ω4(DHS)	ω5(DHS)	ωMbar (DHS)	ωMbar Exptfit
65	-99	-99	-99	-99	-99	0.0103	-99	-99	-99	-99	-99	0.0119	0.01107
66	-99	-99	-99	-99	-99	0.0115	-99	-99	-99	-99	-99	0.0125	0.01153
67	0.00115	0.00196	0.00194	0.00816	0.01168	0.0129	0.00099	0.00172	0.00168	0.00819	0.01240	0.01330	0.01213
68	0.00122	0.00208	0.00212	0.00869	0.01278	0.0140	0.00105	0.00181	0.00183	0.00858	0.01330	0.01410	0.01287
69	0.00130	0.00221	0.00230	0.00924	0.01396	0.0151	0.00111	0.00191	0.00198	0.00899	0.01410	0.01490	0.01374
70	0.00138	0.00235	0.00250	0.00981	0.01524	0.0164	0.00118	0.00201	0.00215	0.00940	0.01500	0.01590	0.01473
71	0.00146	0.00246	0.00269	0.01042	0.01661	0.0177	0.00125	0.00213	0.00233	0.00983	0.01590	0.01670	0.01584
72	0.00166	0.00258	0.00289	0.01105	0.01808	0.0191	0.00141	0.00225	0.00252	0.01027	0.01690	0.01770	0.01706
73	0.00177	0.00270	0.00310	0.01171	0.01966	0.0206	0.00152	0.00238	0.00272	0.01071	0.01790	0.01870	0.01838
74	0.00189	0.00283	0.00332	0.02212	0.02135	0.0225	0.00163	0.00252	0.00294	0.02000	0.01900	0.02010	0.01979
75	0.00201	0.00302	0.00420	0.02328	0.02241	0.0235	0.00175	0.00267	0.00373	0.02119	0.02020	0.02130	0.02128
76	0.00214	0.00322	0.00450	0.02449	0.02351	0.0246	0.00185	0.00284	0.00400	0.02244	0.02140	0.02240	0.02286
77	0.00228	0.00342	0.00481	0.02575	0.02465	0.0259	0.00199	0.00300	0.00429	0.02374	0.02270	0.02380	0.02450
78	0.00243	0.00364	0.00516	0.02704	0.02583	0.0272	0.00214	0.00318	0.00460	0.02510	0.02410	0.02520	0.02620
79	0.00259	0.00391	0.00551	0.02839	0.02704	0.0286	0.00230	0.00342	0.00493	0.02652	0.02550	0.02670	0.02796
80	0.00277	0.00416	0.00586	0.02968	0.02816	0.0298	0.00247	0.00368	0.00527	0.02800	0.02700	0.02830	0.02977
81	0.00296	0.00449	0.00627	0.03109	0.02954	0.0313	0.00265	0.00397	0.00563	0.02960	0.02830	0.02980	0.03161
82	0.00317	0.00485	0.00671	0.03251	0.03096	0.0326	0.00283	0.00428	0.00566	0.03126	0.02960	0.03090	0.03348
83	0.00340	0.00523	0.00715	0.03392	0.03233	0.0341	0.00303	0.00461	0.00619	0.03300	0.03100	0.03260	0.03538
84	0.00364	0.00564	0.00763	0.03554	0.03386	0.0358	0.00324	0.00497	0.00677	0.03484	0.03230	0.03430	0.03729
85	0.00389	0.00607	0.00812	0.03722	0.03543	0.0376	0.00346	0.00534	0.00739	0.03675	0.03370	0.03600	0.03921
86	0.00420	0.00644	0.00881	0.03894	0.03707	0.0393	0.00376	0.00567	0.00806	0.03875	0.03510	0.03780	0.04113

87	0.00452	0.00681	0.00955	0.04062	0.03865	0.0411	0.00408	0.00602	0.00878	0.04083	0.03650	0.03960	0.04304
88	0.00487	0.00721	0.01034	0.04235	0.04028	0.0429	0.00443	0.00638	0.00956	0.04300	0.03800	0.04140	0.04494
89	0.00506	0.00751	0.01128	0.04358	0.04164	0.0442	0.00462	0.00683	0.01054	0.04468	0.03970	0.04320	0.04681
90	0.00529	0.00781	0.01228	0.04483	0.04304	0.0458	0.00497	0.00731	0.01160	0.04641	0.04140	0.04510	0.04865
91	0.00553	0.00815	0.01276	0.04611	0.04446	0.0473	0.00534	0.00783	0.01228	0.04818	0.04320	0.04710	0.05045
92	0.00578	0.00850	0.01326	0.04742	0.04592	0.0488	0.00573	0.00838	0.01300	0.05000	0.04500	0.04910	0.05221

10.4 M shell Coster-Kronig probabilities

Super Coster-Kronig probabilities, sourced from Bambynek et al. (1972) are stored in file

MsubshellSuperSijBambynekat4Mar11.txt

and the Coster-Kronig probabilities, sourced from Chauhan and Puri (2008) are stored in file

MsubshellCKfijsat28Feb11.txt.

10.4.1 File MsubshellSuperSijBambynekat4Mar11.txt

Table 25: M shell Super Coster-Kronig probabilities.

*Origin Interpolated Bambynek Super CK transitions										
*										
*Z	S12	S13	S14	S15	S23	S24	S25	S34	S35	f45
*										
65	0.3020	0.5060	0.0655	0.0950	0.0840	0.5905	0.1285	0.1550	0.7355	0.3885
66	0.2840	0.5165	0.0633	0.0925	0.0950	0.6288	0.1243	0.1500	0.7433	0.3983
67	0.2660	0.5270	0.0610	0.0900	0.1060	0.6670	0.1200	0.1450	0.7510	0.4080
68	0.2680	0.5263	0.0593	0.0903	0.1093	0.6713	0.1150	0.1437	0.7543	0.4317
69	0.2700	0.5257	0.0577	0.0907	0.1127	0.6757	0.1100	0.1423	0.7577	0.4553
70	0.2720	0.5250	0.0560	0.0910	0.1160	0.6800	0.1050	0.1410	0.7610	0.4790
71	0.2470	0.5370	0.0590	0.0990	0.1153	0.6780	0.1053	0.1213	0.7773	0.4563
72	0.2220	0.5490	0.0620	0.1070	0.1147	0.6760	0.1057	0.1017	0.7937	0.4337
73	0.1970	0.5610	0.0650	0.1150	0.1140	0.6740	0.1060	0.0820	0.8100	0.4110
74	0.1850	0.5720	0.0657	0.1130	0.1117	0.6773	0.1033	0.0900	0.7947	0.4133
75	0.1730	0.5830	0.0663	0.1110	0.1093	0.6807	0.1007	0.0980	0.7793	0.4157
76	0.1610	0.5940	0.0670	0.1090	0.1070	0.6840	0.0980	0.1060	0.7640	0.4180
77	0.1567	0.5940	0.0670	0.1100	0.1093	0.6803	0.0970	0.1087	0.7700	0.2940
78	0.1523	0.5940	0.0670	0.1110	0.1117	0.6767	0.0960	0.1113	0.7760	0.1700
79	0.1480	0.5940	0.0670	0.1120	0.1140	0.6730	0.0950	0.1140	0.7820	0.0460
80	0.1383	0.6080	0.0665	0.1078	0.1113	0.6703	0.0920	0.1090	0.7740	0.0433
81	0.1285	0.6220	0.0660	0.1035	0.1085	0.6675	0.0890	0.1040	0.7660	0.0405
82	0.1188	0.6360	0.0655	0.0993	0.1058	0.6648	0.0860	0.0990	0.7580	0.0378

83	0.1090	0.6500	0.0650	0.0950	0.1030	0.6620	0.0830	0.0940	0.7500	0.0350
84	0.1203	0.6310	0.0663	0.0967	0.1113	0.6447	0.0863	0.0867	0.7560	0.0450
85	0.1317	0.6120	0.0677	0.0983	0.1197	0.6273	0.0897	0.0793	0.7620	0.0550
86	0.1430	0.5930	0.0690	0.1000	0.1280	0.6100	0.0930	0.0720	0.7680	0.0650
87	0.1253	0.6173	0.0675	0.0978	0.1250	0.6133	0.0918	0.0783	0.7573	0.0653
88	0.1075	0.6415	0.0660	0.0955	0.1220	0.6165	0.0905	0.0845	0.7465	0.0655
89	0.0898	0.6658	0.0645	0.0933	0.1190	0.6198	0.0893	0.0908	0.7358	0.0658
90	0.0720	0.6900	0.0630	0.0910	0.1160	0.6230	0.0880	0.0970	0.7250	0.0660
91	0.0543	0.7143	0.0615	0.0888	0.1130	0.6263	0.0868	0.1033	0.7143	0.0663
92	0.0365	0.7385	0.0600	0.0865	0.1100	0.6295	0.0855	0.1095	0.7035	0.0665

10.4.2 File MsubshellCKfijsat28Feb11.txt

Table 26: M shell Coster-Kronig probabilities.

*** Y Chauhan, S. Puri, Atomic Data and Nuclear data Tables 94-2008 38-49.**										
***M subshell CK fij**										
*****										
***Z**	**f12**	**f13**	**f14**	**f15**	**f23**	**f24**	**f25**	**f34**	**f35**	**f45**
67	0.292	0.609	0.082	0.114	0.099	0.691	0.136	0.144	0.755	0.388
68	0.250	0.613	0.081	0.114	0.103	0.705	0.133	0.146	0.749	0.399
69	0.215	0.617	0.081	0.113	0.106	0.719	0.131	0.147	0.742	0.409
70	0.185	0.621	0.080	0.113	0.110	0.733	0.128	0.149	0.736	0.420
71	0.160	0.625	0.082	0.115	0.109	0.726	0.125	0.129	0.748	0.431
72	0.146	0.628	0.083	0.117	0.107	0.720	0.121	0.113	0.760	0.442
73	0.144	0.632	0.085	0.119	0.106	0.713	0.118	0.098	0.772	0.453
74	0.142	0.635	0.086	0.121	0.105	0.707	0.115	0.086	0.784	0.039
75	0.140	0.638	0.086	0.121	0.106	0.702	0.113	0.090	0.739	0.041
76	0.138	0.589	0.087	0.121	0.106	0.697	0.111	0.093	0.737	0.042
77	0.137	0.589	0.087	0.121	0.107	0.692	0.110	0.097	0.736	0.044
78	0.135	0.589	0.087	0.121	0.107	0.687	0.108	0.101	0.734	0.045
79	0.132	0.589	0.088	0.122	0.106	0.688	0.107	0.100	0.732	0.047
80	0.130	0.589	0.088	0.122	0.105	0.688	0.107	0.100	0.731	0.049
81	0.126	0.591	0.089	0.122	0.105	0.685	0.108	0.100	0.733	0.052

82	0.121	0.592	0.089	0.123	0.105	0.682	0.109	0.066	0.735	0.054
83	0.117	0.594	0.090	0.123	0.106	0.679	0.110	0.067	0.738	0.057
84	0.114	0.595	0.090	0.124	0.106	0.677	0.111	0.068	0.740	0.058
85	0.110	0.597	0.091	0.124	0.106	0.674	0.112	0.069	0.742	0.059
86	0.107	0.603	0.093	0.126	0.105	0.671	0.112	0.070	0.733	0.060
87	0.104	0.609	0.094	0.127	0.103	0.669	0.111	0.071	0.725	0.061
88	0.101	0.615	0.096	0.129	0.102	0.666	0.111	0.072	0.717	0.062
89	0.077	0.612	0.096	0.129	0.102	0.664	0.112	0.075	0.701	0.068
90	0.078	0.610	0.096	0.129	0.102	0.663	0.114	0.078	0.686	0.074
91	0.079	0.607	0.097	0.129	0.102	0.661	0.113	0.076	0.684	0.081
92	0.080	0.605	0.097	0.129	0.102	0.659	0.113	0.075	0.683	0.088

10.5 M shell characteristic X-ray energies

The M shell X-ray energies have been calculated from the electron binding energies (obtained from the Lawrence Berkeley National Labs). The resulting energies (keV) are stored in the file

MlineEnergies_Calculated.txt.

Table 27: M shell characteristic X-ray energies.

*Z	M5-N3	M5-N7	M5-N6	M5-O3	M4-N2	M4-N3	M4-N6	M4-O3	M4-O2	M3-N1	M3-N2	M3-O1	M3-O45	M3-N5	M3-N4	M3-N67	M2-N1	M2-O1	M2-O4	M2-N4	M1-N23	M1-O23
64	0.9186	1.1810	1.1810	1.1686	0.9359	0.9509	1.2133	1.2009	1.1939	1.1654	1.2580	1.5080	-99	1.4014	1.4023	1.5354	1.3094	1.6520	-99	1.5463	1.6025	1.8565
65	0.9570	1.2387	1.2334	1.2185	0.9545	0.9928	1.2692	1.2543	1.2482	1.2150	1.2886	1.5654	-99	1.4605	1.4605	1.6060	1.3720	1.7224	-99	1.6175	1.6648	1.9424
66	0.9994	1.2883	1.2846	1.2663	0.9995	1.0398	1.3250	1.3067	1.3067	1.2618	1.3425	1.6261	-99	1.5224	1.5224	1.6699	1.4278	1.7921	-99	1.6884	1.7337	2.0207
67	1.0428	1.3458	1.3424	1.3269	1.0485	1.0838	1.3834	1.3679	1.3612	1.3086	1.3975	1.6917	-99	1.5810	1.5810	1.7341	1.4906	1.8737	-99	1.7630	1.8022	2.1006
68	1.0888	1.4043	1.4008	1.3843	1.0868	1.1328	1.4448	1.4283	1.4216	1.3622	1.4458	1.7614	-99	1.6444	1.6444	1.8056	1.5562	1.9554	-99	1.8384	1.8638	2.1790
69	1.1354	1.4634	1.4643	1.4430	1.1291	1.1824	1.5113	1.4900	1.4832	1.4141	1.4991	1.8303	-99	1.7095	1.7095	1.8809	1.6191	2.0353	-99	1.9145	1.9478	2.2786
70	1.1883	1.5267	1.5255	1.5039	1.1873	1.2363	1.5735	1.5519	1.5457	1.4695	1.5613	1.8980	-99	1.7676	1.7588	1.9481	1.6925	2.1210	-99	1.9818	2.0338	2.3708
71	1.2298	1.5815	1.5801	1.5623	1.2266	1.2798	1.6301	1.6123	1.6054	1.5172	1.6116	1.9667	-99	1.8277	1.8179	2.0158	1.7572	2.2067	-99	2.0579	2.1052	2.4609
72	1.2813	1.6478	1.6461	1.6321	1.2778	1.3353	1.7001	1.6861	1.6780	1.5700	1.6698	2.0438	-99	1.8965	1.8880	2.0930	1.8270	2.3008	-99	2.1450	2.1916	2.5671
73	1.3341	1.7134	1.7115	1.7023	1.3296	1.3921	1.7695	1.7603	1.7508	1.6306	1.7306	2.1243	-99	1.9676	1.9561	2.1715	1.9056	2.3993	-99	2.2311	2.2759	2.6706
74	1.3854	1.7776	1.7754	1.7722	1.3816	1.4484	1.8384	1.8352	1.8267	1.6869	1.7906	2.2054	-99	2.0375	2.0251	2.2485	1.9809	2.4994	-99	2.3191	2.3630	2.7790
75	1.4362	1.8425	1.8401	1.8484	1.4303	1.5022	1.9061	1.9144	1.9034	1.7416	1.8483	2.2840	-99	2.1065	2.0931	2.3253	2.0566	2.5990	-99	2.4081	2.4493	2.8919

76	1.4893	1.9093	1.9066	1.9155	1.4819	1.5603	1.9776	1.9865	1.9730	1.7988	1.9079	2.3730	-99	2.1785	2.1639	2.4050	2.1338	2.7080	-99	2.4989	2.5391	2.9978
77	1.5442	1.9792	1.9762	1.9920	1.5382	1.6202	2.0522	2.0680	2.0530	1.8599	1.9732	2.4558	-99	2.2547	2.2391	2.4887	2.2179	2.8138	-99	2.5971	2.6372	3.1185
78	1.6026	2.0508	2.0475	2.0703	1.5929	1.6826	2.1275	2.1503	2.1367	1.9196	2.0359	2.5433	-99	2.3304	2.3134	2.5722	2.3016	2.9253	-99	2.6954	2.7318	3.2375
79	1.6597	2.1220	2.1184	2.1488	1.6483	1.7447	2.2034	2.2338	2.2168	1.9809	2.1003	2.6358	-99	2.4079	2.3898	2.6572	2.3859	3.0408	-99	2.7948	2.8305	3.3593
80	1.7184	2.1951	2.1910	2.2305	1.7048	1.8084	2.2810	2.3205	2.3019	2.0448	2.1668	2.7200	2.8383	2.4882	2.4688	2.7451	2.4768	3.1520	3.2694	2.9008	2.9336	3.4882
81	1.7795	2.2712	2.2668	2.3155	1.7645	1.8755	2.3628	2.4115	2.3904	2.1108	2.2365	2.8210	2.9434	2.5720	2.5513	2.8370	2.5698	3.2800	3.4013	3.0103	3.0390	3.6200
82	1.8405	2.3471	2.3423	2.4007	1.8241	1.9425	2.4443	2.5027	2.4796	2.1742	2.3041	2.9190	3.0466	2.6538	2.6317	2.9267	2.6622	3.4070	3.5333	3.1197	3.1483	3.7562
83	1.9012	2.4230	2.4177	2.4874	1.8828	2.0092	2.5257	2.5954	2.5690	2.2380	2.3718	3.0177	3.1517	2.7369	2.7130	3.0174	2.7570	3.5367	3.6691	3.2320	3.2570	3.8932
84	1.9780	2.4990	2.4990	2.5790	1.9470	2.0930	2.6140	2.6940	2.6660	2.3070	2.4510	3.1250	3.2710	2.8290	2.8020	3.1180	2.8590	3.6770	3.8230	3.3540	3.3710	4.0310
85	2.0470	2.5770	2.5770	2.6720	2.0230	2.1690	2.6990	2.7940	2.7610	2.3840	2.5400	3.2310	3.3860	2.9190	2.8930	3.2160	2.9660	3.8130	3.9680	3.4750	3.5040	4.1855
86	2.1240	2.6540	2.6540	2.7650	2.0930	2.2540	2.7840	2.8950	2.8580	2.4410	2.6090	3.3240	3.4900	2.9970	2.9710	3.3000	3.0620	3.9450	4.1110	3.5920	3.6335	4.3365
87	2.1900	2.7320	2.7320	2.8600	2.1560	2.3260	2.8680	2.9960	2.9540	2.5100	2.6830	3.4290	3.6050	3.0860	3.0600	3.3950	3.1740	4.0930	4.2690	3.7240	3.7570	4.4910
88	2.2260	2.8060	2.8060	2.9520	2.1900	2.3690	2.9490	3.0950	3.0480	2.5840	2.7340	3.5380	3.7240	3.1890	3.1560	3.4930	3.2820	4.2360	4.4220	3.8540	3.8535	4.6455
89	2.3290	2.9000	2.9000	3.0520	2.2900	2.4800	3.0510	3.2030	3.1550	2.6400	2.8290	3.6370	3.8290	3.2700	3.2340	3.5900	3.3870	4.3840	4.5760	3.9810	4.0170	4.8110
90	2.3656	2.9989	2.9896	3.1500	2.3230	2.5246	3.1486	3.3090	3.2620	2.7160	2.8780	3.7560	3.9571	3.3708	3.3339	3.7083	3.5000	4.5400	4.7375	4.1179	4.1148	4.9765
91	2.4350	3.0820	3.0710	3.2100	2.3870	2.6040	3.2400	3.3790	3.3790	2.7870	2.9500	3.8640	4.0800	3.4660	3.4310	3.8085	3.6140	4.6910	4.9070	4.2580	4.2515	5.1350
92	2.5090	3.1746	3.1638	3.3600	2.4570	2.6850	3.3398	3.5360	3.4710	2.8640	3.0320	3.9820	4.2045	3.5668	3.5247	3.9202	3.7430	4.8610	5.0792	4.4037	4.3910	5.3235

The electron binding energies (below) are stored in file

ElectronBindingEnergiesLBLabsZ64_92.txt.

All X-ray energies are in keV.

Table 28: Electron binding energies in keV (part I).

Elt	Z	K	L1	L2	L3	M1	M2	M3	M4	M5	N1	N2	N3	N4	N5	N6	N7
Gd	64	50.239	8.376	7.930	7.243	1.8810	1.6880	1.5440	1.2219	1.1896	0.3786	0.2860	0.2710	0.1418	0.1426	0.0086	0.0086
T	65	51.996	8.708	8.252	7.514	1.9680	1.7680	1.6110	1.2769	1.2411	0.3960	0.3224	0.2841	0.1505	0.1505	0.0077	0.0024
Dy	66	53.789	9.046	8.581	7.790	2.0470	1.8420	1.6760	1.3330	1.2926	0.4142	0.3335	0.2932	0.1536	0.1536	0.0080	0.0043
Ho	67	55.618	9.394	8.918	8.071	2.1280	1.9230	1.7410	1.3920	1.3510	0.4324	0.3435	0.3082	0.1600	0.1600	0.0086	0.0052
Er	68	57.486	9.751	9.264	8.358	2.2070	2.0060	1.8120	1.4530	1.4090	0.4498	0.3662	0.3202	0.1676	0.1676	0.0082	0.0047
Tm	69	59.390	10.116	9.617	8.648	2.3070	2.0900	1.8850	1.5150	1.4680	0.4709	0.3859	0.3326	0.1755	0.1755	0.0037	0.0046
Y	70	61.332	10.486	9.978	8.944	2.3980	2.1730	1.9500	1.5760	1.5280	0.4805	0.3887	0.3397	0.1912	0.1824	0.0025	0.0013
Lu	71	63.314	10.870	10.349	9.244	2.4910	2.2640	2.0240	1.6390	1.5890	0.5068	0.4124	0.3592	0.2061	0.1963	0.0089	0.0075

Hf	72	65.351	11.271	10.739	9.561	2.6010	2.3650	2.1080	1.7160	1.6620	0.5380	0.4382	0.3807	0.2200	0.2115	0.0159	0.0142
Ta	73	67.416	11.682	11.136	9.881	2.7080	2.4690	2.1940	1.7930	1.7350	0.5634	0.4634	0.4009	0.2379	0.2264	0.0235	0.0216
W	74	69.525	12.100	11.544	10.207	2.8200	2.5750	2.2810	1.8720	1.8090	0.5941	0.4904	0.4236	0.2559	0.2435	0.0336	0.0314
Re	75	71.676	12.527	11.959	10.535	2.9320	2.6820	2.3670	1.9490	1.8830	0.6254	0.5187	0.4468	0.2739	0.2605	0.0429	0.0405
Os	76	73.871	12.968	12.385	10.871	3.0490	2.7920	2.4570	2.0310	1.9600	0.6582	0.5491	0.4707	0.2931	0.2785	0.0534	0.0507
Ir	77	76.111	13.419	12.824	11.215	3.1740	2.9090	2.5510	2.1160	2.0400	0.6911	0.5778	0.4958	0.3119	0.2963	0.0638	0.0608
Pt	78	78.395	13.880	13.273	11.564	3.2960	3.0270	2.6450	2.2020	2.1220	0.7254	0.6091	0.5194	0.3316	0.3146	0.0745	0.0712
Au	79	80.725	14.353	13.734	11.919	3.4250	3.1480	2.7430	2.2910	2.2060	0.7621	0.6427	0.5463	0.3532	0.3351	0.0876	0.0840
Hg	80	83.102	14.839	14.209	12.284	3.5620	3.2790	2.8470	2.3850	2.2950	0.8022	0.6802	0.5766	0.3782	0.3588	0.1040	0.0999
Tl	81	85.530	15.347	14.698	12.658	3.7040	3.4160	2.9570	2.4850	2.3890	0.8462	0.7205	0.6095	0.4057	0.3850	0.1222	0.1178
P	82	88.005	15.861	15.200	13.035	3.8510	3.5540	3.0660	2.5860	2.4840	0.8918	0.7619	0.6435	0.4343	0.4122	0.1417	0.1369
Bi	83	90.524	16.388	15.711	13.419	3.9990	3.6960	3.1770	2.6880	2.5800	0.9390	0.8052	0.6788	0.4640	0.4401	0.1623	0.1570
Po	84	93.105	16.939	16.244	13.814	4.1490	3.8540	3.3020	2.7980	2.6830	0.9950	0.8510	0.7050	0.5000	0.4730	0.1840	0.1840
At	85	95.730	17.493	16.785	14.214	4.3170	4.0080	3.4260	2.9090	2.7870	1.0420	0.8860	0.7400	0.5330	0.5070	0.2100	0.2100
Rn	86	98.404	18.049	17.337	14.619	4.4820	4.1590	3.5380	3.0220	2.8920	1.0970	0.9290	0.7680	0.5670	0.5410	0.2380	0.2380
Fr	87	101.137	18.639	17.907	15.031	4.6520	4.3270	3.6630	3.1360	3.0000	1.1530	0.9800	0.8100	0.6030	0.5770	0.2680	0.2680
Ra	88	103.922	19.237	18.484	15.444	4.8220	4.4900	3.7920	3.2480	3.1050	1.2080	1.0580	0.8790	0.6360	0.6030	0.2990	0.2990
Ac	89	106.755	19.840	19.083	15.871	5.0020	4.6560	3.9090	3.3700	3.2190	1.2690	1.0800	0.8900	0.6750	0.6390	0.3190	0.3190
Th	90	109.651	20.472	19.693	16.300	5.1820	4.8300	4.0460	3.4910	3.3320	1.3300	1.1680	0.9664	0.7121	0.6752	0.3424	0.3331
Pa	91	112.601	21.105	20.314	16.733	5.3670	5.0010	4.1740	3.6110	3.4420	1.3870	1.2240	1.0070	0.7430	0.7080	0.3710	0.3600
U	92	115.606	21.757	20.948	17.166	5.5480	5.1820	4.3030	3.7280	3.5520	1.4390	1.2710	1.0430	0.7783	0.7362	0.3882	0.3774

Table 29: Electron binding energies in keV (part II).

Elt	Z	O1	O2	O3	O4	O5	P1	P2	P3
Gd	64	0.0360	0.0280	0.0210	-99	-99	-99	-99	-99
T	65	0.0456	0.0287	0.0226	-99	-99	-99	-99	-99
Dy	66	0.0499	0.0263	0.0263	-99	-99	-99	-99	-99
Ho	67	0.0493	0.0308	0.0241	-99	-99	-99	-99	-99
Er	68	0.0506	0.0314	0.0247	-99	-99	-99	-99	-99
Tm	69	0.0547	0.0318	0.0250	-99	-99	-99	-99	-99
Y	70	0.0520	0.0303	0.0241	-99	-99	-99	-99	-99
Lu	71	0.0573	0.0336	0.0267	-99	-99	-99	-99	-99
Hf	72	0.0642	0.0380	0.0299	-99	-99	-99	-99	-99

Ta	73	0.0697	0.0422	0.0327	-99	-99	-99	-99	-99
W	74	0.0756	0.0453	0.0368	-99	-99	-99	-99	-99
Re	75	0.0830	0.0456	0.0346	-99	-99	-99	-99	-99
Os	76	0.0840	0.0580	0.0445	-99	-99	-99	-99	-99
Ir	77	0.0952	0.0630	0.0480	-99	-99	-99	-99	-99
Pt	78	0.1017	0.0653	0.0517	-99	-99	-99	-99	-99
Au	79	0.1072	0.0742	0.0572	-99	-99	-99	-99	-99
Hg	80	0.1270	0.0831	0.0645	0.0096	0.0078	-99	-99	-99
Tl	81	0.1360	0.0946	0.0735	0.0147	0.0125	-99	-99	-99
P	82	0.1470	0.1064	0.0833	0.0207	0.0181	-99	-99	-99
Bi	83	0.1593	0.1190	0.0926	0.0269	0.0238	-99	-99	-99
Po	84	0.1770	0.1320	0.1040	0.0310	0.0310	-99	-99	-99
At	85	0.1950	0.1480	0.1150	0.0400	0.0400	-99	-99	-99
Rn	86	0.2140	0.1640	0.1270	0.0480	0.0480	0.0260	-99	-99
Fr	87	0.2340	0.1820	0.1400	0.0580	0.0580	0.0340	0.0150	0.0150
Ra	88	0.2540	0.2000	0.1530	0.0680	0.0680	0.0440	0.0190	0.0190
Ac	89	0.2720	0.2150	0.1670	0.0800	0.0800	-99	-99	-99
Th	90	0.2900	0.2290	0.1820	0.0925	0.0854	0.0414	0.0245	0.0166
Pa	91	0.3100	0.2320	0.2320	0.0940	0.0940	-99	-99	-99
U	92	0.3210	0.2570	0.1920	0.1028	0.0942	0.0439	0.0268	0.0168

11 Appendix 4: Miscellaneous input files

Aside from the files specified in Appendix 1 to 3, four additional files are required:

- ***dset4*** – this is a file that is used by PIXAN.
- ***GEOPIXEKabratiosylds16Nov10.txt*** – the GEOPIXE (Ryan et al., 1990) input files.
- ***detector_configuration.txt*** – in this file the detector parameters are specified.

File ***dset4*** contains the information: NAME, UI, Z, ALFAK, EXR, A, WK, where for each element designated NAME, this file contains parameters useful for calculating the X-ray yield by PIXAN. UI is the adsorption edge, A is the element atomic number, ALFAK is the ratio of the reference line to the sum of all lines, EXR is the X-ray energy of the reference line (either Kα or Lα), A is the element atomic weight and ωK is the element fluorescence yield. This file is read in and the quantities ALFAK and ω_K are replaced by the calculated values.

The file ***detector_configuration.txt***, has been included such that the detector efficiency can be calculated for each of the X-ray energies and contains the following information:

- Line 1: detector distance (mm)
- Line 2: Be window, Si dead layer, Gold contact, Thickness, FG, Ice thickness all in microns
- Line 3: filter type 1 for Mylar, 2 for Perspex 3 for Kapton, 4 for Be, 5 for Graphite, 5 graphite, 6 Al, 7 He, 8 Air.
- Line 4: filter thickness (mm) and hole fraction

12 Appendix 5: Output files

The file "***results.csv***" is always generated. It contains a list of the selected options together with a table of relative intensities for each of the K, L and M shells. The files "***xsectionresults.csv***" and "***wbar.csv***" are also generated which contain the line production cross sections and the effective fluorescence yields respectively. The file "***wbar.csv***" also contains the ionisation cross sections and the X-ray production cross-sections for each subshell.

Two additional files "***Lshell_Spectrum.csv***" and "***Mshell_Spectrum.csv***" are optionally generated and contain Gaussian spectral lines for plotting later and the efficiency corrected total spectra for each sub-shell are produced in files "***Lsubshell.csv***" and "***Msubshell.csv***".

12.1 Calculated Intensities – file `results.csv`

The output file "***results.csv***" contains four main sections (illustrated with options specified in section 5.1):

- The options selected for the run
- The K shell intensities
- The L shell intensities
- The M shell intensities

12.1.1 Run options

Calculating for Protons

K shell options

Krause for wk
Salem for K shell emission rates

L shell options Campbell for wL
Scofield for emission rate
Bambynek for wL bar option
M shell options
DF for emission reate
DF for fluorescence yield
Exp for wM_bar
Bambynek for Super C-K transitions
Write Calculated values in dset2

12.1.2 K shell X-ray line intensities for 3 MeV protons

The K shell intensities are generated relative to $(\alpha_1+\alpha_2) = 100$. The average fluorescence yield ω_K is taken from the experimental compilations of Krause 1979.

Table 30: Sample K shell calculates intensities for 3 MeV protons.

Z	Kα1	Kα2	Kα3	Kβ1	Kβ2	Kβ3	Kβ4	Kβ5	Kβ/Kα	Kα/Ktot	ωK
6	67.141	32.859	0	0	0	0	0	0	0	1.00	0.0028
7	67.101	32.899	0	0	0	0	0	0	0	1.00	0.0052
8	67.060	32.940	0	0	0	0	0	0	0	1.00	0.0083
9	67.022	32.978	0	0	0	0	0	0	0	1.00	0.0130
10	66.984	33.016	0	0	0	0	0	0	0	1.00	0.0180
11	66.943	33.057	0	0	0	0	0	0	0	1.00	0.0230
12	66.903	33.097	0	0	0	0	0	0	0	1.00	0.0300
13	66.863	33.137	0	0.826	0	0.722	0	0	0.0155	0.9848	0.0390
14	66.823	33.177	0	1.651	0	0.835	0	0	0.0249	0.9757	0.0500
15	66.785	33.215	0	2.738	0	1.382	0	0	0.0412	0.9604	0.0630

16	66.747	33.253	0	3.825	0	1.929	0	0	0.0575	0.9456	0.0780
17	66.707	33.293	0	5.637	0	2.848	0	0	0.0849	0.9218	0.0970
18	66.667	33.333	0	7.447	0	3.767	0	0	0.1121	0.8992	0.1180
19	66.622	33.378	0	8.251	0	4.177	0	0	0.1243	0.8895	0.1400
20	66.578	33.422	0	9.055	0	4.587	0	0	0.1364	0.8800	0.1630
21	66.556	33.444	0	9.118	0	4.622	0	0	0.1374	0.8792	0.1880
22	66.534	33.466	0	9.182	0	4.657	0	0	0.1384	0.8784	0.2140
23	66.512	33.489	0	9.056	0	4.596	0	0	0.1365	0.8799	0.2430
24	66.489	33.511	0	8.930	0	4.535	0	0	0.1346	0.8813	0.2750
25	66.445	33.555	0	8.794	0	4.468	0	0	0.1326	0.8829	0.3080
26	66.401	33.599	0	8.659	0	4.402	0	0	0.1306	0.8845	0.3400
27	66.357	33.643	0	8.550	0	4.353	0	0	0.1290	0.8857	0.3730
28	66.313	33.687	0	8.442	0	4.304	0	0	0.1275	0.8870	0.4060
29	66.269	33.731	0	8.499	0	4.334	0	0	0.1283	0.8863	0.4400
30	66.225	33.775	0	8.556	0	4.364	0	0	0.1292	0.8856	0.4740
31	66.159	33.841	0	8.760	0.1654	4.472	0	0	0.1340	0.8819	0.5070
32	66.094	33.906	0	8.962	0.3305	4.580	0	0	0.1387	0.8782	0.5350
33	66.050	33.950	0	9.237	0.4789	4.723	0	0	0.1444	0.8738	0.5620
34	66.007	33.993	0	9.512	0.6271	4.865	0	0	0.1500	0.8695	0.5890
35	65.963	34.037	0	9.878	0.9400	5.056	0	0	0.1587	0.8630	0.6180
36	65.920	34.080	0	10.244	1.2525	5.247	0	0	0.1674	0.8566	0.6425
37	65.855	34.146	0	10.240	1.6134	5.252	0	0	0.1711	0.8539	0.6670
38	65.790	34.211	0	10.237	1.9737	5.257	0	0	0.1747	0.8513	0.6900
39	65.725	34.275	0	10.454	2.2018	5.373	0	0	0.1803	0.8473	0.7100
40	65.660	34.340	0	10.670	2.4294	5.489	0	0	0.1859	0.8433	0.7300
41	65.617	34.383	0	10.840	2.5591	5.581	0	0	0.1898	0.8405	0.7470
42	65.574	34.426	0	11.010	2.6885	5.672	0	0	0.1937	0.8377	0.7650
43	65.531	34.469	0	11.173	2.8178	5.763	0	0	0.1975	0.8350	0.7795
44	65.488	34.512	0	11.336	2.9470	5.855	0	0	0.2014	0.8324	0.7940
45	65.445	34.555	0	11.486	3.0432	5.936	0	0	0.2046	0.8301	0.8080
46	65.402	34.598	0	11.635	3.1393	6.017	0	0	0.2079	0.8279	0.8200
47	65.338	34.662	0	11.575	3.2996	5.995	0	0	0.2087	0.8273	0.8310
48	65.274	34.726	0	11.514	3.4595	5.973	0	0	0.2095	0.8268	0.8430
49	65.232	34.768	0	11.735	3.5225	6.089	0	0	0.2135	0.8241	0.8530
50	65.189	34.811	0	11.956	3.5854	6.206	0	0	0.2175	0.8214	0.8620
51	65.125	34.875	0	12.048	3.6796	6.255	0	0	0.2198	0.8198	0.8700

52	65.062	34.938	0	12.141	3.7736	6.305	0	0	0.2222	0.8182	0.8770
53	65.020	34.981	0	12.237	3.9662	6.346	0	0	0.2255	0.8160	0.8840
54	64.977	35.023	0	12.333	4.1585	6.387	0	0	0.2288	0.8138	0.8910
55	64.893	35.107	0	12.333	4.3478	6.389	0	0	0.2307	0.8125	0.8970
56	64.809	35.191	0	12.333	4.5366	6.390	0	0	0.2326	0.8113	0.9020
57	64.746	35.254	0	12.328	4.7264	6.387	0	0	0.2344	0.8101	0.9070
58	64.683	35.317	0	12.322	4.9159	6.384	0	0	0.2362	0.8089	0.9120
59	64.620	35.380	0.0036	12.284	5.1373	6.365	0	0	0.2379	0.8078	0.9170
60	64.558	35.442	0.0071	12.247	5.3583	6.346	0	0	0.2395	0.8068	0.9210
61	64.495	35.505	0.0081	12.241	5.4499	6.337	0	0	0.2403	0.8063	0.9250
62	64.433	35.567	0.0090	12.236	5.5412	6.327	0	0	0.2410	0.8058	0.9290
63	64.350	35.650	0.0100	12.288	5.6049	6.355	0.0273	0.0972	0.2437	0.8041	0.9320
64	64.267	35.733	0.0109	12.339	5.6684	6.382	0.0546	0.1941	0.2464	0.8023	0.9350
65	64.185	35.815	0.0122	12.516	5.6579	6.473	0.0568	0.2073	0.2491	0.8006	0.9380
66	64.103	35.897	0.0135	12.692	5.6474	6.564	0.0590	0.2199	0.2518	0.7989	0.9410
67	64.021	35.980	0.0150	12.804	5.6050	6.626	0.0602	0.2330	0.2532	0.7979	0.9440
68	63.939	36.061	0.0166	12.916	5.5627	6.688	0.0614	0.2462	0.2547	0.7970	0.9470
69	63.877	36.123	0.0179	13.063	5.5254	6.765	0.0639	0.2581	0.2567	0.7957	0.9490
70	63.816	36.184	0.0191	13.210	5.4882	6.841	0.0664	0.2699	0.2587	0.7945	0.9510
71	63.715	36.285	0.0210	13.348	5.4094	6.913	0.0701	0.2823	0.2602	0.7935	0.9530
72	63.613	36.387	0.0229	13.486	5.3308	6.985	0.0738	0.2939	0.2616	0.7926	0.9550
73	63.532	36.468	0.0251	13.596	5.3526	7.043	0.0775	0.3069	0.2637	0.7913	0.9570
74	63.452	36.548	0.0273	13.706	5.3744	7.100	0.0812	0.3198	0.2657	0.7901	0.9580
75	63.371	36.629	0.0298	13.878	5.3961	7.196	0.0862	0.3321	0.2688	0.7881	0.9590
76	63.291	36.709	0.0323	14.051	5.4177	7.291	0.0905	0.3443	0.2719	0.7863	0.9610
77	63.231	36.769	0.0360	14.164	5.5327	7.357	0.0961	0.3566	0.2750	0.7843	0.9620
78	63.171	36.829	0.0398	14.277	5.6475	7.423	0.1017	0.3689	0.2781	0.7824	0.9630
79	63.072	36.928	0.0438	14.317	5.7900	7.446	0.1072	0.3810	0.2803	0.7811	0.9640
80	62.972	37.028	0.0479	14.358	5.9320	7.469	0.1134	0.3929	0.2825	0.7797	0.9650
81	62.873	37.127	0.0525	14.335	6.1050	7.463	0.1201	0.4049	0.2841	0.7787	0.9660
82	62.775	37.225	0.0571	14.313	6.2775	7.458	0.1268	0.4168	0.2857	0.7778	0.9670
83	62.696	37.304	0.0633	14.295	6.4483	7.455	0.1342	0.4295	0.2874	0.7767	0.9680
84	62.617	37.383	0.0701	14.277	6.6187	7.452	0.1415	0.4415	0.2891	0.7757	0.9680
85	62.520	37.481	0.0763	14.255	6.7584	7.446	0.1494	0.4539	0.2904	0.7750	0.9690
86	62.422	37.578	0.0824	14.232	6.8976	7.441	0.1573	0.4669	0.2917	0.7742	0.9690
87	62.305	37.695	0.0903	14.268	7.0000	7.467	0.1657	0.4760	0.2935	0.7731	0.9700

88	62.189	37.811	0.0983	14.304	7.1020	7.494	0.1741	0.4851	0.2953	0.7720	0.9700
89	62.093	37.908	0.1062	14.343	7.1748	7.523	0.1838	0.4986	0.2969	0.7711	0.9710
90	61.996	38.004	0.1147	14.383	7.2474	7.551	0.1940	0.5115	0.2985	0.7701	0.9710
91	61.881	38.119	0.1238	14.418	7.3144	7.584	0.2042	0.5229	0.3001	0.7692	0.9720
92	61.767	38.234	0.1328	14.453	7.3811	7.616	0.2143	0.5343	0.3016	0.7683	0.9720
93	61.652	38.348	0.1418	14.427	7.4476	7.611	0.2244	0.5456	0.3021	0.7680	0.9730
94	61.539	38.462	0.1508	14.400	7.5138	7.606	0.2345	0.5569	0.3027	0.7677	0.9730
95	61.406	38.594	0.1597	14.369	7.5775	7.596	0.2444	0.5680	0.3031	0.7674	0.9740
96	61.275	38.726	0.1685	14.338	7.6409	7.586	0.2543	0.5790	0.3035	0.7672	0.9740
97	61.087	38.913	0.1772	14.417	7.6970	7.642	0.2639	0.5895	0.3055	0.7660	0.9750
98	60.901	39.099	0.1857	14.495	7.7527	7.698	0.2734	0.5999	0.3076	0.7648	0.9750
99	60.790	39.210	0.1945	14.529	7.8176	7.730	0.2833	0.6109	0.3091	0.7639	0.9750
100	60.680	39.320	0.2033	14.563	7.8823	7.761	0.2931	0.6220	0.3106	0.7630	0.9760

12.1.3 L shell intensities

The L shell intensities are generated relative to $(\alpha_1+\alpha_2) = 100$.

Table 31: Sample L shell calculated intensities for 3 MeV protons.

Energy= 3.00 MeVp																			
Z	**Ll**	**Lα1**	**Lα2**	**Lη**	**Lβ1**	**Lβ215**	**Lβ3**	**Lβ4**	**Lβ5**	**Lβ6**	**Lγ1**	**Lγ2**	**Lγ3**	**Lγ44**	**Lγ5**	**Lγ6**	**L1P23**	**Lα/Ltot**	**ωL**
25	10.804	89.738	10.262	4.3570	41.935	0	2.193	1.167	0	0.9647	0	0	0	0	0.3913	0	0	0.6180	0.0037
26	9.452	89.734	10.266	3.8727	42.792	0	1.832	0.978	0	0.8211	0	0	0	0	0.3385	0	0	0.6247	0.0048
28	6.747	89.726	10.274	2.7641	43.392	0	1.454	0.785	0	0.5339	0	0	0	0	0.2200	0	0	0.6415	0.0075
29	6.213	89.734	10.266	2.5531	43.770	0	1.316	0.714	0	0.5124	0	0	0	0	0.2118	0	0	0.6440	0.0091
30	5.679	89.742	10.258	2.6066	49.227	0	1.489	0.812	0	0.4909	0	0	0	0	0.2269	0	0	0.6229	0.0110
32	4.610	89.759	10.242	1.9661	46.591	0	1.994	1.099	0	0.4470	0	0.0269	0.049	0	0.1934	0	0	0.6370	0.0154
33	4.469	89.767	10.233	1.8859	46.416	0	2.036	1.127	0	0.4659	0	0.0521	0.094	0	0.1987	0	0	0.6380	0.0179
34	4.327	89.775	10.225	1.8088	46.321	0	2.099	1.168	0	0.4857	0	0.0791	0.143	0	0.2043	0	0	0.6384	0.0206
35	4.185	89.783	10.217	1.7496	46.681	0	2.108	1.179	0	0.5046	0	0.1050	0.189	0	0.2119	0	0	0.6373	0.0235
36	4.043	89.791	10.209	1.5289	42.588	0	2.536	1.425	0	0.5235	0	0.1570	0.282	0	0.1989	0	0	0.6524	0.0266
37	3.978	89.795	10.205	1.4214	40.578	0	3.619	2.046	0	0.5442	0	0.2481	0.444	0	0.1952	0	0	0.6533	0.0300
38	3.913	89.799	10.201	1.3499	39.527	0	3.888	2.210	0	0.5657	0	0.2923	0.521	0	0.1957	0	0	0.6559	0.0336
39	3.849	89.803	10.197	1.3169	39.582	0.351	4.042	2.311	0	0.5864	0.133	0.3308	0.588	0	0.2019	0	0	0.6524	0.0373

40	3.784	89.807	10.193	1.2217	37.705	1.585	4.154	2.389	0.0834	0.6071	0.598	0.3676	0.651	0	0.1976	0.0272	0	0.6520	0.0413
41	3.759	89.809	10.192	1.1282	35.368	2.819	4.237	2.452	0.0709	0.6233	1.002	0.3894	0.685	0	0.1882	0.0216	0	0.6547	0.0455
42	3.735	89.811	10.189	1.1038	35.152	4.052	4.293	2.501	0.0584	0.6386	1.435	0.4091	0.716	0	0.1902	0.0176	0	0.6481	0.0498
43	3.711	89.813	10.187	1.0851	35.116	5.286	4.381	2.569	0.0458	0.6538	1.872	0.4324	0.752	0	0.1928	0.0137	0	0.6406	0.0544
44	3.687	89.815	10.185	1.0490	34.506	6.521	4.373	2.580	0.0333	0.6700	2.271	0.4465	0.772	0	0.1925	0.0096	0	0.6365	0.0591
45	3.698	89.815	10.185	1.0416	34.501	7.760	4.528	2.692	0.0432	0.6835	2.707	0.4779	0.821	0	0.1942	0.0123	0	0.6283	0.0640
46	3.708	89.815	10.185	1.0327	34.448	9.000	4.542	2.721	0.0531	0.6970	3.138	0.4951	0.846	0	0.1960	0.0149	0	0.6215	0.0692
47	3.718	89.815	10.185	1.0255	34.435	10.239	4.784	2.887	0.0630	0.7104	3.573	0.5380	0.914	0	0.1980	0.0176	0	0.6131	0.0744
48	3.728	89.815	10.185	1.0336	34.953	11.478	4.908	2.984	0.0729	0.7239	4.069	0.5688	0.960	0	0.2027	0.0205	0	0.6035	0.0799
49	3.668	89.823	10.177	1.0213	34.799	12.337	4.957	3.024	0.0839	0.7419	4.357	0.5961	1.001	0	0.2050	0.0233	0	0.5995	0.0855
50	3.609	89.831	10.169	1.1962	41.079	13.196	13.399	8.200	0.0952	0.7609	5.505	1.6694	2.790	0.1391	0.2456	0.0310	0	0.5211	0.0914
51	3.660	89.831	10.169	1.1783	40.717	13.877	13.181	8.133	0.1042	0.7806	5.742	1.6935	2.813	0.2645	0.2472	0.0333	0	0.5197	0.0973
52	3.712	89.831	10.169	1.1518	40.050	14.557	12.902	8.025	0.1141	0.7995	5.929	1.7075	2.821	0.3838	0.2467	0.0353	0	0.5197	0.1035
53	3.764	89.831	10.169	1.1528	40.322	15.238	12.531	7.857	0.1240	0.8193	6.253	1.7071	2.805	0.4941	0.2520	0.0382	0	0.5172	0.1098
54	3.815	89.831	10.169	1.1391	40.096	15.918	12.271	7.755	0.1330	0.8390	6.500	1.7192	2.811	0.6025	0.2542	0.0405	0	0.5157	0.1164
55	3.840	89.827	10.173	1.1387	40.264	16.497	12.031	7.670	0.1455	0.8570	6.768	1.7360	2.819	0.6845	0.2581	0.0439	0	0.5135	0.1231
56	3.864	89.823	10.177	1.1247	39.967	17.075	12.009	7.722	0.1581	0.8758	6.958	1.7833	2.877	0.7770	0.2590	0.0468	0	0.5115	0.1299
57	3.895	89.823	10.177	1.1071	39.495	17.206	11.741	7.624	0.1581	0.8884	6.941	1.7735	2.837	0.7544	0.2567	0.0458	0	0.5136	0.1370
58	3.926	89.823	10.177	1.1022	39.478	17.336	11.585	7.594	0.1590	0.9000	7.002	1.7795	2.822	0.7391	0.2574	0.0458	0	0.5135	0.1442
59	3.957	89.823	10.177	1.1046	39.705	17.466	11.345	7.508	0.1599	0.9126	7.106	1.7715	2.786	0.7187	0.2593	0.0457	0	0.5132	0.1517
60	3.987	89.823	10.177	1.1062	39.922	17.596	10.888	7.274	0.1599	0.9252	7.210	1.7280	2.696	0.6849	0.2615	0.0455	0	0.5142	0.1593
61	4.024	89.823	10.177	1.0988	39.768	17.677	10.599	7.154	0.1608	0.9378	7.228	1.7080	2.640	0.6614	0.2609	0.0449	0	0.5156	0.1672
62	4.062	89.823	10.177	1.0969	39.817	17.758	10.301	7.025	0.1608	0.9494	7.282	1.6852	2.580	0.6376	0.2616	0.0446	0	0.5164	0.1753
63	4.104	89.821	10.179	1.0877	39.567	17.809	9.809	6.765	0.1608	0.9620	7.270	1.6290	2.469	0.6026	0.2603	0.0439	0	0.5194	0.1835
64	4.147	89.817	10.183	1.0806	39.381	17.858	9.433	6.578	0.1617	0.9736	7.269	1.5898	2.386	0.5751	0.2595	0.0433	0	0.5216	0.1921
65	4.189	89.815	10.185	1.0726	39.174	17.909	9.115	6.426	0.1626	0.9862	7.263	1.5586	2.316	0.5514	0.2585	0.0427	0	0.5235	0.2008
66	4.240	89.813	10.187	1.0662	38.985	17.943	8.720	6.226	0.1626	0.9996	7.256	1.5142	2.224	0.5246	0.2577	0.0421	0	0.5259	0.2098
67	4.291	89.812	10.188	1.0420	38.128	17.977	8.285	5.990	0.1635	1.0131	7.124	1.4609	2.122	0.4956	0.2524	0.0412	0	0.5308	0.2191
68	4.342	89.810	10.190	1.0232	37.479	18.011	7.812	5.718	0.1644	1.0274	7.030	1.3981	2.008	0.4646	0.2489	0.0401	0	0.5354	0.2286
69	4.393	89.809	10.192	1.0089	36.981	18.044	7.816	5.792	0.1652	1.0409	6.963	1.4197	2.017	0.4622	0.2459	0.0392	0	0.5365	0.2383
70	4.445	89.807	10.193	0.9912	36.373	18.078	7.297	5.473	0.1661	1.0543	6.875	1.3448	1.891	0.4291	0.2422	0.0382	0	0.5414	0.2484
71	4.505	89.805	10.196	0.9827	36.064	18.264	6.865	5.224	0.1742	1.0732	6.895	1.2915	1.794	0.4279	0.2416	0.0393	0	0.5439	0.2587
72	4.566	89.801	10.199	0.9657	35.427	18.448	6.404	4.944	0.3152	1.0929	6.852	1.2294	1.688	0.4218	0.2384	0.0879	0	0.5474	0.2693
73	4.626	89.799	10.201	0.9470	34.740	18.633	5.939	4.651	0.5945	1.1117	6.795	1.1629	1.579	0.4122	0.2352	0.1932	0	0.5506	0.2802
74	4.694	89.796	10.204	0.9275	33.985	18.832	5.551	4.416	0.8737	1.1341	6.729	1.1121	1.491	0.4024	0.2318	0.2936	0	0.5535	0.2914
75	4.762	89.795	10.205	0.8784	32.141	19.032	4.896	3.956	1.1539	1.1566	6.441	1.0032	1.328	0.3702	0.2208	0.3764	0	0.5627	0.3029
76	4.829	89.792	10.208	0.8705	31.817	19.232	4.405	3.614	1.4340	1.1790	6.453	0.9226	1.206	0.3467	0.2202	0.4706	0	0.5650	0.3147
77	4.897	89.791	10.209	0.8624	31.485	19.431	3.969	3.306	1.7132	1.2014	6.461	0.8493	1.097	0.3247	0.2194	0.5629	0	0.5670	0.3268

78	4.973	89.789	10.211	0.8433	30.732	19.583	2.786	2.364	1.9538	1.2256	6.365	0.6106	0.778	0.2405	0.2157	0.6272	0	0.5770	0.3393
79	5.050	89.788	10.212	0.8284	30.135	19.735	2.576	2.226	2.1935	1.2489	6.298	0.5781	0.727	0.2341	0.2131	0.6916	0	0.5789	0.3520
80	5.125	89.786	10.214	0.8194	29.754	19.888	2.415	2.124	2.4332	1.2732	6.275	0.5544	0.689	0.2304	0.2121	0.7581	0	0.5795	0.3650
81	5.201	89.784	10.216	0.8110	29.395	20.040	2.240	2.006	2.6738	1.2965	6.255	0.5259	0.645	0.2239	0.2111	0.8236	0	0.5802	0.3784
82	5.277	89.783	10.217	0.7970	28.836	20.192	2.075	1.891	2.9134	1.3207	6.191	0.4980	0.604	0.2169	0.2085	0.8809	0.0076	0.5817	0.3920
83	5.364	89.780	10.220	0.7883	28.438	20.365	1.924	1.790	3.1199	1.3476	6.169	0.4742	0.565	0.2103	0.2073	0.9305	0.0141	0.5824	0.4059
84	5.451	89.779	10.221	0.7764	27.929	20.537	1.765	1.677	3.3272	1.3745	6.121	0.4463	0.523	0.2013	0.2053	0.9747	0.0194	0.5837	0.4201
85	5.537	89.776	10.224	0.7632	27.385	20.709	1.612	1.563	3.5327	1.4014	6.062	0.4180	0.482	0.1916	0.2029	1.0152	0.0236	0.5851	0.4345
86	5.624	89.775	10.225	0.7503	26.845	20.882	1.491	1.475	3.7400	1.4283	6.003	0.3962	0.450	0.1843	0.2005	1.0534	0.0272	0.5863	0.4492
87	5.721	89.773	10.227	0.7378	26.293	21.041	1.373	1.394	3.8935	1.4570	5.936	0.3764	0.419	0.1768	0.1982	1.0767	0.0275	0.5878	0.4641
88	5.817	89.772	10.228	0.6267	22.254	21.202	1.266	1.318	4.0478	1.4857	5.073	0.3577	0.390	0.1696	0.1691	0.9491	0.0275	0.6055	0.4792
89	5.914	89.771	10.229	0.7102	25.124	21.361	1.163	1.240	4.2013	1.5153	5.782	0.3381	0.362	0.1616	0.1924	1.1145	0.0273	0.5910	0.4945
90	6.011	89.769	10.231	0.6961	24.528	21.520	1.078	1.178	4.3556	1.5440	5.699	0.3227	0.339	0.1555	0.1896	1.1303	0.0272	0.5925	0.5099
91	6.107	89.768	10.232	0.6486	22.774	21.681	0.994	1.112	4.5100	1.5727	5.341	0.3059	0.315	0.1485	0.1776	1.0881	0.0268	0.5995	0.5255
92	6.204	89.767	10.233	0.6320	22.106	21.840	0.919	1.051	4.6634	1.6014	5.233	0.2903	0.294	0.1419	0.1738	1.0940	0.0264	0.6014	0.5412
93	6.309	89.763	10.237	0.6164	21.464	21.987	0.985	1.159	4.7610	1.6328	5.126	0.3211	0.319	0.1573	0.1702	1.0867	0.0292	0.6020	0.5569
94	6.414	89.759	10.242	0.5275	18.285	22.135	0.926	1.120	4.8586	1.6632	4.405	0.3111	0.303	0.1528	0.1463	0.9466	0.0282	0.6164	0.5727
95	6.519	89.755	10.246	0.5210	17.976	22.282	0.889	1.104	4.9562	1.6946	4.368	0.3077	0.294	0.1514	0.1451	0.9511	0.0279	0.6166	0.5884
96	6.625	89.751	10.250	0.5131	17.626	22.429	0.857	1.092	5.0539	1.7250	4.320	0.3050	0.286	0.1504	0.1435	0.9527	0.0277	0.6169	0.6042

12.1.4 M shell X-ray line intensities for 3 MeV protons

The M shell intensities are generated relative to $(\alpha_1+\alpha_2) = 100$. The following two tables appear side by side in the output file.

Table 32: Sample M shell calculated intensities for 3 MeV protons (part I).

Z	M5-N3	M5-N7	M5-N6	M5-O3	M4-N2	M4-N3	M4-N6	M4-O3	M4-O2	M3-N1	M3-N2	M3-O1	M3-O45	M3-N5
	Mξ	Mα				Mδ	Mβ							
67	8.2571	94.3663	5.6337	0.4624	2.5970	0.3796	33.5970	0.0202	0.1512	0.9280	0.0018	0.1368	0.0000	3.5804
68	7.6055	94.4778	5.5222	0.4346	2.3453	0.3373	32.1279	0.0177	0.1382	0.9153	0.0018	0.1369	0.0000	3.5285
69	6.9523	94.5895	5.4105	0.4067	2.1169	0.2989	30.8134	0.0154	0.1263	0.8976	0.0017	0.1363	0.0000	3.4591
70	6.4205	94.6970	5.3030	0.3835	1.9235	0.2678	29.5915	0.0133	0.1154	0.8891	0.0017	0.1369	0.0000	3.4235
71	5.8874	94.8047	5.1953	0.3603	1.7528	0.2402	28.5943	0.0114	0.1058	0.8858	0.0017	0.1384	0.0000	3.4097
72	5.4427	94.9037	5.0963	0.3369	1.5986	0.2160	27.5147	0.0110	0.0963	0.8824	0.0019	0.1398	0.0187	3.3939
73	4.9971	95.0029	4.9971	0.3135	1.4546	0.1934	26.4959	0.0106	0.0874	0.8693	0.0020	0.1397	0.0685	3.3420

74	4.7431	95.0525	4.9475	0.3232	2.4487	0.3211	46.2015	0.0185	0.1617	0.8553	0.0020	0.1399	0.1167	3.2872
75	4.4888	95.1022	4.8978	0.3329	2.3805	0.3075	46.5842	0.0186	0.1724	1.0292	0.0024	0.1712	0.1997	3.9537
76	4.3699	95.1022	4.8978	0.3852	2.3677	0.3010	47.0242	0.0235	0.2022	1.0473	0.0024	0.1778	0.2634	4.0218
77	4.2511	95.1022	4.8978	0.4375	2.4582	0.3073	49.5611	0.0297	0.2428	1.1209	0.0026	0.1941	0.3465	4.3044
78	4.1419	95.1068	4.8932	0.4946	2.5597	0.3144	52.3991	0.0367	0.3013	1.2055	0.0030	0.2129	0.4794	4.6275
79	4.0327	95.1113	4.8887	0.5516	2.6861	0.3239	55.8446	0.0447	0.3686	1.2988	0.0035	0.2338	0.6317	4.9860
80	3.9522	95.1203	4.8797	0.5707	2.6691	0.3162	55.9562	0.0476	0.3805	1.3367	0.0036	0.2471	0.7060	5.1215
81	3.8718	95.1294	4.8706	0.5898	2.6337	0.3062	55.6797	0.0501	0.3898	1.3730	0.0037	0.2604	0.7823	5.2504
82	3.8006	95.1339	4.8661	0.5993	2.6015	0.2992	55.4104	0.0499	0.4017	1.4089	0.0038	0.2737	0.8557	5.3715
83	3.7294	95.1384	4.8616	0.6089	2.5634	0.2915	55.0078	0.0495	0.4126	1.4408	0.0038	0.2865	0.9291	5.4785
84	3.6722	95.1339	4.8661	0.6231	2.4968	0.2804	53.9273	0.0485	0.4152	1.4317	0.0041	0.2910	0.9667	5.4233
85	3.6149	95.1294	4.8706	0.6374	2.4396	0.2705	53.0347	0.0477	0.4190	1.4376	0.0043	0.2984	1.0139	5.4247
86	3.5674	95.1294	4.8706	0.6469	2.3768	0.2592	51.8387	0.0467	0.4199	1.4897	0.0045	0.3150	1.0959	5.5900
87	3.5198	95.1294	4.8706	0.6564	2.3728	0.2544	51.9221	0.0467	0.4310	1.5597	0.0047	0.3359	1.1947	5.8221
88	3.4484	95.1294	4.8706	0.6611	2.3671	0.2466	51.9107	0.0467	0.4386	1.6294	0.0051	0.3574	1.2763	6.0215
89	3.3771	95.1294	4.8706	0.6659	2.3426	0.2368	51.4857	0.0463	0.4428	1.7453	0.0057	0.3896	1.3966	6.3861
90	3.2916	95.1339	4.8661	0.6564	2.3212	0.2283	51.2968	0.0462	0.4514	1.8623	0.0061	0.4227	1.4991	6.7254
91	3.2062	95.1384	4.8616	0.6469	2.3017	0.2199	51.1497	0.0460	0.4603	1.9027	0.0061	0.4389	1.5405	6.7834
92	3.1208	95.1475	4.8525	0.6375	2.2934	0.2099	51.1922	0.0410	0.4710	1.9400	0.0068	0.4556	1.5807	6.8309

Table 33: Sample M shell calculated intensities for 3 MeV protons (part II).

Z	M3-N4	M3-N67	M2-N1	M2-O1	M2-O4	M2-N4	M1-N23	M1-O23	Mα/Mtot	ωM
	Mγ	Mm1	Mζ	Mm2						
67	0.4361	0.0158	0.3529	0.0556	0	1.7274	0.7657	0.1171	0.6511	0.0121
68	0.4322	0.0171	0.3338	0.0535	0	1.6458	0.7332	0.1143	0.6626	0.0129
69	0.4262	0.0183	0.3170	0.0516	0	1.5741	0.6971	0.1106	0.6738	0.0137
70	0.4242	0.0200	0.3026	0.0501	0	1.5130	0.6668	0.1077	0.6838	0.0147
71	0.4245	0.0218	0.2825	0.0475	0	1.4226	0.6511	0.1071	0.6928	0.0158
72	0.4249	0.0239	0.2645	0.0452	0.0076	1.3411	0.6856	0.1148	0.7015	0.0171
73	0.4208	0.0257	0.2456	0.0426	0.0258	1.2535	0.6753	0.1150	0.7103	0.0184
74	0.4152	0.0271	0.2311	0.0408	0.0421	1.1855	0.6632	0.1156	0.6198	0.0198
75	0.5009	0.0348	0.2293	0.0413	0.0597	1.1822	0.6711	0.1197	0.6155	0.0213
76	0.5104	0.0372	0.2285	0.0419	0.0773	1.1814	0.6796	0.1247	0.6132	0.0229
77	0.5471	0.0418	0.2395	0.0448	0.0999	1.2422	0.7245	0.1367	0.6012	0.0245

78	0.5891	0.0470	0.2490	0.0475	0.1341	1.2951	0.7764	0.1507	0.5880	0.0262
79	0.6352	0.0529	0.2650	0.0516	0.1751	1.3822	0.8369	0.1669	0.5728	0.0280
80	0.6555	0.0566	0.2684	0.0536	0.1893	1.3996	0.8586	0.1763	0.5715	0.0298
81	0.6747	0.0604	0.2705	0.0554	0.2028	1.4102	0.8711	0.1839	0.5717	0.0316
82	0.6924	0.0639	0.2734	0.0574	0.2177	1.4232	0.8804	0.1913	0.5718	0.0335
83	0.7078	0.0674	0.2770	0.0595	0.2335	1.4397	0.8936	0.1996	0.5725	0.0354
84	0.7018	0.0691	0.2816	0.0617	0.2509	1.4592	0.8982	0.2066	0.5763	0.0373
85	0.7025	0.0716	0.2861	0.0640	0.2685	1.4780	0.8927	0.2111	0.5793	0.0392
86	0.7256	0.0763	0.2862	0.0654	0.2817	1.4715	0.8937	0.2167	0.5825	0.0411
87	0.7575	0.0821	0.2812	0.0656	0.2894	1.4392	0.9058	0.2251	0.5808	0.0430
88	0.7870	0.0879	0.2792	0.0661	0.2939	1.4145	0.9220	0.2331	0.5797	0.0449
89	0.8379	0.0964	0.2753	0.0660	0.2962	1.3815	0.9083	0.2335	0.5793	0.0468
90	0.8864	0.1056	0.2723	0.0658	0.2945	1.3487	0.9025	0.2349	0.5783	0.0486
91	0.8981	0.1106	0.2703	0.0658	0.2940	1.3219	0.8917	0.2349	0.5787	0.0505
92	0.9085	0.1154	0.2652	0.0650	0.2900	1.2804	0.8856	0.2360	0.5786	0.0522