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**REVIEW**

# Review and history of photon cross section calculations*

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**Abstract**

Photon (x-ray, gamma-ray, bremsstrahlung) mass attenuation coefficients, $\mu/\rho$, are among the most widely used physical parameters employed in medical diagnostic and therapy computations, as well as in diverse applications in other fields such as nuclear power plant shielding, health physics and industrial irradiation and monitoring, and in x-ray crystallography. This review traces the evolution of this data base from its empirical beginnings totally derived from measurements beginning in 1907 by Barkla and Sadler and continuing up through the 1935 Allen compilation (published virtually unchanged in all editions up through 1971–1972 of the Chemical Rubber Handbook), to the 1949 semi-empirical compilation of Victoreen, as our theoretical understanding of the constituent Compton scattering, photoabsorption and pair production interactions of photons with atoms became more quantitative. The 1950s saw the advent of completely theoretical (guided by available measured data) systematic compilations such as in the works of Davisson and Evans, and by White-Grodstein under the direction of Fano, using mostly theory developed in the 1930s (pre-World War II) by Sauter, Bethe, Heitler and others. Post-World War II new theoretical activity, and the introduction of the electronic automatic computer, led to the more extensive and more accurate compilations in the 1960s and 1970s by Storm and Israel, and by Berger and Hubbell. Today's $\mu/\rho$ compilations by Cullen *et al*, by Seltzer, Berger and Hubbell, and by others, collectively spanning the ten decades of photon energy from 10 eV to 100 GeV, for all elements $Z = 1$ to 100, draw heavily on the 1970s shell-by-shell photoabsorption computations of Scofield, the 1960s coherent and incoherent scattering computations of Cromer *et al*, and the 1980 computations of electron–positron pair and triplet computations of Hubbell, Gimm and Øverbø, these

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names being representative of the vast legions of other researchers whose work fed into these computations.

## 1. Introduction

*Some opening personal remarks*. My first acquaintance with photon (x-ray, gamma-ray, bremsstrahlung) mass attenuation coefficients ($\mu/\rho$) was in the spring of 1950 as a lab exercise measurement of this quantity in Prof. Marc Wiedenbeck's Nuclear Physics Lab course at the University of Michigan in Ann Arbor. I was pursuing an MS (Master of Science) in physics, following an undergraduate degree in engineering physics, having been lured to physics from an electrical engineering (E.E.) curriculum in which I had originally enrolled. I had originally chosen E.E. because my uncle, an E.E., came intact through the Great Depression in the 1930s; my father, a civil engineer, did not, including his untimely death from cancer when I was too young to remember him. My switch to physics, after two years of E.E., I am sure was a result of the sparkling and dramatic physics lectures and demonstrations of Prof. James Cork in his course required for all the engineering undergrads. His textbook *Radioactivity and Nuclear Physics* (Cork 1947) is still at my elbow on my bookshelf. I was one of the many beneficiaries of the United States 'GI Bill' ('GI' for 'government issue' originally applied to army clothing and equipment, later applied to the soldiers themselves) following World War II, providing to the returning veterans a trade school or college education commensurate with one's time in military service, mine including combat, in Europe, and sufficing to carry me through to the MS. As an epilogue to my introduction to $\mu/\rho$ in Marc Wiedenbeck's lab class at Michigan in 1950, after I was established at NBS/NIST (National Bureau of Standards; name changed in 1988 to National Institute of Standards and Technology) and was agressively collecting $\mu/\rho$ measured data from around the globe for undergirding NBS theoretical compilations, Marc went beyond assigning $\mu/\rho$ as a lab exercise, and published his own measurements for 19 elements from Be ($Z = 4$) to Th ($Z = 90$) for photon energies 40 keV to 412 keV (Wiedenbeck 1962). Marc's data points were thus duly added to the NBS/NIST $\mu/\rho$ data collection (see, e.g., Saloman and Hubbell (1986), Saloman *et al* (1988), Hubbell (1994)).

My second major encounter with photon attenuation coefficients, and giving me an inkling of their importance, was in 1952, soon after I joined Ugo Fano's Radiation Theory Group at NBS. The focus of this inkling was a party in Ugo's home on Rodman Street in Washington DC, easy walking distance from NBS, before NBS moved to Gaithersburg in 1965. The party was in celebration of the completion of an 'unpublished' internal report NBS 1003 (1952) by Gladys White (later to use her married name Gladys White Grodstein) 'X ray attenuation coefficients from 10 keV to 100 MeV'. Report NBS 1003 (White 1952) overnight became a global 'best seller' primarily in medical diagnostic and therapy applications, but also in various shielding situations including for civil defense shelters against radioactive fallout from nuclear weaponry, a major national concern through the 'Cold War' which was especially tense through the 1950s and 1960s.

Hence, in the late 1960s when I inherited this NBS data compilation activity 'from the ladies' (besides White (1952), see also, e.g., Nelms (1953), Nelms and Oppenheim (1955), White Grodstein (1957), McGinnies [now Berger] (1959), Berger [R.T.] (1961)), I warmly welcomed this assignment. I have for the subsequent several decades enjoyed my supportive-physics role as a 'middleman' between the producers, both theoretical and experimental, of photon cross section data around the globe, and the x-ray attenuation data user communities, widely dispersed both geographically and by discipline, also from around the globe. In the

remainder of this review, much of the material is taken from and updated from portions of an earlier invited review in this journal (Hubbell 1999).

*Definitions, and new values of the relevant fundamental physical constants.* The mass attenuation coefficient[1] $\mu/\rho$ (cm$^2$ g$^{-1}$) can be defined as

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

in which $t$ is the mass thickness of an absorber layer in units of g cm$^{-2}$. $I_0$ is the intensity of the incident beam of photons measured with the absorber layer removed from the beam, and $I(t)$ is the intensity of the transmitted beam measured with the absorber interposed in the beam, and in which d$x$ is the thickness of a differential layer at distance $x$ into the absorber. $\rho$ is the density of the absorber layer in g cm$^{-3}$ and $\mu$ is the linear attenuation coefficient in cm$^{-1}$. Since $\mu$ is dependent on the sample density $\rho$ which can vary considerably for a given element or compound, for compilation purposes this dependence is removed by tabulating the mass attenuation coefficient $\mu/\rho$.

The fractional reduction of the beam intensity, $-\mathrm{d}I/I$, is proportional to the above mass attenuation coefficient $\mu/\rho$, and to the layer thickness, d$x$, i.e.,

$$-\mathrm{d}I/I = (\mu/\rho)\,\mathrm{d}x. \tag{2}$$

Integrating this equation, one obtains the intensity $I(t)$ transmitted through the slab

$$I(t) = I_0 \exp\left\{-\int_0^t \frac{\mu}{\rho}(x)\,\mathrm{d}x\right\}. \tag{3}$$

For a homogeneous medium, equation (3) reduces to the well-established Bouguer (1729)–Lambert (1760)–Beer (1852) exponential attenuation law

$$I(t) = I_0 \exp\{-(\mu/\rho)t\} \tag{4}$$

from which equation (1) follows.

Calculations of photon interaction data are generally in terms of atomic cross sections, in units of cm$^2$/atom, customarily in units of barns/atom (or b/atom) where 1 barn = $10^{-24}$ cm$^2$. The total atomic cross section $\sigma_{\mathrm{tot}}$ is thus related to the total mass attenuation coefficient according to

$$\begin{aligned}\mu/\rho\ (\mathrm{cm}^2\ \mathrm{g}^{-1}) &= \sigma_{\mathrm{tot}}\ (\mathrm{cm}^2/\mathrm{atom})/\{m_{\mathrm{u}}(\mathrm{g})A\} \\ &= \sigma_{\mathrm{tot}}\ (\mathrm{b/atom}) \times 10^{-24}/\{m_{\mathrm{u}}(\mathrm{g})A\}\end{aligned} \tag{5}$$

where $m_{\mathrm{u}}$ (g) (=1.660 538 86 $\times$ $10^{-24}$ g, formerly with symbol 'u', Mohr and Taylor (2005)) is the atomic mass unit, which is defined as 1/12 of the mass of an atom of the nuclide $^{12}$C, and $A$ is the relative atomic mass of the target element (Martin 1988). It can be noted that $m_{\mathrm{u}}$ (g) = $1/N_{\mathrm{A}}$, where $N_{\mathrm{A}}$ is Avogadro's number (=6.022 1415 $\times$ $10^{23}$ atoms mol$^{-1}$).

The total atomic cross section $\sigma_{\mathrm{tot}}$ can be written as the sum over the cross sections for the most-probable individual processes by which photons interact with atoms

$$\sigma_{\mathrm{tot}} = \sigma_{\mathrm{pe}} + \sigma_{\mathrm{incoh}} + \sigma_{\mathrm{coh}} + \sigma_{\mathrm{pair}} + \sigma_{\mathrm{trip}} + \sigma_{\mathrm{ph.n.}} \tag{6}$$

[1] The quantity $\mu/\rho$ has often been referred to in the literature (e.g., Allen (1935, 1971/1972), Leroux (1960), Victoreen (1943, 1948, 1949), Liebhafsky *et al* (1960), Heinrich (1966, 1986)) as the 'mass absorption coefficient'. However, the term 'mass absorption coefficient' has also been used to refer to the mass energy-transfer coefficient (e.g., Evans (1955, 1968)) and mass energy-absorption coefficient (e.g., Allison (1961)), both having to do with photon energy deposition in the target material. Hence, to avoid confusion, this paper continues to follow the International Commission on Radiation Units and Measurements (ICRU 1980) nomenclature 'mass attenuation coefficient' as used at NBS/NIST by White (1952), White Grodstein (1957) and in subsequent NBS/NIST publications as well as by Leroux and Thinh (1977) to refer to the total probability of the photon interaction processes.

in which $\sigma_{pe}$ (or $\tau$) is the atomic photoeffect cross section, $\sigma_{incoh}$ and $\sigma_{coh}$ are the incoherent (Compton) and coherent (Rayleigh) cross sections, respectively. $\sigma_{pair}$ (or $\kappa_n$) and $\sigma_{trip}$ (or $\kappa_e$) are the cross sections for electron–positron pair production (creation) in the field of the nucleus and in the field of the atomic electrons ('triplet' production), respectively. The photonuclear cross section $\sigma_{ph.n.}$ is a measurable effect (see, e.g., Gimm and Hubbell (1978)). However, this process in which the photon is absorbed by the atomic nucleus and one or more nucleons (neutrons and/or protons) are ejected, is not readily amenable to systematic calculation and tabulation. This is due to a number of factors including its irregular dependence, both in shape and in magnitude, on both $A$ and $Z$, and its sensitivity to isotopic abundances in a given sample of an element (see, e.g., Hayward (1970), Fuller and Hayward (1976) and Dietrich and Berman (1988)). Hence, $\sigma_{ph.n.}$ has been omitted from $\mu/\rho$ compilations up to the present, even though at its giant resonance peak between 5 and 40 MeV it can contribute between 2% (high-$Z$ elements) and 6% (low-$Z$ elements) to the total cross section $\sigma_{tot}$ (see, e.g., the illustrative tables in Hubbell (1969, 1982)).

Hence, current compilations of the mass attenuation coefficient $\mu/\rho$ are derived from theoretical or semi-empirical values of the cross sections for the individual processes according to

$$\mu/\rho = (\sigma_{pe} + \sigma_{incoh} + \sigma_{coh} + \sigma_{pair} + \sigma_{trip})/m_u A \tag{7}$$

referring back to equation (5) for the meaning and units of the conversion factor $1/m_u A$. The cross sections for the individual processes are discussed in section 3, particularly the cross sections obtained or derived, and used, in the recent compilations by Berger and Hubbell (1987), Creagh and Hubbell (1992), Seltzer (1993), Seltzer and Hubbell (1995), Hubbell and Seltzer (1995), Berger and Hubbell (1996/1997) and by Cullen *et al* (1997).

## 2. History

For listings of the available measurements of $\mu/\rho$ beginning with the work of Barkla and Sadler (1907, 1909) up through 2004, for photon energies from 10 eV up to 13.5 GeV in elements $Z = 1$ to 94, one can consult the annotated bibliographies of Hubbell (1994, 1996, 2004). From time to time these measurements have been graphically compared with available theory, in order to evaluate the validity of the various theoretical models for purposes of systematic compilations aimed at medical, biological and other practical applications. Among these evaluations are the graphical comparisons by Hubbell (1971) (10 eV to 100 GeV) and by Saloman *et al* (1988) (100 eV to 100 keV).

The first major general-purpose compilation of $\mu/\rho$ data appears to be that by Allen (1935), covering the photon energy range 30 eV to 2.5 MeV, 32 elements $Z = 1$ to 92 based on his own measurements (e.g., Allen (1924, 1926)), combined with others he found in the literature. First published in the Compton and Allison book (Allen 1935), these tables were soon thereafter published in the Chemical Rubber Handbook, appearing virtually unchanged in all editions from 1935 up through 1971/1972 (Allen 1971/1972). Since no theory was used in constructing the Allen (1935, 1971/1972) compilation, but only the widely scattered measurements found in the literature, there were wide gaps, requiring extensive interpolation and extrapolation across $Z$ and photon energy in order to use this data base in many practical applications.

Following the work of Allen (1935), the next major $\mu/\rho$ compilation was the semi-empirical set by Victoreen (1949), based on his evaluations in Victoreen (1943, 1948) making use of the Klein–Nishina formula for total Compton scattering and some interpretation of the atomic photoeffect and its absorption edges using Sommerfeld (1934) theory, as well as

available $\mu/\rho$ measured data. Davisson and Evans (1952) published tables for 24 elements $Z =$ 1 to 83 and photon energies 102.2 keV to 6.13 MeV (up to 25.54 MeV for $Z = 13$ and 82), obtaining pair production cross sections by graphical integration over the Bethe and Heitler (1934) Born approximation expression.

The National Bureau of Standards (now the National Institute of Standards and Technology) entered this area of collection, evaluation, analysis and compilation of $\mu/\rho$ data with the work of White (1952), Fano (1953a, 1953b), and White Grodstein (1957) and McGinnies [now R.T. Berger] (1959). The White (1952) and White Grodstein (1957) $\mu/\rho$ tables were incorporated into Davisson's (1955a, 1955b, 1965a, 1965b) chapter II appendix in the two editions of the Siegbahn (1955, 1965) book.

New theory and measurements were incorporated by Hubbell and Berger (1968) for tables of $\mu/\rho$ and $\mu_{en}/\rho$ ($\mu_{en}/\rho$ is the mass energy-absorption coefficient: for details, see, e.g. the earlier review in this journal (Hubbell 1999) and accompanying text for an invited contribution to the IAEA (International Atomic Energy Agency) *Engineering Compendium on Radiation Shielding*). With some additional new material, these tables were published by Hubbell (1969) in the National Standard Reference Data System report NSRDS-NBS 29 following their appearance also in the chapter 3 by Evans (1968) in Vol. I (Attix and Roesch, eds.) of the Attix, Roesch and Tochilin, eds. trilogy *Radiation Dosimetry* (2nd Ed., I: 1968, II: 1966, III: 1969).

A collaboration of NBS with the Lawrence Livermore National Laboratory (LLNL) produced extensive tables (McMaster *et al* 1969, 1970, 1969, 1970, Hubbell *et al* 1974) based on a combination of theoretical and measured data, weighted together, and which provided log–log cubic fitting parameters for the individual component cross sections. This effort was in conjunction and collaboration with the LLNL series of $\mu/\rho$ and related tables beginning with Plechaty and Terrall (1966) and extending up through the recent tables by Cullen *et al* (1989, 1997). A somewhat independent tabulation by Storm and Israel (1970), using pair production and some of the scattering data interpolated from NBS, covered all $Z$'s from 1 to 100. Other notable $\mu/\rho$ compilations of this period include, for example, the Boeing compilation by Brown (1966) 1 keV to 10 MeV, $Z = 1$ to 100, the extensive parametric fits by Biggs and Lighthill (1971), the 100 eV to 1 MeV, $Z = 1$ to 94 compilation by Veigele (1973) and the radiology-oriented compilation by Johns and Cunningham (1969, 1983).

The discrepancies and envelope of uncertainty of available $\mu/\rho$ data have been examined from time to time, including the effects of molecular and ionic chemical binding, particularly in the vicinity of absorption edges (e.g. Deslattes (1969)). More recent efforts at such assessments include the International Union for Crystallography (IUCr) project by Creagh and Hubbell (1987, 1990, 1992) and as examined also by Gerward (1993).

Interest in low-energy photon attenuation led to tables by Henke *et al* (1967, 1982) for energies 30 eV to 6 and 10 keV, and more recently the tables by Henke *et al* (1993) for photon energies 50 eV to 30 keV, $Z = 1$ to 92. Responding to low-energy dosimetry standards requirements, Hubbell (1977) developed $\mu/\rho$ and $\mu_{en}/\rho$ data for a few elements and mixtures of particular dosimetric interest, for the range 100 eV to 20 MeV, and later Hubbell (1982) published tables of $\mu/\rho$ and $\mu_{en}/\rho$ for 40 elements and 45 mixtures and compounds over the energy range 1 keV to 20 MeV. The latter tables are still widely used as reference values, but should now be replaced by the Berger and Hubbell (1987 [and updates]) XCOM $\mu/\rho$ values and the $\mu_{en}/\rho$ values of Seltzer (1993) and Hubbell and Seltzer (1995). Extensive new calculations and theoretical tabulations by Chantler (1995) of scattering cross sections and quantities related to $\mu/\rho$ have recently become available for photon energies from a few eV up to 1 MeV or less, for $Z = 1$ to 92. However, this new source of data has yet to be incorporated into general-use $\mu/\rho$ tables for medical, biological and other practical applications.

In the following sections, computations of cross sections for the individual photon–atom interactions, and the growth of our theoretical knowledge of them, will be historically reviewed.

## 3. Atomic photoeffect cross section $\sigma_{pe}$ (or $\tau$)

In the atomic photoeffect, 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, which are the most tightly bound, are the most important in the energy range of medical and biological interest. 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 $\sigma_{pe}$ versus photon energy exhibits the characteristic absorption edges as the binding energy of each electron subshell is attained and a new channel for photo-excitation becomes energetically allowed. Although these absorption edges have superimposed on them some degree of fine structure, discussed in the last two paragraphs in this section, in medical and other general-purpose attenuation coefficient compilations, these edges are idealized as simple sawtooth shapes.

In the early semi-theoretical compilations of $\mu/\rho$, the scattering cross sections were available theoretically to a reasonable approximation from the Klein and Nishina (1929) formula. Thus the photoeffect cross section was obtained by subtracting the theoretical scattering cross sections from measured values of $\mu/\rho$ and interpolating across $Z$ and photon energy, taking care to account for the photoeffect absorption edges shifting in energy with $Z$.

Most of the early calculations of the atomic photoeffect were for the K-shell only, typified by the high-energy work of Pratt (1960) showing 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, including photoelectron angular distributions, for 21 elements $Z = 1$ to 100 for photon energies extending as low as 1 keV ($Z = 1$) to as high as 10 MeV ($Z = 92$).

A significant advance came with the atomic photoeffect cross section calculations by Rakavy and Ron (1965, 1967) for not only the K shell, but also 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 also provide historical reviews of earlier work, are those by Alling and Johnson (1965), Matese and Johnson (1965) and by Schmickley and Pratt (1967). Interpolations from these works, along with the K-shell high-energy asymptotic behaviour provided by Pratt (1960), were helpful in constructing the tables of Hubbell (1969), along with a large body of experimentally determined total photoeffect cross section data obtained by subtracting 'known' theoretical scattering cross sections from measured total cross sections (attenuation coefficients).

However, the 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 HS 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 section results to values expected from a relativistic Dirac–Hartree–Fock (DHF) computation.

This renormalization was performed for two subsequent compilations of $\mu/\rho$ and $\mu_{en}/\rho$ by Hubbell (1977, 1982) and by Hubbell *et al* (1980). However, detailed comparisons (Saloman and Hubbell 1986, Saloman *et al* 1988) with the extensive NBS/NIST $\mu/\rho$ measurement data base tend to favour the unrenormalized $\sigma_{pe}$ Scofield (1973) over the renormalized values. Hence, in subsequent compilations by Berger and Hubbell (1987) and Hubbell and Seltzer (1995), the unrenormalized Scofield (1973) $\sigma_{pe}$ values have been used, accounting for shifts from Hubbell (1977, 1982) of the order of 2% for $Z = 2$ to 54 and photon energies less than 100 keV.

Scofield (1985) later extended these calculations down to 0.1 keV, and these (unrenormalized values) are also included in the comparison by Saloman and Hubbell (1986) and Saloman *et al* (1988), both numerically and graphically, with the NBS/NIST $\mu/\rho$ measurement data base as well as with an experiment-based compilation by Henke *et al* (1982). Values of $\sigma_{pe}$ are also given in the extensive theoretical results of Chantler (1995) computed within a self-consistent Dirac–Hartree–Fock framework, mentioned earlier. For the elements $Z = 1$ to 92, the lower-bound energy varies between 1 eV and 10 eV, and the upper-bound energy varies between 0.4 MeV and 1.0 MeV. Further detailed comparisons with the NBS/NIST measurement data base are needed to consider whether these values could or should supplant the Scofield (1973, 1985) $\sigma_{pe}$ values presently in the NIST (e.g., Hubbell and Seltzer (1995)), LLNL (e.g., Cullen *et al* (1997)) and other currently disseminated $\mu/\rho$ compilations, for medical and biological applications.

*Absorption-edge fine structure*. Oscillatory structures just above absorption edges are well-known (e.g. Sommerfeld (1920), Azároff (1963), Stern (1974)) and can be easily observed with high-resolution spectrometers (e.g. Faessler (1955), Lytle *et al* (1975), Del Grande (1986, 1990)). Above some thresholds, rather dramatic peaks can occur, due to atomic photoionization resonances. For example, in her $\mu/\rho$ measurements just above the K edge for the series of metals Ti ($Z = 22$, $E_{\text{K-edge}} = 4.97$ keV) through Zn ($Z = 30$, $E_{\text{K-edge}} = 9.66$ keV), Del Grande (1986) observed oscillations, confined to within ≈0.5 keV above the edge, of the order of 0.05 keV width with peaks extending ≈5% to ≈10% above the smoothed theoretical values. Fe ($Z = 26$) and Cu ($Z = 29$) each showed one of the series of narrow peaks to be extending ≈20% above the smoothed values.

Superimposed on these can be smaller modulations, of the order of ≈2% or less, of extended x-ray absorption fine structure (EXAFS) associated with chemical binding effects. However, due to their dependence on temperature and other variable atomic environments, these and the above oscillatory structures are currently ignored in $\mu/\rho$ tabulations for medical and biological applications.

## 4. Incoherent (Compton, also inelastic) scattering cross section $\sigma_{\text{incoh}}$

For recent information on the incoherent (Compton) scattering cross section $\sigma_{\text{incoh}}$, 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), resonant Raman scattering by Manninen (1997), applications in biomedical science and industry by Harding (1997) and a historical and status review of incoherent scattering by Hubbell (1997).

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 the nucleus of the target atom. However, the $S$-matrix results and format are not yet particularly 'user-friendly' for medical–biological applications.

The Berger and Hubbell (1987) XCOM PC program, the Hubbell and Seltzer (1995) tabulation and the Cullen *et al* (1997) LLNL data base, still rely on the incoherent scattering function $S(x, Z)$ approach. For these compilations, the incoherent scattering cross section $\sigma_{\text{incoh}}$ was obtained by numerical integration of the Klein and 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 1 to 100, with a span of $x$ values sufficient for computing $\sigma_{\text{incoh}}$ over the photon energy range 100 eV to 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 $\sigma_{\text{incoh}}$.

The Hubbell *et al* (1975) $S(x, Z)$ values were pieced together from 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) ($Z = 7$ to 100, from a non-relativistic Hartree–Fock model). Although giving cross sections differing by up to 2% to 3% 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 $\sigma_{\text{incoh}}$ values still (by default) the reference set used in most medical, biological and other 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 ranges of $x$ and $Z$ as given in the 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 the treatments by Ribberfors and Berggren (1982) and by Namito *et al* (1994, 1995).

## 5. Coherent (Rayleigh, also elastic) scattering cross section $\sigma_{\text{coh}}$

In coherent scattering, photons are scattered by bound electrons in a process 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. Since this scattering is peaked in the forward direction, particularly at high energies, this cross section has sometimes been neglected in photon transport computations. 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, crystal diffraction spectrometry and other areas including studies of molecular structures of biological interest.

The name 'Rayleigh' associated with this process stems from research on the scattering and polarization of visible light by gas molecules ('blue skies, red sunsets') by Strutt [Lord Rayleigh] (1871, 1881). A summary of this and other photon scattering work by Strutt [Lord Rayleigh] has been given in the more recent literature by Young (1982). This process is also sometimes called 'elastic' scattering, and this terminology is used in the extensive review by Kane *et al* (1986).

For recent information on elastic scattering, attention is here also called to a special topical issue of *Radiation Physics and Chemistry* edited by Bradley and Speller (1999) providing in one place a wide-ranging survey of this topic. The all-invited papers in this issue, include, in addition to papers mentioned elsewhere in this section, polarization effects (Fernandez 1999), form factor and dispersion effects (Creagh 1999), magnetic x-ray scattering (Cooper and Stirling 1999), and Delbrück scattering (Schumacher 1999). Other topics in this special issue

include elastic photon–proton scattering (Nathan 1999), photon–atom scattering measurements (Bradley *et al* 1999a, 1999b), magnetic diffraction (Laundy 1999), scattering in polymers and micelles (Fairclough *et al* 1999), collagen x-ray diffraction (Wilkinson and Hukins 1999), tissue molecular cross sections (Tartari 1999), industrial elastic scatter inspection (Luggar and Gilboy 1999), coherent x-ray scatter imaging in biomedical science and industry (Harding and Schreiber 1999), and x-ray diffraction analysis in crystalline and amorphous body tissues (Royle *et al* 1999).

For $\mu/\rho$ compilations in the medical and biological region of interest, the coherent scattering cross section $\sigma_{\mathrm{coh}}$ has been computed by numerical integration of the Thomson (1906) formula 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 again the atomic (charge) number of the nucleus of the target atom.

Theoretical values of $F(x, Z)$ were compared graphically with available measurements in the review and compilation by Hubbell *et al* (1975). Although relativistic Hartree–Fock values were available at that time, the $F(x, Z)$ values tabulated for $7 \leqslant Z \leqslant 100$ were taken from the non-relativistic Hartree–Fock Cromer and Mann (1968) and Cromer (1971) results, in view of the approximate complementarity with $S(x, Z)$, then systematically available only from non-relativistic computations. For $Z = 1$ the $F(x, Z)$ values in Hubbell *et al* (1975) were computed from the 'exact' formula of Pirenne (1946), and for $Z = 2$ to 6 were taken from the configuration interaction calculations by Brown (1970a, 1970b, 1971, 1974). Thus, in the Hubbell *et al* (1975) compilation, both $S(x, Z)$ and $F(x, Z)$ are tabulated for all $Z = 1$ to 100 over the range $0.005\ \text{Å}^{-1} \leqslant x \leqslant 10^9\ \text{Å}^{-1}$, and both $\sigma_{\mathrm{incoh}}$ and $\sigma_{\mathrm{coh}}$ are tabulated for all $Z = 1$ to 100 over the photon energy range 100 eV to 100 MeV.

In the XCOM $\mu/\rho$ data set (Berger and Hubbell 1987), and in the Hubbell and Seltzer (1995) tabulation, the values of $\sigma_{\mathrm{coh}}$ are taken from the relativistic compilation of Hubbell and Øverbø (1979). For these computations, relativistic theoretical values of $F(x, Z)$ were pieced together from Pirenne (1946) for $Z = 1$, and for the other elements, over the different ranges of $x$ and $Z$, from Doyle and Turner (1968), Cromer and Waber (1974) and from Øverbø (1977a, 1978a). Somewhat higher accuracy is anticipated from the relativistic Hartree–Fock–Slater modified atomic form factor (MFF) calculations by Schaupp *et al* (1983) for $F(x, Z)$ for $Z = 1$ to 100, $0 \leqslant x \leqslant 100\ \text{Å}^{-1}$. This compilation was not accompanied by corresponding integrated values of $\sigma_{\mathrm{coh}}$, and these MFF values have not yet found their way into the $\mu/\rho$ compilations for medical and biological applications.

Current theoretical efforts towards improved values of the coherent scattering cross section $\sigma_{\mathrm{coh}}$ are focused on use of the second-order relativistic $S$-matrix 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 absorption edge energies. For example, Zhou *et al* (1992) estimate that anomalous scattering effects can be as much as 15% at the absorption edge (subshell ionization threshold) energy, decreasing to less than 7% at 0.007 keV above the threshold, to less than 5% at 0.045 keV above threshold, and to less than 3% for an incident photon energy 0.35 keV above the threshold. Attention is here called also to recent measurements using synchrotron radiation and hyper-pure germanium (HPGe) detectors, for example those by Hugtenburg *et al* (2002, 2004) disclosing anomalous scattering structures with a few tens of eV below the K-edge energy.

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, $(\mathrm{d}\sigma_{\mathrm{coh}}/\mathrm{d}\Omega)(\theta)(\mathrm{b/sr})$, and total, $\sigma_{\mathrm{coh}}(\mathrm{b})$, for all elements $Z = 13$ to 104, for 14 commonly-used $\gamma$ energies between 50 keV and 1.5 MeV. In their computations, as outlined in an earlier review by Roy *et al*

(1993), the authors have included the amplitudes of the small contributions from nuclear Thomson scattering, Delbrück scattering (see, e.g., Hubbell and Bergstrom (2004)) and nuclear resonance scattering in addition to the Rayleigh amplitudes. Comparisons with some measured differential cross sections are included. Also, the total coherent scattering cross sections, $\sigma_{\rm coh}$, 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% to 3%, and for the highest $Z$ elements and the highest photon energy, 1.5 MeV, differences of the order of 20% are seen. Coherent scattering data in this form, over a more comprehensive energy range, are likely the wave of the future, with modern computers capable of storing the required three-dimensional arrays, in contrast to the two-dimensional arrays sufficing for the $F(x, Z)$ format.

## 6. Pair and triplet production cross sections $\sigma_{\rm pair}$ (or $\kappa_{\rm n}$) and $\sigma_{\rm trip}$ (or $\kappa_{\rm e}$)

### *6.1. Electron–positron pair production*

In this effect, which is the most likely photon interaction at high energies (above ≈10 MeV), a photon disappears in the field of a charged particle, and an electron–positron pair appears. The cross section $\sigma_{\rm pair}$ for pair production in the field of the atomic nucleus varies approximately as the square of the nuclear charge $Z$, i.e.

$$\sigma_{\rm pair} \sim Z^2. \tag{8}$$

The cross section $\sigma_{\rm trip}$ (triplet) in the field of one of the atomic electrons varies as $Z$ times the square of the unit charge, or

$$\sigma_{\rm trip} \sim Z. \tag{9}$$

This cross section is usually called the 'triplet' cross section, since the atomic electron involved in this process is also ejected from the atom, giving rise to a trident signature including the created electron and positron, when observed in a cloud chamber. For $Z = 1$ (hydrogen) $\sigma_{\rm trip}$ is approximately equal to $\sigma_{\rm pair}$, and it becomes progressively less important for higher $Z$ materials, according to

$$\sigma_{\rm trip}/\sigma_{\rm pair} \sim 1/Z. \tag{10}$$

Since biological materials, except for bone, are primarily low $Z$, $\sigma_{\rm trip}$ can be a minor but significant contribution for high-energy photon applications (i.e., above ≈10 MeV).

For some recent developments in pair production research, attention is here called to a special topical issue of *Radiation Physics and Chemistry* edited by Bergstrom (2006) including an over-all historical pair production review by Hubbell (2006), an update by Pratt (2006) on Tseng's low-energy calculations, intermediate-energy distorted wave Born approximation calculations by Sud and Sharma (2006), internal-source absolute pair production cross section measurements by Avignone (2006), the pair production channel in atomic processes by Belkacem and Sørensen (2006), extreme high energy pair production (10 GeV to 10 ZeV) by Klein (2006), relativistic positronium physics by Olsen (2006), and pair production of arbitrary spin particles by electromagnetic fields, by Kruglov (2006).

Both $\sigma_{\rm pair}$ and $\sigma_{\rm trip}$ are extensively reviewed, calculations are performed, and tabulations of these cross sections are provided for all elements $Z = 1$ to 100 over the photon energy range 1 MeV to 100 GeV in Hubbell *et al* (1980). Values from this 1980 publication are still used in current $\mu/\rho$ compilations[2], for example in Berger and Hubbell (1987) (XCOM), Hubbell and

[2] For further and updated NIST photon cross section and attenuation coefficient compilations available electronically, as well as for a variety of other evaluated physical data bases, the reader is encouraged to go to the NIST website: http://physics.nist.gov/PhysRefData/contents.html.

Seltzer (1995) and in Cullen *et al* (1997). Some highlights of how these pair and triplet cross sections were calculated, recently reviewed in more detail by Hubbell and Seltzer (2004) and by Hubbell (2006), are given below.

### *6.2. Pair production cross section (coherent, in screened nuclear field), $\sigma_{\rm pair}$ (or $\kappa_n$)*

In this process, an electron–positron pair is produced in the screened nuclear field (i.e., atomic field), and the atom as a whole recoils without internal excitation. This is in contrast to incoherent (triplet) production $\sigma_{\rm trip}$ in which the atom is either excited or ionized and the target electron recoil significantly affects the dynamics and threshold of the process. In the case of $\sigma_{\rm pair}$, the threshold for this transmutation of electromagnetic energy (a photon) into tangible matter (electron and positron) is just the sum of the rest-mass energies ($m_{\rm e-} = m_{\rm e+} = 9.109\,3826 \times 10^{-28}$ g $= 0.510\,998\,918$ MeV, Mohr and Taylor (2005)) of the two particles, or 1.022 MeV.

The $\sigma_{\rm pair}$ calculation (Hubbell *et al* 1980) begins with the Bethe and Heitler (1934) Born-approximation unscreened pair-production cross section as an initial approximation, to which Coulomb corrections, screening corrections and radiative corrections are applied. The differential Bethe–Heitler unscreened $\sigma_{\rm pair}$ cross section has been cast in forms, suitable for computation, by Bethe and Maximon (1954), Davies *et al* (1954) and by Maximon (1968).

The Coulomb correction for the Hubbell *et al* (1980) computations was pieced together from the low-energy results of Øverbø *et al* (1968, 1973), the intermediate-energy results of Øverbø (1977b) and the high-energy results of Sørenssen (1965, 1966) which in the high energy limit go to the Davies *et al* (1954) extreme relativistic Coulomb correction. Screening corrections were pieced together from the near-threshold results of Tseng and Pratt (1972, 1980) and the intermediate- and high-energy work of Øverbø (1978b). The Øverbø (1978b) work used the Jost *et al* (1950) expression for nuclear-field pair production in the Born approximation for small nuclear recoil but without the extreme high energy approximation. This expression required values of the atomic form factor $F(x, Z)$, for which Øverbø (1978b) used the relativistic $F(x, Z)$ values pieced together from Doyle and Turner (1968), Cromer and Waber (1974) and Øverbø (1977a, 1978a), later published as systematic tabulations by Hubbell and Øverbø (1979). The radiative corrections (Feynman 1949, Mork and Olsen 1960), of the order of $1/137$ and associated with the emission and reabsorption of virtual photons and with the emission of both soft and hard real photons, were obtained from Mork and Olsen (1965).

### *6.3. Triplet production cross section (incoherent pair production, in electron field, with excitation or ionization), $\sigma_{\rm trip}$ (or $\kappa_e$)*

Due to the sharing of photon energy and momentum between the target electron and the created pair, the threshold for this process is 4 $m_e c^2$ (=2.044 MeV). Actually, the process can take place down to 2 $m_e c^2$, since momentum can also be transferred to the atom both in excitation and ionization, but in this region the cross section is negligibly small. Some of the highlights of the calculations and systematic tabulations of $\sigma_{\rm trip}$ by Hubbell *et al* (1980), as a companion to the $\sigma_{\rm pair}$ tabulations therein, are given in the following.

The starting point for these computations of $\sigma_{\rm trip}$ is again the Bethe and Heitler (1934) Born-approximation, now requiring the retardation effect due to the recoil of the target atomic electron. This effect is included in the unscreened formula of Borsellino (1947), improved by including higher terms by Ghizzetti (1947). Corrections for exchange could be obtained as a ratio of results by Haug (1975) to the Borsellino–Ghizzetti results which neglected this effect. A scheme for including screening is given by Wheeler and Lamb (1939) who presented some

results computed using Thomas–Fermi (Thomas 1927, Fermi 1928) statistical-atomic-model values of $S(x, Z)$. In the Hubbell *et al* (1980) computations, screening corrections were obtained by replacing the Thomas–Fermi $S(x, Z)$ values in the Wheeler–Lamb formula by the $S(x, Z)$ values in Hubbell *et al* (1975) based on the configuration-interaction $Z = 2$ to 6 values of Brown (1970a, 1970b, 1972, 1974) and non-relativistic Hartree–Fock $Z = 7$ to 100 values of Cromer and Mann (1967) and Cromer (1969).

## 7. Conclusions and comments

For future tasks, more attention should be paid to the atomic photoeffect absorption edge structure, which will require a much larger and higher-dimensional data base, to accommodate the molecular and other matrix environments of the target atoms. Similarly, for the more-accurate scattering results from the relativistic $S$-matrix theoretical model, to replace the current simplistic and approximate $F(x, Z)$ and $S(x, Z)$ atomic form factor and incoherent scattering function tables, much more extensive and higher-dimensional arrays will be required, as seen in the work by Chatterjee and Roy (1998). However, modern computers continue to take giant steps towards greater computing power, speed and data storage and retrieval, so these objectives should be met within the coming decade, perhaps even including photonuclear data $\sigma_{\text{ph.n.}}$.

At the same time, the experimental capabilities, including more-intense and higher-energy synchrotron light sources, and new detectors with better resolution and higher efficiencies, should provide more-accurate (towards 'underlying reality'?) measured values of $\mu/\rho$ to test and undergird the above theoretical advances. Although it is sometimes said that 'now theory is better than experiment', it is still the belief of this author that 'theory is an interpolation of experiment' for purposes of computing and compiling $\mu/\rho$ tables for medical, biological and other practical applications.

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## Biography

**John Hubbell** (MS, Physics, University of Michigan 1950, and Doctor Honoris Causa, National University of Córdoba, Argentina 1996) is well-known for his evaluations, computations and compilations of photon–atom interaction cross sections and attenuation coefficients, spanning the nine decades of photon energies from 0.1 keV to 100 GeV. John joined NBS/NIST in 1950, and from 1951 to 1988 was a member of the Radiation Theory Group, including a stint 1963 to 1981 as Director of the X-Ray and Ionizing Radiation Data Center (XRIRDC). Although officially retired, he remains professionally active in support of the NIST Radiation Interactions and Dosimetry Group, in particular with the NIST Photon and Charged Particle Data Center (PCPDC). He also served 1992–2001 as Editor-in-Chief of *Radiation Physics and Chemistry*. John enjoys solar eclipse photography, including the travels to the sometimes-exotic locales where they occur.