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Atomic scattering factors and atomic cross-sections in x-ray crystallography

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MASTER THESIS

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Preface

This is the final report of the research work carried as duty to complete the Master thesis in Physics at the University of Stavanger in the 2017 Fall and 2018 Spring semesters. The subject of the research is to provide an overview of the available sets of physical data regarding the atomic scattering factor, the photoeffect cross-section, the incoherent (Compton) cross-section and the coherent (Rayleigh) scattering cross-section.

Stavanger, Norway June 15, 2018

Ioana Andreea Nes

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Nes Ioana Andreea

15 June 2018

Short Summary

Crystallographers as well as other scientists and engineers need reliable sets of physical data. Focus is here set upon the x-ray attenuation coefficients (the atomic photoeffect cross-section, and the incoherent (Compton) and coherent (Rayleigh) scattering cross-sections) and the atomic scattering factor for x-ray. The purpose of this work is to give an overview of the actual state of the existing tabulations for the above mentioned fundamental quantities. Consequently the first part of the work comprises a brief history of the calculations for these fundamental data. The second part focuses on the essential databases. Along the process of assembling information about the existing databases, we have collected and stored the existing tabulations in a number of separate folders.

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1

Introduction

This introductory chapter presents some milestones regarding the compilations of the x-ray attenuation coefficients (the atomic photoeffect cross-section, and the incoherent (Compton) and coherent (Rayleigh) scattering cross-sections) and the atomic scattering factor for x-ray. The litterature regarding these computations is extensive. These computations have developed in the last decades, becoming more extensive and more accurate. In section 1.1 the quantities photoeffect cross-section, incoherent (Compton) and coherent (Rayleigh) cross-sections are presented. These coeffitients are linked with some representative data compilation works. In section 1.2 we focus on the atomic scattering factor. Here as well we mention some important studies regarding tabulations of this quantity. In addition we find it appropriate to give some uncomplex calculations that generate this quantity, like calculations based on Hönl (1933) method and the model of Als-Nielsen and Des McMorrow (2011).

1.1 History of the calculations of the photon cross-sections

Background

After the discovery of x-ray by Röntgen in 1895, Barkla and Sadler (1907, 1909) measured and quantified the transmission of pencil beams through layers of different materials. Accord-

ing to Hubbell (1999) this quantification was in terms of mass attenuation (or absorption) coefficient μ/ρ [cm^2/g] which for nonnarcotic photon can be defined as follows:

$$\frac{\mu}{\rho} = x^{-1} \ln (I_0/I)$$

in which μ is the linear attenuation coefficient in units of [cm^{-1}], ρ is the density of the layer in units [g/cm^3], x is the mass thickness of the layer in units of [g/cm^2], I_0 represents the intensity of the incident and I is the intensity of the beam after it has passed through the layer in units of [e.g. photons/cm^{2}s]. The mass attenuation coefficient μ/ρ is related to the total photon interaction cross section per atom, σ_{tot}, i.e., to the sum of the cross sections for all the elementary scattering and absorption processes, according to the expression given by Hubbell and Berger (1968):

$$\frac{\mu}{\rho} = \sigma_{tot} \frac{N_A}{M}, \qquad (4.1-5)$$

in which N_A is the Avogadro's number ($6.02252 \cdot 10^{23}$ mol^{-1}) and M is the atomic weight of the absorber material in units of [g/mol].

In addition for an isolated atom at photon energies less than 100 keV the total cross section can be expressed through the relation, see Creagh (2006):

$$\sigma_{tot} = \sigma_{pe} + \sigma_{coh} + \sigma_{incoh}. \qquad (4.2.3.6)$$

where σ_{pe} is the photo-effect cross section, σ_{coh} is the Rayleigh cross section and σ_{incoh} is the Compton cross section.

In the next subsections we are going to make a short presentation of the available measurements regarding σ_{pe}, σ_{coh} and σ_{incoh} based on the studies of Hubbell (1969, 1999, 2006).

1.1.1 Outline of some pieces of information about the history of the atomic photoeffect cross section calculations

In the historically review of the photoelectric absorption Hubbell (1999) describes the atomic photoeffect as following: "In the atomic photoeffect, as discussed and historically reviewed in some detail in Hubbell (1969), a photon disappears and an electron is ejected from an

atom. The electron carries away all the energy of the absorbed photon, minus the energy binding the electron to the atom. The K-shell electrons are the most tightly bound, and are the most important contributors to the atomic photoeffect cross-section in most cases. However, if the photon energy drops below the binding energy of a given shell, an electron from that shell cannot be ejected. Hence, particularly for medium- and high-Z elements, a plot of σ_{pe} versus photon energy exhibits the characteristic sawtooth absorption edges as the binding energy of each electron subshell is attained and this process is permitted to occur."

In the beginning the following approach was used in determining the photoeffect cross section, according to Hubbell (2006):
"In the early semi-theoretical compilations of μ/ρ, the scattering cross sections were available theoretically to a reasonable approximation from the Klein-Nishina (1929) formula. Thus the photoeffect cross section was obtained by subtracting the theoretical scattering cross sections from measured values of μ/ρ and interpolating across Z and photon energy, taking care to account for the photoeffect absorption edges shifting in energy with Z."
In addition listing of early calculations of the atomic photoeffect and of the K-shell component of the photoelectric cross section are given by Hubbell (1969). These calculations are characterized as follows by Hubbell (1999):
"Most of these calculations were for the K-shell only, typified by the high-energy work of Pratt (1960) providing the asymptotic behaviour going to arbitrarily high energies and by Pratt, et al. (1964) in the range 200 keV to 2 MeV. Hultberg, et al. (1961, 1968) used the Swedish BESK computer to compute K-shell cross sections...."

A new era began with the works of Rakavy and Ron (1965, 1967) as pointed out by Hubbell (2006):
"A significant advance came with the atomic photoeffect cross section calculations by Rakavy and Ron (1965, 1967) for not only the K shell, but for all the significantly contributing higher subshells ($L_{I-III}, M_{I-V}, N_{I-VII}$ *and* O_{I-III}) over the energy range 1 keV to 2 MeV for $Z =$ 13, 26, 50, 74 and 92. Other important multi-shell photoeffect calculations in this time period, which provide historical reviews of earlier work, are those by Alling and Johnson (1965),

Matese and Johnson (1965) and by Schmickley and Pratt (1967).

Of even of greater importance is the study of Scofield (1973) as outlined by Hubbell (2006): "However, a major advance came with the systematic calculations by Scofield (1973) of the atomic photoeffect cross sections for all subshells, for all elements $Z = 1$ to 101, over the photon energy range 1 keV to 1.5 MeV. These non-relativistic Dirac-Hartree-Slater (DHS) calculations were based on Scofield's solution of the Dirac equation for the orbital electrons moving in a static Hartree-Slater (HS) central potential. In the Hartree-Slater (HS) approximation (Slater (1951)) the electron-electron interaction term is replaced with its average radial value. Hence the model is somewhat less accurate than the full Hartree-Fock (HF) model which requires calculation of the self-consistent field for each term in the Slater product and is thus much more costly than HS in computer time. For $Z = 2$ to 54, Scofield (1973) provided renormalization factors to convert his cross sections results to values expected from a relativistic Dirac-Hartree–Fock (DHF) computation."

Furthermore a discussion around the future use of renormalization is highlighted by Hubbell (2006). The works that include the renormalization factor in their calculations of σ_{pe} are Hubbell (1977, 1982). and Hubbell, et al. (1980). Moreover according to Hubbell (2006) detailed comparisons (Saloman and Hubbell (1986), Saloman, et al. (1988)) with the extensive NBS/NIST[1] μ/ρ measurement database incline to favor the unrenormalized σ_{pe} of Scofield (1973) over the renormalized values. Such that in the subsequent compilations by Berger and Hubbell (1987) and by Seltzer and Hubbell (1995), the σ_{pe} values used are the unrenormalized Scofield (1973) values.

A final remark is given by Hubbell (2006) regarding the values of the photoelectric cross section calculated by Scofield (1973):

"Scofield (1985) later extended these calculations down to 0.1 keV, and these (unrenormalized values) are included in the comparison by Saloman and Hubbell (1986) and Saloman, et al. (1988), both numerically and graphically, with the NBS/NIST μ/ρ measurement data base as well as with an experiment-based compilation by Henke, et al. (1982)."

[1] NBS stands for National Bureau of Standards; named changed in 1988 to NIST National Institute of Standards and Technology according to Hubbell (2006)

More recent values of σ_{pe} are given in the extensive theoretical results of Chantler (1995, 2000) computed within a self-consistent Dirac-Hartree-Fock framework and the values of Cullen, et al. (1997) from Lawrence Livermore National Laboratory (LLNL).

1.1.2 Outline of some pieces of information about the history of the incoherent (Compton, inelastic) scattering cross section calculations

In the historically review of Hubbell (1969) the incoherent scattering cross section is described as follows:

"In Compton scattering, a photon collides with an electron, loses some of its energy and is deflected from its original direction of travel. The basic theory of this effect, assuming the electron to be initially free and at rest, is that of Klein and Nishina (1929). This theory has been well confirmed experimentally (see, for example, Meitner and Hupfeld (1930), ...). Predictions of this theory have been summarized and extensive tabulations have been given by Nelms (1953), ..., and Evans (1958, 1968)."

A current status of the information available on Compton scattering cross-section is provided in Radiation Physics and Chemistry edited by Bradley (1997), according to Hubbell (2006):

"For recent information on the incoherent (Compton) scattering cross-section σ_{incoh}, attention is here called to a special issue of Radiation Physics and Chemistry edited by Bradley (1997) giving collectively a rather comprehensive survey of this topic. The all-invited papers in this issue include an overview of theory by Bergstrom and Pratt (1997) a summary of experiments by Kane (1997), a study of momentum distributions by Cooper (1997), ..., and a historical and status review by Hubbell (1997).

In addition Hubbell (2006) gives the following notification:

"As mentioned in the extensive review by Kane (1992) and in treatments by Bergstrom, et al. (1992, 1993), by Pratt, et al. (1994), and by Bergstrom and Pratt (1997) relativistic

S-matrix calculations are becoming available and will likely supplant the currently-used incoherent scattering function $S(x, Z)$ approach, in which x is a momentum transfer variable related to the incident photon energy and the deflection angle of the scattered photon, and Z is the atomic (charge) number of nucleus of the target atom. However, the S-matrix results and format are not yet particularly 'user-friendly' ...."

Moreover a description of the currently available compilations is given in Hubbell (2006):
"The Berger and Hubbell (1987) XCOM PC program, the Seltzer and Hubbell (1995) tabulation and the Cullen, et al. (1997) LLNL database, still rely on the incoherent scattering function $S(x, Z)$ approach. For these compilations, the incoherent scattering cross-section σ_{incoh} was obtained by numerical integration of the Klein-Nishina (1929) formula weighted by the incoherent scattering function $S(x, Z)$. The values of $S(x, Z)$ were taken from the compilation by Hubbell, et al. (1975) for all Z's from 1 to 100, with a span of x values sufficient for computing σ_{incoh} over the photon energy range 100 eV-100 GeV, which were computed and tabulated in this compilation. Radiative and double-Compton corrections from Mork (1971) were applied to the integrated values for σ_{incoh}."

More details regarding the compilations of the incoherent cross section are given bellow from Hubbell (2006):
"The Hubbell, et al. (1975) $S(x, Z)$ values were pieced together from the data available in the literature, including the work of Pirenne (1946) (Z=1), Brown (1970a, 1970b, 1972, 1974) (Z=2 to 6, with configuration interaction) and by Cromer and Mann (1967) and Cromer (1969) (Z = 7-100, from a nonrelativistic Hartree–Fock model). Although giving cross sections differing by up to 2 to 3 percent from calculations of cross sections for isolated cases using relativistic S-matrix and other more sophisticated models, their compactness and ease of use makes these $S(x, Z)$ and σ_{incoh} values still (by default) the reference set used in most ... practical applications. In the future, use may be made of the relativistic Dirac-Hartree-Fock $S(x, Z)$ values computed by Kahane (1998) over the same range of x and Z as given in Hubbell, et al. (1975) non-relativistic composited set. Some insight into the limitations and use of $S(x, Z)$ tables, and possible refinements, can be found in Ribberfors and Berggren

(1982) and Namito, et al. (1994, 1995)."

1.1.3 Outline of some pieces of information about the history of the coherent (Rayleigh, elastic) scattering cross section calculations

In Hubbell (1999) we find the following explanation for the Rayleigh scattering process:
"Coherent or Rayleigh scattering is a process by which photons are scattered by the bound electrons collectively as a whole, and in which the atom is neither ionized nor excited. The photon loses only a negligible fraction of its energy, since the recoil is by the entire atom including the nucleus, rather than by an individual atomic electron as in the Compton effect, and the scattering is 'coherent' resulting in interference effects.... However, when this coherence is spread over an array of atoms, the interference becomes the Bragg diffraction which is of central importance in x-ray crystallography, ..."
The use of the term "Rayleigh scattering" to identify the contribution to elastic x-ray scattering from atoms due to bound atomic electrons is depicted by Kissel and Pratt (1985) and as well by Hubbell (1999, 2006).

In the work of Hubbell (2006) it is mentioned the special issue of Radiation Physics and Chemistry edited by Bradley and Speller (1999) which includes many studies on elastic scattering (for a detailed listing of the studies see Hubbell (2006)).

Regarding the compilations of the coherent scattering cross section the following explanations from Hubbell (1999) are provided below:
"For general-use compilations of μ/ρ, the coherent scattering cross-section σ_{coh} has been computed by numerical integration of the Thomson (1906) equation weighted by $F^2(x, Z)$, where $F(x, Z)$ is the atomic form factor. As in the somewhat complementary incoherent scattering function $S(x, Z)$, x is the momentum transfer variable dependent on the incident photon energy and the deflection angle of the scattered photon, and Z is the atomic (charge)

number of the nucleus of the target atom, or number of protons."
Next we are going to describe the non-relativistic values of $F(x, Z)$ used to compile the σ_{coh} in the work of Hubbell, et al. (1975). Such that for $Z = 1$ the $F(x, Z)$ values were computed from the 'exact' equation of Pirenne (1946). In addition for $Z = 2$ to 6 the values for $F(x, Z)$ were taken from the configuration interaction calculations by Brown (1970a, 1970b, 1971, 1974). The $F(x, Z)$ values tabulated for $7 \leq Z \leq 100$ were taken from the non-relativistic Hartree-Fock from Cromer and Mann (1968) and Cromer (1971).
In the XCOM, Berger and Hubbell (1987), and in the Seltzer and Hubbell (1995) the values of σ_{coh} are taken from the relativistic compilation of Hubbell and Øverbø (1979). The relativistic theoretical values of $F(x, Z)$ used in these works are for $Z = 1$ the ones from Pirenne (1946) and for the other elements, over the different ranges of x and Z, from Doyle and Turner (1968), Cromer and Waber (1974) and Øverbø (1977a, 1978a).

Other tabulations of $F(x, Z)$ are pointed out and the impact they have on the tabulations of σ_{coh} and μ/ρ is highlighted as follow by Hubbell (1999): "Somewhat higher accuracy is anticipated from the 1983 relativistic Hartree-Fock-Slater modified atomic form factor (MFF) calculations by Schaupp, et al. (1983) for $F(x, Z)$ for $Z = 1$–100, $0\text{Å}^{-1} \leq x \leq 100\text{Å}^{-1}$. This compilation was not accompanied by corresponding integrated values of σ_{coh}, and these MFF values have not yet found their way into the general-use μ/ρ compilations ...."

More recent developments regarding the compilations of the coherent cross section are depicted by Hubbell (2006): " Current theoretical efforts towards improved values of the coherent scattering cross section σ_{coh} are focused on the use of the second -order relativistic formalism (e.g. Kissel, et al. (1980), Pratt, et al. (1994), Kissel (1995)). This formalism is capable of revealing anomalous scattering, particularly in the vicinity of the absorption edge energies.
... A major step in this effort is the Chatterjee and Roy (1998) S-matrix computation and tabulation of the coherent scattering cross section, both differential, $(d\sigma_{coh}/d\Omega(\theta))$, and total, σ_{coh}, for all elements $Z = 13$ to 104, for 14 commonly-used γ energies between 50 keV and 1.5 MeV. [...] Comparisons with some measured differential cross sections are included. The total

coherent scattering cross sections, σ_{coh}, are compared with the corresponding non-relativistic (Hubbell, et al. (1975)) and relativistic (Hubbell and Øverbø (1979)) values. For low Z elements the differences are of the order of 1 percent to 3 percent, and for highest Z elements and the highest photon energy, 1.5 MeV, differences of the order of 20 percent are seen."

1.2 History of the calculations of the atom form factor

1.2.1 Outline of some pieces of information regarding the calculations of the atom form factor

Thoughout history the terms "atomic scattering factor", "atomic form factor" and "atomic structure factor" have all been used in order to describe the elastic scattering of photons by atoms, see Kissel and Pratt (1985). According to Bragg (1955) in the early history around 1924, James R.W. and West J. introduced measurements of absolute intensity as part of the routine of crystal analysis. Further Bragg (1955) mentions that for their work it was needed to know the scattering curves or f curves for all the atoms. At this time Hartree in Cambridge was engaged in calculating the Bohr orbits for a number of atoms, and he used his results to the calculation of the scattering curves, see Bragg (1955). According to Kissel and Pratt (1985) the "atomic scattering factor", f, was defined by Hartree (1925) as the "ration of the amplitude of the wave scattered by this atom to the amplitude scattered by an electron." For further details see Nelms and Oppenheim (1955) who synthesized an historical survey that has its stating point in the initial mentioned attempt of Hartree (1925) to evaluate the charge distribution of the electrons.

A survey of some studies regarding different derivation of the atomic form factor is given by Kissel and Pratt (1985). In this study the following works are mentioned for the classical derivation of the atomic form factor: Hartree (1925), Compton (1930), James (1962). Further non-relativistic quantum-mechanical derivation like Sommerfeld (1939) and James (1962) are noticed. In addition the relativistic quantum-mechanical derivations like for example Franz (1935, 1936), Goldberger and Low (1968), Florescu and Gavrila (1976) are referred.

A review of some more recent form factor theories is given by Creagh (1991). In this study are discussed extension of the classical notions to nonrelativistic quantum mechanics, (see for example Levinger (1952) and Gavrila (1982). In the same study it is mentioned the formula regarding the modified form factor (see Franz (1935) and Brown, et al. (1954, 1954, 1956, 1957)). Further a work of Schaupp, et al. (1988) comprising of relativistic modified form factors is quoted. In addition the work of Cromer and Lieberman (1970) who were the first to use relativistic quantum mechanics to create the tables for the dispersion corrections to the atom scattering factor is discussed as well in the same reference. Other relativistic approximation given by Creagh and McAuley (1991) and Smith (1987) are quoted by Creagh (1991). According to Creagh (1991) a more rigorous approach is provided by Kissel, et al. (1980). This theory is based on S-matrix formalism.
Let us note as well the review of the wide variety of calculations regarding the atomic form factor given by Hubbell, et al. (1975). Hubbell, et al. (1975) and Hubbell and Øverbø (1979) contain comprehensive tabulations of atomic form factors as well.

Herein we are going to present some results that give a functional relation that can be implemented in order to obtain the atomic form factor. Let us now follow some steps in the derivation of the expression of the atomic form factor provided by Kissel and Pratt (1985). The atomic form factor expression is a function of a single variable $\hbar q = 2\frac{\hbar\omega}{c}\sin\frac{\theta}{2}$, the momentum transfer to the atom, instead of $\hbar\omega$ (the photon energy) and θ (the scattering angle is the angle through which the wave vector of the radiation (propagation direction) has been changed). The atomic form factor $f(q)$ is defined for an atom with N electrons as the the matrix element (see, for example, Nelms and Oppenheim (1955)):

$$f(\mathbf{q}) = \int \sum_{n=1}^{N} \exp(i\mathbf{q}\cdot\mathbf{r}_n) |\psi|^2 \, dr_1 \ldots dr_n \qquad (66)$$

where

ψ	is the initial ($\equiv$ final)-state wave function of the atom;
$\hbar\mathbf{q}$	$= \mathbf{k}_i - \mathbf{k}_f$ is the momentum transferred to the atom (here $\mathbf{k}_i$ and $\mathbf{k}_f$ are the initial and final photon momenta; $\hbar$ is $h/2\pi$ where h is Planck's constant);
$\mathbf{r}_n$	are the coordinates of the nth electron.

Now in the model considered the total-atom wave function ψ is written as the product over single-electron wave functions ψ_n,

$$\psi = \prod_{n=1}^{N} \psi_n, \qquad (67)$$

since the electrons are considered independent interacting electrostatically with a single central potential.

Further it is claimed the operator, $\sum_{n=1} \exp(i\mathbf{q}\cdot\mathbf{r}_n)$, is symmetric, it is not needed to symmetrize the state. Such that the form factor can be rewritten in the following way:

$$f(q) = \int \rho(\mathbf{r}) \exp(i\mathbf{q}\cdot\mathbf{r}) d\mathbf{r}, \qquad (68)$$

in which

$$\rho(\mathbf{r}) = \sum_{n=1}^{N} |\psi_n(\mathbf{r})|^2 = \sum_{n=1}^{N} \rho_n(\mathbf{r}), \qquad (69)$$

is the atomic-electron charge density.

Note that the atomic form factor is a Fourier transform of the atomic charge distribution. Further this description of the form factor leads to the classical characterization of electromagnetic radiation from a charge distribution. Now if it assumed that $\rho(r)$ depends only on the magnitude of r, that is $\rho(r)$ is spherically symmetric, then we obtain the following relation for $f(q)$

$$f(q) = 4\pi \int_0^\infty \rho(r) \frac{\sin(qr)}{qr} r^2 dr. \qquad (70)$$

Now we are going to introduce a non-relativistic and a relativistic model for a system of one electron in order to obtain the form factor for e.g. hydrogen. For the non-relativistic model

for the hydrogen hydrogen atom we assume that:

$$\rho(r) = \frac{1}{4\pi} \left| R(Z,n,l,r) \right|^2$$

and

$$R\left(Z,n,l,r\right) = \sqrt{\left(\frac{2}{n\left(\frac{a_0}{Z}\right)}\right)^3 \frac{(n-l-1)!}{2n\left[(n+l)!\right]^3}} e^{-\frac{r}{n\left(\frac{a_0}{Z}\right)}} \left(\frac{2r}{n\left(\frac{a_0}{Z}\right)}\right)^l \left[L_{n-l-1}^{2l+1}\left(\frac{2r}{n\left(\frac{a_0}{Z}\right)}\right)\right],$$

in which

$R\left(Z,n,l,r\right)$	the radial part of the wave function for hydrogen,
Z	the atomic number,
n	the principal quantum-number,
l	the orbital quantum-number; $0, 1, \ldots, n-1$,
a_0	the Bohr radius,
$L_{n-l-1}^{2l+1}\left(\frac{2r}{n\left(\frac{a_0}{Z}\right)}\right)$	Laguerre polynomial.

Further using eq. (70) it is obtained the following relation for the atomic form factor for hydrogen:

$$G0(s) = \int_0^\infty r^2 \left| R\left(Z,n,l,r\right) \right|^2 \frac{\sin 4\pi sr}{4\pi sr} dr$$

where $s = \frac{\sin(\theta/2)}{\lambda}$ (here θ is the scattering angle, the angle between wave vector of the incoming beam and the wave vector towards the point of observation, and λ is the wavelength of the incoming beam).

Further we are going to focus on the relativistic result for the atomic form factor of a one electron system. Now we are going to use the solution to the Dirac equation in order to obtain the relativistic version for the atom form factor for the hydrogen atom. The radial solutions for the Dirac equation are the one derived by Bethe and Salpeter (1977). In this reference we find the explicit expressions for the normalized radial Dirac eigenfunctions:

$$f = \frac{\sqrt{\Gamma\left(2\gamma + n' + 1\right)}}{\Gamma\left(2\gamma+1\right)\sqrt{n'!}} \sqrt{\frac{1-\epsilon}{4N\left(N-\kappa\right)}} \left(\frac{2Z}{Na_0}\right)^{3/2} e^{-\frac{Zr}{Na_0}} \left(\frac{2Zr}{Na_0}\right)^{\gamma-1} \times$$

$$\times \left[n' F\left(-n'+1, 2\gamma+1, \frac{2Zr}{Na_0} \right) + (N-\kappa) F\left(-n', 2\gamma+1, \frac{2Zr}{Na_0} \right) \right],$$

$$g = \frac{\sqrt{\Gamma(2\gamma+n'+1)}}{\Gamma(2\gamma+1)\sqrt{n'!}} \sqrt{\frac{1+\epsilon}{4N(N-\kappa)}} \left(\frac{2Z}{Na_0} \right)^{3/2} e^{-\frac{Zr}{Na_0}} \left(\frac{2Zr}{Na_0} \right)^{\gamma-1} \times$$

$$\times \left[-n' F\left(-n'+1, 2\gamma+1, \frac{2Zr}{Na_0} \right) + (N-\kappa) F\left(-n', 2\gamma+1, \frac{2Zr}{Na_0} \right) \right], \quad (14.37)$$

where

κ is a new quantum number; equation (14.9),
$$\begin{cases} \kappa = -\left(j+\frac{1}{2}\right) = -(l+1) & \text{if} \quad j = l+\frac{1}{2}, \\ \kappa = +\left(j+\frac{1}{2}\right) = l & \text{if} \quad j = l-\frac{1}{2}, \end{cases}$$

γ $= +\sqrt{\kappa^2 - \alpha^2 Z^2}$, equation (14.22),

α the fine structure constant,

a_0 the Bohr radius,

Z is the atomic number,

ϵ $= \left(1 + \left(\frac{\alpha Z}{n-k+\sqrt{k^2-\alpha^2Z^2}}\right)^2\right)^{-\frac{1}{2}}$, equation (14.29) is the formula for the energy for the hydrogen atom,

n' $= n-k$, where $k = |\kappa| = j+\frac{1}{2}$, equation (14.28),

N $= \sqrt{n^2 - 2n'\left(k - \sqrt{k^2-\alpha^2Z^2}\right)}$, is the apparent quantum-number, equation (14.35).

and

Spectral terms	n	l	j
$1S_{1/2}$	1	0	1/2
$2S_{1/2}$	2	0	1/2
$2P_{1/2}$	2	1	1/2
$2P_{3/2}$	2	1	3/2

The above expressions are equations (14.37) from Bethe and Salpeter (1977) with the sign modified. We can use the following formula in order to generate the relativistic form factor for the hydrogen:

$$F0(s) = \int_0^\infty r^2 \left(f(r)^2 + g(r)^2 \right) \frac{\sin 4\pi sr}{4\pi sr} dr.$$

Herein we introduce a graph of the relativistic atom form factor for hydrogen obtained by using the above method. In addtion we include a plot of the ratio between the non relativistic form factor and the relativistic form factor for hydrogen (calculated by the methods described above). We observe that for hydrogen atom the difference in percent is very small. These graphs were taken from the notebook $f0$-hydrogen.nb (2018).

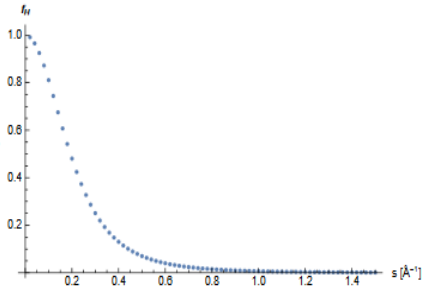

Figure 1.1: The relativistic atom form factor for hydrogen atom, denoted f_h.

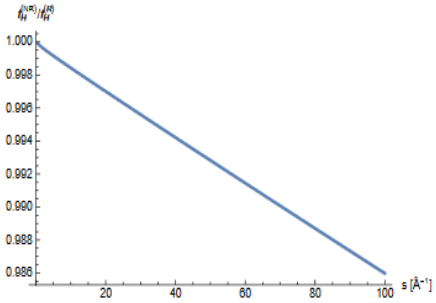

Figure 1.2: The ration between the non relativistic atom form factor and the relativistic atom form factor for hydrogen.

1.2.2 Outline of some pieces of information about the history of the real and imaginary part of the scattering factor calculations

Herein we are going to follow the line presented by James (1962). The total atomic scattering factor for frequency ω_i is given by the formula,

$$f = f_0 + f' + if'', \qquad (4.42)$$

in which f_0 is the atomic scattering factor for frequencies large compared with any atomic absorption frequency, and is independent of the incident frequency, and f', f'' are the real and imaginary parts of f that depend on the frequency.

Further we are going to introduce expressions for f'_K, the contribution to K electrons to the real part of f, denoted f', and f''_K the contribution of the K electrons to the imaginary part of f, denoted f''. The method regarding the derivation of the expression for f'_K and f''_K uses the classic quantum mechanics result for the oscillator strength provided by Hönl (1933). These expression are:

$$f'_K = \frac{2^7 e^{-4}}{9}\left\{\frac{4}{(1-\delta_K)^2}\frac{1}{x^2}\log_e\left|x^2-1\right| - \frac{1}{(1-\delta_K)^3}\left(\frac{2}{x^2}+\frac{1}{x^3}\log_e\left|\frac{x-1}{x+1}\right|\right)\right\},$$

$$f''_K = \frac{2^7 e^{-4}}{9}\pi\left\{\frac{4}{x^2\left(1-\delta_K\right)^2} - \frac{1}{x^3\left(1-\delta_K\right)^3}\right\} \quad \text{if } x>1,\ f''_K = 0 \ \text{ if } x<1. \quad (4.61)$$

where

x	$= \frac{\omega_i}{\omega_K}$ in which ω_i is the frequency of the incident radiation,
ω_K	$= \omega_0(1-\delta_K)$ in which ω_0 is the frequency of the absorption edge for a hydrogen-like atom of nuclear charge $Z-s$,
δ_K	$= \left(A - 911/\lambda_K\right)/A$ equation (4.58a), in which $A = Z_1^2 + 1.33\times 10^{-5}Z_1^4 + 3.55\times 10^{-10}Z_1^6 + 11.7\times 10^{-15}Z_1^8$ equation (4.58b) where $Z_1 = Z - 0.3$ and $911 = 10^8/R$ where R is Rydberg's constant and λ_K is expressed in Ångström units.

Herein we introduce as an example the plots for the real and imaginary part of the scattering form factor for the molybdenum atom calculated using the above expressions. The graphs were taken from the notebook (Hönl-theory-I.nb) (2018).

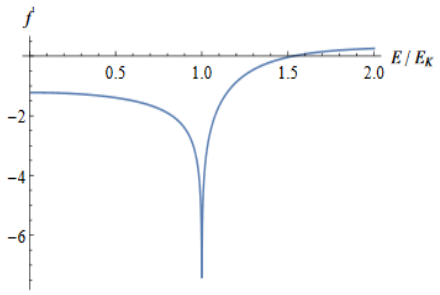

Figure 1.3: The real part of the scattering form factor for the molybdenum atom.

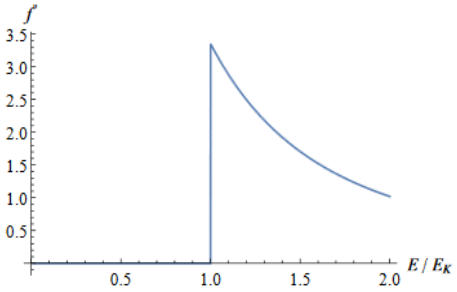

Figure 1.4: The imaginary part of the scattering form factor for the molybdenum atom.

1.2.3 The model outlined by Jens Als-Nielsen and Des McMorrow for the derivation of the real and imaginary part of the scattering factor

The classical oscillator model gives the the real and the imaginary part of the dispersion corrections. In the classical model the electron is bound to an atom. An electron will respond to the driving field of the x-rays as a damped harmonic oscillator, with associated resonant frequency ω_s and damping constant Γ. This is an approximation that let us explore the relationship between the real and the imaginary part of the dispersion corrections. The derivation of this relationship is taken from Als-Nielsen and Des McMorrow (2011).

Let us start by the expression considered for the scattering amplitude of the atom, in units of $-r_0$ (where r_0 is the Thomson scattering length of a single electron, the classical electron radius), can be written in the form:

$$f(\mathbf{Q},\omega) = f^0(\mathbf{Q}) + f'(\omega) + if''(\omega), \qquad (8.1)$$

$f^0(\mathbf{Q})$	the Thomson term depends on the scattering vector $\mathbf{Q}$ (here the $\mathbf{Q}$ dependence is due to the fact that the coherent scattering is produced by all atomic electrons, which have a spatial extent of the same order of magnitude as the X-ray wavelength),
$f'(\omega),\ f''(\omega)$	the real and the imaginary parts of the dispersion corrections which are energy (or equivalently frequency) dependent; (they are known as well as resonant scattering terms or anomalous scattering corrections).

It is worth to notice that the resonant scattering considered here is elastic, meaning that the scattered X-ray has the same energy as that of the incident one.

Now in order to derive the dispersion corrections we need the strength of the radiated electric field. For an observer at distance R and at time t the radiated field is:

$$E_{rad}(R,t) = -r_0 \frac{\omega^2}{\omega^2 - \omega_s^2 + i\omega\Gamma} E_0 e^{-i\omega t} \left(\frac{e^{ikR}}{R}\right)$$

where r_0 is the Thomson scattering length of a single electron, $k = \omega/c$, c is the light velocity, ω_s is the resonant frequency and Γ is the damping constant.

Further we are going to focus on the expression, $\frac{\omega^2}{\omega^2 - \omega_s^2 + i\omega\Gamma}$, which is named the atomic scattering length, f_s. The atomic scattering length, f_s, is defined as the amplitude of the outgoing spherical wave, $\left(\frac{e^{ikR}}{R}\right)$. The atomic scattering length, f_s, has the units of $-r_0$ and the subscript 's' used in the symbol emphasizes that the result is for a single oscillator. In addition let us notice that for frequencies large compared to the resonant frequency, $\omega \gg \omega_s$, the electron can be considered to be free, and the Thomson scattering expression is recovered, i.e. $f_s = 1$.

Next we are going to rearrange the expression for the atomic scattering length as follows:

$$f_s = \frac{\omega^2}{\omega^2 - \omega_s^2 + i\omega\Gamma} \qquad (8.3)$$

$$f_s = 1 + \frac{\omega_s^2 - i\omega\Gamma}{\omega^2 - \omega_s^2 + i\omega\Gamma}$$

Further since Γ is usually very small in comparison with ω_s the $i\omega\Gamma$ will be removed from the numerator but not from the denominator since the denominator can become zero. Such that one gets:

$$f_s \approx 1 + \underbrace{\frac{\omega_s^2}{\omega^2 - \omega_s^2 + i\omega\Gamma}}_{=\chi(\omega)} \quad (8.4)$$

The second term, which is denoted by $\chi(\omega)$ in the expression (8.4), is the dispersion correction to the scattering factor. It can be written as follows:

$$\chi(\omega) = f_s' + if_s'' = \underbrace{\frac{\omega_s^2(\omega^2 - \omega_s^2)}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2}}_{f_s'} + i\underbrace{\frac{(-\omega\Gamma)\omega_s^2}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2}}_{f_s''} \quad (8.6 - 8.7)$$

Now for a single oscillator one can deduce the following relationship between f_s' and f_s'':

$$f_s'(\omega) = \frac{2}{\pi} P \int_0^{+\infty} \frac{\omega' f_s''(\omega')}{\omega'^2 - \omega^2} d\omega'$$

$$f_s''(\omega) = -\frac{2\omega}{\pi} P \int_0^{+\infty} \frac{f_s'(\omega')}{\omega'^2 - \omega^2} d\omega'$$

This relation that (among other pair) exists between f_s' and f_s'' is called the Kramers-Kronig relations. Since $f'(\omega)$ and $f''(\omega)$ are linear superpositions of single oscillators, the Kramers-Kronig relations apply to them as well:

$$f'(\omega) = \frac{2}{\pi} P \int_0^{+\infty} \frac{\omega' f''(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (8.14b)$$

$$f''(\omega) = -\frac{2\omega}{\pi} P \int_0^{+\infty} \frac{f'(\omega')}{\omega'^2 - \omega^2} d\omega' \quad (8.15b)$$

Now in order to derive numerical estimates of $f'(\omega)$ we can use the following procedure. First if one knows (experimentally) the energy dependence of the absorption cross-section, $\sigma_a(\omega)$ it is possible to obtain $f''(\omega)$ using the expression from Als-Nielsen and Des McMorrow (2011):

$$f''(\omega) = -\left(\frac{\omega}{4\pi r_0 c}\right)\sigma_a(\omega) \quad (8.13).$$

Secondly one can use the equation (8.14b) to derive the associated real part of the dispersion

corrections to the scattering amplitude.

Bibliography

[1] Alling W.R. and Johnson W.R. (1965), *Exact calculations of K-shell and L-shell photo-effect*, Phys. Rev. 139, pp. A1050-A1062.

[2] Als-Nielsen J. and Des McMorrow (2011), *Elements of modern X-ray physics*, Second edition, A John Wiley and Sons, Ltd Publication.

[3] Barkla C.G. and Sadler C.A. (1907), *Secondary x-rays and the atomic weight of nickel*, Phil. Mag. 14, pp. 408-422.

[4] Barkla C.G. and Sadler C.A. (1909), *The absorption of Röntgen rays*, Phil. Mag. 17, pp. 739-760.

[5] Brown G. E., Peierls R. E. and Woodward J. B. (1954), *The coherent scattering of γ-rays by K electrons in heavy atoms-I. Method.*, Proc. R. Soc. Lond. A, Vol. 227, No. 1168, pp. 51-58.

[6] Brown G. E., Brenner S. and Woodward J. B. (1954), *The coherent scattering of γ-rays by K electrons in heavy atoms-II. The scattering of 0.32* mc^2 *γ-rays in mercury*, Proc. R. Soc. Lond. A, Vol. 227, No. 1168, pp. 59-72.

[7] Brown G. E. and Mayers D. F. (1956), *The Coherent Scattering of γ-rays by K Electrons in Heavy Atoms. III. The Scattering of 0.64* mc^2 *γ-Rays in Mercury*, Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, pp. 387-390.

[8] Brown G. E. and Mayers D. F. (1957), *The coherent scattering of γ-rays by K electrons in heavy atoms IV. The scattering of 1.28 and 2.56* mc^2 *γ-rays in mercury*, Proc. R. Soc. Lond. A, Vol. 242, No. 1228, pp. 89-95.

[9] Bragg L. (1955), *The crystalline state - a general survey* , Vol. I, G. Bell and Sons Ltd., London.

[10] Bethe H. A. and Salpeter E. E. (1977), *Quantum mechanics of one-and two-electron atoms*, Plenum publishing corporation. New York.

[11] Berger M.J. and Hubbell J.H. (1987), *XCOM: Photon cross sections on a personal computer*, (No. NBSIR-87-3597) National Bureau of Standards, Washington, DC (USA). Center for Radiation Research.

[12] Bergstrom P. M. and Pratt R.H. (1997), *An overview of the theories used in Compton scattering calculations*, Radiat. Phys. Chem. 50, pp. 3-29.

[13] Bergstrom P. M., Surić T., Pisk K. and Pratt R.H. (1992), *Some preliminary calculations of whole atom Compton scattering of unpolarized photons*, Nuclear Inst. and Methods in Physics Research, B, Vol. 71(1), pp. 1-6.

[14] Bergstrom P. M., Surić T., Pisk K. and Pratt R.H. (1993), *Compton scattering of photons from bound electrons: Full relativistic independent-particle-approximation calculations*, Physical Review A, Vol. 48(2), pp. 1134-1162.

[15] Bradley D.A. (ed) (1997), *Inelastic scattering of x-rays and gamma rays*, Radiat. Phys. Chem. 50 (1), (special issue).

[16] Bradley D.A. and Speller R (ed) (1999), *Elastic photon-atom scattering: fundamentals and applications* , Radiat. Phys. Chem. 56 (1–2) (special issue).

[17] Brown R.T. (1970a), *Coherent and incoherent x-ray scattering by bound electrons. I. Helium isoelectronic sequence*, Physical Review A, Vol. 1(5), pp. 1342-1347.

[18] Brown R.T. (1970b), *Coherent and incoherent x-ray scattering by bound electrons. II. Three- and four-electron atoms*, Physical Review A, Vol. 2(3), pp. 614-620.

[19] Brown R.T. (1971), *Atomic form factor for neutral carbon*, The Journal of Chemical Physics, 55(1), pp. 353-355.

[20] Brown R.T. (1972), *Incoherent-scattering function for atomic carbon*, Physical Review A, 5/1972, Vol. 5(5), pp. 2141-2144.

[21] Brown R.T. (1974), *Coherent and incoherent x-ray scattering by bound electrons. III. Five-electron atoms*, Physical Review A, Vol. 10(1), pp. 438-439.

[22] Cromer D.T. and Mann J.B. (1968), *X-ray scattering factors computed from numerical Hartree-Fock wave functions*, Acta Crystallogr. A 24, pp. 321–324.

[23] Cromer D.T. and Mann J.B. (1974), *Compton scattering factors for spherically symmetric free atoms*, LA-3689 UC-34, Los Alamos Scientific Laboratory.

[24] Cromer D.T. and Mann J.B. (1967), *Compton scattering factors for spherically symmetric free atoms*, The Journal of Chemical Physics, 47(6), pp. 1892-1893.

[25] Cromer D.T. (1969), *Compton scattering factors for aspherical free atoms*, J. Chem. Phys. 50, pp. 4857-9.

[26] Cromer D.T. (1971), *Private communication to Veigele W.J. and Hubbell J.H.*

[27] Cromer D.T. and Waber J.T. (1974), *Atomic scattering factors for x-rays, sec. 2.2*, International Tables for X-Ray Crystallography vol. 4 (Birmingham: Kynoch Press), pp. 71-147.

[28] Cromer D.T. and Liberman D. (1970), *Relativistic Calculation of Anomalous Scattering Factors for X Rays*, J. Chem. Phys. 53, pp. 1891-1898.

[29] Cooper M.J. (1997), *Compton scattering and the study of electron momentum density distribution*, Radiat. Phys. Chem. 50, pp. 63-76.

[30] Cullen D.E, Hubbell J.H and Kissel L. (1997), *EPDL97 The Evaluated Data Library, 97 Version*, UCRL-50400, Vol 6, Rev 5.

[31] Chantler C.T. (1995), *Theoretical Form Factor, Attenuation and Scattering Tabulation for Z=1-92 from E=1-10* eV *to E=0.4-1.0* MeV, J. Phys. Chem. Ref. Data 24, pp. 71-643.

[32] Chantler C.T. (2000), *Detailed tabulation of atomic form factors, photoelectric absorption and Scattering Cross Section, Mass Attenuation Coefficients in the vicinity of absorption edges in the soft x-ray (Z=30-36, Z=60-89, E=0.1* keV*-10* keV*), addressing convergence issues of earlier work*, J. Phys. Chem. Ref. Data 29, No. 4, pp. 597-1048, Random House, N.Y.

[33] Chatterjee B.K. and Roy S.C. (1998), *Tables of elastic scattering cross sections of photons in the energy range 50-1500* keV *for all elements in the range* $13 \leq Z \leq 104$, J. Phys. Chem. Ref. Data 27, pp. 1011-1215.

[34] Compton A. H. (1930), *The determination of electron distributions from measurements of scattered x-rays*, Physical Review, 35(8), pp. 925.

[35] Creagh D.C. (1991), *The atomic form factor, the dispersion corrections and their role in x-ray crystallography*, Chinese Journal of Physics, Vol. 29, Issue 4, pp. 299-325.

[36] Creagh D.C. and McAuley W.J. (1995), *X-ray dispersion corrections. Section 4.2.6*, In International Table for X-ray Crystallography, Vol. C, ed. AJC Wilson., pp. 206-219

[37] Doyle P.A. and Turner P.S. (1968), *Relativistic Hartree–Fock x-ray and electron scattering factors*, Acta Crystallogr. A 24, pp. 390-7.

[38] Evans R.D. (1958), *Compton effect. In Corpuscles and Radiation in Matter II (Korpuskeln und Strahlung in Materie II)*, Springer, Berlin, Heidelberg, pp. 218-298.

[39] Evans R.D. (1968), *Radiation Dosimetry in Attix F.H. and Roesch W.C. (eds.)*, Vol. 1, Ch. 3, New York/London: Academic Press.

[40] Florescu V. and Gavrila M., (1976), Phys. Rev. A 14, pp. 211.

[41] Franz W. (1935), Zeitschrift für Physik, 95, pp. 652.

[42] Franz W. (1936), Zeitschrift für Physik, 98, pp. 314.

[43] Goldberger M. L. and Low F. E. (1968), *Photon scattering from bound atomic systems at very high energy*, Physical Review, 176(5), pp. 1778.

[44] Gavrila M. (1982), *Photon-Atom Elastic Scattering*, X-Ray And Atomic Inner-Shell Physics, X-82: 1982 International Conference, Eugene, Oregon (USA) (23–27 August 1982): AIP Conference Proceedings, 01 December 1982, Vol. 94(1), pp. 357-388.

[45] Hönl H. (1933), *Zur Dispersionstheorie der Röntgenstrahlen*, Zeitschrift für Physik, Vol.84(1), pp. 1-16.

[46] Hartree D. R. (1925), *XXIX. The atomic structure factor in the intensity of reflexion of X-rays by crystals*, The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 50(295), pp. 289-306.

[47] Hubbell J.H., Veigele W.J., Briggs E.A., Cromer D.T. and Howerton R.J. (1975), *Atomic Form Factors, Incoherent Scattering Functions, and Photon Scattering Cross Sections*, J. Phys. Chem. Ref. Data 4, pp. 471-538; erratum in 6, pp. 615-616 (1977).

[48] Hubbell J.H. (2006), *Review and history of photon cross section calculations*, Phys. Med. Biol. 51, pp. R245-R252.

[49] Hubbell J.H. (1977), *Photon mass attenuation and mass energy-absorption coefficients for H, C, N, O, Ar, and seven mixtures from 0.1* keV *to 20* MeV, Radiation Research, 70(1), pp. 58-81.

[50] Hubbell J.H. (1999), *Compilation of photon cross-sections: some historical remarks and current status*, X-ray Spectrom. 28, pp. 215-223.

[51] Hubbell J.H. (1977), *Photon mass attenuation and mass energy-absorption coefficients for H, C, N, O, Ar, and seven mixtures from 0.1* keV *to 20* MeV, Radiat. Res. 70, pp. 58-81.

[52] Hubbell J.H. (1969), *Photon cross sections, attenuation coefficients, and energy absorption coefficients from 10* keV *to 100* GeV, NSRDS-NBS 29, pp. 1-80.

[53] Hubbell J.H. (1982), *Photon Mass Attenuation and Energy Absorption Coefficients from 1* keV *to 20* MeV, Int. J. Appl. Radiat Isotopes, 33, pp. 1269-1290.

[54] Hubbell J.H. and Øverbø I. (1979), *Relativistic atomic form factors and photon coherent scattering cross sections*, J. Phys. Chem. Ref. Data 8, pp. 69–105.

[55] Hubbell J.H., Gimm H.A. and Øverbø I. (1980), *Pair, Triplet and Total Atomic Cross Sections (and Mass Attenuation Coefficients) for 1* MeV*-100* GeV *Photons in Elements Z=1 to 100*, J. Phys. Chem. Ref. Data 9, pp. 1023-1147.

[56] Hubbell J.H. and Berger J. (1968), *4.1. Attenuation coefficients, energy absorption coefficients, and related quantities* in Engineering compendium on radiation shielding. Edited by Jaeger R. G. (Editor-in-Chief), Blizard E. P., Chilton A. B., Grotenhuis M., Hönig A., Jaeger Th. A., Eisenlohr H. H.(Coordinating editor). Sponsored by the International Atomic Energy Agency, Vienna. Volume I: Shielding fundamentals and methods. Springer-Verlag, Berlin, Heidelberg, New York (1968).

[57] Henke B.L., Lee P., Tanaka T.J., Schimabukuro R.L. and Fujikawa B.K. (1982), *Low-energy x-ray interaction coefficients: photoabsorption, scattering, and reflection. E=100-2000* eV *Z=1-94*, atomic Data Nucl. Data Tables 27, pp. 1-144.

[58] Hultbergs S., Nagel B. and Olsson P. (1961), *Relativistic differential and total K-shell photoelectric cross-sections and photoelectron polarizations*, Arkiv f. Fysik 20, pp. 555-557.

[59] Hultbergs S., Nagel B. and Olsson P. (1968), *Numerical calculation of K-shell photoeffect*, Arkiv f. Fysik 38, pp. 1-96.

[60] James R.W. (1962), *The Optical Principles of the Diffraction of X-rays*, The crystalline state vol. II, London G. Bell and Sons Ltd.

[61] Kahane S. (1998), *Relativistic Dirac–Hartree–Fock photon incoherent scattering functions*, Atomic Data and Nuclear Data Tables, Vol. 68(2), pp. 323-347.

[62] Kissel L. (1995), *Toward improved photon-atom scattering predictions*, Nucl. Instrum. Methods B 99, pp. 144-147.

[63] Kissel L. and Pratt R.H. (1985), *Rayleigh scattering-Elastic photon scattering by bound Electrons*, in Atomic Inner-Shell Physics, edited by Bernd Crasemann (Plenum Publishing: New York and London).

[64] Kissel L., Pratt R.H. and Roy S.C. (1980), *Rayleigh scattering by neutral atoms, 100* eV *to 10* MeV, Phys. Rev. A 22, pp. 1970-2004.

[65] Kane P.P. (1992), *Inelastic scattering of X-rays and gamma-rays by inner shell electrons*, Physics Reports, Vol. 218(2), pp. 67-139.

[66] Kane P.P. (1997), *Experimental studies of inelastic x-ray and γ-ray scattering*, Pergamon Radiat. Phys. Chem. Vol. 50, No. 1, pp. 31-62.

[67] Klein O. and Nishina Y. (1929), *Über die streuung von strahlung durch freie elektronen nach der neuen relativistischen quanten dynamik von Dirac*, Z. Phys. 52, pp. 853-68.

[68] Levinger J. S. (1952), *Small angle coherent scattering of gammas by bound electrons*, Physical Review, 87(4), pp. 656.

[69] Mork K.J. (1971), *Radiative corrections. II. Compton effect*, Physical Review A, 4(3), pp. 917-927.

[70] Meitner L. and Hupfeld H. (1930), *Über die Prüfung der Streuungsformel von Klein und Nishina an kurzwelliger γ-Strahlung*, Naturwissenschaften, Vol. 18(22), pp. 534-535.

[71] Matese J.J. and Johnson W.R. (1965), *Influence of screening on the atomic photoeffect*, Phys. Rev. 140, pp. A1-A7.

[72] Nelms A. T. (1953), *National Bureau of Standards Circular 542*, US Government Printing Office, Washington, DC.

[73] Nelms A. T. and Oppenheim I.(1955), *Data on the atomic form factor: computation and survey*, J. Res. Nat. Bureau of Standards, 55, pp. 53-62.

[74] Namito Y., Ban S. and Hirayama H. (1994), *Implementation of the Doppler broadening of a Compton-scattered photon into the EGS4 code*, Nuclear Inst. and Methods in Physics Research, A, Vol. 349(2), pp. 489-494.

[75] Namito Y., Ban S., Hirayama H., Nariyama N, Nakashima H., Nakane Y., Sakamoto Y, Asano Y. and Tanaka S. (1995), *Compton scattering of 20- to 40-*keV *photons*, Physical review. A, Atomic, molecular, and optical physics, Vol. 51(4), pp. 3036-3043.

[76] Øverbø I. (1977a), *Atomic form factors for large momentum*, Nuovo Cimento B 40, pp. 330-338.

[77] Øverbø I. (1977b), *The Coulomb correction to electron pair production by intermediate-energy photons*, Phys. Lett. B 71, pp. 412–4.

[78] Pirenne (1946), *The diffraction of x-rays and electrons by free molecules*, (Cambridge: Cambridge University Press) pp. 12-28.

[79] Pratt R.H. (1960), *Atomic photoelectric effect at high energies*, Phys. Rev. 117, pp. 1017-28.

[80] Pratt R. H., Levee R. D., Pexton R. L. and Aron W. (1964), *K-shell photoelectric cross sections from 200* keV *to 2* MeV, Physical Review, 134(4A), pp. A898.

[81] Pratt R.H., Kissel L. and Bergstrom P.M. (1994), *New relativistic S-matrix results for scattering-beyond the usual anomalous factors / beyond impulse approximation*, Resonant Anomalous X-ray Scattering: Theory and Application ed G. Matterlik, C.J. Sparks and K. Fischer (Amsterdam: Elsevier), pp. 9-33.

[82] Ribberfors R. and Berggren K.F. (1982), *Incoherent-x-ray-scattering functions and cross sections* $(d\sigma/d\Omega')_{incoh}$ *by means of a pocket calculator*, Physical Review A, Vol. 26(6), pp. 3325-3333.

[83] Rakavy G. and Ron A. (1965), *Total cross sections of the photoelectric effect for uranium*, Phys. Lett. 19, pp. 207-208.

[84] Rakavy G. and Ron A. (1967), *Atomic photoeffect in the range* E_γ *= 1-2000* keV, Phys. Rev. 159, pp. 50-6.

[85] Schmickley R.D. and Pratt R.H. (1967), *K-, L-, and M-shell atomic photoeffect for screened-potential models*, Phys. Rev. 164, pp. 104-16.

[86] Slater (1951), *A simplification of the Hartree-Fock method*, Phys. Rev. 81, pp. 385-90.

[87] Saloman E.B., Hubbell J.H. and Scofield J.H. (1988), *X-ray Attenuation Cross Sections for Energies 100* eV *to 100* keV *and Elements Z = 1 to Z = 92*, Atomic Data and Nucl. Data Tables 38, pp. 1-197.

[88] Saloman E.B. and Hubbell J.H. (1986), *X-ray Attenuation Coefficients (Total Cross Sections): Comparison of the Experimental Data Base with Recommended Values of Henke and the Theoretical Values of Scofield for Energies between 0.1-100* keV, National Bureau of Standards Report NBSIR 86-3431.

[89] Scofield J.H. (1973), *Theoretical Photoionization Cross Sections from 1 to 1500* keV, Lawrence Livermore National Laboratory Rep. UCRL-51326.

[90] Scofield J.H. (1985), *Private communication to Saloman E.B. and Hubbell J.H.*

[91] Seltzer S.M. and Hubbell J.H. (1995), *Tables of graphs of photon mass attenuation coefficient and mass energy-absorption coefficients for photon energies 1* keV *to 20* MeV *for elements Z=1 to 92 and some dosimetric materials*, https://www.nist.gov/pml/x-ray-mass-attenuation-coefficients.

[92] Schaupp D., Schumacher M., Smend F., Rullhusen P. and Hubbell J.H. (1983), *Small-angle Rayleigh scattering of photons at high energies: tabulations of relativistic HFS modified atomic form factors*, J. Phys. Chem. Ref. Data 12, pp. 467–512.

[93] Sugiura Y. (1927), *Sur le nombre des électrons de dispersion pour les spectres continus et pour les spectres de séries de l'hydrogène*, Journal de Physique et le Radium, Vol. 8(3), pp. 113-124.

[94] Sommerfeld A. (1939), *Atombau und Spektrallinien*, Vol. II.

[95] Schaupp D., Schumacher M., Smend F., Rullhusen P. and Hubbell J.H. (1988), J. Phys. Chem. Ref. Data 12, pp. 467.

[96] Smith D. Y. (1987),*Anomalous x-ray scattering: Relativistic effects in x-ray dispersion analysis*, Physical Review A, 35(8), pp. 3381.

[97] Thomson J.J. (1906), *Conduction of electricity through gases*, (Cambridge: Cambridge University Press) pp. 325.

[98] Thorkildsen G., (2018), *f_0-hydrogen.nb (notebook)*, unpublished manuscript.

[99] Thorkildsen G., (2018), *Hönl-theory-I.nb.nb (notebook)*, unpublished manuscript.

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2

Databases

In this chapter we bring together databases available online, as shown in table 1 from Appendix A. From section 2.1 to 2.17 we present the following databases: the Atomic Scattering Factor Files from Lawrence Berkeley National Laboratory, X-ray Anomalous Scattering database available at Biomolecular Structure Center, X-ray database created by Elam, Ravel and Sieber, FFAST and XCOM databases available at the National Institute of Standards and Technology U.S., the Rayleigh scattering database (RTAB), the X-ray database belonging to the Sasaki laboratory, Xraylib library and the X-ray databases belonging to European Synchroton Radiation Facility (ESRF). The purpose of this chapter is to introduce useful information regardning the datasets comprized in the different databases. In section 2.18, this chapter includes plots obtained from the data sets of some databases.

2.1 X-ray database available at Lawrence Berkeley National Laboratory

The folder 'Berkeleylab' contains tabulations for the atomic scattering factor components from the X-ray database available at Lawrence Berkeley National Laboratory.

2.1.1 A. Availability

The X-ray database is available at Lawrence Berkeley National Laboratory, http://henke.lbl.gov/optical_constants/. Similar tabulations for the atomic scattering factor components, which were generated in 2002 by the code f1f2-Henke.pro, can be found at European Synchroton Radiation Facility (ESRF), http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/, see European Synchroton Radiation Facility (2003).

2.1.2 B. Outline of some pieces of information about the X-ray database

The database is maintained by the Center for X-Ray Optics (CXRO) which is a multidisciplined research group within Lawrence Berkeley National Laboratory's Materials Sciences Division. The tabulations from this database regarding the atomic scattering factors have as starting point the data from the work of Henke, et al. (1993). Since the publication of the tables in 1993, the tabulated values for some elements have been revised, see Center for X-Ray Optics (2011).

2.1.3 C. Outline of some pieces of information regarding the atomic scattering factor components

Herein we give the following quote from the documentation available at European Synchroton Radiation Facility (2003):

"The atomic scattering factors are based upon experimental measurements of the atomic photoabsorption cross section, both from our laboratory and from the literature. The absorption measurements provide values for the imaginary part of the atomic scattering factor.

The real part, which describes the dispersion of radiation as it interacts with matter, is calculated from the absorption measurements using the Kramers-Kronig integral relations."

Further, we include the following text from Henke, et al. (1993):

"From a synthesis of the currently available experimental data and recent theoretical calculations for photoabsorption, the angle-independent, forward-scattering components of the atomic scattering factors have been semiempirically determined and tabulated here for 92 elements and for the region 50-30.000 eV. Atomic scattering factors for all angles of coherent scattering and at the higher photon energies are obtained from these tabulated forward-scattering values by adding a simple angle-dependent form-factor correction."

In addition we introduce the following quote from Henke, et al. (1993) regarding the atomic photoabsorption cross sections, which are used for the calculations of the values of the atomic scattering factor components for the case of forward scattering:

" The experimental photoabsorption data that we have used include those described in the works listed in the INSPEC[1] abstract files of the past 10 years and those which have been recently added to the comprehensive NIST[2] database of experimental values by Saloman, et al. (1988). Best-fit determinations of the photoabsorption cross sections, for 10-10.000 eV, were made relying on both theory and measurements and interpolating across Z for the many elements where few measurements were available. For energies higher than 10 keV, there are several excellent syntheses of photoabsorption cross sections, see Saloman, et al. (1988), Cullen, et al. (1989) and Biggs and Lighthill (1988). We have chosen that of Biggs and Lighthill (1988) as it is based on essentially the same experimental database. In their report, Biggs and Lighthill present four-term polynomial fits in the $(1/E)$[3] variable between absorption edges. Using our photoabsorption best-fit values for the region 10-10.000 eV and those of Biggs and Lighthill (1988) for the higher photon energies, the dispersion integral in

[1] https://www.elsevier.com/__data/assets/pdf_file/0004/56407/IET-Inspec-factsheet.pdf
[2] National Institute of Standards and Technology, Gaithersburg, MD.
[3] where E is photon energy in keV according to Biggs and Lighthill (1988)

(Eq.76) was numerically evaluated to obtain $f_1(0)$[4] in the region 50-30.000 eV."
Our folder 'Berkeleylab' contains the tabulations from Lawrence Berkeley National Laboratory for the angle-independent (forward) atomic scattering factor components in the energy range 50-30.000 eV (0.41 to 248 Å) for the elements with Z=1 (hydrogen) to Z=92 (uranium). The grid used for these tabulations consists of 500+ points on a uniform logarithmic mesh from 10 to 30,000 eV with points added 0.1 eV above and below "sharp" absorption edges, according to Center for X-Ray Optics (2011). Further for some elements data on a finer mesh are included around absorption edges, see Center for X-Ray Optics (2011).

2.2 X-ray Anomalous Scattering database available at Biomolecular Structure Center, University of Washington

The tabulations from the folder 'BrennanCowan' were taken from the X-ray Anomalous Scattering database available at Biomolecular Structure Center, University of Washington, Seattle.

2.2.1 A. Availability

The X-ray Anomalous Scattering database is available at Biomolecular Structure Center, University of Washington at http://skuld.bmsc.washington.edu/. Similar tabulations can be found in a file which is available at European Synchroton Radiation Facility (ESRF), http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

[4] the forward atomic scattering-factor component

2.2.2 B. Outline of some pieces of information about the X-ray database

This dabase was intended mainly for crystallographers' designing experiments based on anomalous scattering, see Merritt (2012).

This database contains tabulations of the characteristic x-ray absorption edge energies, and of the anomalous scattering coefficients f' and f'' as a function of incident x-ray energy. These data are organized in a periodic table for the elements hydrogen through uranium in the energy range 1000 eV (13Å) to 25000 eV (0.50Å). The database gives the possibility to generate plots of the selected scattering coefficients.
Herein we give the following quote from Brennan and Cowan (1992):
"We have created three data bases ... . One data file stores both the Cromer and Liberman f' and f'' values, ... The data bases are accessible through a set of subrutine calls ... . These calls have been packed in a shareable image library."

2.2.3 C. Outline of some pieces of information regarding the anomalous scattering coefficients f' and f''

The data for the anomalous scattering coefficients f' and f'' were calculated using the subrutine library by Brennan and Cowan, see Merritt (2010).
Herein we intoduce a quote from Brennan and Cowan (1992):
"For calculating f' and f'' we use the data of Cromer and Liberman[5] (1981) which follows upon earlier work by the same authors (Cromer (1965) and Cromer and Liberman (1970a)). The imaginary anomalous dispesion term f'' is related to the total photoelectric absorption cross section via the optical theorem. "

[5]" The original data and calling routine for calculating f' and f'' was obtained from D.T. Cromer and P.H. Fuoss as a stack of punch cards. In 1987, during a visit to Hasylab by the authors, the program was converted to F77 and direct access data base format. It has been upgraded extensively since then", according to Brennan and Cowan (1992)

In addition we introduce the following text from the documentation regarding X-ray Anomalous Scattering database, see Merritt (2010):
"The values for f' and f'' are derived using the theoretical approximation developed by Cromer and Liberman. This theory gives accurate values far from an absorption edge but does not account for the effects of neighboring atoms, which can be very substantial near an absorption edge."

The references that were takken into consideration in the developping the tabulations of the the anomalous scattering coefficients f' and f'' from the X-ray Anomalous Scattering database are Cromer (1965), Cromer and Liberman (1970), Cromer and Liberman (1981), Cromer and Mann (1968), Balyuzi (1975), Hoyt, et al. (1984) and Kissel and Pratt (1990) according to Merritt (2006).
Our folder 'BrennanCowan' comprises of the values of f' and f'' for the elements hydrogen through uranium over the range of energy from 1000 eV (13Å) to 25000 eV (0.50Å).

2.3 X-ray database created by Elam, Ravel and Sieber

Tabulations from the folders 'Scatter' and 'Photo' were retrived from the database created by Elam, Ravel and Sieber (NIST[6]version 1.2 from 2001).

2.3.1 A. Availability

The database designed by Elam, Ravel and Sieber is hosted at https://github.com/scikit-beam/XrayDB.

2.3.2 B. Outline of some pieces of information regarding the atomic database

The authors compiled a comprehensive database of atomic parameters dedicated to X-ray spectroscopy which included the best and recent available values, see Elam et al. (2002).
The following is an extract from Elam, et al. (2002):
"Such a selection of necessity involved some subjective judgements, and the result reflects solely the opinion of the authors. ... 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."

2.3.3 C. Outline of some pieces of information regarding the cross sections

Acording to Elam, et al. (2002) the stating point to the cross sections values above 1 keV are the ones given by Berger and Hubbell (1987), which are included in the version 2.1 of the XCOM computer program. Herein, we quote a passage from Elam, et al. (2002):
" These values are checked against the NIST[6] 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. ... 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 used here. ... 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

[6]National Institute of Standards and Technology U.S. Department of Commerce

integration that starts or ends at an absorption edge energy. ... 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 (1986). No interpolation was done; the energy values in the cross section table were simply changed.

... The resulting table contains an energy grid, photoabsorption 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/g."

Our folder 'Photo' contains the resulting table for photoabsoption cross sections for atoms with Z from 1 to 98. In addition our folder 'Scatter' comprises of the table for coherent and incoherent cross sections for atoms with Z from 1 to 98.
Furthermore, we have used a code based on cubic spline interpolation to generate the values of the cross sections between the values given in the tables retrived from this database (for details regarding the interpolation method see Singiresu (2002)).

2.4 X-ray Form Factor, Attenuation and Scattering Tables database (FFAST) available at the National Institute of Standards and Technology U.S.

The data from the folder 'FFAST' were retrived from the X-ray Form Factor, Attenuation and Scattering Tables database (FFAST) available at the National Institute of Standards and Technology U.S. Department of Commerce.

2.4.1 A. Availability

The data base X-ray Form Factor, Attenuation and Scattering Tables database (FFAST) is available at National Institute of Standards and Technology, https://www.nist.gov/pml/x-ray-form-factor-attenuation-and-scattering-tables Similar tabulations can be found in a file which was created in 1996 and is available at European Synchroton Radiation Facility (ESRF), http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

2.4.2 B. Outline of some pieces of information about the X-ray database

This database was created for x-ray diffraction, interferometry, crystallography, and related areas, see National Institute of Standards and Technology (2016). FFAST data base contains data regarding atomic elements from H through U and compounds and covers the energies from 0 to 433 keV, see National Institute of Standards and Technology (2016).

The tabulations and graphs provided by FFAST database regard (in details see National Institute of Standards and Technology (2016)):

- components of the form factors, denoted f_1 and f_2
- component of f_2 relating to the isolated K-shell orbital, denoted f_2, K-shell
- mass photoabsorption coefficient, denoted $[\mu/\rho]_{PE}$
- component of $[\mu/\rho]_{PE}$ relating to the isolated K-shell orbital, denoted $[\mu/\rho]_{PE,K}$
- estimate of coherent and incoherent ($\sigma_{coh} + \sigma_{incoh}$) scattering cross-section sum, denoted $[\sigma/\rho]_{(coh+inc)}$
- mass attenuation coefficient, denoted $[\mu/\rho]_{tot}$

Our folder FFAST contains the above coefficients for atomic elements from H through U in the energy range 2.00 - 433 keV (0.29Å − 6.20Å).

In addition the database FFAST gives tabulations for linear attenuation coefficient, denoted $[\mu]_{tot}$, correction factors (relativistic correction to Re(f), denoted f_{rel}, Nuclear Thomson correction to Re(f), denoted f_{NT}) and the appropriate relativistic correction and conversion factors.

The FFAST data base treats each atom as an isolated system, according to National Institute of Standards and Technology (2016). Moreover, the tabulations from FFAST database are computed within self consistent Dirac-Hartree-Fork framework[7], see National Institute of Standards and Technology (2016).

2.4.3 C. Outline of some pieces of information regarding f_1 and f_2 the components of the form factors and the mass photoabsorption coefficient, $[\mu/\rho]_{PE}$

The tabulations for these coefficients are given in the works of Chantler (1995) and Chantler (2000). Herein we introduce a text from Chantler (2000) regarding these tabulations:

"In this work we use the same formalism as described in Chantler (1995). This follows the DHF (Dirac-Hartree-Fock) SCF (self-consistent field) approach of Cromer and Liberman (1970), Cromer and Liberman (1970), Cromer and Mann (1968) and Cromer and Liberman (1981) and uses the Kohn-Sham potential, see Kohn and Sham (1965), and experimental energy levels to compute partial photoelectric absorption coefficients using the Brysk-Zerby program modified, see Brysk and Zerby (1968). The modifications introduced are to improve computational precision rather than a change of the formalism. We then use f_2 to compute f_1 using standard Kramers-Kronig dispersion formula ... .

Hence, we treat each atom as an isolated system, not influenced by any other atoms or parti-

[7]Grant I. P. (2007) Relativistic Quantum Theory of Atoms and Molecules: Theory and Computation, Springer, New York; Swirles W. (1935), The Relativistic Self-Consistent Field, Ph.D., University of Manchester, http://rspa.royalsocietypublishing.org/content/royprsa/152/877/625.full.pdf; Grant I. P. (1961) Relativistic self-consistent fields, Proc. R. Soc. Lond. A, 262(1311), 555-576.

cles (this is the isolated atom approximation). Additionally, we determine each wave function including correlation according to the DHF (Dirac-Hartree-Fock) procedure, and allow for the electron-electron interactions via the use of the central field and Kohn-Sham potential. In other words, we use Dirac relativistic wave functions with full antisymmetrization of product wave functions within the DHF (Dirac-Hartree-Fock) method.

We make the assumption of the independent particle approximation so that each electron is considered to move in an effective potential of the nucleus with the average repulsive force of the electrons. This effective screening neglects some correlation and neglects the fact that the potential for one electron is really not identical to that of a different electron. This assumption is quite general - the only choice is the selection of the form of the central potential."

Further, for the values in between the tabulations of f_1 from the works of Chantler, one should use linear interpolation, see Chantler (1995, 2000). While in the case of f_2 and $[\mu/\rho]_{PE}$ values linear log-log interpolation is recomanded, see Chantler (1995) and Chantler (2000).

2.4.4 D. Outline of some pieces of information regarding the scattering cross-section sum ($\sigma_{coh} + \sigma_{incoh}$)

Here we give the following quote from Chantler (2000) regarding the coefficients $[\mu/\rho]_{coh}$ and $[\mu/\rho]_{incoh}$:

"These latter two coefficients are angle-dependent and may in part be determined from appropriate structure factors for a given crystal orientation ... . However a column is provided for the sum of these two latter coefficients in an average over-angles for an atomic scatterer, see Veigele (1973) and McMaster et al. (1969). These references should be consulted for details concerning the approximation involved, although the column in the current tabulation is a new computation of the sum (following Chantler (1995))."

2.5 XCOM: Photon Cross Sections Database available at the National Institute of Standards and Technology U.S.

The tabulations from the folder 'Xcomdatany' were calculated by the XCOM program provided by the XCOM: Photon Cross Sections Database.

2.5.1 A. Availability

This database is available at National Institute of Standards and Technology (NIST), https://www.nist.gov/pml/xcom-photon-cross-sections-database. In addition there are available tabulations, from 2009, using XCOM program at European Synchroton Radiation Facility (ESRF) http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

2.5.2 B. Outline of some pieces of information about the X-ray database

XCOM database was developed for radiological physics and dosimetry, see National Institute of Standards and Technology (2016).

According to Berger and Hubbell (1987) the XCOM program can be used to calculate total cross sections and attenuation coefficients as well as partial cross sections for the following processes: incoherent scattering, coherent scattering, photoelectric absorption and pair production in the field of atomic nucleus and in the field of the atomic electrons. These calculations can be done for any element ($Z = 1 - 100$), compound or mixture, at energies from 1 keV to 100 GeV, see Berger and Hubbell (1987).

The XCOM program can calculate cross sections on a standard energy grid, on a grid selected by the user, or for a mix of both grids. XCOM generates two forms of output, such as tables similar to those found in the literature and graphical display of the tabular data, see Berger and Hubbell (1987).

Herein we include the following text from Berger and Hubbell (1987):
" Some limitations should be noted. The cross sections for elements in the XCOM database pertain to isolated neutral atoms, and so do not take into account molecular and solid-state effects which modify the cross sections, especcially in the vicinity of absorption edges."

2.5.3 C. Outline of some information regarding the incoherent and coherent scattering cross sections and the photoelectric cross section

Here we introduce the following quote from Berger and Hubbell (1987):
"A comprehensive database for all elements over a wide range of energies was constructed through the combination of incoherent and coherent scattering cross sections from Hubbell, et al. (1975) and Hubbell, et al. (1979), photoelectric absorption from Scofield (1973), and pair production cross sections from Hubbell, et al. (1980). For scattering and pair production, the same cross sections are used as in other recent tabulations in Hubbell (1977), Hubbell, et al. (1980) and Hubbell (1982), whereas for photoelectric absorption there is a small difference (omission of a renormalization correction) which is discussed below.

The incoherent (Compton) scattering cross sections in Hubbell, et al. (1975) were obtained from a combination of the Klein-Nishina formula and nonrelativistic Hartree-Fock incoherent scattering functions. Radiative and double Compton-scattering corrections[8]were

included. The coherent (Rayleigh) scattering cross sections in Hubbell, et al. (1979) were calculated from a combination of the Thomson formula and relativistic Hartree-Fock atomic form factors. The photoelectric cross sections were obtained by Scofield (1973) by a phase-shift calculation for a central potential and a Hartree-Slater atomic model. Scofield's results extend only up to 1.5 MeV.

... For elements with atomic numbers from 2 to 54, Scofield (1973) presented correction factors for individual atomic subshells, with which the photo-effect cross sections can be renormalized so that they correspond approximately to a relativistic Hartree-Fock model[9] rather than the Hartree-Slater model[10] used in the original calculation. This renormalization is most significant for the outer atomic shells; the total cross section is lowered by no more than 10 percent at energies above 1 keV . Scofield did not actually apply the renormalization to the cross sections given in his tables. The renormalization was used, however, in the tabulations in Hubbell (1977), Hubbell, et al. (1980) and Hubbell (1982). Recent reviews Saloman, et al. (1987) and Saloman, et al. (1986) indicate that, on the whole, agreement with experiment is better when the renormalization is not done. We have therefore omitted the renormalization in the database for the XCOM program."

In addition Berger and Hubbell (1987) note that:
"For the purpose of interpolation with respect to photon energy, the coherent and incoherent scattering cross sections ... are approximated by log-log cubic-spline fits as functions of energy.
... The combined photoelectric absorption cross section for all shells is similarly interpolated with use of log-log cubic-spline fits, but only at energies above the K-shell absorption edge. Below this energy, interpolation is applied to the logarithm of the photoelectric absorption

[8] for details see Hubbell, et al. (1975)

[9] for details regarding the Hartree-Fock model see: Hartree D. R. (1928), The wave mechanics of an atom with a non-coulomb central field. Part II. Some results and discussion, In Mathematical Proceedings of the Cambridge Philosophical Society Vol. 24, No. 1, 111-132, Cambridge University Press; Fock V. (1930), Approximation method for the solution of the quantum mechanical multibody problems, Zeitschrift fur Physik, 61, 126-148.

[10] for details see Slater J. C. (1951), A simplification of the Hartree-Fock method, Physical Review, 81(3), 385-390.

cross section for each separate shell, fitted as a linear function of the logarithm of the photon energy. The separate fitting for each shell is necessary to avoid the error that would be incurred by interpolating across absorption edges. Linear log-log fitting is equivalent to assuming that the photoelectric cross section is proportional to a power of the photon energy, and was found to provide more satisfactory fits than a log-log cubic-spline fit near the absorption edges."

Our tabulations from the forder 'Xcomdatany' were generated by XCOM program using the following grid $\lambda \in \{0.001, 3.000\}$ Å with step 0.001 Å, covering the energy range 4.133 keV - 12.4 MeV . Further these tabulations regard the incoherent and coherent scattering cross sections and photoelectric cross section for our selected grid.

2.6 The database RTAB: the Rayleigh scattering database

The data from the folders 'Data-asf', 'Data-MF', 'Data-NF', 'Data-PE', 'Data-RF', 'Table-asf' were retrived from the database RTAB: the Rayleigh scattering database.

2.6.1 A. Availability

This database is accesible through: http://starship.org/RTAB/RTAB.php. Further a subset of the data included in this database is available at:

- Lawrence Livermore National Laboratory
- ESRF (European Synchroton Radiation Facility): http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/

2.6.2 B. Outline of some pieces of information about the X-ray database

RTAB, the Rayleigh scattering database, was created by Lynn Kissel, who was sustained in her work on elastic photon-atom scattering by Richard Pratt. Their common effort yielded a systematic self-consistent collection of values. According to Kissel (2000), the main goal for preparing the RTAB database was to make extensive tabulations of the differential elastic scattering cross sections and amplitudes readily available. In addition, RTAB includes new tabulations of anomalous scattering factors, total atom form factors[11], total-atom photoeffect cross sections[11], bound-bound oscillator strengths, Dirac-Slater potentials. These values and selected programs that generate or use these tabulations have been collected in this database, named RTAB.

All the quantities of interest for scattering from the RTAB database are computed starting from the same Dirac-Slater potential, see Kissel (2000). A quote from Kissel (2000) is reproduced below :
"The starting point of all our numerical calculations is the model of relativistic single-electron transitions in a local, central potential. We have utilized a modified version of the relativistic Dirac-Slater HEX[12] code (Liberman, et al. (1971)) to evaluate our atomic potentials. Although HEX was used as the basis for these SCF[13] calculations, initiated over 25 years ago, a fresh start today would utilize a more modern code such as DAVID (Liberman and Zangwill (1984)). A copy of the source for RSCF[14] is included in the code folder of the RTAB database for those who wish to duplicate or extend our work."

" The exceptions to this use of a single underlying potential model is the work of other authors (redistributed with their permission) that were included in the RTAB database for completeness and convenience of potential users."

[11] tabulations for shell and subshell are provided as well
[12] Relativistic self-consistent field program for atoms and ions
[13] self-consistent field
[14] according to Kissel (2000) RSCF is a modified version of HEX (Liberman, et al. (1971)), a relativistic Dirac-Slater self consistent potential

2.6.3 C. Outline of some pieces of information about the anomalous scattering factors

The tabulations regarding anomalous scattering factors, from the database RTAB, are for all atoms with the $Z = 1$ throgh $Z = 99$ in the energy range of $0 - 10$ MeV. A quote from Kissel (2000) is provided herein:

"These values are tabulated on a variable grid that allows accurate interpolation to intermediate energies. More details of our ASF calculation are provided in Kissel, et al. (1995).

Two separate tabulations (stored in the folders 'tables-ASF' and 'data-ASF') of our anomalous scattering factors are provided, that differ in how the energy-dependent part of the bound-bound resonances are stored. The values in 'data-ASF' separately tabulate the real and imaginary anomalous scattering factors on independent grids. Further, only the constant contribution of bound-bound transitions is included in the real anomalous scattering factors; an analytic expression and separately tabulated bound-bound oscillator strengths are needed to compute the full result. As a consequence, these values can be accurately interpolated to all intermediate energies using appropriate algorithms, and can be safely used as input for further computations to the ASFTAB[15].

... The tables in 'tables-ASF' explicitly include the full contribution of the bound-bound transitions and have been prepared by ASFTAB[15] from data in 'data-ASF' folder. While these tables are more readily accessible for immediate use without further computations, they cannot be accurately interpolated to intermediate energies in all cases, as one cannot tabulate the full energy dependence of the bound-bound resonances on a dense enough grid.

[15]according to Kissel (2000) ASFTAB was designed to compute the energy-dependent part of the bound-bound contribution to the anomalous scattering factors, and reformats the files in 'data-ASF'; ASFTAB was

In summary, the values in 'data-ASF' have been prepared for subsequent use in further calculations, while the values in 'tables-ASF' have been prepared for direct use without interpolation to intermediate energies.

... An interesting feature of our ASF values that differs from other authors is the explicit inclusion of bound-bound resonant transitions. In our underlying model of single-electron transitions in a potential, a bound-bound resonant transition occurs at a single energy (our levels have no widths), the difference of the energies of the two orbitals involved in the transition. This infinitely narrow transition is manifested as a delta-function spike in the imaginary scattering amplitude and a resonance approaching infinity in the real scattering amplitude. Although these explicit spikes and infinities are unphysical, the underlying strength of the transition is important and contributes significantly to the scattering at low energies."

According to Kissel, et al. (1995), the calculations of the anomalous scattering factors belonging to Cromer and Liberman (1970ab, 1976, 1981), Cromer (1974, 1983) and Henke, et al. (1981, 1982, 1993) do not include the contribution from the bound-bound transitions.
Tabulations of the relativistic multipole bound-bound oscilator strengths presented in the RTAB database are the ones given by the formulation of Scofield (1975).
Our folder 'Data-asf' contains the tabulations for the real and imaginary part of the anomalous scattering factor from the folder 'data-ASF' from RTAB database. In addition our folder 'Table-asf' contains the values for the anomalous scattering factors from the folder 'tables-ASF' belonging to RTAB database.

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used as well to prepare the files in the 'table-ASF' folder of RTAB

2.6.4 D. Outline some pieces of information about the atomic form factor

RTAB databse provides tabulations for the modified relativistic form factor (MF) and relativistic form factor (RF). These tabulations are found in our folders 'Data-MF' and 'Data-RF' for all atoms with the $Z = 1$ throgh $Z = 99$.

Herein we give the following quote form Kissel (2000) regarding these data sets:

"Our total-atom and K-shell modified relativistic form factors are found to agree closely with the values published by Schaupp, et al. (1983). Similarly, our total-atom relativistic form factors agree closely with the values published by Hubbell and Øverbø (1979)." Besides these tabulations of form factors, the database RTAB includes the non-relativistic form factors (NF) of Hubbell, et al. (1975) as a conveniece to users. These values are found in our folder 'Data-NF' for all atoms with the $Z = 1$ throgh $Z = 99$.

2.6.5 E. Outline some pieces of information about the photoeffect cross section

In the following we are giving a quote from Kissel (2000):

"Our evaluation of the real anomalous scattering factors proceeds from the relativistic dispersion relation, requiring an integral over all energies of the imaginary scattering amplitude. Using the optical theorem, we note that the photoeffect cross section dominates the imaginary scattering amplitude for x-ray and low-energy γ-ray energies. Our evaluation of the photoeffect cross section starts with a modified version of the PIXS[16] code due to Scofield (see, for example, Saloman, et al. (1988)). We directly compute subshell photoeffect cross sections in our potential to obtain total-atom cross sections up to several hundred keV."

In our folder 'Data-PE' we stored these values of the photoeffect cross sections in the energy range 0 to 50 MeV for all atoms with the $Z = 1$ throgh $Z = 99$.

[16] Phonon inelastic x-ray scattering

2.6.6 F. Outline some pieces of information about selected work of other authors

In the following we are giving a quote from Kissel (2000):
"As a convenience to potential users, we have included selected work of other authors.

- Cromer and Liberman - the pioneering anomalous-scattering-factor code FPRIME and associated database due to Cromer and Liberman (1970a,b). We include a modified version of the 1983 code (Cromer, 1983) where we have included our high-energy-limit corrections (Kissel and Pratt (1990)).
- Henke, et al. (1993) – $1 - 30$ keV anomalous scattering factors based on experimental photoeffect cross sections.
- Scofield (1973) – a copy of the UCRL report with Dirac-Slater total-atom, shell and subshell photoeffect cross sections for $Z = 1 - 101$, $E = 1 - 1500$ keV."

2.7 X-ray database belonging to the Sasaki laboratory

The tabulations from the folders 'Sasakidataf' and 'Sasakidatafpfpp' were retrived from the X-ray database belonging to the Sasaki laboratory.

2.7.1 A. Availability

The X-ray database is available at Sasaki laboratory at http://www.sasakiken.net/indexe.html. In addition the same tabulations for the anomalous scattering factors are available as well at European Synchroton Radiation Facility (ESRF) http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

2.7.2 B. Outline of some pieces of information about the X-ray database

At Sasaki laboratory can be found the numerical tabulations among others for:

- anomalous scattering factors, f' and f''
- atomic form factor (the frequency-independent Thomson scattering factor), f.

According to Sasaki (1989) the anomalous scattering effect is of interest for applications like absorption and scattering experiments, phase determination of crystal structures, and x-ray dispersion experiment itself.

2.7.3 C. Outline of some pieces of information regarding the anomalous scattering factors data

The tabulations, belonging to the Sasaki Laboratory X-ray database, for anomalous scattering factors and atomic form factor are structured in tables and reports. The tables, named Numerical Tables of Anomalous Scattering Factors Calculated by the Cromer and Liberman's Method, contain the f' and f'' values for the atoms Li trough Bi, plus U in the wavelenght-range from 0.1 to 2.89 Å in intervals of 0.01 Å. This grid for the values allows linear interpolation between the data, which is reasonably accurate in the general case, according to Sasaki (1989). The f' values for wavelenghts shorter than 0.15 Å are not included for elements larger than $Z = 79$. Furthermore, the values of the real anomalous factors, f', were calculated without the Jensen's correction term on the magnetic scattering, see Sasaki (1989). In addition, there are tabulations for the values of f' and f'' at 0.0001 Å intervals in the neighborhood of the K, L_1, L_2, L_3 absorption edges. The values for the wavelength for the respective absorption edges are taken from Bearden (1974) according to Sasaki (1989).

The tables of anomalous scattering factors are calculated from the photoelectric cross sections by numerical integration using a modified version of the program FPRIME[17]according to Sasaki (1989). Herein we introduce a quote from Sasaki (1989):
"The cross sections were calculated from Dirac-Slater wavefunctions based on Brysk and Zerby (1968). The cross section data exclude outer orbitals other than those of the ground state. Therefore, the result may not be reasonably accurate for the longer wavelengths, if the outer-most orbital has a significant contribution for such wavelengths. We suggest that this calculation should be valid in the x-ray region with wavelengths shorter than and on the order of Cr$K_\alpha(\lambda = 2.3\text{Å})$[17]."

Herein, we include a quote from Brysk and Zerby (1968) regarding the photoelectric cross section calculation:
"The present calculation is relativistic ... . It uses for the bound-state wave functions the potential output (on tape) of a self-consistent-field calculation, see Liberman, Waber and Cromer (1965), in the Dirac relativistic version with the Slater density approximation for exchange ... ."
In addition, according to Brysk and Zerby (1968) a complete description of the program used to compute the photoelectric cross section is given in Brysk and Zerby (1967).
In our folder 'Sasakidatafpfpp' we have stored these tabulations from the Sasaki laboratory for the anomalous scattering factors.

2.7.4 D. Outline of some pieces of information regarding the form factor data

Tabulations for Thomson scattering factor are given in the table Contents of atomic scattering factors' table at Sasaki Laboratory. The table contains values for the atomic scattering factor for for the atoms Li through Bi, plus U and some ions. Herein we include the quote from

[17]see Cromer D.T.: private communication (1983)

Sasaki (1987):

"Atomic scattering factors for each atom (or ion) are taken from the reported tables (1) to (5) or calculated using the program ASF (Sasaki, unpublished). Most of data are interpolated to obtain 150 values per atom from $\sin\theta/\lambda = 0$ to 1.49 Å^{-1}." The reported tables from (1) to (5) are Ibers (1962), Cromer and Waber (1974), Fukamachi (1971), Tokonami (1965), Sasaki, et al. (1979), according to Sasaki (1987).

In our folder 'Sasakidataf' we have included these tabulations available at Sasaki laboratory for the atomic form factor.

2.8 Xraylib library

The folders 'Csb-Photo', 'Csb-Rayl', 'Csb-Compt', 'fpfpp' contain data from the xraylib library.

2.8.1 A. Availability

The xraylib library is available at ESFR (European Synchroton Radiation Facility), http://ftp.esrf.fr/pub/scisoft/xraylib/. Furthermore xraylib is hosted on https://github.com/tschoonj/xraylib.

2.8.2 B. Outline of some pieces of information regarding the x-ray library

Xraylib is a software library created for X-ray fluorescence applications, see Brunetti, et al. (2004). According to Schoonjans (2014), xraylib was created by Bruno Golosio to support his work on Monte-Carlo simulations and X-ray fluorescence tomography reconstructions. The same source refers to other authors who brought contributions to the development of the

xraylib like Manuel Sanchez del Rio and Alexandre Simionovici. Although xraylib is dedicated to X-ray fluorescence applications, data for cross sections like photoionization, coherent scattering and Compton scattering, form factors and anomalous scattering functions are as well available through this library, see Brunetti, et al. (2004).

Herein we give the following quote from Schoonjans, et al. (2011) about the data contained in xraylib:
"It is important to note that the included databases were selected by the authors and reflect their personal preferences, based on their experiences. The authors have never striven to produce datasets of their own, whether through experiments or computational work ... ."
Furthermore we provide the following text from Golosio, et al. (2017):
"Xraylib provides access to some of the most respected databases of physical data in the field of X-rays. The core of xraylib is a library, ... , containing over 40 functions to be used to retrieve data from these databases."

2.8.3 C. Outline of some pieces of information about the cross section data

Here we refer to the following text from Schoonjans, et al. (2011) which provides information about the cross section data from the xraylib version 2.15.0:
"The three main photon-matter interaction types in the 0.1-1000 keV energy range are Compton (inelastic) scattering, Rayleigh (elastic) scattering and photoionization. The tabulations of the scattering cross sections found in xraylib are taken from Elam, et al. (2002). The photoionization cross sections are taken from Kissel (2000), and are calculated as the weighed sum of individual partial (subshell) photoionization cross sections. The weights in this case correspond to the electronic occupation of the different subshells. Since these databases consist, for each element, of an array of energies with the corresponding cross sections, interpolation is required to determine cross sections at any arbitrary energy. In xraylib, this is

accomplished using a cubic spline interpolation routine[18], which requires access to the second derivative values of the cross sections and are stored in the library. Since the photoionization cross section profiles display discontinuous behavior at the absorption edges, care has to be taken to avoid erroneous interpolation near these energies. This has been accomplished by setting the second derivatives to zero at the edge energies."

Our folders 'Csb-photo', 'Csb-Rayl' and 'Csb-Compt' contain the photoionization, coherent scattering and Compton scattering cross section for the elements with Z between 1 to 98 covering the energy range 4.133 keV - 12.4 MeV or $\lambda \in \{0.001, 3.000\}$ Å with the step 0.001 Å and the step 0.0001 Å near the absorption edges.

2.8.4 D. Outline of some pieces of information regarding form factor and scattering function

Herein we include a quote from Brunetti, et al. (2004) regarding the form factor and scattering function from xraylib:
" The form factor and scattering function come from the Hubbell, et al. (1975) and Cullen, et al. (1997) compilations. The forms factors are the non-relativistic data calculated by Hubbell. He calculated the relativistic and relativistic modified form factors. However, he recommended to use the nonrelativistic data because they are closer to the experimental data. The anomalous scattering functions are due to Cullen, et al. (1997) who evaluated them from photoionization cross sections using the relativistic dispersion relation."

Our folder 'fpfpp' contains the anomalous scattering factors for energy range 4.133 keV - 12.4 MeV or $\lambda \in \{0.001, 3.000\}$ Å for the elements with $Z = 1$ through $Z = 98$. The following grid was used $\lambda \in \{0.001, 3.000\}$ Å with the step 0.001 Å and the step 0.0001 Å near the absorption edges.

[18] for details see for example Singiresu S. R. (2002), Applied numerical methods for engineers and scientists, Prentice Hall, Upper Saddle River, NJ 07458

2.9 X-ray database belonging to European Synchroton Radiation Facility (ESRF)

The tabulations from the folder 'Cross-Sec-BrennanCowan' were retrived from a file belonging to European Synchroton Radiation Facility (ESRF).

2.9.1 A. Availability

The tabulations are available at European Synchroton Radiation Facility (ESRF), http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

2.9.2 B. Outline of some pieces of information regarding photo-electric cross sections and Compton and Rayleigh cross sections

The cross section factors available at European Synchroton Radiation Facility have been calculated using the subrutine library by Brennan and Cowan (1992), according to the documentation available at European Synchroton Radiation Facility (2003). Regarding the programs developed by Brennan and Cowan we give here a quote from Brennan and Cowan (1992):
"We have created three data bases for the VMS operating system. ... The second contains the parametrized Compton and Rayleigh cross sections. The data bases are accessible through a set of subrutine calls ... . These calls have been packaged in a shareable image library."

Herein we introduce the following text from the documentation available at European Synchroton Radiation Facility (2003):
"The photo-electric cross section is calculated using the theoretical approximation developed by Cromer and Liberman. This theory gives accurate values far from an absorption edge but

does not account for the effects of neighboring atoms, which can be critical near an absorption edge."
In addition it is mentioned in the same reference that the data regarding the Compton cross section are generated using the method described by Balyuzi (1975).

The folder 'Cross-Sec-BrennanCowan' comprises these values of the photoelectric cross section, Compton cross section and Rayleigh cross section and the total cross section. These values are for the elements with Z from $Z = 3$ to 92 at a grid that contains 520 energy points in a logarithmic scale, according to documentation available at European Synchroton Radiation Facility (2003).

2.10 X-ray database belonging to European Synchroton Radiation Facility (ESRF)

The tabulations from the folder 'CrossSec-Compton-IntegrHubbell' were retrived from a file belonging to European Synchroton Radiation Facility (ESRF). This file has been created using CrossSec-Compton.pro in 2003, according to the documentation available at European Synchroton Radiation Facility (2003).

2.10.1 A. Availability

The tabulations for the Compton cross sections are available at European Synchroton Radiation Facility (ESRF), http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

2.10.2 B. Outline of some pieces of information regarding Compton cross sections

Herein we give the following quote from the documentation available at European Synchroton Radiation Facility (2003):

" Data in this file has been calculated by:

- i) using the Klein-Nishina formula of cross section versus θ in a grid of 360 pts in $[0, \pi]$ rad (using code kn-angle.pro). See for example the formula 16 in Davisson and Evans (1952).
- ii) use the inelastic scattering function (calculated using isf-calc-rib.pro) versus x, where $x = \sin(\theta)/\lambda$, λ is the incident photon wavelength.
- Multiply i) times ii) times $2*\pi*\sin(\theta)$ and integrate numerically using int-tabulated.pro"

Our folder 'CrossSec-Compton-IntegrHubbell' comprises of these values of the Compton cross sections calculated for the energy range 10 eV to 10 MeV ($\lambda \in \{0.00124, 1240\}$ Å) with a 500 points logarithmic grid for the elements $Z = 1$ - 90, according to documentation available at European Synchroton Radiation Facility (2003).

2.11 X-ray database belonging to European Synchroton Radiation Facility (ESRF)

The tabulations from the folder 'CrossSec-Compton-IntegrXop' were retrived from a file belonging to European Synchroton Radiation Facility (ESRF). This file has been created using CrossSec-Compton.pro in 2003, according to the documentation available at European Synchroton Radiation Facility (2003).

2.11.1 A. Availability

The tabulations are available at European Synchroton Radiation Facility (ESRF), http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

2.11.2 B. Outline of some pieces of information regarding the Compton cross sections

Herein we give the following quote from the documentation available at European Synchroton Radiation Facility (2003):

" Data in this file has been calculated by:

- i) using the Klein-Nishina formula of cross section versus θ in a grid of 360 pts in $[0, \pi]$ rad (using code kn-angle.pro). See for example the formula 16 in Davisson and Evans (1952).
- ii) use the inelastic scattering function (calculated using isf-calc-rib.pro) versus x, where $x = \sin(\theta)/\lambda$, λ is the incident photon wavelength.
- Multiply i) times ii) times $2*\pi*\sin(\theta)$ and integrate numerically using int-tabulated.pro"

In our folder 'CrossSec-Compton-IntegrXop' comprises of these values of the Compton cross sections calculated in the energy range 10 eV to 10 MeV ($\lambda \in \{0.00124, 1240\}$ Å) with a 500 points logarithmic grid for the elements $Z = 1$ - 90, according to the documentation available at European Synchroton Radiation Facility (2003).

2.12 X-ray database belonging to European Synchroton Radiation Facility (ESRF)

The tabulations from the folder 'CrossSec-Compton-KleinNishina' were retrived from a file belonging to European Synchroton Radiation Facility (ESRF). This file has been creadted using CrossSec-Compton-KleinNishina.pro in 2003, according to the documentation available at European Synchroton Radiation Facility (2003).

2.12.1 A. Availability

The tabulations are available at European Synchroton Radiation Facility (ESRF), http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

2.12.2 B. Outline of some pieces of information regarding the Compton cross sections

Herein we give the following quote from the documentation available at European Synchroton Radiation Facility (2003):

" Data in this file has been calculated using the Klein-Nishina formula. It is valid for describing the Compton scattering by free electrons. See for example the formula 19 in Davisson and Evans (1952)."

Our folder 'CrossSec-Compton-KleinNishina' comprises of these values of the Compton cross sections calculated in the energy range 1 keV to 10 MeV ($\lambda \in \{0.00124, 12400\}$ Å) with a 500 points logarithmic grid for the elements $Z = 1$ - 90, according to the documentation available at European Synchroton Radiation Facility (2003).

2.13 X-ray database belonging to European Synchroton Radiation Facility (ESRF)

The tabulations from the folder 'CrossSec-McMaster' were retrived from a file belonging to European Synchroton Radiation Facility (ESRF).

2.13.1 A. Availability

The tabulations are available at European Synchroton Radiation Facility (ESRF), http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

2.13.2 B. Outline of some pieces of information regarding the photoelectric cross section, the Rayleigh and Compton cross section

This tabulations set contains data calculated on 2001 by using mucal (a subroutine to calculate x-ray cross sections) by Pathikrit Badyopadhyay, according to the documentation available at European Synchroton Radiation Facility (2003). Calculations are based on data from the reference McMaster, et al. (1969). In this reference data are not available for the following elements: 84 (Po), 85 (At), 87 (Fr), 88 (Ra), 89 (Ac), 91 (Pa), 93 (Np).
Futher, a Periodic Table WWW interface can be access at Center for Synchrotron Radiation Research and Instrumentation, Illinois Institute of Technology.
Our folder 'CrossSec-McMaster' comprises of the values for the photoelectric cross section, the Rayleigh and Compton cross section and total cross section calculated by using the mucal subrutine. Such that our folder includes data for all elements with Z=1 to Z=94 with the following exceptions notified above. The values for the cross section are given for the

following energy range from 30.0 eV (410Å) to 69.4 keV (0.179Å).

2.14 X-ray database belonging to European Synchroton Radiation Facility (ESRF)

The tabulations from the folder 'Cross-Sec-PE-Scofield' were retrived from a file belonging to European Synchroton Radiation Facility (ESRF). The file provided by European Synchroton Radiation Facility was created using CrossSec-Scofield.pro on 2003, see European Synchroton Radiation Facility (2003).

2.14.1 A. Availability

The tabulations are available at European Synchroton Radiation Facility (ESRF), http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

Furthermore data from this file are available in the RTAB database[19], according to the documentation available at European Synchroton Radiation Facility (2003).

2.14.2 B. Outline of some pieces of information regarding photoelectric cross sections

The tabulations for the photoelectric cross sections belonging to European Synchroton Radiation Facility come from Scofield tables, see Scofield (1973).
Herein we introduce the following text from Scofield (1973):
" The bulk of the present report lists the calculated photoionization cross sections for ionization of neutral atoms with Z's from 1 to 101 by photons energies from 1 to 1500 keV. The

[19] http://starship.org/RTAB/files/others/index-lvl2.php

cross sections for the ionization from the individual subshells are listed.
In the calculation of the cross section, the electrons are treated relativistaically and are assumed to be moving in the same Hartree-Slater central potential[20] both before and after the absorption of the photon.
... In the high-energy region the present results could be renormalized by using the renormalizations derived from a more accurate atomic model. In the present report such renormalization has not been performed; however, in the Table A1 of the Appendix we list the normalizations derived from a relativistic Hartree-Fork calculations for Z=1 to 54."

Our folder 'Cross-Sec-PE-Scofield' comprises the values of the photoelectric cross sections, the cross section for the ionization from the K, L and M shells as well as that from the individual subshells. These values are for the elements with Z from Z= 1 to 100 for a set of photon energies from 1.0 keV to 1.5 MeV ($\lambda \in \{0.008, 12.40\}$ Å).

2.15 X-ray database belonging to European Synchroton Radiation Facility (ESRF)

The tabulations from the folder 'CrossSec-StormIsrael' were retrived from a file belonging to European Synchroton Radiation Facility (ESRF). The file provided by European Synchroton Radiation Facility was created using CrossSec-StormIsrael.pro on 2002, see European Synchroton Radiation Facility (2003).

2.15.1 A. Availability

The tabulations are available at European Synchroton Radiation Facility (ESRF), http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

[20] for details see Scofield (1973)

2.15.2 B. Outline of some pieces of information regarding photo-electric cross sections, Compton cross sections and Rayleigh cross sections

The tabulations for the cross sections factors belonging to European Synchroton Radiation Facility come from Storm and Israel tables, see Storm and Israel (1970).
In their tables for incoherent interaction only the bound-electron cross section are given, according to Storm and Israel (1970). In the same reference the following details regarding the incoherent scattering functions used in the calculation of total incoherent cross section for bound electrons are imparted:

" Cromer and Mann(1967) have calculated incoherent scattering functions for all spherically symmetric free atoms using Hartree-Fock-Slater wavefunctions with exchange terms. Cromer (1969) has extended these calculations to include the aspherical atoms. Recently Brown (1969) has calculated incoherent and coherent scattering functions for low-Z elements using wavefunctions of Weiss (1967). The incoherent scattering functions of Cromer and Brown were used ... to calculate the total incoherent cross section for a bound electron."

Concerning the tabulations of coherent scattering cross sections the following information about the form factor needed in the calculations of these cross sections is given by Storm and Israel (1970):

According to Scofield (1973) and Storm and Israel (1970) the tabular results for photo-electric cross section comprised in the latter study are based on the computer code of Brysk and Zerby (1968) up to 200 keV and on the results of Rakavy and Ron (1965), Rakavy and Ron (1967) and Schmickley and Pratt (1967) for higher energies.

Our folder 'CrossSec-StormIsrael' comprises of the values of the incoherent and coherent cross

sections and photoelectric cross sections. These values are for the elements with Z from $Z = 1$ to 100 for a set of photon energies from 1.0 keV to 100 MeV ($\lambda \in \{0.00124, 12.40\}$ Å). In addition our folder contains values for Compton absorption (incoherent) cross section, pair production (nuclear field) cross section, pair production (electron field), pair production (absorption) cross section, photo electric absorption cross section, total cross section, total cross section absorption, total cross section energy absorption.

2.16 X-ray database belonging to European Synchroton Radiation Facility (ESRF)

The tabulations from the folder 'f1f2-CromerLiberman' were retrived from a file belonging to European Synchroton Radiation Facility (ESRF). This tabulation set contains data that were calculated with a Cromer and Liberman program on 2002, according to the documentation available at European Synchroton Radiation Facility (2003).

2.16.1 A. Availability

The tabulations are available at European Synchroton Radiation Facility (ESRF), http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

2.16.2 B. Outline of some pieces of information regarding the anomalous scattering factors

This tabulations set of anomalous scattering factors contains values calculated with the code from Cromer and Liberman (1983) with the high energy limit corrections by Kissel and Pratt (1990), according to the documentation available at European Synchroton Radiation Facility (2003). In addition this program can be found in the RTAB database, see Kissel (2000),

according to the European Synchroton Radiation Facility (2003).
Further in the documentation available at European Synchroton Radiation Facility (2003) there are pointed out the following references that characterize this data set: Cromer (1983), Cromer and Liberman (1970a), Cromer and Liberman (1970b), Cromer and Liberman (1976) and Cromer and Liberman (1981).
Our folder 'f1f2-CromerLiberman' comprises of the values for the anomalous scattering factors calculated with the above mentioned code for all elements with Z=3 to Z=93 in the energy interval 1 keV (12.40Å) to 70 keV (0.177Å). In addition the data set is given for a grid that contains 1024 points in log scale, according to the documentation available at European Synchroton Radiation Facility (2003).

2.17 X-ray database belonging to European Synchroton Radiation Facility (ESRF)

The tabulations from the folders 'CrossSec-EPDL97', 'f0-EPDL97' and 'f1f2-EPDL97' were retrived from files belonging to European Synchroton Radiation Facility (ESRF).

2.17.1 A. Availability

The tabulations are available at European Synchroton Radiation Facility (ESRF), http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

In addition similar tabulations can be found:

- In USA: at Lawrence Livermore National Laboratory, https://wci.llnl.gov/codes/tart/photons.html

- In Europe, Korea and Japan: at Nuclear Energy Agency https://www-nds.iaea.org/epdl97/za1to100.htm

2.17.2 B. Outline of some pieces of information about the X-ray database

The Evaluated Photon Data Library (EPDL), version (EPDL97), was created at Lawrence Livermore National Laboratory for the use in photon transport calculations, see Cullen, et al. (1975). This library includes data for all elements with atomic number between $Z = 1$ and $Z = 100$ regarding among others:

- photoionization [21]
- coherent and incoherent scattering cross sections
- form factor, scattering functions, anomalous scattering functions

According to Cullen, et al. (1997) the data from this library regarding the atomic processes like photoionization, coherent and incoherent scattering are applicable to cold, neutral, isolated atoms.
Further Cullen, et al. (1997) comes with the subsequent details regading the use of data from the EPDL97:
"All of the EPDL97 data is in the form of tabulated data with a defined method of interpolation between tabulated values. Cross sections, form factors and scattering functions are log-log interpolable ... ."

"You can safely and accurately use this data down to about 1 keV."

[21] include cross sections for all subshell

2.17.3 C. Outline of some pieces of information about the photoionization, coherent and incoherent scattering cross sections tabulations

Herein we give the following quote from Cullen, et al. (1997) regarding the photoionization cross sections:

"The sources of photoionization data include data calculated by Kissel using Scofield's subshell cross sections (see Saloman, et al. (1988)) from the edge energy up to 1 MeV and Hubbell's (see Saloman, et al. (1988), Hubbell and Seltzer (1995), Hubbell and Veigele (1976)) total photoionization cross sections from 1 keV to 100 GeV. These two sets of data have been combined to define subshell cross sections from the edge energy to 100 GeV. From the edge to 1 MeV, the subshell cross sections and total, defined as the sum of the subshells, are based on Scofield's data. From 1 MeV to 100 GeV the total is based on Hubbell's data (see Hubbell, et al. (1980)). At 1 MeV the total photoionization is identical from both sources, so that joining the two sets could be done in a consistent manner."

In the following we introduce a text from Cullen, et al. (1997) regading the coherent and incoherent scattering cross sections:

"In the specific case of EPDL97, we will define incoherent scattering, our only inelastic scattering process, as Compton scattering by bound electrons. Similarly we will define coherent scattering, our only elastic scattering processing, as Rayleigh scattering from the bound electrons. These are the only scattering processes included in EPDL97. Therefore in the specific case of EPDL97 the terms coherent, elastic and incoherent, inelastic can be used interchangeably".

Furthermore the following quotes are given from Cullen, et al. (1997) regarding the coherent and incoherent cross sections:

“The coherent cross sections are those of Cullen based on the combination of Thomson scattering, form factors, and anomalous scattering factors, which were numerically integrated to define the cross sections. Coherent scattering cross sections are included from 1 eV up to 100 GeV.”

“The incoherent cross sections are those of Cullen based on the combination of Compton scattering described by the Klein-Nishina formula and scattering functions that were numerically integrated to define the cross sections. Incoherent scattering cross sections are included from 1 eV up to 100 GeV.”

Our folder ’CrossSec-EPDL97’ includes these tabulations for the photoelectric cross section, Rayleigh cross section and Compton cross section in the energy range 1.0 eV to 1.0 MeV ($\lambda \in \{0.0124, 12400\}$ Å) for the elements $Z = 1$ to $Z = 100$. Futhermore our folder ’CrossSec-EPDL97’ contains tabulations regarding total cross sections, energy-transfer coefficients like photo electric energy transfer coefficients and incoherent energy transfer coefficients (for details see Hubbell and Seltzer (1995)).

2.17.4 D. Outline of some pieces of information about the form factor

The facts about the form factor tabulations given by Cullen, et al. (1997) are cited below:

“Hubbell has calculated nonrelativistic, relativistic, and modified relativistic form factors. Based on Hubbell’s recommendation the data included in EPDL97 are his nonrelativistic form factors, which are currently the most widely used of Hubbell’s form factors.”
Such that the data in our folder ’f0-EPDL97’ are the tabulations from the reference Hubbell, et al. (1975).

2.17.5 E. Outline of some pieces of information about the anomalous scattering factors

Herein we give the following quote from Cullen, et al. (1997) about the anomalous scattering factors:

"Anomalous scattering factors are those of Cullen (1989) computed using the relativistic dispersion relation as detailed in Pratt, et al. (1994) in conjunction with the EPDL97 photoionization and photoexcitation data. Since the relativistic photoelectric cross section varies as $1/E$ at high energies, the relativistic dispersion integral is not convergent without considering other contributing effects. As Pratt, et al. (1994) note, contributions from bound-electron pair production contribute to the same order and must be included for convergence of the integral. We estimate this contribution to the dispersion integral using analytic semi-relativistic expressions due to Costescu, et al. (1994). For more details on our utilization of bound-electron pair production (wherein the electron of the pair is created in a bound state of the atom) in evaluation of the relativistic dispersion relation, see Kissel, et al. (1995). The resulting anomalous scattering factors vary from a value of $-Z$ at zero photon energy to a non-zero high energy limit as defined by Kissel and Pratt (1990)."

Our foulder 'f1f2-EPDL97' comprises of these anomalous scattering factors from 1 eV to 10 MeV ($\lambda \in \{0.00124, 12400\}$ Å) for the elements $Z = 1 - 100$.

2.18 Plots with data from different databases

Herein we introduce some graphics illustrating the tabulations from the databases presented in the above sections. For the photoeffect cross section and for the incoherent and coherent cross section we provide the following plots for the elements sodium and molybdenum. For the real part of the atomic form factor and the imaginary part of the atomic form factor we give the plots for elements carbon and iron. It can be observed that the above graphs do not show significant differences between the databases.

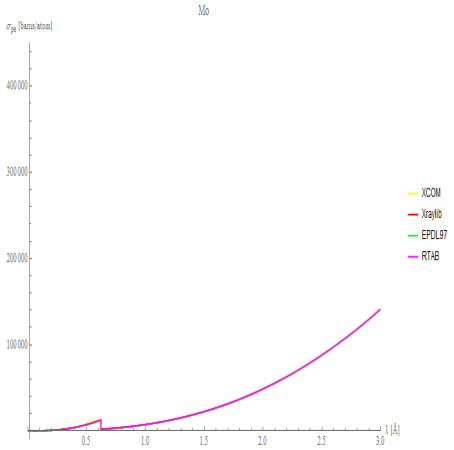

Figure 2.1: The photoeffect cross section the molybdenum atom.

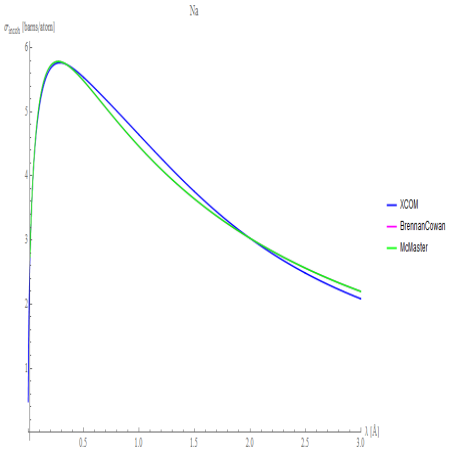

Figure 2.2: The incoherent (Compton) scattering cross section for sodium atom.

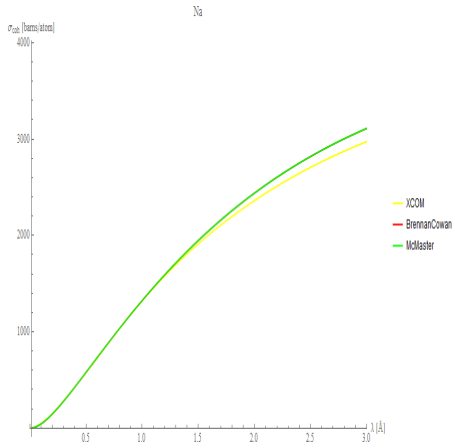

Figure 2.3: The coherent (Rayleigh) scattering cross section for sodium atom.

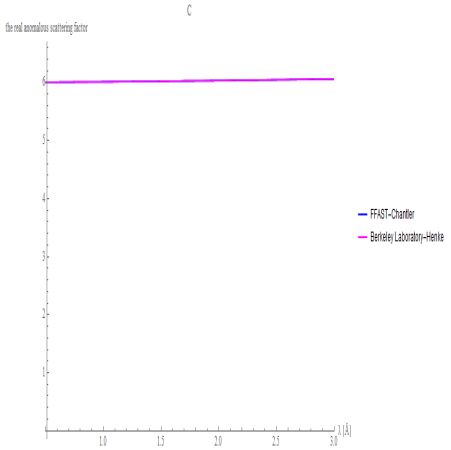

Figure 2.4: The real part of the atom form factor for the carbon atom.

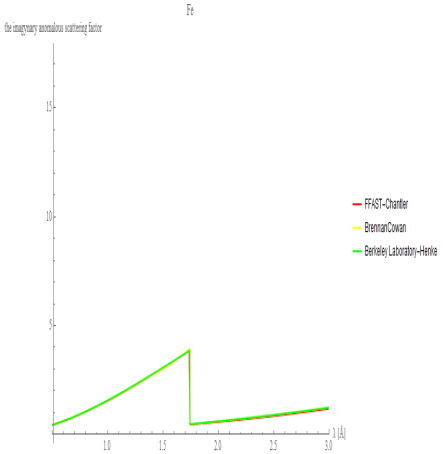

Figure 2.5: The imaginary part of the atomic form factor the iron atom.

Bibliography

[1] Brunetti A., Sanchez del Rio M., Golosio B., Simionovici A. and Somogyy A. (2004), *A library for X-ray-matter interaction cross sections for X-ray fluorescence applications*, Spectrochimics Acta Part B59, pp. 1725-1731.

[2] Bearden J.A. (1974), *International Tables For X-ray Crystallography vol. IV*, Birmingham: kynoch Press, England, pp. 5-43.

[3] Brysk H. and Zerby C.D. (1967), *Low-energy photoelectric cross sections calculations*, Union Carbide Corporation Report No. UCC/DSSD-299, (unpublished).

[4] Brysk H. and Zerby C.D. (1968), *Photoelectric Cross Sections in the* keV *range* Phys. Rev., Volume 171, Number 2, pp. 292-298.

[5] Berger M. J. and Hubbell J. H. (1987), *XCOM: Photon Cross Sections on a Personal Computer*, Publication NBSIR 87-3597, National Bureau of Standards, Gaithersburg, MD.

[6] Brown R.T. (1969), EG and G, Inc., Report L-958 and unpublished data.

[7] Brennan S. and Cowan P.L. (1992), *A suite of programs for calculating x-ray absorption, reflection and diffraction performance for a variety of materials at arbitrary wavelengths*, Rev. Sci. Instrum. 63, pp. 850-853.

[8] Balyuzi H.H.M. (1975), *Analytic approximations to incoherently scattered X-ray intensities*, Acta Cryst A31, pp. 600-602.

[9] Biggs F. and Lighthill R. (1988), *Analytical Approximations for X-Ray Cross Sections III*, Sandia Report SAND87—0070, pp. 1-143.

[10] Center for X-Ray Optics (2011), *Updates to the atomic scattering factors*, http://henke.lbl.gov/optical_constants/update.html.

[11] Center for X-Ray Optics (2011), *The Atomic Scattering Factor Files*, http://henke.lbl.gov/optical_constants/asf.html.

[12] Chantler C.T. (1995), *Theoretical Form Factor, Attenuation and Scattering Tabulation for Z=1-92 from E=1-10* eV *to E=0.4-1.0* MeV, J. Phys. Chem. Ref. Data 24, pp. 71-643.

[13] Chantler C.T. (2000), *Detailed tabulation of atomic form factors, photoelectric absorption and Scattering Cross Section, Mass Attenuation Coefficients in the vicinity of absorption edges in the soft x-ray (Z=30-36, Z=60-89, E=0.1* keV*-10* keV*), addresing convergence issues of earlier work*, J. Phys. Chem. Ref. Data 29, No. 4, pp. 597-1048 Random House, N.Y.

[14] Costescu A. (1994), *Retardation and Multipole Effects in Rayleigh Scattering by Hydrogen-like Ions at Low and X-Ray Photon Energies*, Phys. Rev. A 50, pp. 1390-1398.

[15] Cullen D.E, Hubbell J.H and Kissel L. (1997), *EPDL97 The Evaluated Data Library, 97 Version*, UCRL-50400, Vol 6, Rev 5.

[16] Cullen D.E (1989), *Program SCATMAN: A Code Designed to Calculate Photon Coherent Scattering Anomalous Scattering Factors and Cross Sections*, Lawrence Livermore National Laboratory.

[17] Cullen D.E., Chen M.H., Hubbell J.H., Perkins S.T., Plechaty E.F., Rathkopf J.A. and Scofield J.H.(1989), *Tables and graphs of photon-interaction cross sections from 10* eV *to 100* GeV *derived from the LLNL Evaluated Photon Data Library (EPDL)* UCRL-50400 Vol. 6.

[18] Cromer D.T. and Mann J.B. (1967), *Compton scattering factors for spherically symmetric free atoms*, LA-DC-8819 (Los Alamos Scientific Laboratory, LA-3689).

[19] Cromer D.T. and Mann J.B. (1968), *X-ray scattering factors computed from numerical Hartree-Fork wave functions*, Acta Cryst A24, pp. 321-324.

[20] Cromer D.T. (1969), *Compton scattering factors for aspherical free atoms*, The Journal of Chemical Physics 50, pp. 4857-4859.

[21] Cromer D.T. (1965), *Anomalous Dispersion Corrections Computed from Self-Consistent Field Relativistic Dirac-Slater Wave Functions*, Acta Cryst. 18, pp. 17-23.

[22] Cromer D.T. and Liberman D. (1970a), *Relativistic Calculation of Anomalous Scattering Factors for X Rays*, J. Chem. Phys. 53, pp. 1891-1898.

[23] Cromer D.T. and Liberman D. (1970b), *Relativistic Calculation of Anomalous Scattering Factors for X Rays*, Los Alamos Scientific Laboratory Report LA-4403, Los Alamos, New Mexico, pp. 163.

[24] Cromer D.T. and Liberman D. (1981), *Anomalous Dispersion Calculations Near to and on the Long-wavelength side of an absorption edge*, Acta Cryst. A37, pp. 267-268.

[25] Cromer D.T. and Liberman D. (1976), *Anomalous scattering factors for Co Kα1 radiation*, Acta Cryst. A32, pp. 339-340.

[26] Cromer D. T. (1983), *Calculation of anomalous scattering factors at arbitrary wavelengths*, J. Appl. Cryst.16, pp. 437-437.

[27] Cromer D.T. (1974), International tables for X-ray Crystallography, Vol. IV, edited by J.A. Ibers and W.C. Wilson, pp. 148-150. Birmingham: Kynoch Press.

[28] Davisson C. M. and Evans R. D., (1952), *Gamma-Ray Absorption Coefficients*, Reviews of Modern Physics, 24, pp. 79-109.

[29] Elam W.T., Ravel B.D. and Sieber J.R. (2002), *A new atomic database for X-ray spectroscopic calculations*, Radiation Physics and Chemistry 63 (2002), pp. 121-128.

[30] European Synchroton Radiation Facility (2003), *Documentation*, http://ftp.esrf.fr/pub/scisoft/xop2.3/DabaxFiles/.

[31] Fukamachi T. (1971), *Mean X-ray scattering factors calculated from analytical Roothaan-Hartree-Fock wave functions by Clementi*, Tech. Rep. B12, Institute for Solid State Physics, The University of Tokyo.

[32] Golosio B., Brunetti A., Sanchez del Rio M., Ikonen T, Schoonjans T., Wormington M. and Sagan D. (2017), *The definitive manual. Version 3.3.0.*, Ghent University, Belgium.

[33] Hoyt J.J., De Fontaine D., and Warburton W.K. (1984), *Determination of the Anomalous Scattering Factors for Cu, Ni and Ti using Dispersion Relation*, J. Appl. Cryst. 17, pp. 344-351.

[34] Hubbell J. H., Veigele W. J., Briggs E. A., Brown R. T., Cromer D. T. and Howerton R. J. (1975), *Atomic form factors, incoherent scattering functions, and photon scattering cross sections*, J. Phys. Chem. Ref. Data 4, 471-538; erratum (1977) 6, pp. 615-16.

[35] Hubbell J.H. and Øverbø I. (1979), *Relativistic Atomic Form Factors and Photon Coherent Scattering Cross Sections*, J. Phys. Chem. Ref. Data 8, pp. 69-105.

[36] Hubbell J.H. and Seltzer S.M. (1995), *Tables of X-RAY Mass Attenuation Coefficients and Mass Energy-Absorption Coefficients 1* keV *to 20* MeV *for Elements Z = 1 to 92 and 48 Additional Substances of Dosimetric Interest*, NISTIR 5632, National Institute of Standards and Technology.

[37] Hubbell J.H. and Veigele W.J. (1976), *Comparison of Theoretical and Experimental Photoeffect Data 0.1* keV *to 1.5* MeV, National Bureau of Standards Tech. Note 901.

[38] Hubbell J.H. (1977), *Photon mass attenuation and mass energy-absorption coefficients for H, C, N, O, Ar, and seven mixtures from 0.1* keV *to 20* MeV, Radiat. Res. 70, pp. 58-81.

[39] Hubbell J.H. (1982), *Photon Mass Attenuation and Energy Absorption Coefficients from 1* keV *to 20* MeV, Int. J. Appl. Radiat Isotopes, 33, pp. 1269-1290.

[40] Hubbell J.H., Gimm H.A. and I. Øverbø (1980), *Pair, Triplet, and Total Cross Sections (and Mass Attenuation Coefficients) for 1* MeV-*100* GeV *Photons in Elements Z = 1 to 100*, J. Phys. Ref. Data, Vol. 9, No. 4, pp. 1023-1147.

[41] Hanson H. P., Herman F., Lea J. D. and Skillman S. (1964), *HFS Atomic Scattering Factors*, Acta Cryst. 17, pp. 1040.

[42] Henke B. L., Lee P., Tanaka T. J., Shimabukuro R. L. and Fujikawa B. K. (1981), *Low Energy X-ray Diagnostics-1981*, Ed. DT Attwood and BL Henke. In AIP Conference Proceedings, New York, Vol. 75, p. 340-388.

[43] Henke B. L., Lee P., Tanaka T. J., Shimabukuro R. L. and Fujikawa B. K. (1982), *Low-energy X-ray interaction coefficients: Photoabsorption, scattering, and reflection: E= 100–2000* eV *Z= 1–94*, Atomic data and nuclear data tables, 27(1), pp. 1-144.

[44] Henke B. L., Gullikson E. M. and Davis J. C. (1993), *X-ray interactions: photoabsorption, scattering, transmission, and reflection at E=50-30.000* eV*, Z=1-92*, Atomic Data Nuclear Data Tables Vol. 54, No. 2, pp. 181-342.

[45] Ibers J.A. (1962), *Atomic scattering factors for x-ray (corrected to november 1961). Section 3.3.1.*, International tables for X-ray Crystallography, Vol. III, Birmingham: Kynoch Press, England.

[46] Kane P.P., Kissel L., Pratt R.H. (1985), *Elastic scattering of γ-rays and x-ray by atoms*, Physical Reports, 140, No. 2, pp. 75-159.

[47] Kohn W. and Sham L.J. (1965), *Self-consistent equations including exchange and correlation effects*, Physical review, 140(4A), pp. 1133-1138.

[48] Kissel L., Zhou B., Roy S.C., Sen Gupta S.K. and Pratt R.H (1995), *The valdity of form-factor, modified-form factor and anomalous-scattering-factor approximations n elastic scattering calculations* , Acta Cryst. A51, pp. 271-288.

[49] Kissel L. and Pratt R. H. (1985), *Rayleigh scattering - Elastic photon scattering by bound electrons*, Atomic Inner-Shell Physics, edited by Bernd Crasemann (Plenum Publishing: New York).

[50] Kissel L. and Pratt R. H. (1990), *Corrections to tabulated anomalous scattering factors*, Acta Cryst. A46, pp. 170-175.

[51] Kissel L. (2000), *RTAB: the Rayleighscattering database*, Radiat. Phys. Chem. 59, pp. 185-200.

[52] Kissel L. and Pratt R.H (1990), *Corrections to Tabulated Anomalous-Scattering Factors*, Acta Cryst. A46, pp. 170-175.

[53] Liberman D., Waber J.T. and Cromer D.T (1965), *Self-consistent-field Dirac-Slater wave functions for atoms and ions. I Comparison with previous calculations*, Physical Review, Vol 137, No. 1A., pp. 27-34.

[54] Liberman D. A., Cromer D. T. and Waber J. T. (1971), *Relativistic self-consistent field program for atoms and ions*, Comput. Phys. Commun. 2, pp. 107-13.

[55] Liberman D. A. and Zangwill A. (1984), *A relativistic program for optical response in atoms using a timedependent local density approximation*, Comput. Phys. Commun. 32, pp. 75-82.

[56] McMaster W.H., Del Grande N.K., Mallett J.H. and Hubbell J.H.,(section I 1970, section II 1969, section III 1969 and section IV 1969) *Compilation of x-ray cross sections*, Lawrence Livermore National Laboratory Report UCRL-50174.

[57] National Institute for Standards and Technology (2016), *Note on NIST X-ray Attenuation Databases*, https://www.nist.gov/pml/note-nist-x-ray-attenuation-databases.

[58] National Institute for Standards and Technology (2016), *Note on NIST X-ray Attenuation Databases*, https://www.nist.gov/pml/note-nist-x-ray-attenuation-databases.

[59] National Institute for Standards and Technology (2016), *Database Holdings*, https://physics.nist.gov/PhysRefData/FFast/html/holdings.html.

[60] Pratt R.H., Kissel L. and Bergstrom P.M. Jr. (1994), *New relativistic S-Matrix results for scattering - beyond the usual anomalous factors/ beyond impulse approximation," in Resonant Anomalous X-Ray Scattering*, G. Materlik, C.J. Sparks and K. Fischer, eds. (Elsevier Science Publishers, Amsterdam, 1994), pp. 9-33.

[61] Merritt A. E. (2006), *Anomalous Scattering References*, http://skuld.bmsc.washington.edu/scatter/AS_references.html#edge_refs.

[62] Merritt A. E. (2012), *X-ray anomalous scattering*, http://skuld.bmsc.washington.edu/scatter/AS_index.html.

[63] Merritt A. E. (2010), *X-ray Absorption Edges*, http://skuld.bmsc.washington.edu/scatter/AS_periodic.html.

[64] Rakavy G. and Ron A. (1967), *Atomic Photoeffect in the range* $E_\gamma = 1 - 2000keV$ Phys. Rev., Volume 159, Number 1, pp. 50-56.

[65] Rakavy G. and Ron A. (1965), *Total cross sections of the photoelectric effect for uranium* Physics Letters, 19(3), pp. 207-208.

[66] Saloman E.B., Hubbell J.H. and Scofield J.H. (1988), *X-ray attenuation cross sections for energies 100* eV *to 100* keV *and elements Z=1 to Z=92*, Atomic Data Nuclear Data Tables Vol. 38, pp. 1-197.

[67] Saloman E.B. and Hubbell J.H. (1987), *Critical Analysis of Soft X-ray Cross Section Data*, Nucl. Instr. Meth. A255, pp. 38-42.

[68] Saloman E.B. and Hubbell J.H. (1986), *X-ray Attenuation Coefficients (Total Cross Sections): Comparison of the Experimental DataBase with Recommended Values of Henke and the Theoretical Values of Scofield for Energies between 0.1-100* keV, National Bureau of Standards Report NBSIR 86-3431.

[69] Scofield J. H. (1973), *Theoretical Photoionization Cross Sections from 1 to 1500* keV, Lawrence Livermore Laboratory Report UCRL-51326, Livermore, California.

[70] Scofield J.H. (1975), *Radiative transitions, in Atomic Inner-Shell Processes*, edited by B. Crasemann Academic Press, New York, pp. 265-292.

[71] Schmickley R. D. and Pratt R. H. (1967), *K-, L-, and M-Shell Atomic Photoeffect for Screened-Potential Models* Phys. Rev., Volume 164, Number 1, pp. 104-116.

[72] Storm E. and Israel H.I. (1970), *Photon Cross Sections from 1* keV *to 100* MeV *for elements Z=1 to Z=100*, Nuclear Data Tables A7, pp. 565-681.

[73] Schaupp D., Schumacher M., Smend F., Rullhusen P. and Hubbell J. H. (1983), *Small-angle Rayleigh scattering of photons at high energies: Tabulations of relativistic HFS modified atomic form factors*, J. Phys. Chem. Ref. Data 12, pp. 467-512.

[74] Singiresu S.R. (2002), *Applied numerical methods for engineers and scientists*, Prentice Hall Upper Saddle River, NJ 07458.

[75] Sasaki S. (1987), *RADY: A Fortran program for the least-squares refinement of crystal structures*, Photon Factory, National Laboratory for High Energy Physics Oho-machi, Tsukuba-gun, Ibaraki, 305, Japan, http://www.sasakiken.sakura.ne.jp/reports/RADY-KEKintRep1987.pdf.

[76] Sasaki S., Fujino K. and Takéuchi Y. (1979)*X-ray determination of electron-density distributions in oxides, MgO, MnO, CoO, and NiO, and atomic scattering factors of their constituent atoms*, Proceedings of the Japan Academy, Series B, 55(2), pp. 43-48.

[77] Sasaki S. (1989) *Numerical tables of anomalous scattering factors calculated by the Cromer and Liberman's method*, National Laboratory for High Energy Physics Oho 1-1, Tsukuba 305, Japan, http://www.sasakiken.sakura.ne.jp/reports/fp-KEKrep(88-14)1989text.pdf.

[78] Schoonjans T.,Brunetti A., Golosio B., Sanchez del Rio M., Solé V.A., Ferrero C. and Vincze L. (2011), *The xraylib library for X-ray-matter interactions. Recent developments.*, Spectrochimics Acta Part B66, pp. 776-784.

[79] Schoonjans T. (2014), *The xraylib library for X-ray –matter interaction cross sections, Monte Carlo simulation tools for X-ray imaging and fluorescence* , Monte Carlo simulation tools for X-ray imaging and fluorescence Workshop 24 - 25 February.

[80] Veigele W.J. (1973), *Photon cross sections from 0.1* keV *to 1* MeV *for elements Z=1 to Z=94*, At. Dat. Tables 5, pp. 51-111.

[81] Tokonami M. (1965), *Atomic scattering factor of* O_2, Acta Crystallographica, 19(3), pp. 486-486.

[82] Williams G.P. (1986), *Electron binding energies of the elements*, Weast, R.C. (Ed.), CRC Handbook of Chemistry and Physics, 67th Edition. CRC Press, Boca Raton, pp. F163-F166.

[83] Weiss A. W. (1967), J. Res. Nat. Bur. Stand. Sect. A, pp. 71-157.

Appendix A

X-ray databases

Table 1 provide an overview of the databases presented in chapter 2. The web source information includes the url of each database as active hyperlinks. Table 2 links databases with its main authors. Table 3 provides an overview of each database file. Finally headings are provided for each file.

Table 1. X-ray database

Databases' name	**Web source of information**
The Atomic Scattering Factor Files	Lawrence Berkeley National Laboratory's (LBNL)
X-ray Anomalous Scattering	University of Washington Biomolecular Structure Center
Elam	GitHub
FFAST	National Institute of Standards and Technology (NIST)
XCOM	National Institute of Standards and Technology (NIST)
RTAB	Rayleigh Scattering database
X-ray database	Sasaki Laboratory
Xraylib	European Synchroton Radiation Facility (ESRF)
ESRF (DABAX libray)	European Synchroton Radiation Facility (ESRF)

Table 2. X-ray database.

Databases' name	**Main referance**
The Atomic Scattering Factor Files	Henke, et al. (1993)
X-ray Anomalous Scattering	Brennan and Cowan (1992)
Elam	Elam, et al. (2002)
FFAST	Chantler C.T. (1995, 2000)
XCOM	Berger and Hubbell (1987)
RTAB	Kissel (2000)
X-ray database	Sasaki (1989)
Xraylib	Brunetti, et al. (2004)
ESRF (DABAX library)	Brennan and Cowan (1992)
ESRF (DABAX library)	EPDL97 database - Cullen, et al. (1997)
ESRF (DABAX library)	McMaster et al. (1969, 1970)
ESRF (DABAX library)	Scofield's (1973)
ESRF (DABAX library)	Storm and Israel (1970)
ESRF (DABAX library)	Cromer and Liberman (1970a)

Table 3. Folders of the x-ray databases

Database	**Folder**
The Atomic Scattering Factor Files	Berkeleylab
X-ray Anomalous Scattering	BrennanCowan
Elam	Photo
Elam	Scatter
FFAST	FFAST
XCOM	Xcomdatany
RTAB	Dataasf
RTAB	DataMF
RTAB	DataNF
RTAB	DataPE
RTAB	DataRF
RTAB	Tableasf
Sasaki	Sasakidataf
Sasaki	Sasakidatafpfpp
Xraylib	CsbPhoto
Xraylib	CsbRayl
Xraylib	CsbCompt
Xraylib	fpfpp

Folders of the x-ray databases (Continued)

Databases	**Folder**
ESRF (DABAX library)	CrossSecBrennanCowan
ESRF (DABAX library)	CrossSecComptonIntegrHubbell
ESRF (DABAX library)	CrossSecComptonIntegrXop
ESRF (DABAX library)	CrossSecComptonKleinNishina
ESRF (DABAX library)	CrossSecEPDL97
ESRF (DABAX library)	CrossSecMcMaster
ESRF (DABAX library)	CrossSecScofield
ESRF (DABAX library)	CrossSecStormIsrael
ESRF (DABAX library)	f0EPDL97
ESRF (DABAX library)	f1f2CromerLiberman
ESRF (DABAX library)	f1f2EPDL97

Heading for the files in the folder Berkeleylab:

1. Energy [eV]
2. $f1$ [dimensionless]
3. $f2$ [dimensionless]

Heading for the files in the folder BrennanCowan:

1. Energy [eV]
2. $f1$ [dimensionless]
3. $f2$ [dimensionless]

Heading for the files in the folder Photo:

1. Energy [eV] (values are logarithms and become eV when exponentiated)
2. photo-absorption-log-value [cm^2/g] (values are logarithms and become cm^2/g when exponentiated)
3. photo-absorption-spline (values are logarithms and become cm^2/g when exponentiated)

Heading for the files in the folder Scatter:

1. Energy [eV] (values are logarithms and become eV when exponentiated)
2. coherent-scatter-log-value [cm^2/g] (values are logarithms and become cm^2/g when exponentiated)
3. coherent-scatter-spline (values are logarithms and become cm^2/g when exponentiated)
4. incoherent-scatter-log-value [cm^2/g] (values are logarithms and become cm^2/g when exponentiated)
5. incoherent-scatter-spline (values are logarithms and become cm^2/g when exponentiated)

Heading for the files in the folder FFAST:

1. Energy [keV]
2. $f1$ [e $atom^{-1}$]
3. $f2$ [e $atom^{-1}$]
4. Photoelectric $[\mu/\rho]$ [cm^2/g]
5. Coh+inc $[\sigma/\rho]$ [cm^2/g]
6. Total $[\mu/\rho]$ [cm^2/g]
7. $[\mu/\rho]_K$ [cm^2/g]
8. Wavelength [nm]

Heading for the files in the folder Xcomdatany:

1. Photon Energy [MeV]
2. Scattering Coherent [barns/atom]
3. Scattering Incoherent [barns/atom]
4. Photoelectric Absorption [barns/atom]

Heading for the files in the folder Dataasf/Imaginary anomalous scattering factor:

1. Photon Energy [keV]
2. $g'' = f''$ (according to Kissel, et al. (1995))
3. CS-RATIO = total cross section / photoeffect cross section
4. σ_{PE}, photoeffect cross section [barns]

Heading for the files in the folder Dataasf/Real anomalous scattering factor:

1. Photon energy [keV]
2. $G' = g'$ (the real anomalous scattering factor)
3. $F' = f'$ (the real anomalous scattering factor)

Heading for the files in the folder DataMF:

1. $X(1/A) = \sin(\theta/2)/\lambda$ [1/Å]
2. $MF/ELECTRON$ = modified relativistic form factor (MF) [form factor per electron]

Note: θ (scattering angle) = 2*Bragg angle.
Note: in order to retrive the value of the MF the values from the column 2 should be multiplied by the appropriate number of electrons.

Heading for the files in the folder DataNF:

1. $X(1/A) = \sin(\theta/2)/\lambda$ [1/Å]
2. $F(X)$ = form factor, f
3. $S(X)$ = incoherent scattering factor, S

Note: θ (scattering angle) = 2*Bragg angle.

Heading for the files in the folder DataPE:

1. Photon energy [keV]
2. Total-Atom Photoeffect Cross Section [barns/atom]

Heading for the files in the folder DataRF:

1. $X(1/A) = \sin(\theta/2)/\lambda$ [1/Å]
2. $RF/ELECTRO$ = relativistic atomic form factors [form factor per electron]

Note: θ (scattering angle) = 2*Braggs angle.
Note: in order to retrive the value of the RF the values from the column 2 should be multiplied by the appropriate number of electrons.

Heading for the files in the folder Tableasf:

1. Photon energy [keV]
2. $g'' = -f''_{CL} = -f2$, the imaginary part of the anomalous scattering factor (for details see Kissel (2000))
3. g'= the real part of the anomalous scattering factor (for details see Kissel, et al. (1995))
4. f'= the real part of the anomalous scattering factor (for details see Kissel, et al. (1995))
5. $f1$ (for details see Kissel (2000))

Heading for the files in the folder Sasakidataf:

1. $\sin\theta/\lambda$ [1/Å]
2. f [dimensionless]

Note: θ is Bragg angle.

Heading for the files in the folder Sasakidatafpfpp:

1. Wavelength [Å]
2. Energy [keV]
3. f'[dimensionless]
4. f'' [dimensionless]

Heading for the files in the folder CsbCompt:

1. Wavelength [Å]
2. Compton scattering cross section [barn/atom]

Heading for the files in the folder CsbPhoto:

1. Wavelength [Å]
2. Photoionization cross section [barn/atom]

Heading for the files in the folder CsbRayl:

1. Wavelength [Å]
2. Rayleigh scattering cross section [barn/atom]

Heading for the files in the folder fpfpp:

1. Wavelength [Å]
2. The anomalous scattering factor f' [dimensionless]
3. The anomalous scattering factor f'' [dimensionless]

Heading for the files in the folder CrossSecBrennanCowan:

1. Photon Energy [eV]
2. Photo Electric [barn/atom]
3. Compton (incoherent) [barn/atom]
4. Rayleigh (coherent) [barn/atom]
5. Total Cross Section [barn/atom]

Heading for the files in the folder CrossSecComptonIntegrHubbell:

1. Photon Energy [kev]
2. Compton (incoherent) [barn/atom]

Heading for the files in the folder CrossSecComptonIntegrXop:

1. Photon Energy [kev]
2. Compton (incoherent) [barn/atom]

Heading for the files in the folder CrossSecComptonKleinNishina:

1. Photon Energy [kev]
2. Compton (incoherent) [barn/atom]

Heading for the files in the folder CrossSecEPDL97:

1. Photon Energy [eV]
2. Total Cross Section [barn/atom]
3. Photo Electric [barn/atom]
4. Photo Electric Energy Transfer [barn/atom]
5. Rayleigh (coherent) [barn/atom]
6. Compton (incoherent) [barn/atom]
7. Compton (incoherent) Energy Transfer [barn/atom]

Heading for the files in the folder CrossSecMcMaster:

1. Photon Energy [eV]
2. Photoelectric Cross Section [barn/atom]
3. Coherent Cross Section [barn/atom]
4. Incoherent Cross Section [barn/atom]
5. Total cross-section [barn/atom]

Heading for the files in the folder CrossSecScofield:

1. Photon Energy [kev]
2. Total Cross Section [barn/atom]
3. Individual shells (K-shell,L -shell, M-shell,...) i+1: all other i+2,... Partial cross sections for individual shells: 1s1/2, 2s1/2, etc.

Heading for the files in the folder CrossSecStormIsrael:

1. Photon Energy [keV]
2. Compton (incoherent) [barn/atom]
3. Compton Absorption (incoherent) [barn/atom]
4. Rayleigh (coherent) [barn/atom]
5. Pair Production (NuclearField) [barn/atom]
6. Pair Production (ElectronField) [barn/atom]
7. Pair Production (Absorption) [barn/atom]
8. Photo Electric [barn/atom]
9. Photo Electric Absorption [barn/atom]
10. Total Cross Section [barn/atom]
11. Total Cross Section Absorption [barn/atom]
12. Total Cross Section Energy Absorption [barn/atom]

Heading for the files in the folder f0EPDL97:

1. $X(1/A) = \sin(\theta/2)/\lambda$ [cm $^{-}1$]
2. $f0$ = form factor [electron units]

Note: θ (scattering angle) = 2*Braggs angle .

Heading for the files in the folder f1f2CromerLiberman:

1. Photon Energy [eV]
2. $f1$ [dimensionless]
3. $f2$ [dimensionless]

Heading for the files in the folder f1f2EPDL97:

1. Photon Energy [eV]
2. $f1$ [dimensionless]
3. $f2$ [dimensionless]

Bibliography

[1] Berger M. J. and Hubbell J. H. (1987), *XCOM: Photon Cross Sections on a Personal Computer*, Publication NBSIR 87-3597, National Bureau of Standards, Gaithersburg, MD.

[2] Brunetti A., Sanchez del Rio M., Golosio B., Simionovici A. and Somogyy A. (2004), *A library for X-ray-matter interaction cross sections for X-ray fluorescence applications*, Spectrochimics Acta Part B59, pp. 1725-1731.

[3] Brennan S. and Cowan P.L. (1992), *A suite of programs for calculating x-ray absorption, reflection and diffraction performance for a variety of materials at arbitrary wavelengths*, Rev. Sci. Instrum. 63, pp. 850-853.

[4] Chantler C.T. (1995), *Theoretical Form Factor, Attenuation and Scattering Tabulation for Z=1-92 from E=1-10* eV *to E=0.4-1.0* MeV, J. Phys. Chem. Ref. Data 24, pp. 71-643.

[5] Chantler C.T. (2000), *Detailed tabulation of atomic form factors, photoelectric absorption and Scattering Cross Section, Mass Attenuation Coefficients in the vicinity of absorption edges in the soft x-ray (Z=30-36, Z=60-89, E=0.1* keV*-10* keV*), addresing convergence issues of earlier work*, J. Phys. Chem. Ref. Data 29, No. 4, pp. 597-1048 Random House, N.Y.

[6] Cullen D.E, Hubbell J.H and Kissel L. (1997), *EPDL97 The Evaluated Data Library, 97 Version*, UCRL-50400, Vol 6, Rev 5.

[7] Cromer D.T. and Liberman D. (1970a), *Relativistic Calculation of Anomalous Scattering Factors for X Rays*, J. Chem. Phys. 53, pp. 1891-1898.

[8] Elam W.T., Ravel B.D. and Sieber J.R. (2002), *A new atomic database for X-ray spectroscopic calculations*, Radiation Physics and Chemistry 63 (2002), pp. 121-128.

[9] Henke B. L., Gullikson E. M. and Davis J. C. (1993), *X-ray interactions: photoabsorption, scattering, transmission, and reflection at E=50-30.000* eV*, Z=1-92*, Atomic Data Nuclear Data Tables Vol. 54, No. 2, pp. 181-342.

[10] Kissel L. (2000), *RTAB: the Rayleighscattering database*, Radiat. Phys. Chem. 59, pp. 185-200.

[11] Kissel L., Zhou B., Roy S.C., Sen Gupta S.K. and Pratt R.H (1995), *The valdity of form-factor, modified-form factor and anomalous-scattering-factor approximations n elastic scattering calculations* , Acta Cryst. A51, pp. 271-288.

[12] McMaster W.H., Del Grande N.K., Mallett J.H. and Hubbell J.H.,(section I 1970, section II 1969, section III 1969 and section IV 1969) *Compilation of x-ray cross sections*, Lawrence Livermore National Laboratory Report UCRL-50174.

[13] Scofield J. H. (1973), *Theoretical Photoionization Cross Sections from 1 to 1500* keV, Lawrence Livermore Laboratory Report UCRL-51326, Livermore, California.

[14] Storm E. and Israel H.I. (1970), *Photon Cross Sections from 1* keV *to 100* MeV *for elements Z=1 to Z=100*, Nuclear Data Tables A7, pp. 565-681.

[15] Sasaki S. (1989) *Numerical tables of anomalous scattering factors calculated by the Cromer and Liberman's method*, National Laboratory for High Energy Physics Oho 1-1, Tsukuba 305, Japan, http://www.sasakiken.sakura.ne.jp/reports/fp-KEKrep(88-14)1989text.pdf.

Appendix B

Formula

Herein we include SI and CGS units tables and physical contants and conversion factors taken from Waseda, et al. (2011). In addition we provide some expressions used to calculate the photo-effect cross section, incoherent and coherent cross sections and the scattering atom form factor given in some representative works, like Hubbell et al. (1995), Hubbell and Øverbø (1979), Henke, et al. (1993), Kissel, et al. (1995), Creagh and Hubbell (2006) and Cromer and Lieberman (1970). In addition it is included a formula from Singiresu (2002).

Units frequently used with SI units and derived SI units				
Quantity	Symbol	Value	Units SI	Units CGS
electron volt	eV	1.60219	10^{19}J	10^{-12}erg
angstrom	Å		0.1nm=10^{-10}m	10^{-8}cm
barn	b		10^{-28}m^2	10^{-24} cm^2
Energy	J		m^2·kg·s^{-2}	
Frequency	Hz		s^{-1}	
Electric charge	C		s·A	
Electric capacity	F		m^{-2}·kg^{-1}·s^2·A^2	
Plane angle	rad			
Solid angle	sr			

Physical constants and conversion factors				
Quantity	Symbol	Value	Units SI	Units CGS
Velocity of light i vacuum	c	2.997925	10^{8}m/s	10^{10}cm/s
Planck's constant	h	6.6260	10^{-34}J/s	10^{-27}erg/s
Planck's constant (reduced)	$\hbar$	$= h/2\pi$		
Atomic number	Z			
Charge of electron	e	1.60219	10^{-19}C	10^{-20}emu
Electron rest mass	m_e	9.10956	10^{-31}g	10^{-28}g
Electron radius	r_e	2.81794	10^{-15}m	10^{-13}cm
Bohr radius	a_0	5.29177	10^{-11}m	10^{-9}cm
Fine structure constant	α	7.29735	10^{-3}	10^{-3}
Avogadro's number	N_A	6.02217	10^{23}/mol	10^{23}/mol
Permittivity of vacuum free space	ε_0	8.854188	10^{-12}F/m	
Rydberg constant	R_∞	1.09737	10^{7}/m	10^{5}/m

X-ray database available at Lawrence Berkeley National Laboratory

Herein we follow the line chosen by Henke, et al. (1993).

The dispersion equations used for calculating the forward atomic scattering-factor components, $f_1(0)$ and $f_2(0)$ are:

$$f_1(0) = Z^* + C\int_0^\infty \frac{\epsilon^2 \mu_a(\epsilon)\, d\epsilon}{E^2 - \epsilon^2}, \qquad (76)$$

$$f_2(0) = \frac{\pi}{2} CE\mu_a(E), \qquad (77)$$

and

$$Z^* = Z - (Z/82.5)^{2.37}, \qquad (78)$$

where

Symbol	Name or definition	Units	Where used
$f_1(0)$	angle-independent component of the atomic scattering factor based primarily upon the measured photoabsorption data (μ_a)	dimensionless	eq.(76)
$f_2(0)$	angle-independent component of the atomic scattering factor based primarily upon the measured photoabsorption data (μ_a)	dimensionless	eq.(77)
Z^*	limiting value of $f_1(0)$ taking relativistic effects into account	dimensionless	eq.(76-78)
C	constant equal to $= (\pi r_e hc)^{-1} = 0.9111$	(eV Å^2)$^{-1}$	eq.(76-78)
E	photon energy	eV	eq.(76-77)
$\mu_a(E)$	is the atomic photoabsorption cross section at the incident photon energy, E	barns/atom	eq.(76-77)

XCOM database: Photon Cross Sections Database

Here we are going to follow the work of Hubbell, et al. (1975). The values for the incoherent scattering cross section, σ_{inc}, were obtained by using the following equations:

$$\sigma_{inc} = \int_{\theta=0}^{\theta=\pi} \mathrm{d}\sigma_{KN}(\theta)\, S(x, Z), \qquad (8)$$

$$\begin{aligned}\sigma_{KN} &= \int_{\theta=0}^{\theta=\pi} \mathrm{d}\sigma_{KN}(\theta) \\ &= 2\pi r_e^2 \left\{ \frac{1+k}{k^2} \left[\frac{2(1+k)}{1+2k} - \frac{\ln(1+2k)}{k} \right] + \frac{\ln(1+2k)}{2k} - \frac{1+3k}{(1+2k)^2} \right\}, \quad (7)\end{aligned}$$

$$\frac{\mathrm{d}\sigma_{KN}(\theta)}{d\Omega} = \frac{r_e^2}{2} \left[1 + k(1-\cos\theta)\right]^{-2} \times \left[1 + \cos^2\theta + \frac{k^2(1-\cos\theta)^2}{1+k(1-\cos\theta)} \right], \quad (5)$$

where

Symbol	Name or definition	Units	Where used
σ_{inc}	total incoherent (bound-electron Compton) scattering cross section per atom	barn/atom	eq.(8)
k	photon energy in units of electron rest mass energy (i.e.,mc^2units), $= 1/\lambda = E(\mathrm{eV})/511003.4$		eq.(5-7)
λ	photon wavelength in Compton units, $= 1/k = 511003.4/E(\mathrm{eV})$		
E	photon energy	eV	
$\mathrm{d}\Omega$	$= 2\pi\sin\theta \mathrm{d}\theta$ (in steradians)		

Symbol	Name or definition	Units	Where used
$\frac{\mathrm{d}\sigma_{KN}(\theta)}{\mathrm{d}\Omega}$	differential Klein-Nishina (free-electron Compton) collision cross section per electron	$\frac{\text{barn/atom}}{\text{steradian}}$	eq.(5-7)
θ	the angle between the photon directions of travel prior to and following a scattering interaction (in rad)		eq.(5-7-8)
$S(x, Z)$	non-relativistic Hartree-Fock values of the incoherent scattering function	dimensionless	eq.(8)
x	$\sin(\theta/2)/\lambda\left(\text{Å}\right)$	Å^{-1}	eq.(8)
λ(Å)	photon wavelength in angstroms = $12398.520/E$ (eV)	Å	
σ_{KN}	total Compton collision cross section per electron as given by the eq.(5)	barn/atom	eq.(7)

In addition the radiative and double Compton-scattering corrections were included in the total incoherent scattering cross section and the following formula was used:

$$\sigma_{inc}^{M} \simeq \sigma_{inc} \cdot \left(1 + \triangle\sigma_{KN}^{M}\right) \qquad (10)$$

where

σ_{inc}^{M} total incoherent (bound-electron Compton) scattering cross section per atom including radiative and double-Compton corrections in units of [barns/atom]

σ_{inc} total incoherent (bound-electron Compton) scattering cross section per atom in units of [barns/atom]

$\triangle\sigma_{KN}^{M}$ combined radiative and double-Compton correction given by Mork (1971).

Herein we are going to use the work of Hubbell and Øverbø (1979). The coherent (Rayleigh)

scattering cross section was calculated from a combination of the Thompson formula and relativistic Hartree-Fock atomic form factors. The following formulas were used:

$$\sigma_{coh} = \int_{\theta=0}^{\theta=\pi} \mathrm{d}\sigma_T(\theta)\left[F(x,Z)\right]^2, \quad (3)$$

$$= \frac{3}{8}\sigma_T \int_{-1}^{+1} \left(1+\cos^2\theta\right)\left[F(x,Z)\right]^2 \mathrm{d}(\cos\theta), \quad (4)$$

$$\mathrm{d}\sigma_T(\theta)/\mathrm{d}\Omega = \frac{r_e^2}{2}\left(1+\cos^2\theta\right), \quad (2)$$

where

Symbol	Name or definition	Units	Where used
σ_{coh}	coherent (Rayleigh) scattering cross section per atom	barn/atom	eq.(3-4)
E	photon energy	eV	
$\mathrm{d}\Omega$	$= 2\pi\sin\theta\mathrm{d}\theta$ (in steradians)		
$\frac{\mathrm{d}\sigma_T(\theta)}{\mathrm{d}\Omega}$	differential Thomson scattering cross section per electron	$\frac{\text{barn/atom}}{\text{steradian}}$	eq.(2)
θ	the angle between the photon directions of travel prior to and following a scattering interaction (in rad)		eq.(2-3-4)
$F(x,Z)$	atomic from factor	dimensionless	eq.(3)
x	$\sin(\theta/2)/\lambda\left(\text{Å}\right)$	Å^{-1}	eq.(3)
$\lambda(\text{Å})$	photon wavelength in angstroms, $= 12398.520/E(\text{eV})$	Å	
σ_T	cross section for classical Thomson scattering from an electron $= 8\pi r_e^2/3$=0.6652448 b	barn	eq.(4)

Elam database

In order to obtain the values of the cross section in between the values retrived from Elam database the cubic spline interpolation is used. The formula used by this interpolation method according to Singiresu (2002) is:

$$f_i(x) = f''(x_{i-1})\frac{(-x_i + x)^3}{6(-x_i + x_{i-1})} + f''(x_i)\frac{(x - x_{i-1})^3}{6(x_i - x_{i-1})} +$$

$$+ \left\{ \frac{f(x_{i-1})}{x_i - x_{i-1}} - f''(x_{i-1}) \left(\frac{x_i - x_{i-1}}{6} \right) \right\} (x_i - x) +$$

$$+ \left\{ \frac{f(x_i)}{(x_i - x_{i-1})} - f''(x_i) \left(\frac{x_i - x_{i-1}}{6} \right) \right\} (x - x_{i-1})$$

$$x_{i-1} \leq x \leq x_i;\ i = 1, 2, \ldots, n. \qquad (5.93)$$

FFAST: X-ray Form Factor, Attenuation and Scattering Tables

Here we will highlight the formalism chosen by Chantler (2000). The following relations characterizes the real and the imaginary part of the atom from factor, f, here denoted by $\mathrm{Re}(f)$ and $\mathrm{Im}(f)$:

$$\mathrm{Re}(f) = f_0 + f' + f_{NT}, \quad f' = f_1 + f_{rel} - Z, \qquad (4)$$

$$f_0(q, Z) = 4\pi \int_0^\infty \frac{\rho(r)\sin(qr)r^2 \mathrm{d}r}{qr}, \qquad (5)$$

$$q = |\mathbf{K} - \mathbf{K}'| = 4\pi \sin(\theta/2)/\lambda, \qquad (3)$$

$$f'(E, Z) = f'(\infty) - \frac{2}{\pi} P \int_0^\infty \frac{\varepsilon' f''(\varepsilon')}{E^2 - (\varepsilon')^2}\, \mathrm{d}\varepsilon', \qquad (6)$$

$$\mathrm{Im}(f) = f''(E) = f_2(E) = \frac{E\sigma_{PE}(E)}{2hcr_e}, \qquad (7)$$

where

Symbol	Name or definition	Units	Where used
f_{rel}	a small relativistic correction term	e/atom	eq.(4)
f_{NT}	the small nuclear Thomson term	e/atom	eq.(4)
f_0	the angular form factor, for the expression see, for example, Kissel and Pratt (1985)	e/atom	eq.(4-5)
f'	the real "anomalous" scattering factor (depending on x-ray energy E and the atomic number Z)	e/atom	eq.(4-6)
q	momentum transfer	$Å^{-1}$	eq.(3-5)
E	photon energy	keV	eq.(6-7)
P	represents the pricipal value		eq.(6)
σ_{PE}	is the photoeffect cross section at photon energy E	cm^2/g	eq.(7)

RTAB database

The total-atom modified form factor is refered by Kissel, et al. (1995) as:

$$g(q) = \sum_n g_n(q) = 4\pi \sum_n \int_0^\infty \rho_n(r)(\sin qr/qr) \left\{ \frac{mc^2}{[E_n - V(r)]} \right\} r^2 \mathrm{d}r \quad (19)$$

where

$g(q)$ is the total-atom modified form factor

n the number of the electrons

According to Kane, et al. (1986) the following description of the modified form factor was given by Franz:

$$g_i(q) = 4\pi \int_0^\infty \rho_i(r) \frac{\sin(qr)}{(qr)} \left[\frac{mc^2}{E_i - V(r)} \right] r^2 \mathrm{d}r \quad (2.2.13)$$

where

$g_i(q)$	is the modified form factor,
ρ_i	is the charge distributon,
$\hbar q$	is the momentum transfer $K = K_f - K_i \equiv \hbar q$,
E_i	the total energy (including rest mass energy) of the ith electron,
$V(r)$	is the potential energy of a charge e at position r due to nucleus and (other) atomic electrons.

In addition the following clarification is given by Kissel, et al. (1995):
"Unlike FF (form-factor), owing to the presence of E_n, MF (the modified-form-factor) cannot be calculated directly from the total electron charge distribution; instead, contributions from electrons of each subshell must be calculated and summed."
According to Kane, et al (1986) the modified relativistic form-factor approximation gives the following corrections, the anomalous scattering factors g' and g''. The following quote regading the anomalous scattering factors g' and g'' can be found at Kissel, et al. (1995):
"These anomalous scattering factors are closely related to anomalous scattering factors f' and f'' conventionaly defined in reference to the nonrelativistic high-energy limit, $-Nr_e$, as

$$g' = f' + \left\{N + \left[ReA^R(\infty, 0)/r_e\right]\right\}, \;\; g'' = f''. \qquad (24)''$$

where,

N	the number of bound electrons (for a neutral atom $N = Z$)
$ReA^R(\infty, 0)$	the real part of the amplitude for elastic (Rayleigh) scattering, which in nonrelativistic dipole approximaton becomes $ReA^R(\infty, 0) = -Nr_e$.

Theoretical Rayleigh scattering data, σ_{coh} and the theoretical Compton scattering, σ_{inc}

Herein we are going to provide the expression for theoretical σ_{coh} and σ_{inc} data outlined

by Creagh and Hubbell (2006):

$$\sigma_{coh} = \pi r_e^2 \int_{-1}^{1} (1 + \cos^2\theta) f^2(q, Z) \mathrm{d}(\cos\theta), \qquad (4.2.4.6)$$

$$\sigma_{inc} = \pi r_e^2 \int_{-1}^{1} \left(\frac{1 + \cos^2\theta + \frac{k^2(1-\cos\theta)^2}{1+k(1-\cos\theta)}}{(1 + k(1 - \cos\theta))^2} \right) \times S(q, Z) \mathrm{d}(\cos\theta), \quad (4.2.4.10)$$

where

Symbol	Name or definition	Units	Where used
σ_{coh}	the bound-electron Compton scattering cross section	barn/atom	eq.(4.2.4.10)
σ_{inc}	the bound-electron Compton scattering cross section	barn/atom	eq.(4.2.4.10)
k	$= \hbar\omega/mc^2$		eq.(4.2.4.10)
θ	the angle between the photon directions of travel prior to and following a scattering interaction (in rad)		eq.(4.2.4.6)-(4.2.4.10)
$S\,(q, Z)$	the incoherent scattering function	dimensionless	eq.(4.2.4.10)
$f(q, Z)$	is the atomic scattering factor as defined by Cromer and Waber (1974)	dimensionless	eq.(4.2.4.6)
$2\pi d(\cos\theta)$	is the solid angle between cones angles θ and $\theta + d\theta$ (in steradian)		eq.(4.2.4.6)-(4.2.4.10)
q	$= \sin(\theta/2)/\lambda$, is the momentum transfer parameter(here λ is expressed in Å)	Å^{-1}	eq.(4.2.4.6)

Outline some steps regarding the formalism developped by Cromer and Lieberman (1970)

Herein we will use the work of Cromer and Lieberman (1970). Making use of the relativistic quantum mechanics the scattering factor for light by a bound electron (one electron system) is written as:

$$f = mc^2 \sum_{n^+} \left\{ \frac{\langle 2|\mathbf{e}_2 \cdot \boldsymbol{\alpha} e^{-i\mathbf{k}_2\cdot\mathbf{r}}|n^+\rangle\langle n^+|\mathbf{e}_1 \cdot \boldsymbol{\alpha} e^{i\mathbf{k}_1\cdot\mathbf{r}}|1\rangle}{\epsilon_1 - \epsilon_n^+ + \hbar\omega_1} + \frac{\langle 2|\mathbf{e}_1 \cdot \boldsymbol{\alpha} e^{i\mathbf{k}_1\cdot\mathbf{r}}|n^+\rangle\langle n^+|\mathbf{e}_2 \cdot \boldsymbol{\alpha} e^{-i\mathbf{k}_2\cdot\mathbf{r}}|1\rangle}{\epsilon_1 - \epsilon_n^+ - \hbar\omega_2} \right\}$$
$$+ mc^2 \sum_{n^-} \left\{ \frac{\langle 2|\mathbf{e}_2 \cdot \boldsymbol{\alpha} e^{-i\mathbf{k}_2\cdot\mathbf{r}}|n^+\rangle\langle n^+|\mathbf{e}_1 \cdot \boldsymbol{\alpha} e^{i\mathbf{k}_1\cdot\mathbf{r}}|1\rangle}{\epsilon_2 + |\epsilon_n^-| + \hbar\omega_2} + \frac{\langle 2|\mathbf{e}_1 \cdot \boldsymbol{\alpha} e^{i\mathbf{k}_1\cdot\mathbf{r}}|n^+\rangle\langle n^+|\mathbf{e}_2 \cdot \boldsymbol{\alpha} e^{-i\mathbf{k}_2\cdot\mathbf{r}}|1\rangle}{\epsilon_2 + |\epsilon_n^-| - \hbar\omega_1} \right\} \quad (2)$$

where

$1, 2$	indicate the initial and final states of the electron,
n^+, n^-	indicate intermediate electron states of positive and negative energy,
$\mathbf{e}_1$, $\mathbf{e}_2$	the polarization vectors,
$c\boldsymbol{\alpha}$	the Dirac velocity operator,
$\mathbf{k}_1, \mathbf{k}_2$	the wave vectors of the incident and scattered light, respectively.
ω_1, ω_2	the corresponding angular frequencies,
ϵ_1, ϵ_2	binding energy for the electron initial and final states,
ϵ_n^+	positive energy intermediate states for the electron,
ϵ_n^-	$= -\left\|\epsilon_n^-\right\|$, negative energy intermediate states for the electron,
$\hbar\omega_1, \hbar\omega_2$	the initial and final energy state of the x-ray.

Here the Kramers-Kronig relations are:

$$f^+ = \left(\frac{mc}{2\pi\hbar e^2}\right) P \int_{mc^2}^{\infty} \frac{\left(\epsilon^+ - \epsilon_1\right)^2 \sigma\left(\epsilon^+ - \epsilon_1\right) d\epsilon^+}{\left(\hbar\omega\right)^2 - \left(\epsilon^+ - \epsilon_1\right)^2} \quad (26)$$

$$f'' = \left(\frac{mc}{4\pi\hbar e^2}\right) \left(\hbar\omega\right) \sigma\left(\hbar\omega\right) \quad (25)$$

where

f^+	$= f'$, the real part of the dispersion corrections,
f''	the imaginary part of the dispersion corrections,
ϵ_1	the initial binding energy for the electron ,
$\sigma\left(\hbar\omega\right)$	the photoabsorption cross section or the total cross section .

Bibliography

[1] Berant Z., Moreh R. and Kahane S. (1977), *Nuclear Thomson scattering of 5.5–7.2* MeV *photons* , Physics Letters B, Vol. 69(3), pp. 281-283.

[2] Creagh D.C. and Hubbell J.H. (2006), *X-ray absorption (or attenuation) coefficients). Section 4.2.4.*, International Tables for Crystallography, Vol. C, Section 4.2.4, pp. 220-229.

[3] Chantler C.T. (2000), *Detailed tabulation of atomic form factors, photoelectric absorption and Scattering Cross Section, Mass Attenuation Coefficients in the vicinity of absorption edges in the soft x-ray (Z=30-36, Z=60-89, E=0.1* keV*-10* keV*), addresing convergence issues of earlier work*, J. Phys. Chem. Ref. Data 29, No. 4, pp. 597-1048 Random House, N.Y.

[4] Cromer D.T. and Waber J.T. (1974), *Atomic scattering factors for x-rays. Section 2.2.*, International Tables for X-ray Crystallography, Vol IV, edited by Ibers J. A. and Hamilton W. C. at The Kynoch Press Birmingham, England, pp. 71-147.

[5] Cromer D.T. and Liberman D. (1970), *Relativistic calculation of anomalous scattering factors for X-Rays*, J. Chem. Phys., 53, pp. 1891-1898.

[6] Cromer D.T. and Liberman D. (1981), *Anomalous dispersion calculations near to and on the long-wavelenght side of an absorption edge*, Acta Crys., A37, pp. 267-268.

[7] Cullen D.E, Hubbell J.H and Kissel L. (1975), *EPDL97 The Evaluated Data Library, 97 Version*, UCRL-50400, Vol 6, Rev 5.

[8] Davisson C. M. and Evans R. D. (1952), *Gamma-Ray Absorption Coefficients*, Reviews of Modern Physics, 24, pp. 79-109.

[9] Ericson T. E. O. and Hüfner, J. (1973), *Low-frequency photon scattering by nuclei*, Nuclear Physics B, 57(2), pp. 604-616.

[10] Henke B. L., Gullikson E. M. and Davis J. C. (1993), *X-ray interactions: photoabsorption, scattering, transmission, and reflection at E=50-30.000* eV*, Z=1-92*, Atomic Data Nuclear Data Tables Vol. 54, No. 2, pp. 181-342.

[11] Hubbell J.H., Veigele W.J., Briggs E.A., Cromer D.T. and Howerton R.J. (1975), *Atomic Form Factors, Incoherent Scattering Functions, and Photon Scattering Cross Sections*, J. Phys. Chem. Ref. Data 4, pp. 471-538; erratum in 6, pp. 615-616. (1977)

[12] Hubbell, J.H. and Øverbø I. (1979), *Relativistic Atomic Form Factors and Photon Coherent Scattering Cross Sections*, J. Phys. Chem. Ref. Data 8, pp. 69-105.

[13] Hubbell J.H., Gimm H.A. and Øverbø I (1980), *Pair, Triplet and Total Atomic Cross Sections (and Mass Attenuation Coefficients) for 1* MeV*-100* GeV *Photons in Elements Z=1 to 100*, J. Phys. Chem. Ref. Data 9, pp. 1023-1147.

[14] Hubbell J.H. (1982), *Photon Mass Attenuation and Energy Absorption Coefficients from 1* keV *to 20* MeV, Int. J. Appl. RadiatIsotopes, 33, pp. 1269-1290.

[15] Kissel L. and Pratt R. H. (1985), *Rayleigh scattering - Elastic photon scattering by bound electrons*, Atomic Inner-Shell Physics, edited by Bernd Crasemann (Plenum Publishing: New York).

[16] Kissel L., Zhou B., Roy S.C., Sen Gupta S.K. and Pratt R.H (1995), *The valdity of form-factor, modified-form factor and anomalous-scattering-factor approximations n elastic scattering calculations* , Acta Cryst. A51, pp. 271-288.

[17] Kissel L. and Pratt R. H. (1990), *Corrections to tabulated anomalous scattering factors*, Acta Cryst. A46, pp. 170-5.

[18] Klein O. and Nishina T. (1929), *Über die Streuung von Strahlung durch freie Elektronen nach der neuen relativistischen Quantendynamik von Dirac*, Zeitschrift vfür Physik, 1929, Vol.52(11), pp. 853-868.

[19] James R.W. (1982), *The Optical Priciples of the Diffraction of X-ray*, Ox Bow Press, Connecticicut, U.S.A.(originally published as The Crystalline State Vol. II in 1948, Bell and Hyman Ltd. England).

[20] Jensen M.S. (1979), *Some remarks on the anomalous scattering factors for X-rays*, Physics Letters A, Volume 74, Issues 1–2, pp. 41-44.

[21] Mork K.J. (1971), *Radiative Corrections. II. Compton Effect*, Phys. Rev. A 4., pp. 917-927.

[22] Parratt L.G. and Hempstead C.F. (1954), *Anomalous dispersion and scattering x-rays*, Physical Review Vol 94, No.6, pp. 1593-1600.

[23] Sasaki S. (1989), *Numerical tables of anomalous scattering factors calculated by the Cromer and Liberman's method* National Laboratory for High Energy Physics Oho 1-1, Tsukuba 305, Japan, http://www.sasakiken.sakura.ne.jp/reports/fp-KEKrep(88-14)1989text.pdf.

[24] Saloman E.B. and Hubbell J.H. (1987), *Critical Analysis of Soft X-ray Cross Section Data*, Nucl. Instr. Meth. A255, pp. 38-42.

[25] Saloman E.B. and Hubbell J.H. (1986), *X-ay Attenuation Coefficients (Total Cross Sections): Comparison of the Experimental DataBase with Recommended Values of Henke and the Theoretical Values of Scofield for Energies between 0.1-100* keV, National Bureau of Standards Report NBSIR 86-3431.

[26] Singiresu S.R. (2002), *Applied numerical methods for engineers and scientists*, Prentice Hall Upper Saddle River, NJ 07458.

[27] Scofield J.H., (1973) *Theoretical Photoionization Cross Sections from 1 to 1500* keV Lawrence Livermore National Laboratory Rep. UCRL-51326.

[28] Storm E. and Israel H.I. (1970), *Photon Cross Sections from 1* keV *to 100* MeV *for elements Z=1 to Z=100*, Nuclear Data Tables A7, pp. 565-681.

[29] Schaupp D., Schumacher M., Smend F., Rullhusen P. and Hubbell J. H. (1983), *Small-Angle Rayleigh Scattering of Photons at High Energies: Tabulations of Relativistic HFS Modified Atomic Form Factors*, Journal of Physical and Chemical Reference Data, Vol. 12(3), pp. 467-512.

[30] Waseda Y., Matsubara E. and Shinoda K. (2011), *X-ray diffraction crystallography*, Springer-Verlag, Berlin Heidelberg.

Appendix C

The stucture of the zip file

We provide the structure of the database used in the paper as a zip-file. Following is an overview of its structure.

Table 1. Stucture of the zip file attached to this paper.

Name database	Folder name i Database	Description of contents
The Atomic Scattering Factor Files	Berkeleylab	Data001(H)–Data092(U)
X-ray Anomalous Scattering	BrennanCowan	Data001 (H)–Data092(U)
Elam	Elam/Photo	Data001(H)–Data098(Cf)
Elam	Elam/Scatter	Data001(H)–Data098(Cf)
FFAST	NIST/FFAST	Data001 (H)–Data092(U)
XCOM	NIST/Xcomdatany	Data001 (H)–Data099(Es)

Name database	Folder name i Database	Description of contents
RTAB	RTAB/Dataasf/Imaginary Anomalous Scattering Factor	Data001 (H)–Data099(Es)
RTAB	RTAB/Dataasf/Real Anomalous Scattering Factor	Data001 (H)–Data099(Es)
RTAB	RTAB/DataMF	Data001 (H)–Data099(Es)
RTAB	RTAB/DataNF	Data001 (H)–Data099(Es)
RTAB	RTAB/DataPE	Data001 (H)–Data099(Es)
RTAB	RTAB/DataRF	Data001 (H)–Data099(Es)
RTAB	RTAB/Tableasf	Data001 (H)–Data099(Es)
Sasaki	Sasaki/Sasakidataf	Data003 (Li)–Data083(Bi); Data092(U)
Sasaki	Sasaki/Sasakidatafpfpp	Data003 (Li)–Data083(Bi); Data092(U)(∗)
Xraylib	Xraylib/CsbPhoto	Data001 (H)–Data098(Cf)
Xraylib	Xraylib/CsbRayl	Data001 (H)–Data098(Cf)
Xraylib	Xraylib/CsbCompt	Data001 (H)–Data098(Cf)
Xraylib	Xraylib/fpfpp	Data001 (H)–Data098(Cf)

Name database	Folder name i Database	Description of contents
ESRF	ESRF/CrossSecBrennanCowan	Data003 (Li)–Data099(Es)
ESRF	ESRF/CrossSecComptonIntegrHubbell	Data001 (H)–Data090(Th)
ESRF	ESRF/CrossSecComptonIntegrXop	Data001 (H)–Data090(Th)
ESRF	ESRF/CrossSecComptonKleinNishina	Data001 (H)–Data090(Th)
ESRF	ESRF/CrossSecEPDL97	Data001 (H)–Data100(Fm)
ESRF	ESRF/CrossSecMcMaster	Data001 (H)–Data94(Pu) (∗∗)
ESRF	ESRF/CrossSecScofield	Data001 (H)–Data100(Fm)
ESRF	ESRF/CrossSecStormIsrael	Data001 (H)–Data100(Fm)
ESRF	ESRF/f0EPDL97	Data001 (H)–Data100(Fm)
ESRF	ESRF/f1f2CromerLiberman	Data003 (Li)–Data093(Np)
ESRF	ESRF/ f1f2EPDL97	Data001 (H)–Data100(Fm)

(∗)(includes as well data files with values of the scattering anomalous factors in the neighborhood of K, L_1, L_2, L_3 absorption edges denoted for example Data015K)

(∗∗)(without data for 84(Po), 85(At), 87(Fr), 88(Ac), 91 (Pa), 93 (Np))