

TOPICAL REVIEW

Review of photon interaction cross section data in the medical and biological context*

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Abstract. The probability of a photon (x-ray, gamma-ray, bremsstrahlung, etc) of a given energy E undergoing absorption or scattering when traversing a layer of material Z can be expressed quantitatively in terms of a linear attenuation coefficient μ (cm^{-1}). Since μ is dependent on the material's density, ρ (g cm^{-3}), which can be variable, the quantity usually tabulated is the mass attenuation coefficient μ/ρ ($\text{cm}^2 \text{g}^{-1}$) in which the dependence on the density has been removed. μ/ρ , in turn, can be obtained as the sum of the different types of possible interactions of photons with atoms of the material. For photon energies below 1 MeV the major interaction processes to be considered are incoherent (Compton) scattering, coherent (Rayleigh) scattering and atomic photoeffect absorption. Above 1 MeV one must also include nuclear-field pair production and atomic-field (triplet) production, and above 5 MeV one in principle should include photonuclear absorption, although the latter is neglected in data tabulations up to the present time. This review includes a selective history of measurements and theory relating to μ/ρ from the turn of the century up to the present time, and is intended to provide a basis for further calculations and critical tabulations of photon cross section data, particularly as required by users in radiation medicine and biology. The mass energy-absorption coefficient μ_{en}/ρ is also briefly discussed.

1. Introduction

In medical physics and in radiation biology, as well as in many other areas of human enterprise, few sets of physical data are as ubiquitous and widely needed and used as data on the transmission and absorption of x-rays in biological, shielding and dosimetric materials.

Within a very few years after the discovery of x-rays by Röntgen (1895), the transmission of a narrow (parallel) beam of x-rays through layers of different materials was measured and quantified with respect to photon‡ incident energy and atomic number of the material by Barkla and Sadler (1907, 1909). This quantification is in terms of the mass attenuation coefficient§

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‡ In this work the generic term 'photon' will be frequently used, which includes gamma rays, bremsstrahlung and other electromagnetic radiation as well as x-rays.

§ The quantity μ/ρ has often been referred to in the literature (e.g., Allen 1935, 1971/1972, Leroux 1960, Victoreen 1943, 1948, 1949, Liebhafski *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.

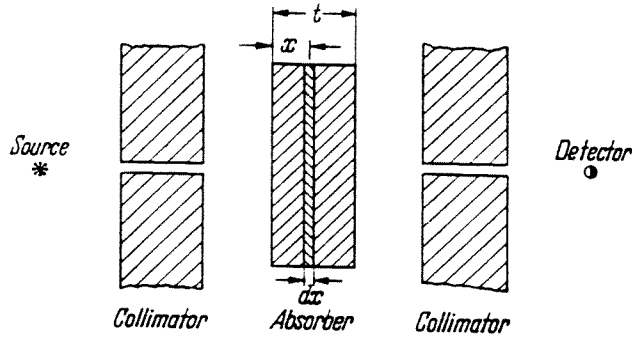


Figure 1. Arrangement for experimental determination of narrow-beam attenuation coefficients. The absorber is a slab of thickness t with plane parallel faces normal to the beam defined by the source, collimators and detector, and dx is a differential layer at distance x into the absorber.

μ/ρ ($\text{cm}^2 \text{g}^{-1}$) which can be defined as

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

in which t is the mass thickness of the 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 as shown schematically in figure 1, in which dx is the thickness of a differential layer at distance x into the absorber. ρ is the density of the absorber layer in g cm^{-3} and μ is the linear attenuation coefficient in cm^{-1} . Since μ is dependent on the sample density ρ which can vary considerably for a given element or compound, for compilation purposes this dependency is removed by tabulating the mass attenuation coefficient μ/ρ .

As described in more detail in Hubbell (1969), the fractional reduction of the beam intensity, $-dI/I$, is proportional to the above mass attenuation coefficient μ/ρ , and to the layer thickness, dx , i.e.

$$-dI/I = (\mu/\rho) dx. \quad (2)$$

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

$$I(t) = I_0 \exp\left(-\int_0^t (\mu/\rho)(x) dx\right). \quad (3)$$

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

$$I(t) = I_0 \exp[-(\mu/\rho)t] \quad (4)$$

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 σ_{tot} is thus related to the total mass attenuation coefficient according to

$$\mu/\rho(\text{cm}^2 \text{g}^{-1}) = \sigma_{\text{tot}}(\text{cm}^2/\text{atom})/(u(\text{g})A) = \sigma_{\text{tot}}(\text{b/atom}) \times 10^{-24}/(u(\text{g})A) \quad (5)$$

where $u(\text{g}) (= 1.6605402 \times 10^{-24} \text{g})$ (Cohen and Taylor 1986, 1997) 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 $u(\text{g}) = 1/N_A$, where N_A is Avogadro's number ($= 6.0221367 \times 10^{23} \text{atoms/mol}$).

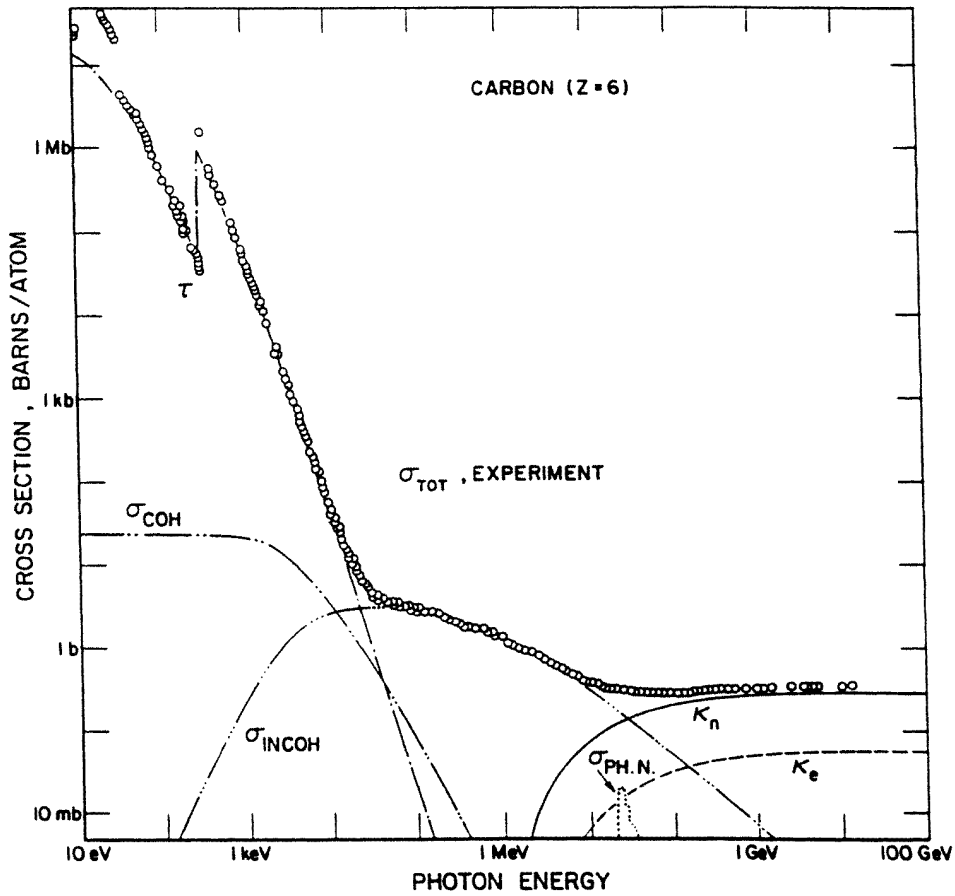


Figure 2. Contributions of atomic photoeffect, τ , coherent scattering, σ_{COH} , incoherent (Compton) scattering, σ_{INCOH} , nuclear-field pair production, κ_n , electron-field pair production (triplet), κ_e , and nuclear photoabsorption, $\sigma_{\text{PH.N.}}$, to the total measured cross section, σ_{TOT} (circles) in carbon over the photon energy range 10 eV to 100 GeV. The measured σ_{TOT} points, taken from 90 independent literature references, are not all shown in regions of high measurement density.

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

$$\sigma_{\text{tot}} = \sigma_{\text{pe}} + \sigma_{\text{incoh}} + \sigma_{\text{coh}} + \sigma_{\text{pair}} + \sigma_{\text{trip}} + \sigma_{\text{ph.n.}} \quad (6)$$

in which σ_{pe} (or τ) is the atomic photoeffect cross section, σ_{incoh} and σ_{coh} are the incoherent (Compton) and coherent (Rayleigh) cross sections respectively. σ_{pair} (or κ_n) and σ_{trip} (or κ_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. Finally, $\sigma_{\text{ph.n.}}$ is the nuclear photoeffect cross section discussed in the following paragraphs. All of these individual processes are shown in figures 2 and 3 for C ($Z = 6$) and Pb ($Z = 82$) respectively, from Hubbell *et al* (1980).

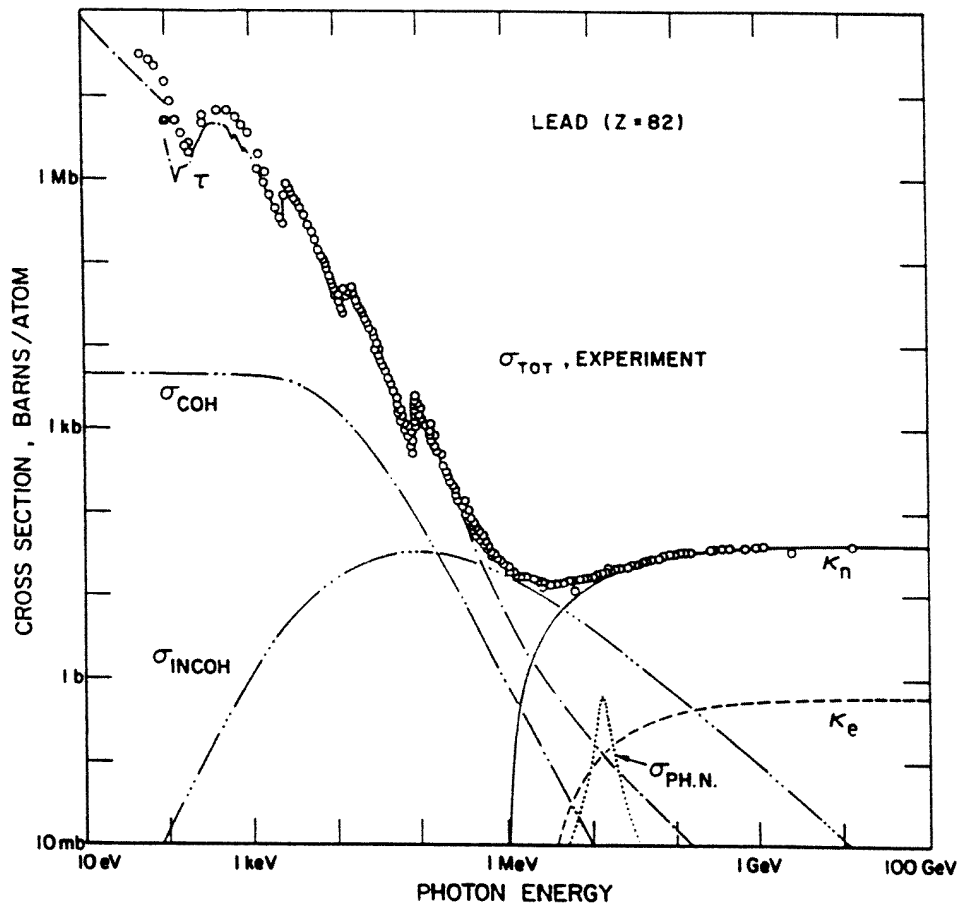


Figure 3. Contributions of atomic photoeffect, τ , coherent scattering, σ_{COH} , incoherent (Compton) scattering, σ_{INCOH} , nuclear-field pair production, κ_n , electron-field pair production (triplet), κ_e , and nuclear photoabsorption, $\sigma_{\text{PH.N.}}$, to the total measured cross section, σ_{TOT} (circles), in lead over the photon energy range 10 eV to 100 GeV. The measured σ_{TOT} points, taken from 121 independent literature references, are not all shown in regions of high measurement density.

1.1. Nuclear photoeffect, $\sigma_{\text{ph.n.}}$

In equation (6), the photonuclear cross section $\sigma_{\text{ph.n.}}$ is a measurable effect (see, for example, 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 shape and magnitude, on both A and Z , and its sensitivity to isotopic abundances in a given sample of an element (see, for example, Hayward 1970, Fuller and Hayward 1976, Dietrich and Berman 1988). Hence, $\sigma_{\text{ph.n.}}$ has been omitted from μ/ρ 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 σ_{tot} (see the illustrative tables in Hubbell 1969, 1982).

Hence, current compilations of the mass attenuation coefficient μ/ρ are derived from theoretical or semiempirical values of the cross sections for the individual processes according

to

$$\mu/\rho = (\sigma_{\text{pe}} + \sigma_{\text{incoh}} + \sigma_{\text{coh}} + \sigma_{\text{pair}} + \sigma_{\text{trip}})/uA \quad (7)$$

referring back to equation (5) for the meaning and units of the conversion factor $1/uA$. 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 (1998/1999) and by Cullen *et al* (1997).

2. History

For a listing of the available measurements of μ/ρ beginning with the above work of Barkla and Sadler (1907, 1909) up to 1995, 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). From time to time these measurements have been graphically compared with available theory, in order to evaluate the theory 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).

The first major compilation of μ/ρ 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 (for example 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 published thereafter in the Chemical Rubber Handbook, appearing virtually unchanged in all editions up to 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.

In graphing the Allen (1935) μ/ρ data versus Z at constant photon energy to compare with some new measurements (Hubbell 1953), significant departures from Z -smoothness were noted, particularly in the vicinity of Ni ($Z = 28$), in agreement with the very early observation of this anomaly by Barkla and Sadler (1907). These departures from Z -smoothness are attributable to the fact that the relative atomic mass A is not a smooth monotonically increasing function of Z , but depends on the isotopic mix for each element. These mixes, of cosmogenic origin (or since the atomic age altered by isotopic separation, such as for Li), are irregular. The function A versus Z even reverses for the Co(27)–Ni(28)–Cu(29) sequence, as well as for the Ar(18)–K(19)–Ca(20) sequence.

These departures from Z -smoothness (even where atomic photoeffect absorption edge discontinuities (section 3.1) are not involved) have been a limitation on the accuracy of some μ/ρ fitted compilations where Z -smoothness was assumed for interpolation purposes. Such compilations include, for example, those of Leroux (1960), Leroux and Thinh (1977) and Heinrich (1966, 1986). In his later compilation Heinrich (1986) acknowledged this problem, but considered the A -irregularity (versus Z) to be within the spread of the uncertainties of the available measured data to which the compilation was fitted.

Following the work of Allen (1935), the next major μ/ρ compilation was the semiempirical 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 μ/ρ

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–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 μ/ρ data with the work of Fano (1953), White (1952), White-Grodstein (1957) and McGinnies (now R T Berger) (1959). The White (1952) and White-Grodstein (1957) μ/ρ tables were incorporated into Davisson's (1955, 1965) Chapter II appendix in two editions of the Siegbahn book.

Building on this, White (1952), White-Grodstein (1957) and McGinnies (Berger) (1959) foundation work, new theory and measurements were incorporated by Hubbell and Berger (1968) for tables of μ/ρ and μ_{en}/ρ (μ_{en}/ρ is the mass energy-absorption coefficient, briefly described in section 4) and accompanying text for an invited contribution to the IAEA *Engineering Compendium on Radiation Shielding*. With some additional new material, these tables were published by Hubbell (1969) in the NSRDS-NBS 29 report following their appearance also in the chapter by Evans (1968) in the Attix–Roesch book *Radiation Dosimetry* (2nd edition, vol 1).

At the same time, a collaboration of NBS with the Lawrence Livermore National Laboratory (LLNL) produced extensive tables (McMaster *et al* 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 μ/ρ 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 Zs from 1 to 100. Other notable μ/ρ 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 Vegele (1973) and the radiology-oriented compilation by Johns and Cunningham (1969, 1983).

The discrepancies and envelope of uncertainty of available μ/ρ data have been examined from time to time, including the effects of molecular and ionic chemical binding, particularly in the vicinity of absorption edges (for example 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 reviewed 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, $Z = 1$ –92. Responding to low-energy dosimetry standards requirements, Hubbell (1977) developed μ/ρ and μ_{en}/ρ 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 μ/ρ and μ_{en}/ρ 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–Hubbell (1987 (and updates)) XCOM μ/ρ values and the μ_{en}/ρ 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 μ/ρ have recently become available for photon energies from a few eV up to 1 MeV or less, for $Z = 1$ –92. However, it is not yet clear how to incorporate this new source of data into μ/ρ tables for medical, biological and other practical applications.

3. The individual photon interaction processes

3.1. The atomic photoeffect cross section σ_{pe} (or τ)

As discussed and historically reviewed in some detail in Hubbell (1969), 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 σ_{pe} versus photon energy exhibits the characteristic absorption edges as the binding energy of each electron subshell is attained and a new channel for photoexcitation becomes energetically allowed. Although these absorption edges have superimposed on them some degree of fine structure, discussed in the last paragraph in this section, in medical and other general-purpose attenuation coefficient compilations, these edges are idealized as simple sawtooth shapes.

In the early semitheoretical 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 .

For a more extensive listing of the early calculations of the atomic photoeffect, the reader is referred to Hubbell (1969). 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, 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 breakthrough 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 multishell 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).

A greater breakthrough 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 calculations were based on his solution of the Dirac equation for the orbital electrons moving in a static Hartree–Slater central potential. For $Z = 2$ to 54, Scofield (1973) provided renormalization factors to convert to values expected from a relativistic Hartree–Fock model.

This renormalization was performed for two subsequent compilations of μ/ρ and μ_{en}/ρ 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 μ/ρ measurement data base (Hubbell 1971, 1994, 1996, Hubbell *et al* 1986) tend to favour the unrenormalized Scofield

(1973) σ_{pe} over the renormalized values. Hence, in subsequent compilations by Berger and Hubbell (1987) and Hubbell and Seltzer (1995), the unrenormalized Scofield (1973) σ_{pe} values have been used.

In a private communication to Saloman and Hubbell, Scofield (1985) 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 μ/ρ measurement data base as well as with an experimentally based compilation by Henke *et al* (1982). Values of σ_{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 and 10 eV, and the upper-bound energy varies between 0.4 and 1.0 MeV. Further detailed comparisons with the NBS/NIST measurement data base are under way to consider whether these values could or should supplant the Scofield (1973, 1985) σ_{pe} values in the NIST (for example Hubbell and Seltzer 1995) and LLNL (for example Cullen *et al* 1997) currently disseminated μ/ρ compilations for medical and biological applications.

3.1.1. Absorption-edge fine structure. Oscillatory structures just above absorption edges are well known (for example Sommerfeld 1920, Azároff 1963, Stern 1974) and can be easily observed with high-resolution spectrometers (for example 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 μ/ρ measurements just above the K edge for the series of metals Ti ($Z = 22$, $E_{K-edge} = 4.97$ keV) to Zn ($Z = 30$, $E_{K-edge} = 9.66$ 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 $\sim 5\%$ to $\sim 10\%$ above the smoothed theoretical values. Fe ($Z = 26$) and Cu ($Z = 29$) each showed one of the series of narrow peaks to be extending $\sim 20\%$ above the smoothed values.

Superimposed on these can be smaller modulations, of the order of $\sim 2\%$ 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 μ/ρ tabulations for medical and biological applications.

3.2. Incoherent (Compton) and coherent (Rayleigh) scattering, σ_{incoh} and σ_{coh}

3.2.1. Incoherent/Compton/inelastic scattering σ_{incoh} . For up-to-date 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), resonant Raman scattering by Manninen (1997), applications in biomedical science and industry by Harding (1997) and an historical and status review by Hubbell (1997).

As mentioned by Bergstrom and Pratt (1997) and earlier in the extensive review by Kane (1992) and in treatments by Bergstrom *et al* (1992, 1993) and Pratt *et al* (1994), relativistic S -matrix calculations are becoming available and will probably 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. However, the S -matrix results are not yet particularly ‘user-friendly’ for medical–biological applications.

Current μ/ρ compilations such as the Berger–Hubbell (1987) XCOM PC program, the Hubbell–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 σ_{incoh} was obtained by numerical integration of the Klein–Nishina (1929) formula weighted by the incoherent scattering function $S(x, Z)$. The required 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 σ_{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 σ_{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, b, 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 2–3% 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 σ_{incoh} values still (by default) the reference set used in most medical, biological and other practical applications. 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).

3.2.2. Coherent/Rayleigh/elastic scattering σ_{coh} . Rayleigh scattering is a process by which photons are scattered by bound electrons 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. 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 association of the name ‘Rayleigh’ with this process stems from researches 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 compilations of μ/ρ in the medical and biological region of interest, the coherent scattering cross section σ_{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 the atomic (charge) number of the nucleus of the target atom.

Measured values of $F(x, Z)$ were compared graphically with theory 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 $7 \leq Z \leq 100$ 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 Pirene (1946), and for $Z = 2$ to 6 were taken from the configuration interaction calculations by Brown (1970a, b, 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 $0.005 \text{ \AA}^{-1} \leq x \leq 10^9 \text{ \AA}^{-1}$, and both σ_{incoh} and σ_{coh} are tabulated for all $Z = 1$ to 100 over the photon energy range 100 eV to 100 MeV.

In the Berger–Hubbell (1987) XCOM μ/ρ data set, and in the Hubbell–Seltzer (1995) tabulation, the values of σ_{coh} are taken the relativistic compilation of Hubbell and Øverbø (1979). For these computations, relativistic theoretical values of $F(x, Z)$ were pieced together from Pirene (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, $0 \leq x \leq 100 \text{ \AA}^{-1}$. This compilation was not accompanied by corresponding integrated values of σ_{coh} , and these MFF values have not yet found their way into the μ/ρ compilations for medical and biological applications.

Current theoretical efforts toward improved values of the coherent scattering cross section σ_{coh} are focused on use of the second-order relativistic S -matrix formalism (for example 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 5% at 0.045 keV above threshold, and to less than 3% for an incident photon energy 0.35 keV above the threshold. However, one loses the convenience and ease of application of the atomic form factor approach, although these details may be of more interest in the future.

3.3. Pair and triplet production, σ_{pair} (or κ_n) and σ_{trip} (or κ_e)

3.3.1. 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 σ_{pair} for pair production in the field of the atomic nucleus varies approximately as the square of the nuclear charge Z , i.e.

$$\sigma_{\text{pair}} \propto \sim Z^2. \quad (8)$$

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

$$\sigma_{\text{trip}} \propto \sim Z. \quad (9)$$

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) σ_{trip} is approximately equal to σ_{pair} , and it becomes progressively less important for higher Z materials, according to

$$\sigma_{\text{trip}}/\sigma_{\text{pair}} \approx 1/Z. \quad (10)$$

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

Both σ_{pair} and σ_{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 μ/ρ compilations, for example Berger and Hubbell (1987) (XCOM), Hubbell and Seltzer (1995) and Cullen *et al* (1997). Some highlights of how these pair and triplet cross sections were calculated are given below.

3.3.2. *Pair production cross section (coherent, in screened nuclear field), σ_{pair} (or κ_n).* In coherent production, 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 σ_{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 σ_{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 ($m_{e^-} = m_{e^+} = 9.109\,3897 \times 10^{-28} \text{ g} = 0.510\,999\,06 \text{ MeV}$ (Cohen and Taylor 1986)) of the two particles, or 1.022 MeV.

The σ_{pair} calculation (Hubbell *et al* 1980) begins with the Bethe–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 σ_{pair} cross section has been cast in forms suitable for computation by Bethe and Maximon (1954), Davies *et al* (1954) and 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 Sørensen (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).

3.3.3. *Triplet production cross section (incoherent pair production, in electron field, with excitation or ionization), σ_{trip} (or κ_e).* Due to the sharing of photon energy and momentum between the target electron and the created pair, the threshold for this process is $4m_e c^2 (= 2.044 \text{ MeV})$. Actually, the process can take place down to $2m_e c^2$, 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 σ_{trip} by Hubbell *et al* (1980), as a companion to the σ_{pair} tabulations therein, are given in the following.

The starting point for these computations of σ_{trip} is again the Bethe–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, b, 1972, 1974) and non-relativistic Hartree–Fock $Z = 7$ to 100 values of Cromer and Mann (1967) and Cromer (1969).

4. The mass energy-absorption coefficient μ_{en}/ρ

A companion coefficient to μ/ρ of particular interest in medical and biological applications is the mass energy-absorption coefficient μ_{en}/ρ , used for computing the energy deposition (ionization, excitation, heat, etc) at a site (a ‘volume of interest’) within a mass of irradiated target material. For detailed discussions and the mathematical expressions for computing this coefficient, the reader is referred particularly to the definitive work of Berger (1961), also to the work of Hubbell (1982) widely used as a reference standard, and to the more recent works of Seltzer (1993) and Hubbell and Seltzer (1995).

Here, μ_{en}/ρ will be defined pictorially in figure 4 (from Hubbell 1977, which is also the source of the following text), in terms of the progressively more-detailed quantities μ/ρ , μ_a/ρ , μ_{tr}/ρ and μ_{en}/ρ , reading from left to right across the bottom of the diagram. Each of the photon interaction cross sections appearing in the sum on the right-hand side of equation (6) is represented schematically on the vertical left-hand side of figure 4 as the base dimension of a broad arrow. Moving from left to right along each of these arrows representing an interaction process, upward-branching arrows have been drawn to represent the fraction of the initial photon energy lost to the volume of interest in the form of secondary photons.

These secondary photons can include not only scattered and fluorescence photons from the primary event, but also bremsstrahlung and annihilation radiation from the charged-particle products of the primary event. The remaining fractional photon energy is assumed to be available for deposit in the volume of interest via the various charged-particle energy-dissipation mechanisms (see, for example, Seltzer 1993). For application to absorbed-dose calculations, information on this available energy can be represented by the various approximate coefficients μ_a/ρ , μ_{tr}/ρ and μ_{en}/ρ listed across the bottom of figure 4. Each of these coefficients has the same dimensions (for example $\text{cm}^2 \text{g}^{-1}$) as the mass attenuation coefficient μ/ρ but is reduced by a fraction which takes into account a specified combination of secondary photon energy losses as schematically indicated by the connecting broken lines in figure 4.

4.1. The mass absorption coefficient μ_a/ρ

The simplest of these approximate coefficients, μ_a/ρ , referred to by Evans (1955, 1968) as the ‘mass absorption coefficient’, assumes, as indicated in figure 4, that only scattered photons, both coherent and incoherent, leave the volume of interest. Usually included in this approximation is the assumption that incoherent (Compton) scattering is adequately described by the Klein–Nishina (1929) equations which assume the target electrons to be initially free and at rest.

4.2. The mass energy-transfer coefficient μ_{tr}/ρ

The next approximation, discussed in ICRU Report 33 (ICRU 1980), is the ‘mass energy-transfer coefficient’ μ_{tr}/ρ symbolized by the broken line in figure 4 connecting to this quantity.

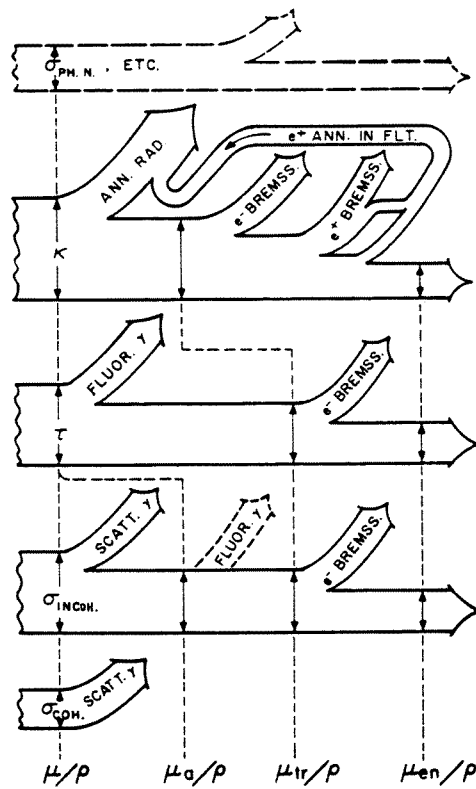


Figure 4. Schematic representation of the mass attenuation coefficient μ/ρ , the mass absorption coefficient μ_a/ρ , the mass energy-transfer coefficient μ_{tr}/ρ , and the mass energy-absorption coefficient μ_{en}/ρ in terms of the cross sections for coherent (σ_{COH}) and incoherent (σ_{INCOH}) scattering, atomic photoeffect (τ), pair production (κ), and photonuclear reactions ($\sigma_{PH.N.}$). The upward-branching arrows represent the fraction, of the incident photon energy, lost to the volume of interest in the form of secondary photons such as positron annihilation radiation (ANN. RAD.), bremsstrahlung (e^- , e^+ BREMSS.), fluorescence x-rays (FLUOR. γ) and scattered photons (SCATT. γ). The enhancement of annihilation photon energies due to positron annihilation in flight (e^+ ANN. IN FLT.) at the expense of positron bremsstrahlung and energy deposition is also indicated.

This coefficient assumes that *all* secondary photons from the primary event, fluorescence as well as scattered photons, are lost to the volume of interest. In addition, although born subsequent to the primary interaction at a distance determined by the positron travel prior to annihilation, annihilation radiation (two 0.511 MeV photons, here assuming annihilation to take place only after the positron has come to rest) is included in the fractional energy subtractions in computing μ_{tr}/ρ .

4.3. The mass energy-absorption coefficient μ_{en}/ρ

The further-reduced ‘mass energy-absorption coefficient’ μ_{en}/ρ indicated symbolically as the broken line at the extreme right edge of figure 4, is still a somewhat inexact quantity due to the arbitrariness of the ‘volume of interest’ and other factors, but is an improvement over the above

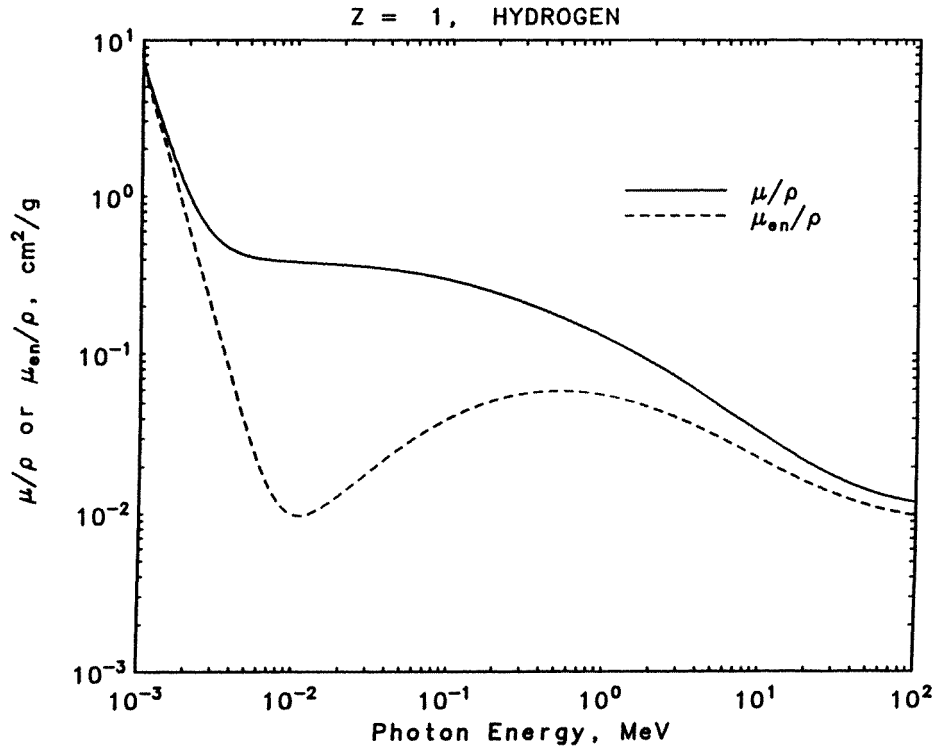


Figure 5. The mass attenuation coefficient μ/ρ and mass energy absorption coefficient μ_{en}/ρ for hydrogen for photon energies 1 keV to 100 MeV.

coefficients if one is to use this general approach in computing energy deposition. Seltzer's (1993) calculations address all the criticisms by Carlsson (1971) of earlier μ_{en}/ρ computations, by taking into account (i) electron binding effects on the Compton-scattered photon distribution, (ii) the complete cascade of fluorescence emission after ionization events in any atomic subshell, including those associated with incoherent scattering and triplet production, and (iii) the radiative energy losses of the secondary electrons and positrons slowing down in the medium, including the emission of bremsstrahlung, characteristic x-rays from impact ionization, and positron in-flight as well as at-rest annihilation quanta. His consideration of the processes in (iii) goes beyond the continuous-slowing-down approximation and includes the effects of energy-loss straggling.

Figures 5, 6 and 7 from Hubbell and Seltzer (1995) show some sample results for μ_{en}/ρ for H ($Z = 1$), water and Cu ($Z = 29$), compared with μ/ρ taken from the Berger-Hubbell (1987) XCOM PC data base. It is clear that for low- Z materials, in which incoherent scattering is the dominant process in the energy range of interest in medicine and biology, the fraction of photon energy deposited in the medium is small, but increases for higher- Z materials where photoelectric absorption is more significant. For compounds and mixtures, it should be pointed out that μ_{en}/ρ values cannot be simply added together according to fractions by weight, as in the case of μ/ρ , due to the matrix effect (secondary radiations produced by atoms differing from the original target atom) on the calculation.

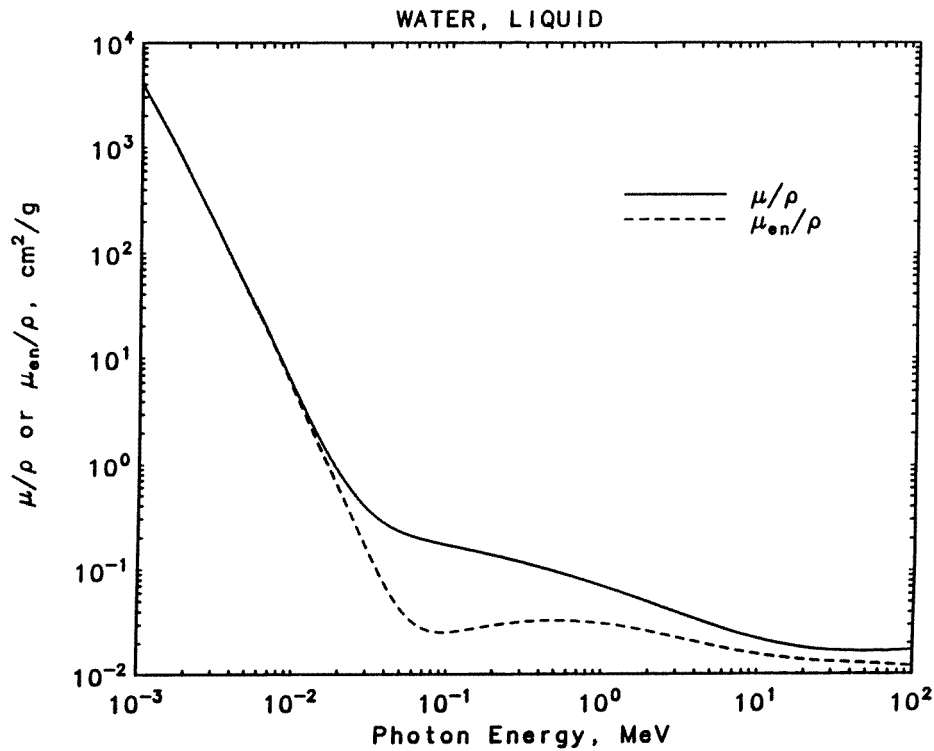


Figure 6. The mass attenuation coefficient μ/ρ and mass energy absorption coefficient μ_{en}/ρ for water for photon energies 1 keV to 100 MeV.

5. Current status and future tasks, particularly for medical and biological applications

It is clear from the above account that the μ/ρ tables used in medical, biological and other applications are indebted to a great army of theoretical physicists, working on the many pieces of the puzzle, from the time of Röntgen (1895) to the present. These tables are further indebted to the even greater army of experimental physicists listed in the Hubbell (1994) bibliography whose results the theory must reproduce at the points where comparison is possible. If such reproduction is achieved, within the uncertainties of the theoretical models and the experimental measurements, then we feel we have some understanding of the underlying reality of the physical entities and processes involved in the interactions of the photons with tangible matter.

Many of the above calculations and computations, still used in current μ/ρ compilations, were performed on rather rudimentary computers, compared with what are available today. Hence, new computations are anticipated, to replace the old, using newer approaches such as the relativistic S -matrix formalism. One would hope that the value of μ/ρ obtained from improved measurements and better theoretical models, for any given combination of Z and incident photon energy, is converging in time asymptotically, as the years pass, to an 'underlying reality' μ/ρ , although there have been some notable divergences in the past. Hence it has been difficult to establish an 'envelope of uncertainty' as desired by workers in radiation dosimetry reference standards.

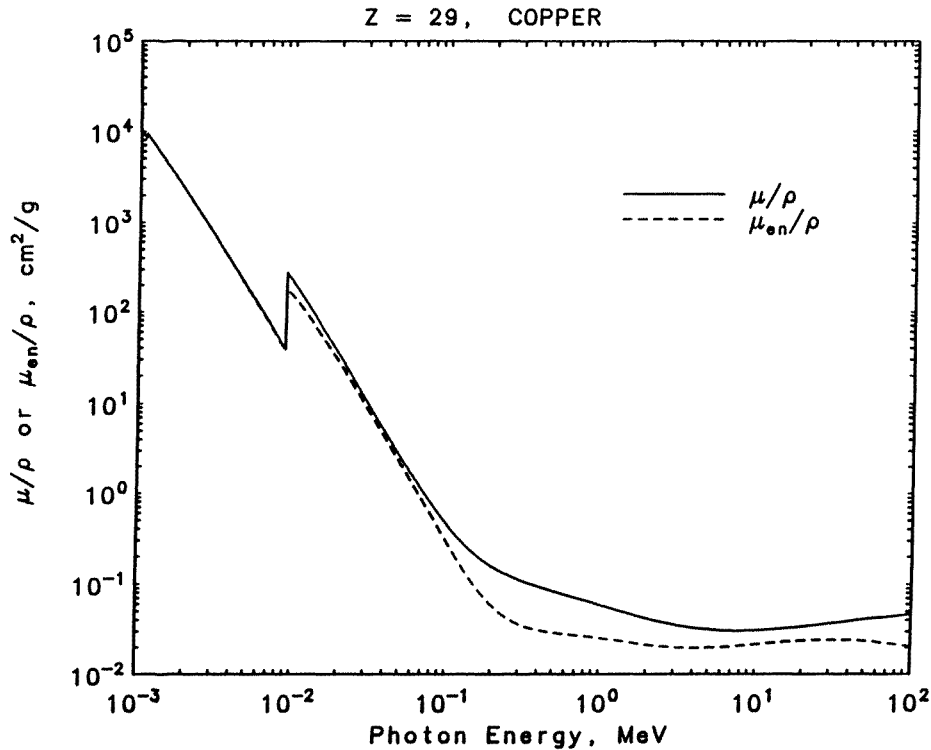


Figure 7. The mass attenuation coefficient μ/ρ and mass energy absorption coefficient μ_{en}/ρ for copper for photon energies 1 keV to 100 MeV.

Table 1. EPDL97 photoionization cross section estimated uncertainties (1σ assumed).

Photon energy range	Solid	Gas
1 eV–10 eV	?	?
10 eV–100 eV	1000%	20%
100 eV–0.5 keV	100%–200%	10%–20%
0.5 keV–1.0 keV	10%–20%	5%
1.0 keV–5.0 keV	5%	5%
5 keV–100 keV	2%	2%
100 keV–10 MeV	1%–2%	1%–2%
10 MeV–100 GeV	2%–5%	2%–5%

For the photoionization cross section, an attempt has been made in EPDL97 (Cullen *et al* 1997) to provide some rough estimates of the envelope of uncertainty, over the ranges of photon energies encompassed in that data base (table 1). Since photoionization or atomic photoeffect is the dominant interaction at low photon energies, where the uncertainties are the largest, these very approximate and subjective percent uncertainties can be taken as a rough guide to the uncertainties of the total photon cross section σ_{tot} or the mass attenuation coefficient μ/ρ . In the region 5 MeV to 30 MeV where the photonuclear giant dipole resonance occurs in the photonuclear cross section $\sigma_{\text{ph.n.}}$, neglect of this cross section can make errors in μ/ρ in excess of 5%, at the peak of this resonance. This $\sigma_{\text{ph.n.}}$ peak energy varies with both Z and the particular isotope of that element.

From this we can see that in the photon energy range of most interest in medical and biology applications, 5 keV to a few MeV, the envelope of uncertainty of μ/ρ , judging from the above estimates, is of the order of 1% to 2%. For the photon energy range 1 keV to 50 MeV, of most interest to medical physicists, attention is here called to a recently assembled electronic data base, including values of μ_{en}/ρ , developed by Boone and Chavez (1996).

Some notion of the convergence of μ/ρ as a function of time may be had by selecting a photon energy, here 40 keV, and two elements, here carbon and lead, and following the variations in these μ/ρ values from the first compilation to use a standard energy grid (White 1952), through to the values given by Hubbell and Seltzer (1995) and by Boone and Chavez (1996) (table 2).

Table 2. Variance of compiled values of μ/ρ as a function of time.

Compilation (at 40 keV)	μ/ρ (cm ² g ⁻¹) ('with coherent')	
	C (Z = 6)	Pb (Z = 82)
White (1952)	0.202	10.5
White Grodstein (1957)	0.205	10.5
McGinnies (1959)	0.205	15.1
Allison (1961)	—	14.3
Brown (1966)	0.193	14.3
Plechaty and Terrall (1966)	0.208	13.2
Hubbell (1969)	0.206	14.0
McMaster <i>et al</i> (1969)	0.205	14.1
Johns and Cunningham (1969)	0.205	13.8
Storm and Israel (1970)	0.207	14.2
Veigele (1973)	0.209	14.2
Hubbell (1982)	0.207	14.4
Hubbell and Seltzer (1995)	0.208	14.4
Boone and Chavez (1996)	0.207	14.3

The stability of the μ/ρ values beginning in the 1960s, particularly for Pb for which 40 keV is below the K-shell photoabsorption edge (only L and higher shells contributing) can be attributed to a combination of the higher-shell photoeffect cross section calculations by Rakavy and Ron (1965, 1967) and by Scofield (1973), with a flurry of new measurements in this time period.

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. However, modern computers continue to take giant steps toward 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 (toward 'underlying reality'?) measured values of μ/ρ to test and undergird the above theoretical advances. Although it is sometimes said that 'now theory is better than experiment', the belief of this author is that 'theory is an interpolation of experiment' for purposes of compiling μ/ρ tables for medical, biological and other practical applications.

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