



A new atomic database for X-ray spectroscopic calculations

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Abstract

The authors undertook to compile a database of recent values of the atomic parameters required for fundamental parameters (FP) calculation of X-ray fluorescence (XRF) spectra, calculation of X-ray absorption in crystals and other samples, and correction of X-ray absorption spectra for self-absorption effects. All values were obtained from published sources and include the elements hydrogen (atomic number 1) through californium (atomic number 98). The data were collected into a single unstructured ASCII text file. Published by Elsevier Science Ltd.

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1. Introduction

The authors are in the process of writing and updating several computer codes used for analysis of X-ray spectra. These include codes for fundamental parameters calculation of X-ray fluorescence (XRF) spectra, calculation of X-ray absorption in crystals and other samples, and correction of X-ray absorption spectra for self-absorption in the sample. All of these applications require X-ray absorption cross sections and several other atomic parameters. The authors compiled a database of recent values of the parameters required for their various applications and compared the resulting database to other, similar compilations.

This paper discusses the details of the information included in the database. The parameters included in the

database were those necessary to compute X-ray absorption and X-ray emission for each element in the periodic table, from atomic number 1 to 98. Information was included for each atomic energy level with energies in the X-ray range, which is above 100 eV. Details given in this paper include the sources of the data, the motivations for the choices made concerning what data to include, and any manipulation made to the data before inclusion. The paper is organized into sections for each major parameter in the database.

An earlier compilation for this same purpose was made by DeBoer (1989). An excellent and more recent compilation by Joy (1999) contains information on some of these parameters even though it principally concerns X-ray generation by electrons. A comprehensive database intended for photon transport calculations is described by Cullen et al. (1997).

2. Results

The goal of this project was to compile a comprehensive database of atomic parameters relevant to X-ray spectroscopy which included the best available values. Such a selection of necessity involved some subjective

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¹Copies of the database (machine readable) are available from J.R. Sieber, National Institute of Standards and Technology, 100 Bureau Dr., Stop 8391, Gaithersburg, MD 20899-8391.

judgements, and the result reflects solely the opinion of the authors. Where possible the values chosen were based on experiment and reflected the most recent information available, such as recent measurements of fluorescence yields and Coster–Kronig transition rates measured by selective photoionization using synchrotron radiation from Jitschin (1990). All values were obtained from published sources; the authors collected no data. This work is solely a compilation whose product will be a set of values that is in a common source. A secondary goal was to convert values for these parameters from other authors who have compiled similar databases to a common format, both for comparisons and for use in computer codes. In this way, a user may select the particular set of parameters to use in a calculation, as well as compare the results of a calculation with different parameter sets. The first such compilation to be converted to the common format is the X-ray cross section fits of McMaster et al. (1969).

2.1. Overall organization

The parameters included in the database are listed in Table 1. The database was organized by element, then by X-ray absorption edges for each element. These edges correspond to the atomic “diagram levels” as defined by the International Union of Pure and Applied Chemistry (IUPAC) in the description for their recommended notation for X-ray lines published by Jenkins et al. (1991). This paper will adhere to both the IUPAC and Siegbahn conventions for designating emission lines. Each X-ray emission line is included below the X-ray

edge whose vacancy causes the line to be emitted. The term X-ray edge will usually be used in place of X-ray level in this context. Because the energy resolution of X-ray spectra is continuously improving, all X-ray emission lines are included in the database and the user can combine lines as necessary to compare with a particular experimental resolution. The final list of included lines was limited by the relative intensity values available in the literature. Only those lines with a reasonably reliable non-zero relative intensity were included.

The sources of each of the parameters will be discussed in turn, along with any manipulation of the data performed by the authors before inclusion. The elements hydrogen (atomic number 1) through californium (atomic number 98) were included. Many of the parameters for transuranic elements are only available from theoretical calculations. The limiting factor that precluded inclusion of elements above Cf was the availability of X-ray absorption cross sections below 1000 eV. Atomic weights from several sources were compared and agreement was generally found to within single-precision computer arithmetic (about 7 digits). Pure element densities were likewise compared among several sources and agreement was found to be within 0.01% (except for technetium, where the disagreement was about 1%). The final values included were those of Berger and Hubbell (1987).

2.2. Edge energies

X-ray absorption edge energies were obtained from the table compiled by Williams (1986). Values for some edges below 10 eV were added to allow calculation of the X-ray emission line energies by subtracting the appropriate edge energies (see discussion under X-ray emission line energies). The values from Williams were compared to the values of Berger and Hubbell and most agreed to within 1 eV. An error was found in the values of Berger and Hubbell for the M5 edge of rhenium, where the tables of Berger and Hubbell had 1822 eV and other tables had 1883 eV. The value of 1883 eV was used for this work. Various other edges (37 in all) had disagreements larger than 1 eV, ranging up to 6 eV.

2.3. Fluorescence yields

Fluorescence yields for K edges were calculated from the fits given by Hubbell et al. (1994). Since Hubbell et al. do not give subshell yields, their values could not be used for the other edges. Also, Hubbell et al. do not recommend their fits for atomic numbers below 11. For K edges of elements lighter than atomic number 11 and for L edges, the values of Krause (1979) were used, with modifications proposed by Jitschin (1990). The Krause values for the fluorescence yield of the L1 edge for atomic numbers 85 and higher were increased. The

Table 1
Parameters included in the database

Element
Symbol
Atomic number
Atomic weight
Pure element density (cm ³ /g)
X-ray absorption edge
Designation
Energy (eV)
Jump ratio
Fluorescence yield
Coster–Kronig transition probabilities
Total Coster–Kronig transition probabilities (see text)
X-ray emission lines
IUPAC designation
Siegbahn designation
Energy (eV)
Relative intensity
Photoabsorption cross sections (versus energy, cm ² /g)
Coherent scattering cross section (versus energy, cm ² /g)
Incoherent scattering cross section (versus energy, cm ² /g)

increases started with 3% at atomic number 85 and rose smoothly to 25% at atomic number 90 and remained there for higher atomic numbers. The values for light elements in condensed matter from Table 1 in the reference by Krause were used. Subshell fluorescence yields for M shells were taken from the theoretical calculations of McGuire (1972). The authors judged these values to be in best agreement with experimental values given by Hubbell et al. Values for N shells were only available from the calculations of McGuire (1974). The values for $Z = 38$ to 50 were adjusted by multiplying the values by the ratio of the linewidth given in parentheses in Table 1 of McGuire (1974) to the non-parenthetical linewidth. The reader is referred to the discussions by McGuire at the end of Section IV.a. (p. 1845) and the last sentence of the conclusions for the reasons for this choice.

2.4. Coster–Kronig transition probabilities

Coster–Kronig transition probabilities for the K and L shells were taken from the work of Krause (1979). Again, the modifications recommended by Jitschin (1990) were incorporated into the values of the L1 to L2 transition probabilities. The dip in the Krause values starting at atomic number 72 was shifted to higher atomic number and made less pronounced, rejoining the original Krause values at atomic number 96. Other modifications suggested by Jitschin were deemed subjective and too difficult to implement quantitatively. Again, values from Table 1 of Krause, values for light elements in condensed matter, were used. The use of these values for the L2 to L3 transition probability results in a discontinuous change at atomic number 30. The reader is referred to the discussion by Krause in Section 5.3, L2 Subshell, and the last paragraph of Section 7 for reasons why this is expected. Values for M and N shells were taken from the same works of McGuire as the fluorescence yields. Where necessary, all values were linearly interpolated as a function of atomic number.

2.5. Total Coster–Kronig transition probabilities

Vacancies in L, M, and N shells may travel to lower-energy subshells in the same shell via multiple Coster–Kronig transitions. The simplest example is the transition of an L1 vacancy to the L2 shell and then to the L3 shell. Thus the total probability of an L1 vacancy winding up as an L3 vacancy is the sum of the L1 to L3 transition probability plus the product of the L1 to L2 and L2 to L3 probabilities. For the M and N subshells, the possible transitions are more numerous and calculating the total probabilities is more arduous. The authors have included in the computer program that generates the database an algorithm that enumerates

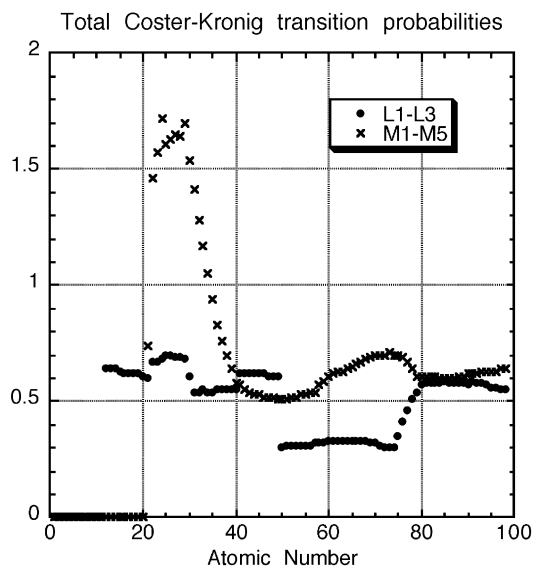


Fig. 1. Total Coster–Kronig transition probabilities including transitions via intermediate levels. Values are greater than unity for some very low energy levels, where the higher levels in the same shell can ionize the lower level and produce more than one vacancy.

all of the possible routes that a vacancy could take from any subshell to a given lower-energy subshell. The total Coster–Kronig transition probability for a pair of subshells can be calculated using this enumeration. This calculation is included in the database using the single-shell transition probabilities. The results of this calculation are plotted in Fig. 1. Note that for some very low energy levels, where the higher levels in the same shell can ionize the lower level, more than one vacancy is produced in some transitions.

2.6. X-ray emission lines

X-ray emission lines occur when a vacancy is filled from an occupied shell. The IUPAC nomenclature for the lines consists of the designations of the shells, or energy levels, separated by a hyphen. The Siegbahn notation for emission lines groups them by energy range. The major contribution to the energy is the shell (not subshell) with the vacancy, so the IUPAC and Siegbahn notations agree on the first term in the designation as the shell (K, L, etc.) with the vacancy. The Siegbahn notation then groups the lines by energy and designates the groups by Greek letter. Individual lines are given an arbitrary Arabic numeral suffix. This work groups lines with the energy level, which contains the vacancy that causes emission of the line. The energy level is associated with an X-ray absorption edge, so the line is grouped under that edge. Both the IUPAC and Siegbahn

notations are given where applicable. The Siegbahn notation has deviations from the scheme described above (such as the l lines) and has no designation for some weak lines. Thus the Siegbahn notation is omitted for these lines.

The energy of the emission line is the difference in energy between the level that contains the vacancy and the level that contributes an electron to fill the vacancy. For this database, the line energies are taken as the difference between the energies of the X-ray absorption edges. Some of the edge values below 10 eV, which were omitted in the table from Williams (1986), were added by the authors to provide better agreement for some line energies. The line energies used to calculate the very small edge energies were taken from the CRC Handbook, which contains a compilation by Bearden (1967). In principle, any shell of lower energy can contribute an electron to fill the vacancy, making the number of possible emission lines very large. Selection rules reduce the number somewhat, but even lines forbidden by selection rules sometimes have very weak but measurable intensities. For this work lines were included if a non-zero value for the relative intensity could be found in the literature. The intensities of the lines from a given energy level were forced to sum to unity. Values of the relative intensity for K and L lines were taken from Salem et al. (1974). Since the data were given for alternate values of atomic number, these values were fit to polynomials varying from second order to fourth order. The lowest order that gave an acceptable fit (judged by eye) was used. Where necessary the fits were split into two atomic number ranges, which were fit separately. For the $K-N_{3,2}$ ($K_{\beta 2}$) line, the structure versus atomic number was too complex for a satisfactory polynomial fit. Since this structure was also visible in the calculations presented in the paper by Salem et al., this structure was deemed real and retained. The full data set from the Salem et al. table was included with linear interpolation for odd values of atomic number. All of the data were extrapolated to low atomic numbers, where data were missing in the work of Salem et al., using linear extrapolation of the lowest few data points. Salem et al. did not give the relative intensities for lines originating from the M levels. Schrieber and Wims (1982) recommend a value of 0.65 for the relative intensity of $M_5-N_{6,7}$ (M_{α}) line for all elements. Values of 1% and 0.1% were used for the M_3-N_5 (M_{γ}) and $M_{4,5}-N_{6,7}$ (M_{ϵ}) lines, respectively, to provide some small intensity for these lines and to make them distinguishable from each other. The remaining intensity was assigned to the M_4-N_6 (M_{β}) line.

The intensity of the L_2-N_4 ($L_{\gamma 1}$) line for palladium (atomic number 46) in Table 3 of Salem et al. (1974), which is 10.67%, is out of line with the nearby values in the table. No corresponding feature was visible in the

plot of this parameter versus atomic number at the top of page 104. Since the remainder of the data agreed with the curves in the plots, an interpolated value of 8.96 % was used for the intensity ratio of the L_2-N_4 ($L_{\gamma 1}$) line of palladium.

2.7. X-ray absorption cross sections (above 1 keV)

The majority of the actual data in the database consists of values for the absorption and scattering cross sections for each element as a function of energy. The starting point for these values was the tabulation of Berger and Hubbell (1987) included in version 2.1 of the XCOM computer program. These values are checked against the NIST database of measured values and were deemed by the authors to be the best available. Values from 1 keV to 1 MeV were used directly from this tabulation. Pair production was neglected for this work, necessitating restricting energy values to below the pair production threshold at 1.022 MeV. Cubic spline interpolation of the logarithm of the cross section versus logarithm of the energy values is used by Berger and Hubbell in their computer program and was also used here.

A compact and efficient cubic spline algorithm is available in *Numerical Recipes* by Press et al. (1986). This algorithm has two distinct advantages. First, it only requires storing one number for each energy value in addition to the cross section. Most algorithms require storing all four coefficients of the spline for each interval, although the coefficients in successive intervals are not independent. For the particular algorithm used here, this extra stored value is the second derivative of the interpolatory polynomial, chosen to make the first derivative continuous at the interval boundaries. If this extra value is zero, then the algorithm reduces to linear interpolation. Second, its search method can handle distinct regions of separate splines provided pairs of identical energy values are included to separate the regions. The extra (second derivative) value is made equal to zero at the end points of a spline region. This is useful for absorption edges, where the cross section values are discontinuous. These two advantages allow storage of a single table with three numbers per entry, where the cross section value for any energy can be obtained by a single call to the spline interpolation algorithm. Berger and Hubbell found that spline interpolation was too unstable to use between absorption edges, where there are not enough energy points. Linear interpolation of the log of the values was used below the K edge of each element, with values found in separate tables in the XCOM database. This work incorporated these linearly interpolated values in a single table.

The locations of the edge discontinuities in the table of photoabsorption cross sections must match exactly

the edge energies in the database. For example, many calculations involve an integration that starts or ends at an absorption edge energy. A user typically requests the edge energy and then calculates using the cross sections up to that energy. If the edge discontinuity is at a different value in the cross section table, then serious numerical errors may result. To ensure that the cross section tables agree with the edge energies in the database, the edge energy values from Berger and Hubbell were adjusted to match the values in the table of Williams. No interpolation was done; the energy values in the cross section table were simply changed. The discrepancies were discussed in the paragraph on edge energies above.

The resulting table contains an energy grid, photo-absorption cross section values, and spline second derivative values for each element. There is a separate energy grid for the scattering cross sections together with values for the coherent and incoherent cross sections. All values in the table are log values and must be exponentiated to get the actual values, which are given in units of eV and cm^2/gm .

2.8. X-ray absorption cross sections (below 1 keV)

The table of scattering values from Berger and Hubbell was used without modification. Since it stops at 1 keV, another source was used to extend the database to lower energies. The data that were most compatible with the Berger and Hubbell tables was a 1981 compilation by Plechaty et al. (1981), which was available in machine-readable form from Brown (1998). The values of the edge jumps in the photo-absorption cross sections calculated from this table joined smoothly to the values calculated from the Berger and Hubbell data. The Plechaty et al. table is in units of barns per atom and was converted to cm^2/gm using the conversion factor of 0.60221367, which is Avogadro's number times 10^{-24} barns/ cm^2 divided by the atomic weight in the Plechaty et al. data. To provide a smooth connection to the values above 1000 eV, all three cross sections from Plechaty et al. were multiplied by the ratio of the corresponding XCOM value to the Plechaty et al. value at 1000 eV (actually performed by adding the difference of the log values). These normalization ratios are plotted in Fig. 2. The interpolatory splines for the values above and below the crossover were kept separate and each was terminated by a zero second derivative at the crossover energy. At the crossover energy, a duplicate set of data points was used to terminate both splines and to ensure that the table would give the correct value for any energy with Berger and Hubbell values used above and at the crossover and the adjusted Plechaty et al. values used below the crossover.

The most difficult part of reading the Plechaty et al. table and incorporating it into the new database was

reconciling the edge energies to the values of Williams. Since the machine-readable version of the Plechaty et al. table did not contain separate values for the edge energies, they had to be extracted from the data. Since a pair of energy points separated by about 1.4 eV represented the edge values, this produced many exceptions where discontinuities spanned grid points. Most of these exceptions were handled by special cases in the code to read the table, but some of them had to be corrected by hand. In some cases, the Plechaty et al. table had only one edge discontinuity where there are actually two close together, such as the L2 and L3 edges for atomic numbers below 30 (when both edges occur at less than 1000 eV). For these cases, two edge discontinuities were included in the new database with the edge jump for one of the edges taken as a fixed value obtained from nearby elements in the Berger and Hubbell data. The other edge jump comes from the discontinuity in the Plechaty et al. data divided by the fixed value. In all cases, the edge jump that had the least atomic number dependence was transferred from the Berger and Hubbell data. For the N_{6,7} and O_{5,6} edges, the edge jump was split between the edges by taking the square root of the jump in the Plechaty et al. data. One data point was missing for Cs, atomic number 55, which precluded obtaining the edge jump for the M₅ edge. A value of 1.55 was used, which was obtained by interpolating between adjacent atomic numbers. This also caused the

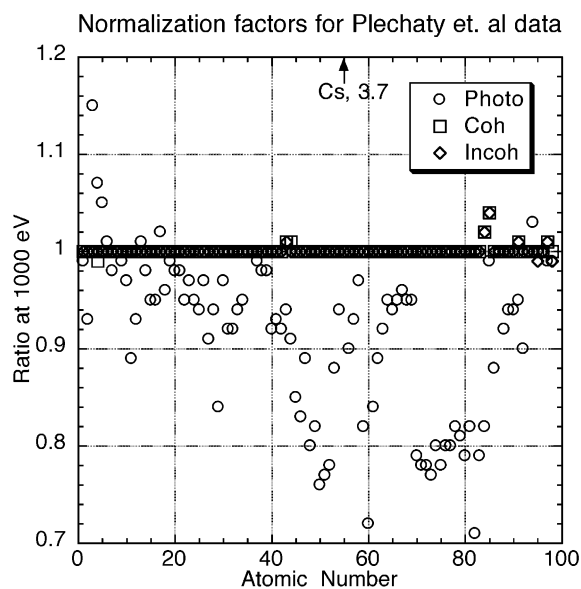


Fig. 2. Normalization factors used to match the Plechaty et al. cross sections to the Berger and Hubbell values at 1000 eV. Values are found by dividing the value from the Berger and Hubbell table at 1000 eV by the value from the Plechaty et al. table at the same energy. The large value for Cs, atomic number 55, results from a missing point in the original data.

normalization to the Berger and Hubbell data at 1000 eV to be unusually large (see Fig. 2), but the values after all adjustments agreed well with the Plechaty et al. values below the Cs M5 edge.

As with the Berger and Hubbell data, the energy of the edge discontinuities from the Plechaty et al. data were forced to agree with the edge energies in the Williams table. Unlike the Berger and Hubbell data, however, the disagreements were too significant and the energy dependence of the cross sections at these low energies were too great to simply shift the edge energies. The smoothly varying background cross section (with the edge discontinuities removed) was interpolated to obtain values at the new edge energies. These new values were then used as the values below the corresponding edges and the values above the edge energy were multiplied by the edge jump. This process was repeated for each edge of the element being calculated, working from lowest to highest in energy. The resulting data were then adjusted to match the Berger and Hubbell data at 1000 eV, as described above, and included in the new database. For a very few cases, the Plechaty et al. table had no discontinuity for a given edge, mostly where the edge energy was very near the 100 eV lower limit of the table. In these cases, the edge discontinuity was omitted in the new database even though the edge energy in the Williams table was above 100 eV.

For many elements, the cross sections of Plechaty et al. increase as a function of energy in the region below 250 eV. This may be an artifact in the method used to calculate the cross sections. The authors believe that the cross sections below about 250 eV should be regarded as unreliable. They were included because they were available and may be of some use. The fact that the values were adjusted to match the Berger and Hubbell values at 1000 eV and thus simply used to extrapolate the Berger and Hubbell values to the region below 1000 eV should make the cross sections between 250 eV and 1000 eV fairly accurate.

In summary, the database in this work contains two tables of log cross section values versus log energy, plus a second derivative of the spline interpolation function. One table contains the information for the photoabsorption cross section and the second contains coherent and incoherent scattering cross sections. The photoabsorption table is discontinuous at the absorption edge energies. The discontinuity is implemented using a pair of successive, identical log energy values in the table. These energies agree with the values of the absorption edges given earlier in the database. The spline functions are calculated separately for each region between edges, with linear interpolation used for some regions. The choice of linear or spline interpolation is handled automatically via the value of the second derivative in the table. Thus, once the tables for a particular element have been stored in computer memory, the only

operations needed to obtain the cross section for that element at a given energy are to perform the spline interpolation on the table at the log of the given energy (in eV) and to exponentiate the result. The cross section is then obtained in cm^2/g .

3. Discussion

The database containing all of the above-described information has been collected into a single data file. The basic data is stored as an unstructured ASCII text file, ordered by element. The data for each element is ordered by X-ray absorption edge energy, followed by cross section tables. The authors have prepared computer codes to use the data, written (thus far) in the C++, Perl, and Fortran computer languages. The use of a common text file format allows this and other databases to be used by the several computer programs for a variety of calculations. Thus, the results of using different values for the relevant parameters can be compared. As a check of the database prepared for this work, the cross section values above 1000 eV were extensively compared to those of McMaster et al. The substantial majority of the discrepancies discovered were due to disagreements in the locations of absorption edge discontinuities. A few other discrepancies were discovered, traced to coding errors, and corrected. Most of the data for fluorescence yields, Coster–Kronig transition probabilities, and emission line intensities were typed in by hand. To check the accuracy of the data, plots of each parameter were made versus atomic number. Any points that appeared to be visibly out of line or any discontinuities visible by eye were investigated. In all cases, the data were checked for agreement with the published values, and forced to agree with the published values even if discontinuities remained except as noted in the text.

The database was first implemented in the C++ computer language as a series of classes. The classes were Element, XrayEdge, XrayLines, and XrayXsect Table. The simplest class was the Element class, whose private data contained only the atomic number. An object of this class represented a specific element, and the member functions of the class provided the atomic number, symbol, atomic weight, and density of the element. The constructors of the Element class require either the atomic number or the atomic symbol. Objects of the XrayEdge class represent an X-ray absorption edge of a given element, so their constructor requires an element object and a unique designator of an absorption edge of that element, such as the energy, letter symbol, or a numerical index. Once instantiated, an XrayEdge object has member functions that provide the edge energy, the fluorescence yield and Coster–Kronig transition probabilities as well as other parameters,

and such information as the quantum numbers of the electron energy level associated with the absorption edge. The XrayEdge objects thus represent both an X-ray absorption edge and the electron energy level, which produces the jump in X-ray absorption at the edge. In addition, there is a static function for this class that returns a list of edges for a given element whose energies fall below a given energy. This list is thus the edges of a given element that will be excited at a given excitation energy. Static functions are available before any objects of the class are instantiated. The XrayLines class provides information about the emission lines produced by excitation of a given X-ray edge, such as the line energy, relative intensity, and the line symbol in IUPAC and Siegbahn notations. The member functions of these classes all contain the raw data from the literature or fits to the data, and interpolate or calculate the individual values as needed. The C++ container classes can be used to create groups of these objects, such as the elements found in a sample or the edges excited under a given set of spectroscopic conditions.

Objects of the final class, XrayXsectTable, contain the photoelectric, coherent, and incoherent cross section values for a given element as a function of energy. This class is unique in that the member functions contain no data. The data for the particular element are read from a file when the object is created. The member functions of the object operate on the table of cross sections contained in the object. This allows for efficient utilization of memory, since only the tables used in a particular calculation will be created and loaded from the file.

The unstructured ASCII text file version of the database is created by instantiating all available objects for each element in turn, calling the member functions to obtain the required values for that element, and writing the values to the ASCII file. Our choice to present the data as an unstructured ASCII text file offers flexibility in its application. This text file is readily converted into a form usable by any programming language. Along with the C++ implementation described above, the authors have implemented interfaces in Perl and Fortran. For the Perl version, the text file is converted into a network-ordered binary file. A Perl module has been written to access this file efficiently and included in an object-oriented interface to atomic data, including absorption coefficients and anomalous scattering factors. For the Fortran version, the text file is converted into data statements and embedded in a subroutine that can be compiled against any Fortran program.

In conclusion, a new database of atomic parameters has been constructed from values available in the literature. The database is comprehensive regarding the parameters relevant to X-ray spectroscopy, and can easily be extended to include other parameters as needed. The format is standardized and in text form,

which makes it readable by a variety of computer programs.

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References

- Bearden, J.A., 1967. X-ray wavelengths. *Rev. Mod. Phys.* 39, 78–124.
- Berger, M.J., Hubbell, J.H., 1987. XCOM: Photon Cross Sections on a Personal Computer. National Bureau of Standards Publication NBSIR 87-3597, Gaithersburg, MD, July 1987. Web version available at <http://physics.nist.gov/xcom>
- Brown, D.B., 1998. Private communication.
- Cullen, D.E., Hubbell, J.H., Kissel, L., 1997. EPDL97: The evaluated photon data library, '97 Version. Lawrence Livermore National Laboratory Report UCRL-50400, Vol. 6, Rev. 5.
- DeBoer, D.K.G., 1989. Fundamental parameters for X-ray fluorescence analysis. *Spectrochim. Acta* 44B, 1171–1190.
- Hubbell, J.H., Trehan, P.N., Singh, N., Chand., B., Mehta, D., Garg, M.L., Garg, R.R., Singh, S., Puri, S., 1994. A review, bibliography, and tabulation of K, L, and higher atomic shell X-ray fluorescence yields. *J. Chem. Phys. Ref. Data* 23, 339–364.
- Krause, M.O., 1979. Atomic radiative and radiationless yields for K and L shells. *J. Phys. Chem. Ref. Data* 8, 307–327.
- Jenkins, R., Manne, R., Robin, J., Senemaud, C., 1991. Nomenclature system for X-ray spectroscopy. *Pure Appl. Chem.* 63, 735–746.
- Jitschin, W., 1990. Progress in measurements of L-subshell fluorescence, Coster–Kronig, and auger values. In: Carlson, T.A., Krause, M.O., Manson, S.T. (Eds.), *AIP Conference Proceedings* 215, X-ray and Inner-Shell Processes, Knoxville, TN, 1990, American Institute of Physics, New York, pp. 408–423.
- Joy, D.C., 1999. Fundamental constants for quantitative X-ray microanalysis. *Microsc. Microanal.* 5 (Suppl. 2), 564–565; *Microsc. Microanal.*, 2000, to appear.
- McGuire, E.J., 1972. Atomic Coster–Kronig, auger, and radiative rates, and fluorescence yields for Ca–Th. *Phys. Rev. A* 5, 1043–1047.
- McGuire, E.J., 1974. Atomic N-shell Coster–Kronig, auger, and radiative rates and fluorescence yields for $38 \leq Z \leq 103$. *Phys. Rev. A* 9, 1840–1851.
- McMaster, W.H., Kerr Del Grande, N., Mallett, J.H., Hubbell, J.H., 1969. Compilation of X-ray cross sections. Lawrence Livermore National Laboratory Report UCRL-50174, Sec. II, Rev. 1.
- Plechaty, E.F., Cullen, D.E., Howerton, R.J., 1981. Tables and graphs of photon interaction cross sections from 0.1 keV to

- 100 MeV derived from the LLL evaluated nuclear data library. Lawrence Livermore National Laboratory Report UCRL-50400, Vol. 6, Rev. 3. (Available from the National Technical Information Service, Springfield, VA as DE82-004819.)
- Press, W.H., Flannery, B.P., Teukolsky, S.A., Vetterling, W.T., 1986. *Numerical Recipes*. Cambridge University Press, Cambridge, pp. 86–89.
- Salem, S.I., Panossian, S.L., Krause, R.A., 1974. Experimental X-ray emission rates. *At. Data Nucl. Data Tables* 14, 92–109.
- Schrieber, T.P., Wims, A.M., 1982. Relative intensity factors for K, L, and M shell X-ray lines. *X-ray Spectrometry* 11, 42–45.
- Williams, G.P., 1986. Electron binding energies of the elements. In: Weast, R.C. (Ed.), *CRC Handbook of Chemistry and Physics*, 67th Edition. CRC Press, Boca Raton, pp. F163–166.