1.1 Brief historical background on photon interaction

In the study of interaction of radiation (photon) with matter, the overall behavior of an absorber or scatterer may be inferred by considering it as a collection of individual atoms. Each atom interacts with the incident photon independently. Each of these processes is associated with an individual atom and hence may be characterized by measure of the probability of interaction called atomic cross section.

The process involved during interaction of a photon with an atom may be principally scattering or absorption. During scattering, a photon may be scattered elastically or inelastically.

**Elastic scattering:** In this process, the incident photon does not impart any energy to the atom and the electron remains in the same energy state. There is a definite phase relationship between the scattered photons from different electrons of the same atom and hence the elastic scattering is also said to be coherent.

**Inelastic scattering:** In this process, part of the incident photon energy is imparted to the atom. In this case there is no phase relationship between photons scattered by the different electrons of the same atom and hence it is also said to be incoherent.

**Absorption:** During absorption, the entire energy of the photon is transferred to the interacting atom. Consequently an electron is emitted. This process is called atomic photoeffect. In cases where energy of the incident photon exceeds a threshold of 1.02 MeV, energy manifests itself into matter in the vicinity of the nucleus of the atom with which the photon interacts. This process is called pair production.

Whichever be the process involved in the interaction of the primary photons with the absorber or scatterer through which they pass, the interacting photons will be removed from the primary beam in a single event (provided the beam is well collimated). Therefore the amount of total attenuation of the transmitted beam is a measure of the interaction occurring in the absorber. In a well collimated narrow beam of photons passing through a homogeneous material of thickness \( t \), the ratio of the intensity of transmitted beam along the incident direction, to the incident intensity is given by the Beer-Lambert's law

\[
I = I_0 e^{-\mu t} \tag{1.1}
\]
where $\mu$ is the linear attenuation coefficient of the sample. $(\mu / \rho)$ is called the total mass attenuation coefficient of the sample whose density is $\rho$. It is related to the total attenuation cross section $\sigma_{\text{tot}}$ per atom or molecule of the target by the relation

$$\sigma_{\text{tot}} = \frac{A \mu}{N_0 \rho}$$

(1.2)

where $N_0$ is the Avogadro number and $A$ is the atomic weight or molecular weight of the target. In the energy region below 1 MeV, the contribution of pair production to the total attenuation cross section is very small and hence can be neglected. Thus we can write

$$\sigma_{\text{tot}} = \sigma_{\text{coh}} + \sigma_{\text{inccoh}} + \sigma_{\text{photo}}$$

(1.3)

The mixture rule (Deslattes (1969)) provides a very convenient and effective way to calculate the mass attenuation coefficient of a chemical compound or homogeneous mixture from the weighted sum of the coefficients for the constituent elements. Any change in the atomic wave functions as a result of the molecular, chemical and crystalline environments are neglected in the mixture rule. The errors are expected to be generally less than a few percent for photon energies above 10 keV and less than 2% at energy 1 keV or more away from an absorption edge. Near the absorption edge there may be considerable fine structure, which varies with the chemical composition and the state of aggregation.

1.2 Survey of theoretical studies on total attenuation cross sections

Many tabulations of total attenuation cross sections are available in literature. These compilations are either purely theoretical, purely experimental or a combination of both theoretical and experimental information. Davisson and Evans (1951,1952) have reviewed both theoretical and experimental work and compiled a report on attenuation coefficient measurements till 1952. Grodstein (1957) and Davisson (1955) separately reviewed and compared the theoretical and experimental works.

Hubbell (1969) tabulated attenuation coefficients for 23 elements ($Z=1$ to 92) between 10 keV and 100 GeV and for air, water and 7 elements up to 100 MeV. It contains detailed information on the individual predominant processes of interactions,
and their cross sections between 10 keV and 100 GeV for 23 elements and for 13 compounds and mixtures.

Storm and Israel (1970) have tabulated attenuation and energy absorption coefficients of all elements from $Z=1$ to 100 for photon energies in the range 1 keV to 100 MeV.

Hubbell (1971) has provided a bibliography of 290 references containing absolute photon total cross section data above 10 eV, covering the period 1909 to 1971 for $Z=1$ to 94. Graphs are presented for 17 elements ($Z=10$ to 92) over the energy range 100 eV to 10 MeV comparing some attenuation coefficient tabulations by the Lawrence Livermore Radiation Laboratory, National Bureau of Standards, Los Alamos Scientific Laboratory, and others, with the above documented data points.

Biggs and Lighthill (1971) have provided a compact parameterization of attenuation coefficient data extending down to 0.01 keV. They have derived empirical formulae for the attenuation coefficients of mixtures by fitting data with sums of polynomials or exponential functions. By the very nature of their empirical formulae, they are valid only in the fitted range of $Z$ and $E$.

Simmons and Hubbell (1973) used Biggs and Lighthill parameters and formulae to compute an explicit tabulation data set, synthesized from available compilations. These compilations are of attenuation and energy absorption coefficients for pure elements barring a few exceptions.

Veigele (1973) compiled experimental photon attenuation cross sections for elements with $Z=1$ to 94 for energies in the range 0.1 keV to 1 MeV, from literature available to the end of 1970. Scattering cross sections calculated by relativistic self-consistent-field methods, were subtracted from total attenuation data, and the resulting Photoeffect and measured Photoeffect cross sections from 1 keV to 1 MeV were fitted by a least squares procedure. The theoretical scattering cross sections were then added to the resulting values to obtain total attenuation coefficients. From 0.1 keV to between 1 keV and 10 keV, non-relativistic, self-consistent-field, independent-electron theory was used to calculate Photoeffect cross sections. Theoretical scattering values were added to obtain total attenuation cross sections. Uncertainties were estimated.
Hubbell et al (1974) has reviewed, the developments in theoretical and experimental cross sections for the basic photon interactions, photoeffect, coherent and incoherent scattering and electron-positron pair production - with emphasis given to the extensive total and sub shell photoeffect calculation by Scofield (1973) and atomic form factor and incoherent scattering function data calculated by Cromer and Mann (1967,1968) and Brown (1970, 1971, 1972, 1974). Some comparisons of these theoretical results with available explicit cross sections and total attenuation coefficient measurements are presented. The results are presented graphically.

Kim (1974) and White & Fitzgerald (1977) have computed attenuation and energy absorption coefficients for human organs and tissues using average chemical compositions.

Cho et al (1975), Mc Cullong (1975) and Rutherford et al (1976) applied the equation for total attenuation coefficient of a single element, which is a function of atomic number Z, photon energy E and electron density nZ (where n is the number of atoms per unit volume), in which functions of Z and E have been obtained by fitting data at several energies to complex materials. It has led to various definitions of effective atomic number and effective electron density.

Hubbell and Veigele (1976) used experimental values of total attenuation cross sections, available in the literature, to derive photoeffect cross sections in the energy range 0.1 keV to 1.5 MeV. The results both calculated and experimental, were presented graphically as a function of photon energy for all elements from Z=1 to 94. The calculated results presented are (1) the non-relativistic Hartree-Fock self-consistent-field (SCF) results of Veigele. Over the range 0.1 keV to between 1 and 8 keV for all elements Z=1 to 94 and (2) the relativistic Hartree-Slater SCF results of Scofield over the range 1 keV to 1.5 MeV for all elements Z=1 to 101.

Plechaty et al (1978) made tabulation of attenuation and energy absorption coefficients similar to that of Storm and Israel (1970) but extending the energy down to 0.1 keV. They have combined the tabulations of McMaster et al (1969), Veigele et al (1971) and other data sources.

Jackson and Hawkes (1981) have reviewed the status of mass attenuation coefficients for pure elements and mixtures. They derived parameterizations for individual processes of interaction and thus derived an accurate parameterization for
the atomic total attenuation cross sections. They have used accurate parameterization
to determine the physical parameters of a complex medium, such as electron density
in the mixture in comparison with that in the standard element, difference between
mean atomic number and the atomic number of the standard element etc. It also yields
information regarding changes in the physical characteristics of the medium, such as
density or state of aggregation or physical changes arising from changes in chemical
composition or structure etc. They conclude that definition of one or two effective
atomic numbers characterizing a mixture, such as tissue, is not valid over wide energy
ranges or for mixtures containing elements of much different atomic number.
Although it provides a very useful approximation for a variety of radiation studies and
leads to consistent results in certain cases of greater importance the conclusion is that
the neglect of the coherent cross section which leads to the definition of a single
effective atomic number, is extremely suspect in the energy region relevant to
diagnostic X-rays and is not satisfactory for accurate work with mixtures containing
elements of low atomic number, such as biological tissue.

Hubbell (1982) has provided a very useful and extensive tabulation of mass
attenuation coefficients and mass energy-absorption coefficients for 40 elements
ranging from Z=1 to 92 in the energy range 1 keV to 20 MeV and for 45 mixtures and
compounds of dosimetric interest in the same energy range. The data given for pure
elements have been used to derive the corresponding data for the mixtures and
compounds. The tabulation is based on the calculated photoeffect cross sections of
Scofield (1973), modified for Z=1-54 using the relativistic Hartree - Fock
renormalization factors supplied by Scofield (1973).

A computerized photon attenuation data base has been developed by NBS
Photon and Charged Particle Data Center for the photon energy range 10 eV to 100
GeV and for elements, with Z=1-94. The data-base permits easier statistical analysis
of the measured $\mu/\rho$ values, as well as a variety of computer-graphics aids for the
critical evaluation of the best set theoretical or quasi-theoretical compiled data.

Schaupp et al (1983) have presented tabulations of relativistic Hartree-Fock-
Slater modified form factors for the momentum transfer range 0-100 Å⁻¹ for all
elements. These represent the atomic Rayleigh scattering amplitudes with good
accuracy at energies well above the absorption edges and suggest that the modified
form factors should replace the relativistic Hartree - Fock values in the MeV range.
Hubbell et al (1986) have presented a bibliography of papers reporting absolute measurements of photon total attenuation coefficients for elements and some compounds. It covers an energy range 10 eV to 10 GeV and the period from 1907 to 1986. The bibliography includes about 500 nonduplicative references to a total of about 20,000 data points, available in machine-readable form.

Saloman and Hubbell (1986) have presented for the energy range 0.1 to 100 keV the National Bureau of Standards data base of experimental X-ray attenuation coefficients and cross sections calculated using a relativistic Hartree-Slater model for the photoeffect cross sections for elements of atomic number Z=1 to 92. The information is displayed in both tabular and graphical form. The cross sections obtained using the semi-emperical set of recommended values of Henke and co-workers are also shown graphically.

Berger and Hubbell (1987) have developed a computer program, XCOM and data base, which can be used to calculate with a personal computer, photon cross sections for scattering, photo effect, pair production as also the total attenuation cross sections in elements, compounds or mixtures at energies from 1 keV to 100 GeV. The program is based on conclusions developed from comparison with measurements in Saloman et al (1988) and uses the unrenormalized photoeffect cross sections of Scofield (1973).

Saloman et al (1988) and Manson (1989) have reviewed the existing experimental data situation for X-ray attenuation coefficients of the elements in the energy range from 0.1 to 100 keV.

Gerward (1993) has presented the state of knowledge of X-ray attenuation coefficients in the photon energy range 1 to 100 keV, which includes several new sources of experimental and theoretical data, compilations, tables and other useful tools for calculation of X-ray attenuation in matter.

The International Union of Crystallography (IUCr) has started a project aimed at improving the techniques for the measurements of attenuation coefficients and for producing better sets of tables for experimenters, and following it some papers have been published (Creagh and Hubbell, 1987, 1990).

Creagh and McAuley (1992) and Chantler (1995) have also calculated theoretical photo effect cross sections. The data of Creagh and McAuley (1992) were

Chantler (2000) addresses the key discrepancies arising due to the smoothening of edge structure, the use of non relativistic wave functions, and the lack of appropriate convergence of wave functions and derives new theoretical results of substantially higher accuracy in near-edge soft x-ray regions. The high-energy limitations of such an approach have also been illustrated. The energy range covered is 0.1 to 10 keV. It is observed that discrepancies of the order of 200% exist among currently used theoretical approaches for numerous elements from 1 to 3 keV X-ray energies. The associated figures and tabulation demonstrate the comparison with an alternate theory and with available experimental data. It is concluded in this paper that, in general, experimental data are not accurate enough to establish the errors and inadequacies of theory. It is opined that new developments in experimental measurement hold great promise in making critical comparisons with theory in the near future.

1.3 Survey of experimental work on total attenuation cross sections

Experimental work on total attenuation cross sections has been carried out on elements, certain mixtures, compounds and alloys in good geometry set-up producing satisfactory agreement of experimental results with corresponding theoretical results.

Wiedenbeck (1962) has measured total attenuation coefficients for Be, C, Al, Fe, Co, Ni, Cu, Nb, Mo, Ag, Cd, In, Sn, Ta, W, Pt, Au, Pb, and Th in the energy range 39.52 to 412 keV. The DuMond bent crystal spectrometer was used for the analysis of the scattered radiation. The photons so analysed were detected by a 3 inch NaI(Tl) crystal with an energy resolution of 12%. The influence of the position of the absorber from the source was investigated and it was found that the measured counting rate of the transmitted radiation was independent of the absorber position. The results obtained were in general agreement with earlier tabulation at energies above the K-edge, but were higher than most estimates at energies below the K-edge.

McCrary et al (1967) have measured total attenuation coefficients of Be, C, Mg, Al, S, Ti, Fe, Ni, Cu, Zn, Zr, Nb, Mo, Ag, Sn, La, Gd, Hf, W, Au, Pb, Th, U and Pu in a narrow beam geometry with a Bragg diffraction monochromator, in the energy
range 24 to 131 keV. The results obtained are in good agreement with the results of Deslattes (1958) and Bearden (1966) in the energy region 25 to 30 keV.

Grimvall and Persson (1969) made use of an X-ray double-crystal spectrometer, which has been described by Brogren (1951), for the measurement of absorption coefficient of germanium for energies 5.415 to 41.33 keV. They have calculated the oscillator strength for the K-electrons from the photoeffect cross sections so obtained. There was good agreement between experimental and theoretical values.

Conner et al (1970) have measured mass attenuation coefficients of Air, Neon, Argon, Krypton and Xenon in the energy range 4.508 to 145.43 keV, in a narrow beam geometry and have calculated photoeffect, coherent and incoherent cross sections theoretically also. The photoeffect cross sections were computed by a modified version of the Brysk and Zerby (1968) computer code, which uses bound-state wave functions and potentials from relativistic Dirac-Slater self-consistent field calculations of Liberman et al (1965). McCrory et al (1967) used an improved treatment of the Slater exchange term with experimentally measured values of electron binding energies by Bearden (1967). The total incoherent cross section for bound electrons was calculated using the Klein-Nishina equation. The coherent scattering cross section was calculated by numerical integration of differential scattering cross section. There was a good agreement between experimental and theoretical values.

Gopal and Sanjeevaiah (1973a) have studied the variation of percentage resolution of the scintillation spectrometer, by interposing absorbers, (C, Al, Cu, Sn and Pb) with different thickness. They employed the counting sequence of Conner et al (1970) and obtained attenuation coefficients at 661.6 keV gamma rays, using an experimental arrangement similar to that of Davisson and Evans (1951) with little modifications. The angle of acceptance was 16 minute. They observed an increase in percentage resolution and total attenuation cross sections with increase in $\mu t$ above 1. With increase in $\mu t$ above unity, the lower energy side of the photopeak was found to broaden which increased with $\mu t$. The effects were shown graphically for elements of lowest and highest Z used. The changes were attributed to the increase in multiple scattering effects with the increase in attenuator thickness. However the multiple
scattering effect was found to be negligible when $\mu < 1$. They carried out the investigation for values of $\mu t$ up to 4.2.

Gopal and Sanjeevaiah (1973b) have measured the total attenuation coefficient of absorbers for 84 keV gamma rays. The broadening of the lower energy side of the photopeak also was shown graphically. They have concluded that the accuracy in the measurement of total attenuation coefficient may be increased to a great extent by using the criterion $\mu t < 1$ and the counting sequence of Conner et al (1970) which will effectively reduce the effect of multiple scattering to a minimum. Adopting this method they have measured total attenuation coefficients of carbon, aluminum, copper, tin and lead at gamma energies 84 keV to 411.8 keV. The results were in general agreement with the values of Conner et al (1970) except at certain cases, where disparities could be observed. The disparity is attributed to the fact that they have not chosen the criterion $\mu t < 1$ in all the cases. In certain cases $\mu t$ has gone up to 2.3 in their measurements.

Goswami and Chaudhuri (1973) made an accurate measurement of attenuation coefficients using a highly collimated narrow beam transmission method which effectively excluded corrections due to small-angle and multiple scattering of photons and reported for 34 elements with $Z=1$ to 82 in the energy range 662 keV to 1332 keV. The angle of acceptance for the scattered photons was 24 minutes. A 2.5 cm NaI(Tl) crystal detector was employed for the study. For elements, which were not available in the foil, powder or liquid forms, their compounds (in the form of powder) have been used. They derived the attenuation cross sections of Hydrogen from the measured attenuation cross sections of some hydrocarbons in the liquid form, applying the mixture rule. The total attenuation cross sections of some elements obtained experimentally were in satisfactory agreement with the corresponding values of Conner et al (1970), Colgate (1952), Davisson and Evans (1952).

Parthasaradhi and Hansön (1974) reported total photon attenuation cross sections at a series of energies from 3.3 to 165.8 keV for the elements Al, V, Cu, Mo, Sn, Ta, Au, and Pb. They have used Ge(Li) and Si(Li) detectors in a good geometry set-up in their study. A 5% deviation was observed with the results obtained. The photoeffect cross sections have been derived by the subtraction method and the authors claim an accuracy within 3%, for the results obtained.
Ramakrishna Gowda and Sanjeevaiah (1974) used a NaI(Tl) crystal detector in a narrow beam geometry set-up and measured the total attenuation coefficients of Al, Cu, Zr, Ag, Sn, Ta, Au and Pb for 72.1 keV photons of $^{203}$Hg. They followed the counting sequence of McCrary et al (1967) along with the condition, $\mu t < 1$ (Gopal and Sanjeevaiah, 1973), for minimising multiple scattering effects. Except for Au and Pb the experimental values were in agreement with the interpolated values of McCrary et al. The photoeffect cross sections were derived from the measured total attenuation cross sections by subtracting the theoretical values of scattering contributions.

Reddy et al (1976) obtained total attenuation cross sections of U, Th, Pb, and Au at energies 30.9, 35.9 and 55.4 keV. They used a Krypton-filled proportional counter for the detection of transmitted photons. In this case they modified the narrow beam setup so as to have more angle of acceptance for scattered photons, to compensate for the low efficiency of the proportional counter and applied corrections for small angle coherent and incoherent contributions. The total attenuation cross sections obtained were compared with the values of McCrary et al (1967), Perkin & Douglas (1967) and Wiedenbeck (1962), and deviations reported. Photoelectric cross sections for the samples used are derived from the measured total attenuation cross sections by the subtraction method.

Canada et al (1977) have measured the mass attenuation coefficients of Plutonium for various energies between 96.7 keV to 199 keV. There was an average deviation of 4% between the measured values of attenuation coefficients and the values of Veigele (1973), below the edge. However the deviation above the edge was less than 1%. They obtained the K-absorption edge value of plutonium to be 121.795 ± 0.014 keV.

Kane et al (1977) used a good resolution Ge(Li) detector in a narrow beam geometry and measured attenuation coefficients of lead, tantalum and molybdenum in the energy range 662 to 1330 keV. They studied the multiple scattering effects on the dependence of the percentage resolution, gamma ray attenuation coefficients and broadening of the lower energy side of the photopeak on the attenuator thickness, reported by Gopal et al (1973) and found to be small up to the corresponding mean free path of the gamma ray.
Rajendra Prasad (1978, 1980) studied the total attenuation cross sections of elements Al, Fe, Mo, Ag, W, Pt, Ca, V, Ni, Zn, Y, Cd, In and Nd for energy below 100 keV and 4% deviation was recorded by comparing the results obtained with the available theoretical values. The photoeffect cross sections of the elements were obtained from the experimental total attenuation cross sections by the subtraction method.

Hubbell and Øverbø (1979) and Hubbell et al (1975) have tabulated Rayleigh and incoherent cross section data. The tables cover all the elements and energies from 100 eV to 100 MeV. These calculations respectively utilize the relativistic and non-relativistic self-consistent field Hartree-Fock model for the charge distribution within the atom, for the calculation of the form factor and incoherent scattering function.

Berry and Lawrence (1979) reported X-ray attenuation coefficients of graphite for energies up to 31.07 keV using the method adopted by Lawrence and Mathieson (1976). The International Tables for X-ray Cryst. (1974) from which they have obtained theoretical values for comparison of experimental values, contains information on full contributions from Bragg scattering. The experimental values are slightly higher due to the Bragg scattering.

Lawrence (1979) has measured mass attenuation coefficients of polycrystalline samples of magnesium and aluminum in the energy range 9.68 to 40.52 keV and estimated the contributions of Bragg, thermal diffuse, Compton scattering and derived the photoeffect coefficients for the two elements. The dependence of mass absorption coefficients on wavelength has been studied and found to be the same for the polycrystalline samples of both the elements. An excellent agreement is reported between the experimental values and those of Miller and Greening (1974). However their results are higher by 2% from the values of International Tables for X-ray Cryst. (1974).

Puttaswamy et al (1979) measured total attenuation cross sections of the elements C, Al, S, Cu, Zr, Ag, Sn, Ta, Au and Pb for photon energy range 5 to 150 keV using proportional counter filled with Krypton gas and a thin NaI(Tl) detector in the energy ranges 5 to 25 keV and 30 to 130 keV respectively. The total attenuation cross sections obtained are compared with other experimental values available in the literature. In most of the cases there values were higher particularly at energies 32 and
36.9 keV. An improvement in agreement was observed with increase in Z and energy. Photoeffect cross sections were derived by subtracting the theoretical scattering contributions from the measured total attenuation cross sections. The values so obtained were in good agreement with the corresponding values of Scofield (1973).

Ramakrishna Gowda et al (1979) noticed a trend of decrease in error in the total attenuation cross section measurements of several elements like carbon, by many investigators. In view of the fact that the convergence of the measured values was to be determined, they measured total attenuation cross sections of carbon with radio active sources which emit in the energy range 5-14.4 keV X-rays using a Krypton filled proportional counter in a good geometry set-up. The values so obtained were compared and discussed with values available in the literature.

Puttaswamy et al (1981) extracted total attenuation cross sections, total and K-shell photoeffect cross sections, K-jump ratios and total to K-shell photoeffect cross section ratios at the K-edges of the elements Cu, Zr, Ag, Sn, Ta, Au, and Pb, from their earlier studies on total attenuation cross sections [Ramakrishna Gowda et al (1976), Puttaswamy et al (1979), (1981), Puttaswamy (1980)]. The derived photoeffect cross sections were in good agreement with corresponding values of Scofield (1973). They obtained empirical relations for K-edge cross sections and ratios, which were found to reproduce the values to accuracy better than 1%.

Umesh et al (1981) studied the total attenuation cross sections of a number of compounds and derived the incoherent scattering cross sections of low and medium Z elements for energies in the range 279.2 to 1115.5 keV. The compounds used are LiOH, MgO, NaF, NaCl, NaNO₂, KCl, NiO, CuO, TiO₂, NaHCO₃, NaNO₃, MnO₂, CuCl, CrO₃, Al₂O₃, Na₂CO₃, KBr, RbCl, ZrO₂, SrF₂, KH₂PO₄, Na₂SO₄, AgCl, BaO, KI, CdI₂. The attenuation cross sections of Al, Cu, Zr and Ag foils also have been measured. The binding effects of electrons were discussed.

Umesh et al (1982) extended their earlier work and measured total attenuation cross sections of some compounds containing rare earth and high Z elements and derived the incoherent scattering cross sections of several constituent elements in the energy range 279.2 to 1115.5 keV. In the measurement of the total attenuation cross section, an extrapolation method was used to correct for the multiple scattering effects. The compounds La₂O₃, CeO₂, PrO₂, Nd₂O₃, Sm₂O₃, Gd₂O₃, Dy₂O₃, HO₂O₃,
Er$_2$O$_3$, Ta$_2$O$_5$, Bi$_2$O$_3$, (HCOO)$_2$Pb were used in the investigation. The incoherent scattering cross sections of La, Ce, Pr, Nd, Sm, Gd, Dy, Ho, Er, Ta, H, Pb, and Bi have been derived.

Nageswara Rao et al (1984) reported the measurement of total attenuation coefficients in compounds containing the elements C, Al, S, Ni, Cu, Zn, Se, Mo, Ag, Cd, In, Sn, Sb, Te, I, Hg, Pb and Bi in the energy range 32.1 to 661.6 keV, by employing a NaI(Tl) scintillation spectrometer in a good geometry set-up. From these values they have derived the photoeffect cross sections for low and high Z elements, by the subtraction method, with the aid of mixture rule in the energy range 30 to 280 keV. Analysis in terms of effective atomic numbers and photoelectric cross sections is given.

Umesh et al (1984) have measured total attenuation cross sections of 38 compounds at energies 1170 and 1330 keV. The whole-atom integral incoherent scattering cross sections were derived for 38 elements using mixture rule and an extrapolation method.

Umesh and Ranganathaiah (1984) derived a simple method for the determination of the photoeffect cross sections of elements from the measured total attenuation cross sections of their compounds. The investigation involves the measurement of total attenuation cross sections of the compounds AgCl, KI, BaO, La$_2$O$_3$, CeO$_2$, PrO$_2$, Nd$_2$O$_3$, Sm$_2$O$_3$, Gd$_2$O$_3$, Dy$_2$O$_3$, Ho$_2$O$_3$, Er$_2$O$_3$, Ta$_2$O$_5$, (HCOO)$_2$Pb, and Bi$_2$O$_3$. From these values the total photoeffect cross sections of elements have been derived in the energy range 514 to 1332.5 keV using the new method.

Parthasaradhi (1985) carried out total attenuation cross section measurements near the edges of some elements and compounds. Analysis in terms of photoelectric cross sections was given. Deviations were reported by comparing the data obtained for compounds with the available theoretical data.

Reddy et al (1985) made a study of total attenuation cross sections of several alloys in the energy range 32.1 to 661.6 keV using a NaI(Tl) detector in a good geometry set-up. The photoeffect and scattering cross sections at appropriate photon energies were obtained by using the subtraction method. The total and partial
effective atomic numbers were also derived. The results were in agreement with the theoretical values.

Umesh et al (1985) measured total attenuation cross sections of several compounds and by applying the mixture rule the total attenuation cross sections of some constituent elements were derived at the energy 145.4 keV in a good geometry set up. Photoeffect cross sections of the corresponding elements have been derived from their total attenuation cross sections by using the subtraction method. The compounds used were NaNO₂, NaNO₃, La₂O₃, CeO₂, PrO₂, Nd₂O₃, Sm₂O₃, Gd₂O₃, Dy₂O, HO₂O₃ and Er₂O₃.

Bradley et al (1986) made photon absorption studies of some elements, mixtures and substances of biomedical interest in the energy range 33.1 to 662 keV. The elements C, Al, S, compounds H₂O, CaCO₃, and substances dry bone, bone standard, wax, polyethylene, polyisoprene, dried lean meat, fat, coconut oil, corn oil, ghee were used.

Seetharami Reddy et al (1987) used a high resolution Si(li) detector to resolve the gamma ray doublet with 79.623 and 80.999 keV energies of ¹³³Ba source. The total attenuation cross sections of Cu, Pt and Au were measured for the above gamma rays. They have adopted the experimental set-up and method of measurement reported by Smiles et al (1982) and Kane et al (1977). They have measured total attenuation coefficients at the doublet energies and obtained the cross section for the intensity weighted average energy 80.905 keV by using two methods. In the first method, they interpolated the cross section corresponding to the lower edge (80.923 keV) of Scofield (1973) down to 80.905 keV which yielded a highly underestimated value for cross section. In the second method, the lower edge was totally neglected and the data of Scofield below the upper edge (81.57 keV) extrapolated to 80.905 keV. The value of cross section so obtained is lower than the corresponding value of Storm and Israel (1970) by about 12%. The results except for Au at 80.905 keV were in agreement with values of Storm and Israel (1970) and Hubbell et al (1975, 1979). They have reported a steady fall in total attenuation cross sections at 80.905 keV with increase of μ. The disagreement at 80.905 keV is attributed to (1) the dilution of the transmitted intensity due to 79.623 keV photons and (2) effect of the finite level width of Au K-edge which falls between the doublets.
Ghosh and Das (1990) have measured total attenuation cross sections of several elements with Z=6 to 92 in the energy range 43 to 1330 keV mainly in the vicinity of the shell edges by using a NaI(Tl) detector in a good geometry set-up. The angle of acceptance for the scattered photon was 0.3°.

Umesh et al (1992) measured total attenuation cross sections of the oxides of rare-earth elements such as La, Ce, Pr, Nd, Sm, Gd, Dy, Ho and Er and also NaNO3 and NaNO2 in a narrow beam geometry set-up at 323 keV. The total attenuation cross section for oxygen was obtained as the difference in NaNO3 and NaNO2 cross sections. Using this, the total attenuation cross sections of the individual lanthanides were obtained with the aid of mixture rule. Photoeffect cross sections were derived from these values by subtracting the scattering contributions.

Gopinathan Nair et al (1994) have measured the total attenuation cross sections of several amino acids and several sugars using a high resolution hyper pure germanium detector in the energy range 30 to 1500 keV which is found to be most useful in medical and biological fields. Their studies indicate that the chemical structure of the compounds has little or no effect on the gamma ray attenuation coefficient in them and there exists a unique value of mass attenuation coefficient for all the compounds at each energy of interest.

Roy et al (1997) gives a complete analysis of the estimated photoelectric cross-sections from the measured total photon attenuation coefficients of several atoms (41 ≤ Z ≤ 92) at two photon energies, 43 and 59.5 keV. These energies fall close to K-absorption edges of some of the elements studied. Here they examine the role of using coherent scattering cross-sections derived from various sources such as the state-of-the-art precise theoretical calculations, commonly used form factor approximations and form factors with anomalous corrections in estimating the photoelectric cross-section. Comparison of theoretical and other available experimental results are also made with the measured and estimated values. It has been found that an overall change of 5% in the total mass attenuation is expected while using the precise coherent scattering cross-sections.

Cunhale Silva et al (2000) reports the application of an alternative methodology for the linear attenuation coefficient determination of irregular shape samples, in such a way that it is not necessary to know the sample thickness. Based on
this method, indigenous archaeological ceramic fragments from the region of Londrina, north of Parana State in Brazil, were studied. On the other hand, theoretical mass attenuation coefficient values were determined with the XCOM computer code. With the results obtained, it was concluded that the two media method works very well for the linear attenuation coefficient measurement of irregular-shaped ceramic samples, which makes it suitable, especially, for archaeometric studies.

Gagandeep et al (2000) reports the linear attenuation coefficients in aqueous solutions of three carbohydrates, glucose (\(C_6H_{12}O_6\)), maltose monohydrate (\(C_{12}H_{22}O_{11}H_2O\)), and sucrose (\(C_{12}H_{22}O_{11}\)). The values were determined at 81, 356, 511, 662, 1173, and 1332 keV by the gamma-ray transmission method in a good geometry set-up. From the precisely measured densities of these solutions, mass attenuation coefficients were then obtained that varied systematically with the corresponding changes in the concentrations (g/cm\(^3\)) of these solutions. The experimental results were used in terms of effective atomic numbers and electron densities. A comparison between experimental and theoretical values of attenuation coefficients has proven that the study has a potential application for the determination of attenuation coefficients of solid solutes from their solutions without obtaining them in pure crystalline form.

Gagandeep Kaur et al (2000) have reported the attenuation coefficients of aqueous solutions of alkali metal chlorides viz. LiCl, NaCl and KCl having different concentrations. These values have been determined at 81, 356, 511, 662, 1173 and 1332 keV gamma photons using narrow beam transmission method. The experimental results were analysed in terms of total cross sections, effective atomic numbers and electron density values of these solutions. In addition, molar extinction coefficients, interaction cross-sections and interaction radii for the solid solutes in aqueous solutions have also been calculated at these energies and concentrations. The mixture rule is applied to examine the compatibility of the results.

Materna et al (2000) have measured the X-ray attenuation coefficients of bismuth and of uranium in the regions of 40-240 and 70-240 keV, respectively, using a tunable hard X-ray source based on the linear electron accelerator at the University of Ghent. Results were compared with the semi-empirical values of Storm and Israel and to the theoretical values of Berger and Hubbell. They have also proposed a simple function for the attenuation coefficient in the vicinity of the K-edge for uranium and
in an extended range of energy for bismuth. The set-up of the source at Ghent is described and the future improvements are explained.

Measurements have been made by Abdel-Rahman et al (2000) to determine γ-rays attenuation coefficients very accurately by using an extremely narrow-collimated-beam transmission method. The effect of the sample thickness on the measured values of the mass attenuation coefficients (μ/ρ) cm²/g of perspex, bakelite, paraffin, Al, Cu, Pb and Hg have been investigated at three different γ-ray energies (59.54, 661.6 and 1332.5 keV). It was seen that for these chosen materials (μ/ρ) was in good agreement with the theoretical values up to 3 mean free paths and after that (μ/ρ) values for Cu, Pb and Hg decreased with a further increase in the absorber thickness. This result might be attributed to the increase in the number of coherent small-angle scattering photons, which reach the detector.

As it is inconvenient to use elements like hydrogen, carbon and oxygen in pure form for measurement of their gamma mass-attenuation coefficient, the measurements are to be done indirectly, by using compounds of the elements or a mixture of them. Teli et al (2000) have given a simple method of measuring the total mass-attenuation coefficients μ/ρ of the elements in a compound simultaneously and in a single experiment through the measurements of the μ/ρ values of the concerned compounds and using the mixture rule. The method was applied for the measurement of μ/ρ of hydrogen, carbon and oxygen by using acetone, ethanol and 1-propanol. Results (for E=0.123-1.33 MeV) were seen to be in better agreement with the theoretical values of Hubbell and Seltzer (1995).

Peele et al (2002) have outlined a precision measurement of the mass attenuation coefficients for air at various energies using two types of detectors and a simple test of detector response. They discuss whether sufficient accuracy could be obtained using these data to distinguish between competing theoretical estimates. In the process, they have investigated the intensity response of two common synchrotron X-ray detectors, a X-ray to optical charge-coupled device camera using a crystal scintillator and a X-ray sensitive photodiode.

Tran et al (2003) compared new experimental X-ray total mass attenuation coefficients of silicon obtained with the X-ray extended range technique (XERT) from 5 to 20 keV with theoretical calculations and earlier experimental measurements over 5 to 50 keV energy range. The accuracy of between 0.27% and 0.5% of the XERT data allows us to probe alternate atomic and solid state wave function
calculations and to test dominant scattering mechanisms. Discrepancies between experimental results and theoretical computations of the order of 5% are discussed in detail. No single theoretical computation is currently able to reproduce the experimental results over the entire 5 to 50 keV energy ranges investigated.

Prem Singh et al (2004) measured the K-L and K-M resonant Raman scattering (RRS) cross-sections for the first time at the 59.536 keV photon energy in the $^{70}\text{Yb}$ ($B_K=61.332$ keV), $^{71}\text{Lu}$ ($B_K=63.316$ keV) and $^{72}\text{Hf}$ ($B_K=65.345$ keV) elements; $B_K$ being the K-shell binding energy. The K-L and K-M RRS measurements have been performed at the 59° and 133° angles, respectively, to avoid interference of the Compton-scatter peak. The Rayleigh and Compton scattering cross-sections for the 59.536 keV γ-rays have also been measured at both the angles in the atomic region $Z=1$-92. Measurements were performed using the reflection-mode geometrical arrangements involving the $^{241}\text{Am}$ radioisotope as photon source and planar Si(Li) and HPGe detectors. Ratios of the K-M and K-L RRS cross-sections in Yb, Lu and Hf are in general lower than that of the fluorescent $K\beta_{1,3,5}$ (K-M) and $K\alpha$ (K-L) X-ray transition probabilities. Theoretical Rayleigh scattering cross-sections based on the modified form-factors (MFs) corrected for the anomalous scattering factors (ASFs) and the S-matrix calculations are on an average 15% and 6% higher, respectively, at the 133° angle and exhibit good agreement with the measured data at the 59° angle. Larger deviations 30% and 20%, respectively, are observed at the 133° angle for the $^{64}\text{Gd}$, $^{66}\text{Dy}$, $^{67}\text{Ho}$ and $^{70}\text{Yb}$ elements having the K-shell binding energy in the vicinity of the incident photon energy. The measured Compton scattering cross-sections are in general agreements with those calculated using the Klein–Nishina cross-sections and the incoherent scattering function.

Midgley (2005) has reported the X-ray linear attenuation coefficients measured for materials containing elements hydrogen to calcium. Characteristic X-rays with energies 32-66 keV were produced by X-ray fluorescence using a secondary target system, and 140 keV gamma rays were obtained from an unsealed $^{99m}\text{Tc}$ source. The photon beams were highly collimated and recorded using energy dispersive detection. A high-purity germanium detector was utilized to distinguish between measurements with $K\alpha$ and $K\beta$ characteristic X-rays and the gamma ray measurements used a sodium iodide detector. Samples were selected on the basis of their known composition and mass densities were measured using a pycnometer. The samples comprised six plastics, seven crystalline materials, three tissue substitute
materials, three liquids and six salt solutions. Their results have an uncertainty of less than 2% and were a few percent lower than values predicted by the tabulations.

1.4 Survey of theoretical studies on photoeffect cross sections

Exact theoretical analysis of the photoeffect is difficult and tedious. The final state wave functions, which are the solutions of the relativistic Dirac equation for outgoing electron, cannot be obtained in finite terms. The actual difficulty associated with the theoretical development is in the choice of wave functions of initial state and the final ejected photoelectron and the calculation of the matrix element. The theoretical developments can be divided into three energy regions (1) below 0.35 MeV (2) from 0.35 to 2 MeV and (iii) above 2 MeV. In the energy region from 0.35 to 2 MeV Hulme et al (1935) have carried out rigorous numerical calculations of K-shell photoeffect cross sections assuming that each K electron is independent of the other.

Heitler (1947) gave the relation for the K-shell photoeffect cross sections using non-relativistic quantum mechanics and the Born approximations and hydrogen like wave functions for the atomic electron. Sauter (1931a, 1931b) and Hulme (1931) have calculated photoeffect cross sections in the relativistic region where binding energies can be neglected using the Born approximation and relativistic wave functions for the atomic electrons. Neither Hulme's values nor values from Sauter's equations fit smoothly into the more accurate values of Hulme et al (1935) at high energies. However, the agreement is better if Stobbe's (1930) non-relativistic correction factor is considered in the Sauter's work.

Contribution from higher shells to the total cross section were accounted for by multiplying K-shell cross sections by $5/4$ and subsequent work has shown that the effective $Z$ approximation is poor. The numerical work of Hulme et al (1935) has been verified and the $5/4$ rule has been found to be fair enough only for high $Z$. Because of the restricted and approximate character of the theoretical results, the quantitative aspects of the photoeffect are largely empirical.

Gavrila (1959) has obtained expressions in non-relativistic limits and relativistic limits for the total and differential photoeffect cross sections, correct to first order in $\alpha Z$, assuming the contribution from K-shell electrons only. It agrees to zeroth order of Heitler (1947) and differs from the high-energy result of Hall (1936).
Pratt (1960) has used approximate Coulomb wave functions to obtain photoeffect cross sections from the K-shell of an atom of arbitrary charge in the limit of high energies. He obtained a term corresponding to the Stobbe correction factor and another term arising from the use of Coulomb, rather than plane wave functions. Pratt numerically evaluated his expression for the total cross section to within an accuracy of 0.1%. He also expanded the cross section in powers of $\alpha Z$ to obtain an approximate analytical formula incorporating the energy dependence of Gavrila's results to encompass the entire high-energy region.

Nagel (1960) was the first to deduce expression for the calculation of photoeffect cross sections applicable to all elements at all energies. He analysed the K-shell photoeffect, including all polarization effects, in a way which can serve as a convenient starting point both for approximate analytical treatment and exact numerical calculations. Using Sommerfield-Maue wave functions in order to surmount the difficulty of divergence that occurs in second order, when one applies Born approximation to the Coulomb potential, Nagel analysed the photoeffect in terms of four reaction amplitudes which describe the process completely. He explained these reaction amplitudes in terms of quantities, which correspond to absorption of definite electric or magnetic multipole components of the incident radiation.

Hultberg et al (1961) made numerical calculations using these expressions and reported the exhaustive data on K-shell cross sections in various elements.

Rakavy and Ron (1965, 1967) performed calculations using Thomas-Fermi and Fermi-Amaldi potentials and found that the differences between the two sets of cross sections are not more than 1.5% in general. Data calculated using the modified Fermi-Amaldi potential and the Thomas-Fermi potential for the heaviest atoms in the energy region 1-2000 keV are reported.

Schmickley and Pratt (1967) have calculated the total photoeffect cross sections for the K-shell through M-sub shells, assuming Coulomb, Thomas-Fermi, Kerner and Yukawa central potentials. The decrease in total cross sections was found to be expressible by means of a renormalization factor equal to the square of the ratio of screened to Coulomb bound state wave functions. The results are consistent with...
other earlier calculations and are at variance with the total cross sections of the K- and L- shells reported by Matese and Johnson (1965).

Hultberg et al (1958) and Brysk and Zerby (1968) have carried out the relativistic calculations treating the electrons as moving in a Coulomb field.

Brysk and Zerby (1968) have developed the computer code and obtained results for the Hartree-Slater model.

Storm and Israel (1970), Barfield et al (1972) and McGuire (1967) have also used the Hartree-Slater model for an extensive set of non-relativistic calculations.

Scofield (1973) has calculated the photoeffect cross sections for elements with Z=1-101 and for photon energies from 1 to 1500 keV. In the calculation, the electrons were treated relativistically and are assumed to be moving in the Hartree-Slater central potential both before and after the absorption of the photon. All the multipole contribution and retardation effects are included in the treatment of the radiation field. The Scofield’s cross sections are in good agreement with the values of Schmickley and Pratt (1967). Scofield has also provided correction factors for individual atomic sub shells for elements with atomic number from Z=2-54. Using these factors, the photoeffect cross sections can be renormalized so that they correspond to a relativistic Hartree-Fock model rather than the Hartree-Slater model used in the original calculation. Gerward (1993) has shown that there is a difference in the total photoeffect cross sections calculated using the above two models only below 50 keV and is of the order of 1 to 4%.

Pratt et al (1973) has reviewed the status on photoeffect for incident photon energies above 10 keV. In this review article, the theoretical development for the last two decades and the basic assumptions underlying the photoeffect calculations are described and pertinent atomic models are discussed.

Hubbell and Veigele (1976) have made a graphical comparison of calculated and experimental photoeffect cross sections as a function of photon energy 0.1 keV to 1.5 MeV for all elements Z=1-94. They have used the non-relativistic Hartree-Fock self consistent field (SCF) results of Veigele (1973), Henry et al (1972) over the range 0.1 and 8.0 keV for all elements Z=1-94 and the relativistic Hartree-Slater self consistent field results of Scofield over the range 1.0 keV to 1.5 MeV for all elements Z=1-101. They used the experimental data obtained by subtracting theoretically
calculated scattering cross sections from the measured total attenuation cross sections available in the literature. The differences between theoretical and experimental photoeffect data are found to be typically a factor of two from 0.1 to 1 keV, 5 to 10 percent from 5 keV up to energies ranging from 20 keV for carbon up to 500 keV for lead, above which the photoeffect cross section becomes fractionally too small to be accurately determined from the total attenuation cross sections.

1.5 Survey of experimental work on photoeffect cross sections

In the early experiments on photoeffect the ionization produced in the gas by the photoelectrons emitted was measured. Later during the years (1920-1935) the cloud chamber was the most frequently used instrument to study the photoeffect as it allowed a study of the number of photoelectrons emitted, shapes of their tracks and of their ranges in air. This method was inadequate because of poor statistics. Experiments in 1921 by Robinson, deBroglie and Simon in the X-ray region and Ellis in the gamma ray region finally established the existence of groups of photoelectrons with different energies for every photon of energy $h\nu$. Several experimental investigations on the photoeffect were carried out in the year's 1924-1931. A detailed account of the investigations carried out before 1928 are found in the comprehensive article by Kirchner (1930).

The availability of various types of gamma ray sources also made it possible to obtain more information on the photoeffect. The experimental determination of photoeffect cross sections can be classified into five important methods: (1) the direct method (2) the internal - external conversion method (3) X-ray fluorescence method (4) X-ray photoelectron coincidence method and (5) the indirect method.

1.5a The direct method

In this method, the photoelectrons produced in the sample material by the gamma rays are detected directly using either a beta ray spectrometer or a beta ray scintillation spectrometer. If a beta ray spectrometer is used the number of photoelectrons has to be integrated over all angles to get the total whereas in the case of scintillation spectrometer the total number of photoelectrons may be obtained over $4\pi$ geometry by making a through hole or well in the scintillator. The competing partial process, the incoherent scattering effect is to be corrected for in order to obtain the absolute number of photoelectrons. This is accomplished by making use of a pure
incoherent scatterer. But practically no pure incoherent scatterer is available. As such aluminum sample is used as a pure incoherent scatterer since the photoeffect cross section is negligible in the gamma ray region. So an aluminum sample having the same number of electrons as in the experimental sample is used to subtract the Compton contribution. The coherent scattering effect is very small if a through hole scintillator is used, because then the coherent scattering would be confined to the forward direction.

Davidson and Latyshev (1942) made one of the earliest measurements of the photoeffect cross sections using beta ray spectrometer. They have measured the photoeffect cross sections for 2.62 MeV gamma rays in lead, tantalum, silver and copper with an error of about 30%. They also studied the angular distribution of photoelectrons and the Z-dependence of photoeffect cross sections. They also measured the photoeffect cross section ratios for Cu, Ag, Ta and Pa, which are in good agreement with the theoretical values of Schmickley and Pratt (1967). Later Hedgran (1952), Hedgran and Hultberg (1954) and Hultberg (1955) improved the beta ray spectrometer methods. In order to obtain the true angular distribution the experimental curves were corrected for geometrical distortion and multiple scattering in the sample foil. The angular distributions were measured and the cross section ratios for the various sub shells were estimated.

Hultberg (1959), Marty (1952), Bergkervisk (1964), Boyd et al (1965), Jansen et al (1962), Herrlander et al (1960), Ryde and Sujkowski (1962), Frey et al (1963), Sujkowski (1961), Grigoryev and Zolotavin (1959) have measured the different shell and sub shell cross section ratios using the high resolution beta ray spectrometers at different energies. Their measurements are mainly restricted to heavier atoms.

Titus (1959, 1965) was the first to use the plastic scintillator in the determination of photoeffect cross sections. He used a through hole plastic scintillator of 5/8 inch diameter and 3/2 inch in length with an axial hole 5/32 inch in diameter in which the experimental sample was placed and irradiated by highly collimated gamma rays of energy 661.6 keV and 2.62 MeV. The scintillator was coupled to a photomultiplier through a Lucite light guide 6 inch long and the pulses were counted in the usual way. To correct for incoherent scattering, an equivalent aluminum was used in an auxiliary experiment. The cross sections were estimated for copper, molybdenum, silver, tantalum and gold. The data of Titus were consistently below the
theoretical values of Schmickley and Pratt (1967). Subsequently Parthasaradhi et al (1964a, 1964b, 1965, 1966) employed this method at lower energies. They have used the plastic scintillator of 1 inch diameter, 1/8 inch thickness having a well of 1/16 inch depth and 3/8 inch diameter and measured the photoeffect cross sections in copper, silver, tin, tantalum, platinum and lead for 145, 320 and 661.6 keV gamma rays. The errors are as high as 10% and also there is a wide discrepancy in the cross sections of high Z materials between the measured values and the theoretical values of Schmickley and Pratt (1967).

Ramakrishana Gowda, and Sanjeevaiah (1973a, 1973b, 1974a, 1974b, 1974c, 1975) and Ranganthaiah et al (1977) have employed a well type plastic scintillator to measure the total and K-shell photoeffect cross sections in Al, Cu, Zr, Ag, Sn, Ta, Au and Pb for 145, 279, 323, 412 and 661.6 keV gamma rays. They used aluminum as the pure Compton scatterer for subtracting the unresolved Compton electrons to obtain the resolved photoelectron spectrum. A gaussian was fitted to the main photoelectron peak to estimate the K-shell cross sections. The errors mainly due to subtraction are of the order of 4 to 6%. Their results are in fairly good agreement with the theoretical values of Schmickley (1967) and Scofield (1973).

The photoeffect cross sections of 279.1 and 661.6 keV gamma rays in Y, Ce, Dy and Yb was measured by Manna and Visweswara Rao (1985) using a well type plastic scintillator. The experimental values were found to be more or less in agreement with the interpolated theoretical values of Storm and Israel (1970) and of Scofield (1973) and with the values of Veigele (1971) which were mostly based on previous experimental results.

1.5b The internal-external conversion method

The internal-external conversion method like the direct method involves the detection of photoelectrons emitted but is restricted to some special cases where the source emits both conversion electrons and gamma rays. Hultberg and Stockendal (1958) and Hultberg (1959) first established this method using a beta ray spectrometer. By measuring the conversion electron and photoelectron spectra and using the internal conversion coefficients, the photoeffect cross sections are determined by comparing the intensities of the two. If the instrument provides the
necessary resolution, it is also possible to determine the different shell and sub shell photoeffect cross sections by this method.

Hultberg and Stockendal (1959), Bleeker et al (1962) and Boyd et al (1965) have used the high-resolution beta ray spectrometers and determined the photoeffect cross sections. The values of Hultberg and Stockendal, and Bleeker et al are too high for the predicted values of Schmickley and Pratt (1967) and also for the values of Scofield (1973). Boyd et al determined the L-sub shell photoeffect cross sections of 122 keV photons in uranium with iron free magnetic spectrometer.

Raja Rao et al (1968, 1969) has also measured the photoeffect cross sections at 662 keV and 279 keV in copper, cadmium and tantalum. The errors on these are about 10%. Hager and Seltzer (1968) and Raman et al (1972) have also estimated the absolute photoeffect cross sections using the calculated internal conversion coefficients of Sliv and Band (1956).

1.5c X-Ray fluorescence method

This method involves the measurement of X-ray intensity following the photoelectron emission for known photon intensity. The X-ray emission following the photoelectron emission is assumed to be isotropic. After correcting for the fluorescence yield and interfering effects due to scattering etc., the intensity of X-rays is integrated over the total solid angle.

This X-ray fluorescence method has been used extensively by Dilazzaro and Missoni (1965), Oberai et al (1965), Ghumman et al (1967, 1968), Sahota (1970) but the accuracy attained in all these experiments is rather poor. The K-shell, L-shell and higher shell photoeffect cross sections have been measured in various elements by Singh and Sood (1971, 1972), Allawadhi and Sood (1975), Allawadhi et al (1973, 1976, 1977, 1978) using X-rays in the energy range 18 to 74 keV as well as gamma rays of energy 84, 145 and 279 keV. A fairly good agreement within the experimental uncertainties is obtained with calculated values of Schmickley and Pratt (1967) except in a very few cases. The L-shell cross sections at 32.8 keV were found to be higher than the theoretical values.

1.5d X-Ray photoelectron coincidence method

Seeman (1956) has measured the K-shell photoeffect cross sections of lead using annihilation radiation (0.511 MeV) from the positron source $^{22}$Na. A
coincidence technique was used in conjunction with the K-X-rays that follow the emission of K-shell electrons. The measured cross sections were found to be higher than the values of Schmickley and Pratt (1967).

Ranganathaiah et al (1978, 1979) have used the fast-slow coincidence technique for the measurement of K-shell photoeffect cross sections in Sn, Ta, Au, Pb, Bi, Th and U at 515, 661, 840, 960, 1110, 1117 and 1330 keV gamma rays. They have used a thin beryllium window NaI(Tl) detector as an X-ray detector and a plastic scintillator as an electron detector. A fairly good agreement with the latest theoretical values of Scofield (1973) was reported in all the cases.

1.5e The indirect method (subtraction technique)

This method involves the measurement of the total attenuation cross sections in a good geometry set up and then subtracting the contribution of all other partial interfering processes such as the coherent and incoherent scattering. The scattering cross sections are calculated from the theoretically computed tables (Veigele 1973, Hubbell et al 1975, Hubbell and Overbo1979, Hubbell 1982) using form factors and incoherent scattering functions. The photoeffect process is dominant at low photon energies compared to other photon interactions. The scattering cross sections, below 100 keV, in all elements except for very low Z elements are usually less than 10% of the total cross sections. The estimation of photoeffect cross section by subtracting the scattering cross sections from the measured total attenuation cross sections is therefore justified at energies below 100 keV as it does not impair the over all accuracy to be obtained. At energies greater than 100 keV and less than 300 keV, the photoeffect more or less matches the scattering contribution. Hence this method can be effectively used upto 300 keV. But as the energy increases (beyond 300 keV), the scattering contribution dominates and this method fails to yield accurate values.

In a narrow beam collimation experiment, the total attenuation cross sections can be determined to an accuracy of less than one percent. Therefore, the photoeffect cross section can be estimated to the same accuracy in the region where the scattering cross sections are known very accurately and are of smaller magnitude. The photoeffect cross sections so estimated are in good agreement with the theoretical values but as the K shell threshold is reached, the disagreement becomes as high as about 10% or even more.
Millar and Greening (1974) have estimated the photoeffect cross sections for C, N, F, Ne, Mg, Al, S, Cl and Ar by a curve fitting method from the measured total attenuation cross sections of CO, N, O, CF, Ne, H S, HCl, Ar, air, Mg, Al, SiO and (C H) PO in the energy range from 4.5 to 25.2 keV using Bremsstrahlung radiation from X-ray tubes.

Parthasaradhi and Hansen (1974) have also estimated the photoeffect cross sections for the elements Al, V, Cu, Mo, Ag, Sn, Ta, Au and Pb in the energy range from 5 to 160 keV using radioactive isotopes as sources of photons.

Nageswara Rao et al (1984) have measured the photon attenuation cross sections in 18 elements and 29 compounds for gamma energies in the energy range 30-660 keV. They report the atomic photoeffect cross sections in medium and high Z elements in energy range 30-280 keV and are compared with the theoretical values.

Parthasaradhi (1985), Dattatreya Reddy et al (1985) have reported the photoeffect cross sections around K-edges in certain elements derived from the attenuation cross sections of suitable elements and compounds by subtracting the coherent and incoherent scattering cross sections as well as other elemental cross sections in the cases of compounds. They report satisfactory agreement of their experimental values with the theoretical cross sections of Storm and Israel (1970) and Scofield (1973).

Photoeffect cross sections for Cd and In at 22.2, 59.6 and 88.8 keV was reported by Prasad (1985), Machali et al (1979, 1981, 1987) have reported the cross sections of gamma rays in the energy range 43 to 152 keV, 187 to 662 keV for elements Al, Cu, Zn, Ag, Pt, Au and Pb. They show agreement between experimental values and the available theoretical data.

Rao et al (1981) has measured the photoeffect cross sections for X-ray photons in low and medium Z elements.

Gerward (1989) measured the atomic photoeffect cross sections for Be, C, Si and Cu from 5 to 20 keV. Systematic results in their experimental values suggest that the Scofield theoretical values with and without the Hartree-Slater to Hartree-Fock renormalization can be used as lower and upper limits of the experimental photoeffect cross sections.
Anasuya et al (1994), Shylaja Kumari et al (1994), Channegowda et al (1995) have used new methods to determine coherent, incoherent and photoeffect cross sections of elements by measuring the total attenuation cross sections of their mixtures, keeping them at two different positions using a well type NaI(Tl) detector. The salient feature of this method is that it does not depend on any theoretical assumptions or values. First the sample is kept outside the detector (narrow beam geometry) in such a way that no scattered photons enter in to the detector. Next the sample is kept inside the well of the detector (4π geometry) in such a way that almost all the scattered photons enter into the detector. The attenuation cross section measured at first position contains contributions due to all possible types of interactions at the energy of interest, where as at the second position it contains contributions only due to photoeffect. This idea was used in their measurements.

Basavaraju and Kane (1994) have determined differential cross sections using high-purity germanium detector for the elastic scattering of 81-keV gamma rays by aluminum, nickel, tantalum, gold, and lead through angles of 60°, 90°, 120° and 133°. The atomic Rayleigh scattering amplitudes were obtained in the independent-particle approximation by calculations of modified relativistic form factors (MF's), a combination of MF's and angle-independent `anomalous' scattering factors (ASF's), and the relativistic second-order S matrix. Most experimental cross sections for gold and lead are found to be slightly smaller than the calculations in the S matrix or the MF-ASF approaches, the differences being larger in the latter case. The calculated cross sections based on MF's are enormously larger than these values. The tantalum data are in good agreement with S-matrix calculations. The data for Al show agreement with the different calculations, which differ by less than about 6%.

Ömer Sögüt (2002) have reported the total atomic photoelectric cross-sections and total atomic attenuation cross-sections in the atomic range 22 ≤ Z ≤ 58 for 59.5 keV photons by using a Si(Li) solid state detector. Experimental results have been compared with the theoretical values.

1.6 Survey of theoretical studies on the anomalous scattering factors (dispersion corrections to the forward Rayleigh scattering amplitudes)

Photons both X-rays and gamma rays, are produced during electronic and nuclear transitions respectively. X-rays were discovered by Röntgen in 1895 where as gamma rays were discovered by Villard in 1900. When a photon interacts with an
atom several absorption and scattering process may occur. The primary interactions of photoabsorption, scattering, diffraction and reflection of the low energy photons can be effectively described by using the atomic scattering factor. Atomic scattering factor is a measure of the amplitude of radiation scattered by an atom when radiation of the given amplitude falls upon it. It is expressed in terms of the amplitude scattered by a single classical electron under the same conditions by an electron scattering according to Thomson formula.

Max Von Laue (1912) introduced it formally into his equations while studying X-ray diffraction and Darwin used it in his early papers, and indicated clearly that it must depend on the spatial arrangement of the electrons in atom.

W. L. Bragg and W. H. Bragg (1912) took the amplitude scattered by an atom as proportional to the atomic weight, but Sir William Bragg in his Bakerian lecture of (1915) expressed clearly the importance of taking into account the effect of the distribution of electrons over the region whose dimensions are comparable with the wavelength of the radiation employed.

Debye (1915) pointed out that atoms irregularly arranged, as in a gas, must still produce diffraction effects with X-rays, because of grouping of the electrons which are responsible for the scattering about the atomic nuclei. In a very important paper, which laid the foundations of subsequent work on the scattering of X-rays by gases, he showed how to calculate the scattering factor with certain assumptions regarding the electronic arrangements.

Compton (1917) calculated the scattering factors for certain simple configurations of electrons, and used them to estimate the dimensions of the atoms in calcite and rock salt by comparison of observed and calculated intensities of spectra. Debye and Scherrer also made similar estimates in (1918). In all their work the scattering of X-rays by the electrons were based on the classical theory but it was unsatisfactory. Existence of the diffraction of X-rays by crystals showed definitely that coherent radiation forms an important part of the total scattering. Older quantum theory provided no means of calculating the scattering of coherent radiation by electrons.

Kramers and Heisenberg (1925) first gave the quantum dispersion formula on the basis of the correspondence principle. It was first obtained in terms of the
concepts of wave mechanics by Schrödinger (1926) and was extended to include X-ray frequencies by Ivan Waller (1927).

Waller (1927) derived a general formula for the dispersion of X-rays in atoms on the basis of a non-relativistic quantum mechanical radiation theory. This formula accounts for the coherent and incoherent scattering of X-rays by atoms. Here, however, we are concerned with the coherent scattering. Waller's formula includes retardation effects and differs therefore from Kramers and Heisenberg's dispersion formula which had been derived by application of the correspondence principle to the classical dispersion formula (Ramasheshan and Abrahams 1975). Retardation effects are of importance for X-rays, because the wavelengths of X-rays are of the same order as the spatial extensions of atoms. Several authors have solved Waller's dispersion formula by different theoretical methods.

Anomalous scattering of photons arises due to binding of electron to the atom and it is defined as the difference between the actual electronic Rayleigh scattering and the classical free-electron Thomson value. One can express the anomalous scattering factors or dispersion corrections in the forward direction through the relation

\[ f(E) = f_0 + f'(E) + if^*(E) \]  

\[ (1.5) \]

where \( f(E) \) is the scattering factor, \( f_0 \) is form factor, \( f'(E) \) and \( f^*(E) \) are called real and imaginary part of the anomalous scattering factor. The quantity \( (f(E) - f_0) \) is called anomalous scattering factor. Anomalous scattering of photons arises due to electron binding effects to the atom. The form factor \( f_0 \) represents Thomson's classical free electron value for scattering factor.

The first papers on the evaluation of dispersion corrections were published by Hönl (1933a, b). Hönl evaluated Waller's dispersion formula by means of hydrogen-like eigen functions in a non-relativistic approach. He calculated the matrix elements for the transition probabilities, which are contained in the oscillator strengths on the photoelectric absorption cross sections by means of hydrogen-like eigen functions. He expanded these matrix elements into electromagnetic multipole transitions and so obtained the angular dependence of \( f' \) and \( f^* \) as well. The calculations gave good results for medium energy X-rays and elements of relatively low atomic numbers. Under these circumstances mainly the electrons in the K-shell cause dispersion effects.
and one therefore needs only fairly good estimates for the contributions of the electrons in the higher atomic shells. For this particular case hydrogen-like eigenfunctions are a good enough approximation. This, however, does not hold for elements with high atomic numbers, because then the outer shells contribute substantially to the dispersion corrections. Hönl's approach gives the angular dependence of the dispersion corrections. The initial calculations have been restricted to the electrons of the K-shell only.

An extension to other electron shells and numerical computations have been carried out by Eisenlohr and Müller (1954). Guttman and Wagenfeld (1966), Wagenfeld, Guttman and Kühn (1973) and Williams (1934).

Parratt and Hempstead (1954) and Cromer and Libermann (1970) have used other methods. The calculations made by the other authors apply to pure forward scattering only. The equivalence of the quantum mechanical and the classical theories of X-rays led Parratt and Hempstead (1954) to develop a semi-emperical approach described by a power law to the problem. The angular dependence of the dispersion corrections were calculated. The necessity of including the anomalous effects of more than one shell of electrons is pointed out with the correlative conclusion that there is practically no region of normal X-ray dispersion. Damping has been retained, its effect evaluated and shown to be negligible except close to the edge. With damping neglected, universal dispersion curves were given from which one can readily deduce the atomic scattering factor.

Levinger et al (1957) have proposed relativistic corrections to the Dipole sum rule to evaluate $f'$. They have calculated the summed oscillator strengths to the order of $(v/c)^2$ for a Dirac electron in a central force field. The suggested corrections to $f'$ were due to retardation and relativistic effects for the core electrons. They have obtained the value for relativistic multipole corrections with retardation effects as $({E_{tot}/mc})^2$.

Cromer (1965) attempted to re-evaluate the dispersion corrections using Parratt and Hempstead's theory and concluded that the measured values of the mass absorption coefficient were unreliable to be used in his calculations. Cromer determined the absorption cross sections at the absorption edge by means of the sum rule of Thomas, Reiche and Kühn. This can be done in the following manner. $\sigma(\omega)$ is
directly proportional to the continuum part of the oscillator strengths for a certain electron. In order to obtain the oscillator strengths for the discrete spectrum, one has to calculate all possible and finite transition probabilities within the discrete spectrum. Cromer used for this calculation, self consistent field relativistic Slater-Dirac wave functions. An uncertainty still remains within these calculations which is based on the Parratt and Hempstead’s theory but the numerical results show in some cases good agreement with experimental data.

Cromer and Liberman (1970) have carried out calculations for $f'$ and $f^*$ pointing out the basic flaw in using the power law which is an approximation concerning the variation of the photoelectric absorption coefficient with energy. They used for the calculations of the oscillator densities the results of photoelectric absorption calculations of Brysk and Zerby (1968) which are based on the relativistic Dirac-Slater wave functions. They obtained the relativistic self energy correction term $5/3(E_{tot}/mc^2)$ for $f'$ in the dipole approximation.

Jensen (1979) has pointed out that for high values of photon energies there is an additional energy dependent, magnetic term $-\langle 1/2 \rangle Z^2 \omega mc^2$ in addition to Cromer and Liberman’s relativistic dipole correction term to be considered to calculate $f'$. It corresponds to scattering from the magnetic moments of the electrons. The theoretical objections have been made by Creagh (1984), Smith (1987) and Sasaki (1989) about the Jensen’s correction due to magnetic scattering and shown that it is negligible when higher order multipolar expansions and retardation are considered and the total self-energy correction becomes $(E_{tot}/mc^2)$ rather than $5/3(E_{tot}/mc^2)$.

Kissel et al (1980) have developed a computer program based on the second order scattering matrix formalism suggested by Brown et al (1955) to predict accurately the total atom Rayleigh scattering amplitudes. Their model treats the elastic scattering as the sum of bound electron, nuclear and Delbrück scattering cross sections and treats the Rayleigh scattering by considering second order single electron transitions from electrons bound in a relativistic self-consistent central potential. This potential was Dirac Hartee Fock Slater potential and exchange was included by use of the Kohn and Sham exchange model. They have omitted radiative corrections.

Kissel et al (1980) have developed a computer program for accurate evaluation of the total-atom Rayleigh scattering amplitude using the relativistic
second order S-matrix of quantum electrodynamics. The S-matrix formalism is considered to be the most rigorous of all the available methods. In practice, the contributions from inner shell electrons are calculated using S-matrix formalism while those of the outer shells are evaluated using form factor approximations.

The S-matrix prediction represents the state-of-the-art calculations for atomic scattering of low energy X-rays. The amplitude for elastic scattering of a photon is obtained from a specified atomic sub-shell, within the framework of external field quantum electrodynamics and a description of independent bound atomic electron states in a relativistic self consistent central potential. The S-matrix approach is based on Furry's extension of the Feynman-Dyson formulation of quantum electrodynamics, in which the interaction of electrons and positrons with the atomic field is included in the unperturbed Hamiltonian.

Sasaki (1989) has given extensive tabulations of anomalous scattering factors close to the K- and L-absorption edges which cover the wavelength range of synchrotron radiation using the relativistic treatment described by Cromer and Libermann (1970), neglecting Jensen's correction term on the magnetic scattering.

Smith (1987) as well as Creagh and McAuley (1992) have pointed out that in the non-relativistic dispersion analysis values of $f'$ lie above the direct interferometric measurements and as calculated from attenuation measurements indicating the expected relativistic reduction. The effect is clearly overestimated by the dipole only approximation. Inclusion of retardation and higher multipole terms $(E_{tot}/mc^2)$ in dispersion analysis resolves reported conflicts between values of the anomalous scattering factor as measured interferometrically and as calculated from attenuation measurements. Relativistic term is important for a dispersion analysis even when calculating scattering factors for soft X-rays. While relativistic effects are negligible in absorption process at these low energies, they contribute to the dispersion, which involves the sum of virtual processes at all energies, including those involving relativistic core states.

Wang and Pratt (1983) as well as Wang (1986) have pointed out that, in both theoretical and experimental studies, it was assumed that the contribution to $f'$ from allowed bound-bound transitions in $f^*$ is small and may be neglected. This approach is generally acceptable as long as the photon energy is sufficiently far away from the
resonance which occurs at the bound-bound transition energies. For heavy elements the bound-bound contribution is important only within a very small energy interval, compared with the magnitude of the resonance energy, around the position of resonance. At least for isolated atoms, this is not the case for light elements—particularly for Z<10 and the omission of the bound-bound contribution may lead to significant errors both below and above the edge. One reason for this different behavior for light elements is that there are less electrons to scatter off, so the bound-bound contribution to the scattering amplitude becomes relatively more important. Contribution due to bound-bound transitions in the dispersion calculation reduces the total amplitude below the edge and enhances the total amplitude above the K-edge. The effect on the real part of the anomalous scattering is more prominent. A 5% contribution to \( f' \) can be seen for photon energies as high as three times the K-threshold. On the other hand, the bound-bound contribution in heavy neutral atoms in their ground state always involves a virtual transition to a higher quantum state. Such oscillator strengths are smaller than for a transition between low quantum state, and so for this reason also the bound-bound contribution is relatively unimportant for heavy elements.

Kissel and Pratt (1990) have suggested a \( Z \) dependent, energy independent correction term to the high-energy limit based on the S-matrix calculations. They have also given a correction term that is to be added to Cromer-Liberman's values to get the appropriate value of \( f' \). The predicted values of dispersion corrections are commensurate with those of Creagh and McAuley's relativistic multipole correction term for very low \( Z \) elements and are different by about 6% to 7% for \( Z>20 \).

Zhou et al (1992) have studied the effect of many-electron correlation on anomalous scattering factors in Rayleigh scattering, in the case of the Ar atom, using dispersion relations and the relativistic random-phase approximation (RRPA). The correlation effect changes the Ar 3s-subshell photoionization cross sections significantly compared with the corresponding independent-particle approximation calculations; thereby the anomalous scattering factors of Rayleigh scattering from this sub-shell also experience marked structural changes. But the Ar 3p sub-shells dominate the coherent total-atom scattering amplitude so that sub-shell structural changes in the Ar 3s sub-shell due to many-electron correlation effects are not seen in the total-atom scattering cross section or the total-atom anomalous scattering factors,
which are the physical observable in Rayleigh-scattering experiments. One anticipates this outcome generally for closed-shell atoms, while in the case of open shells one can anticipate a greater importance for the many-electron-correlation effects.

Chantler (1995) has provided extensive tabulations of theoretical form factor, attenuation and scattering data for elements of $Z=1$ to 92 from $E=1$-10 eV to $E=0.4$-1 MeV. Here, the primary interactions of X-rays with isolated atoms are described and computed within the self-consistent Dirac-Hartee-Fock framework. Form factors are evaluated with the inclusion of relativistic multipole correction term ($E_{tot}/mc^2$). The S-matrix channels of nuclear photoeffect (dipole resonance), nuclear pair production, electron pair production, Delbrück scattering and other smaller effects are typically neglected, providing upper limits in energy for the validity of these syntheses.

Kissel et al (1995) have discussed the validity of form-factor, modified form-factor and anomalous scattering factor in predictions of elastic photon-atom scattering and assessed with the aid of the state-of-the-art numerical calculation of Rayleigh scattering obtained using the second-order S-matrix theory, in the photon energy range from 100 eV to 1 MeV. In general, relativistic form factor (RF) and relativistic modified form factor (MF) are high-photon-energy and small-momentum-transfer approximations. They provide good predictions of small-angle differential cross sections for photon energies above the K-shell photoeffect threshold, while they fail at all angles for photon energies below the K-threshold and at large angles for photon energies well above the K-threshold for high-Z elements.

Both RF and MF can provide good predictions for the angle-integrated cross section above the K-threshold but not below. The MF value in the forward direction is very close to the correct high-energy limit of the forward-angle-Rayleigh scattering amplitude. The importance of bound-bound contributions and the angle dependence of the anomalous scattering factors were discussed. With starting point as the many-body elastic scattering amplitude, a detailed discussion is presented of the partitioning of the elastic scattering amplitude into Rayleigh and Delbrück scattering components. This partion of the optical theorem reveals contributions from bound-bound atomic transitions, bound pair annihilation and bound pair production that are not usually associated with elastic scattering. Numerical S-matrix calculations appear at forward angles approaches the relativistic modified form factor at high energy.
Cullen et al (1997) have provided a photon data library (EPDL97) which is available from IAEA on a CD-ROM. This library includes photon interaction data for all elements with atomic number between 1-100 over 1eV to 100 GeV. \( f' \) and \( f'' \) values have also been provided. The relativistic correction term used was the one calculated by Kissel and Pratt (1995).

Roy et al (1999) have discussed the photon scattering from bound electrons of atoms with special emphasis to Rayleigh scattering. General features of the many-body scattering amplitude and its partitioning into Rayleigh and Delbrück (and nuclear) single-electron transition scattering amplitudes are examined. The use of the state-of-the-art precise second-order S-matrix calculations of Rayleigh scattering in terms of single-electron transition-amplitudes has led to significant progress in the understanding of the scattering process. The importance of relativistic, higher multipole, and bound-bound contributions in calculating anomalous scattering factor deviations from form factor amplitudes must be emphasized. Accurate interpolation of cross sections in the three-dimensional space of scattering angle, photon energy, and atomic number, utilizing the available published S-matrix data, has permitted extensive tabulation of differential scattering cross sections. S-matrix results may be compared with experiments to assess their validity; they may be compared with simpler but more approximate approaches, to identify the extent of the utility of such approaches and to develop simpler prescription schemes, which can give results comparable to the S-matrix results. In spite of their many successes, the present second order S-matrix methods also have limitations and shortcomings, observed in certain recent experiments. The explanation of these experiments in terms of a composite theory, which also incorporates non-local exchange and correlation effects, is provided along with a discussion of other future issues.

Kissel (2000) has provided systematic tabulated the differential scattering cross sections for all atoms for photon energies 0.0543–2754.1 keV in various approximations with a focus on the S-matrix approach of Kissel and Pratt. New tabulations are also being made available of (anomalous scattering factors for 0-10 MeV) total-atom, shell and sub shell form factors; bound-bound oscillator strengths total-atom, shell and sub shell photoeffect cross sections, and Dirac-Slater potentials. Accurate interpolation of S-matrix cross sections to intermediate energies has also...
been investigated. Selected computer codes that generate or use these data are described.

Chantler (2000) addresses the key discrepancies arising due to the smoothening of edge structure, the use of non-relativistic wave functions, and the lack of appropriate convergence of wave functions and derives new theoretical results of substantially higher accuracy in near-edge soft X-ray regions. The high-energy limitations of such an approach have also been illustrated. The energy range covered is 0.1 to 10 keV. It is observed that discrepancies of the order of 200% exist among currently used theoretical approaches for numerous elements from 1 to 3 keV X-ray energies. The associated figures and tabulation demonstrate the comparison with an alternate theory and with available experimental data. It is concluded in this paper that, in general, experimental data are not accurate enough to establish the errors and inadequacies of theory. It is opined that new developments in experimental measurement hold great promise in making critical comparisons with theory in the near future.

1.7 Survey of experimental work on the anomalous scattering factors (Dispersion correction to the forward Rayleigh scattering amplitudes)

On the experimental side it can be noticed that different techniques have been employed to determine the anomalous scattering factors ($f'$ and $f''$). Among those there are two important techniques, namely

a) Interferometer technique  b) Attenuation coefficient technique

1.7a Interferometer technique

X-ray interferometer techniques are used extensively for the measurement of the refractive index of materials and hence to evaluate $f'$ and $f''$. All the interferometers are transmission geometry type and initially they were used to measure the X-ray refractive indices by means of phase shifts of certain materials, which is directly related to the real part of the atomic scattering factor, using the characteristic radiation emitted by sealed X-ray tubes. There are basically two different types of interferometer used for these measurements. The first type is LLL type interferometer and the second type is Angstrom ruler interferometer.

The first LLL (Laue-Laue-Laue) type X-ray interferometer invented by Bonse and Hart (1965) allowed a new approach to the measurement of X-ray refractive
indices. It was manufactured from a monolithic boule of perfect single crystal silicon, which is machined to produce three rigid wafers linked at the base. The thickness of each wafer is adjusted to ensure that the intensity in the Laue diffracted beam is comparable with that of the forward transmitted beam. The second wafer further diffracts these two beams which emerge from the first wafer. These beams proceed towards the second wafer where they undergo further Laue diffraction. Two of these phase coherent beams converge towards the third wafer where they interfere with one another. It is the position of this standing wave pattern with respect to the third wafer, which determines the contrast in the beams, which emerge from the third wafer. The insertion of objects in one of these beams causes a shift in the position of the standing wave pattern with respect to the Bragg planes of the third wafer and hence a change of contrast in the beams which emerge from the interferometer. This phase shift is related directly to the X-ray refractive index, which in turn is related to the dispersion corrections. Although a variety of materials have been studied, these have been restricted mainly to alkali halides at some characteristic wavelengths.

Bonse and Hellkötter (1969) determined $f'$ using a prism shaped specimen. Creagh and Hart (1970) made measurements using parallel-sided specimens. By using parallel sided specimen they were able to eliminate the effect of specimen absorption on the measurement and hence could give values for the real part of the X-ray dispersion correction. Bonse has extended this technique. The values are in reasonable agreement with Hönl's theory.

Bonse and Hartmann-Lotsch (1984) made a direct measurement of the energy dependence of the atomic scattering factor $f'(E)$ near absorption edges using X-ray interferometer. $f'(E)$ may be determined at identical specimen position either from the contrast of measured interference fringes or by measuring the absorption of a noninterfering beam. Measured $f'(E)$ values complemented by extrapolated values obtained from the literature were transformed to $f'(E)$ by using the Kramers-Kronig transform for Co, Ni and Cu near their K-edge.

Creagh (1980) pointed out that a major source of inaccuracy in the LLL type interferometric technique is associated with the precision to which fringe shifts can be measured. It is difficult to measure fringe shifts to a precision of better than 0.2%, which implies that the error in $(Z+f')$ is of the same order. Thus, the precision
attainable using this technique is not high. One can not discriminate among the relativistic and non-relativistic theories with such an interferometer.

The second type of interferometer called Ångström ruler interferometer, (Hart 1968), offers a significant improvement in the precision to which $f'$ can be measured. This interferometer is similar to the first interferometer except that it is fabricated such that the third wafer can be moved with respect to the standing wave field. Shifts in phase are monitored using counter techniques. When the third wafer is moved a cosinusoidal variation in intensity be observed. If the object is placed in one beam, the position of the standing wave field with respect to the wafers is changed. Further motion of the third wafer establishes the new position of the standing wave field and the phase shift can be directly measured.

Cusatis and Hart (1975, 1977) used this technique to determine $f'$ for zirconium in the region of its K-edge. Siddons and Hart (1979) repeated the experiments using niobium and molybdenum foils to an accuracy of about 1%. Buras & Tazzari (1985) made measurements of $f'(0, 0)$ using Ångström ruler interferometer with solid state detector. This type of interferometer enables direct measurements of the refractive index and the linear attenuation coefficient.

For Ångström ruler type interferometric measurements specimens usually have to be small and very thin for measurements near an absorption edge. There are difficulties with the measurements of specimen thickness, with homogeneity and with surface finish for the specimen and also with the device stability. Absorption of the primary beam by the interferometer limits the maximum wavelengths, which can be used. Pendellösung effects in the beams and small lattice twists can also cause problems to the experimentalists.

Despite the fact that the X-ray dispersion corrections are extensively used in X-ray diffraction studies, very few reliable measurements have been made. The few laboratories capable of making X-ray interferometer measurements are producing data very slowly. However, the results, which have been forthcoming from these experiments, do not support the contention that the relativistic theory gives a better description of the X-ray scattering process than the non-relativistic theory.

One could say in general that the interferometer experiments have been successful at measuring X-ray refractive indices very precisely. However, the
refractive index as measured is related to the real part of the structure factor \( (f_0 + f') \). The error in the structure factor measurement becomes the error in the computed dispersion correction. Also, the value of \( f_0 \) can be in error if the thermal parameters are not well defined, and this adds to the probable error in \( f'(E) \). The interferometer technique has not yet provided the accurate measurements of \( f'(E) \) which X-ray crystallographers require to resolve their experimental data.

Determination of \( f'(\omega, \Delta) \), where \( \Delta \) is called scattering wave vector, is based on measurement of the geometrical structure factors. The dynamical theory of X-ray diffraction (Pendellösung technique and measurement of reflectivity of perfect crystals in Laue-or Bragg-reflection) and Friedel- and Bijvoet-pair techniques have been employed.

Ewald (1916) showed that there is an interchange in energy between the transmitted and the reflected beam propagating in a crystal structure. This phenomenon is known as Pendellösung. The first observation of Pendellösung was by Kato and Lang (1959) in perfect crystals of silicon. The intensity of the wavefield, which results from the interference of the incident and diffracted beam (i.e., the period of the standing wave pattern), is related to the geometrical structure factor. If a crystalline defect exists, the periodicity of the Pendellösung fringe is modified. Aldred & Hart (1973a,b) measured the atomic scattering factor \( f(\omega, \Delta) \) using Pendellösung technique for Silicon. From these data, Price et al (1978) was able to refine values of \( f'(\omega, \Delta) \) for a number of photons. Deutsch & Hart (1985) were able to extend the determination of the form factor to higher values of momentum transfer. The success of this technique depends upon the availability of large, strain-free crystals, which limits the range of materials, which can be investigated.

A number of experiments have attempted to measure Pendellösung fringes for parallel-sided specimens illuminated by white radiation. Takama et al (1980) have studied silicon, Takama & Sato (1982) have studied copper, Takama et al (1982) have studied aluminum with solid state detector, Takama & Sato (1984) have studied germanium. A feature of this technique is that it can be used with small crystals.

Another technique using the dynamical theory of X-ray diffraction determines the integrated reflectivity for a Bragg-case reflection, which uses the expression for integrated reflectivity given by Zachariasen (1945). Using this approach.
Measurements of intensity are difficult to make and this is not capable of yielding results having the precisions of the Pendellösung techniques.

Bijvoet et al (1951) used Bijvoet pair technique to study the phase problem in the solution of crystal structures by measuring intensity ratios for noncentrosymmetric crystals. Measurement of as many as several hundred values for the diffracted intensities $I_{hkl}$ for a crystal may be made. When these were analysed, Cole & Stemple (1962) observed that the ratio of the intensities scattered in the Bijvoet or Friedel pair is independent of the state of the crystal is assumed to hold. This is a necessary assumption since in a large number of structure analyses radiation damage occurs during the course of an experiment. Measurements on a set of Bijvoet pairs gave rise to a set of simultaneous equations with $f'$ and $f''$ as the solutions. This technique is based on the assumption that no angular dependence of anomalous dispersion corrections exists. Agreement between theory and experiment is not outstanding in these techniques largely because of the practical difficulties in measuring the intensities of the related pairs.

Hosoya (1975) has outlined a number of ways in which values of $f'(\omega, g_{hh})$ and $f''(\omega, g_{hh})$ may be extracted from the Friedel-pair ratios and made measurements for simple structure of atoms such as gallium, indium, arsenic and selenium. In more complicated crystal structures and for which the positional parameters are known attempts have been made to determine the dispersion corrections by least squares refinement techniques for a number of atoms by Templeton & Templeton (1978), Philips et al (1978), Templeton et al (1980), Philips & Hodson (1985), and Chapuis (1985). This approach requires a measurement of intensities accurately for a large period of time and based on the assumption that specimen perfection does not affect the intensity ratio. Also, factors such as crystal shape and primary and secondary extinction may adversely affect the ability to measure intensity ratios correctly.

Fukamachi and Hosoya (1975) and Fukamachi et al (1977) have combined measurements of the ratio of intensities between Friedel pairs in polar materials (GaAs, GaP) for which the structure is known with linear attenuation coefficient measurements to derive the variation of the anomalous dispersion corrections as a function of photon energy. Their measurements were made in the vicinity of the K-absorption edges of gallium and arsenic. The analysis of their data depends on the
assumption that the imaginary part of the dispersion correction has no angular dependence. They have outlined a number of ways in which values of $f' (\omega, g_{kl})$ and $f^* (\omega, g_{kh})$ may be extracted from Friedel-pair ratios.

Fukamachi et al (1978) used Bragg reflection to measure refractive indices and hence $f' (\omega, 0)$ for copper in the neighbourhood of its K-absorption edge. Ishida & Katoh (1982) have described the use of a multiple-reflection diffractometer for the determination of X-ray refractive indices. Later Katoh et al (1985a, b) described its use for the measurement of $f' (\omega, 0)$ for Li and KCl at a wavelength near that of MoK $\alpha_1$ and for germanium in the neighbourhood of its K-absorption edge.

In many experiments the dispersion corrections have been deduced from the measurements of the X-ray refractive index. Larsson (1929) used a technique in which the deviation of an X-ray beam by a prism of calcite was detected. From the deviation he was able to test the Hönls theory of dispersion for a wavelength range which included the absorption edges. This technique was extended by Bearden (1932). Later Davis and Slack (1925) and Authier et al (1968) were able to improve the precision of measurement by the use of double crystal spectrometers. Unfortunately the use of prism shaped specimen does not enable the separation of the real part from the imaginary part of a dispersion correction.

1.7b Attenuation coefficient technique

Another important technique to measure $f'$ and $f^*$ is the attenuation coefficient technique and it is expected that this should result in improved quality of data. In addition X-ray attenuation experiments do not suffer from the problems associated with the specimen dimensions and device stability which X-ray interferometer experiments experience. Measurements can be made for a large range of atomic numbers over a wide range of photon wavelengths.

Tirsell et al (1975) have measured absolute coherent scattering cross sections of 25-75 keV filtered fluorescence K$\alpha$ radiation from thin Sn, Sm, Ta, Pt and Au foils by attenuation method. With high-resolution Ge (Li) spectrometers, they have separated the coherent X-rays from the incoherently scattered X-ray background and thus have directly measured coherent differential scattering cross sections over a range of 0.5 to 5.5 Å$^{-1}$ for scattering angles from $45^0$ to $135^0$ and hence obtained the
atomic scattering factors for five incident energies and compared with Cromer's (1965) form factor calculations obtained from relativistic Dirac-Slater wave functions for the electrons with and without corrections for anomalous dispersion. The real part of the dispersion correction was evaluated by using both numerical method as well as non-relativistic approximations and electric dipole contributions were included. The photoeffect cross sections calculated from the computed values of \( f^* \) were within 4% of those obtained experimentally.

Creagh (1975,1977,1978,1980) employed the computer fitting of data acquired in X-ray attenuation measurement for the determination of \( f' \) for alkali and alkaline earth halides using characteristic radiations.

Gerward et al (1979) has measured X-ray anomalous scattering factors for silicon and germanium using attenuation method for a wide range of photon energies including K-shell absorption edge. The evaluation of the integral for the real part requires that the photoeffect cross-section is known over as large an energy gap as possible. The contributions due to Compton scattering and thermal diffuse scattering have been calculated and subtracted from the experimental values to obtain the linear photoelectric absorption coefficient. Extrapolation technique was used to obtain \( \sigma_k \) from which oscillator strength \( g_k \) was obtained. Using \( \sigma_k \), dispersion integral was solved analytically. The use of the direct integration technique to determine \( f' \) for germanium and silicon in the vicinity of L3 -edges was described by Fouss (1980) and Fouss et al (1981).

Henke et al (1982) have evaluated the atomic scattering factors for \( Z=1 \) to 94 for 100 eV to 2 keV photon energy region by fitting the best available experimental and theoretical photoabsorption cross section data. For the shorter wavelengths and for the larger angles of scattering, the accuracy of these atomic scattering factors were improved by the inclusion of two correction terms for relativistic and charge distribution effects which are attributed to anomalous dispersion. They have used relativistic dipole correction term \( 5/3(E_{tot}/3mc^2) \) and the charge distribution correction term equal to \( (Z-f_0) \) where \( f_0 \) is the atomic form factor which has been tabulated by Hubbell and Øverbø.

Dreier et al (1984) have measured dispersion correction for Ni, Cu, Zn and Zr close to their K-edges and Ta, W, Pt and Au near their respective L-edges. Absolute
attenuation coefficients were obtained from measured relative spectral distributions normalised to known absolute cross-sections. They have followed a fitting procedure of the experimental data with precise published cross-sections far away from an absorption edge. During fitting procedure it turned out to be necessary to correct the experimental spectra for an additional weak energy dependent term. Therefore a small component \((a+bE)\), where \(E\) is the photon energy, was added to the measured absorption. For an accurate calculation of the dispersion correction the experimental data had to be extrapolated up to 1 MeV and down to 0.1 keV. Their results were of high precision and hence it was possible to predict the fine structure in the near edge region.

Hoyt et al (1984) have measured X-ray absorption spectra about the \(K\) edges of Ni, Cu and Ti at the Stanford Synchrotron Radiation Laboratory. The imaginary part of the atomic scattering factor \(f^*\) was determined using the optical theorem and the real part \(f'\) computed by the Kramers-Kronig dispersion relation. Methods for evaluating this integral as well as the effects on \(f'\) of various experimental errors are investigated. The \(f'\) results for Cu and Ni are compared to data from interferometry.

Barkyoumb et al (1990) have measured the forward X-ray scattering factor of Cu over an extended energy range using dispersion analysis of the measured absorption. The analysis required that this scattering factor should have the relativistic correct high-energy and low-energy limits. Uncertainty in the total oscillator strength was eliminated within the experimental error. Near edge structures at both \(L_{II}\), \(L_{III}\) and \(K\)-edges with relativistic second order corrections were considered. It was pointed out that the magnitude of the scattering is influenced by the net absorption strength in all portions of the spectrum.

Barkyoumb and Smith (1990) have calculated the X-ray scattering factors of metallic aluminum from a self-consistent X-ray attenuation database. The best-fit tabulation of the optical absorption of aluminum is modified to include K-edge extended X-ray absorption fine structures (XAFS) and other near-edge structures (XANES). Sum rules and comparisons with optical and electron energy-loss experiments are used to check the consistency of the modifications to the absorption spectrum. The forward scattering factor is calculated from the modified spectrum and a significant difference in \(f^*(\omega, 0)\) is found between the original and the modified.
data sets near the K-edge and it is largely attributed to resonant effects in the near edge absorption structure of aluminum.

Kefi et al (1992) have utilised a power law $\mu = kE^n$ to fit the variation of the experimentally observed mass attenuation coefficient as a function of the photon energy to evaluate the anomalous scattering factors of medium-Z elements Pd, Ag, Cd, In, Sn, I and Xe around their K-edge, between 15 and 45 keV. An analytic expression involving Gauss hypergeometric functions was used to evaluate the dispersion term. They have derived a relativistic correction term which is smaller than that proposed by Cromer and Libermann (1970) and agrees with that proposed by Levinger et al (1957) for the summed oscillator strength.

Henke et al (1993) have extended their earlier work and tabulated the atomic scattering factors for Z=1 to 92 in the energy range 50 eV to 30 keV by obtaining the best fit values for the photoabsorption cross sections based on a semi-empirical approach using theoretical-experimental attenuation data base with the inclusion of relativistic multipole correction term ($E_{tot} / mc^2$), which was obtained by fitting tabulated values of Kissel and Pratt (1990), equal to $(Z/82.5)^{2.37}$. They have used the available experimental data in the region 10 eV -10 keV, and for interpolating in the region 10 eV-1 keV, the theoretical calculations of Doolen and Liberman (1987) that are based upon a relativistic, time-dependent, local density approximation which can account for the important collective effects which become large at these low energies. The experimental photo absorption data include those given in INSPEC abstract files and those which have been added to the comprehensive NIST database of experimental values by Saloman et al (1987). Above 10 keV they have chosen that of Biggs and Lighthill (1988). At energies near the absorption edges the photoabsorption is found to depend on the chemical environment of the atom since transitions are to weakly bound excited states or to unbound shape resonance giving rise to near-edge X-ray absorption fine structure (NEXAFS). At energies somewhat higher than this there are weaker oscillations in the cross section as a function of energy resulting from the back scattering of the outgoing wave function of the photoelectron (EXAFS) from neighboring atoms.

In the work of Basavaraju and Kane (1994) it is mentioned that the anomalous scattering corrections to Rayleigh scattering amplitudes calculated in the form factor approximation are of considerable interest in the study of elastic- scattering of $\gamma$-rays.
and X-rays. When photon energies are close to binding energies of atomic inner shell electrons, the corrections have relatively large magnitudes. But under such conditions, the comparatively weak elastic-scattering contribution cannot be resolved even with semiconductor detectors from most of the components of target Kβ' X-rays. It was shown that elastic-scattering in such an interesting energy regime can be determined with the help of a least-squares-fitting procedure for the composite spectrum. The procedure is illustrated with a detailed study of 81.0 keV γ-ray scattering from gold having a K-shell binding energy of 80.723 keV. Data were obtained at several angles with gold and other targets of different atomic number Z.

Sandiego et al. (1997) have evaluated the dispersion corrections for the elements Cu and Ag. Umesh et al. (1998) have evaluated the dispersion correction Zr and Sn in the energy range 5-85 keV using the attenuation coefficient method. Using nearly mono energetic unpolarized Kα X-rays with energies E=17.44-42.75 keV, Rao et al. (1998) have measured differential elastic scattering cross sections for Cd, In, Sn and Sb at an angle of 90° to assess the contribution of anomalous dispersion in the vicinity of K-absorption edges. An X-ray tube with a secondary target arrangement was used to obtain the mono energetic radiation. A new method is developed to estimate the degree of monochromaticity, geometrical effects of the measuring system, solid angle correction and some considerations which are necessary in experiments using an X-ray tube with secondary target arrangement. Experimental results are compared with theoretical elastic scattering cross sections calculated using relativistic form factors (RFFs), relativistic modified form factors (RMFs), a combination of RFFs, RMFs and angle-independent anomalous scattering factors (ASFs), and relativistic numerical calculations based on multipole expansion of the second order S-matrix approach. Fairly good correspondence was observed between the experimental results and a combination of RFFs with ASFs above and below the edges. The experimental results were in excellent agreement with S-matrix values and a combination of RMFs with ASFs above and below the edges of Cd, In, Sn and Sb. However, the differences were larger nearer to the edges indicating the importance of anomalous terms in reproducing anomalous behaviour of the K-shell regions.

Sasaki et al. (1998) with X-ray wavelengths close to an absorption edge have determined independently the behavior of ions in different valence states. The anomalous scattering factors of Fe(2+) and Fe(3+) obtained from both absorption and
diffraction data have a large difference in $f$ between the two kinds of ions. Using a valence-difference contrast method, Bragg and diffuse scattering measurements were carried out for single crystals of Fe(3)O(4) at low temperatures. The results demonstrated the ability of the contrast method to resolve charge ordering and valence fluctuation details.

Rao et al (1998) have measured using nearly mono energetic unpolarised Ka radiation, the elastic scattering cross sections for Pt, Au and Pb in the energy region $5.41 \leq E \leq 9.23$ keV. The experimental results for Pt, Au and Pb are new. A new X-ray scattering system was assembled using an X-ray tube and secondary targets. In order to improve the peak-to-background ratio and the efficiency of the detection system, particularly in the low-energy region, excitation source, sample and detector assembly were placed in a vacuum chamber at a pressure of $10^{-2}$ mbar. The employed system helped considerably in reducing the scattering and background effects and in removing the interference of Ar K X-rays, which fall in the investigated regions. A new method was developed to estimate the degree of monochromaticity, geometrical effects of the measuring system, solid angle correction and some considerations which are necessary in experiments using X-ray tube with secondary target arrangement. Experimental elastic scattering cross sections were compared with theoretical estimates, a combination of relativistic modified form factors with angle independent anomalous scattering factors (RMF + ASFs) and recent theoretical estimates based on the multipole expansion of the second order S-matrix approach. Deviations were observed around the edges (high-energy side) indicating the importance of the dispersion correction terms. The experimental results were useful taking into account that the available calculated values describe the free atom and deviations for a solid have to be expected. This was due to the difference of the electronic structure of the solid in comparison to the free atom as a base for theoretical estimations. However, the comparison of experimental results with theoretical estimated indicates the importance of numerical calculations based on the multipole expansion of the second order S-matrix approach and high energy limit values (RMF + ASFs).

Takeshi et al (1999) have made Synchrotron anomalous scattering experiments with X-ray wavelengths at the Fe $K$ absorption edge possible to distinguish between ions having different valence states in magnetite at low temperatures. Using a large difference in anomalous scattering factors between Fe21 and Fe31, the valence-difference contrast method was applied for the intensity
measurements of fundamental and super lattice reflections of magnetite at low temperature. Reflections with half-integer indices, such as 0 4 7/2 and 4 4 9/2, were observe data 102 K, showing that magnetite transformed to a lower symmetry form. The energy dependence in the diffracted intensity was clearly observed at the Fe K-edge for the 0 47/2 super lattice reflection at 102 K. A sharp minimum of the normalized intensity at 57.122 keV was explained by the valence contrast between Fe ions occupied in the respective upper and lower parts of the double cell. Thus, their results strongly suggest the existence of charge ordering between ferrous and ferric ions in magnetite at low temperatures.

Bradley et al (1999) demonstrated that elastic photon-atom scattering can be important in a variety of biomedical applications. These include solving for the crystal structure of a macromolecule, imaging, and radiation dose calculations. To the extent that scattering is significant, it is important to remember that there are a number of effects which go beyond the form-factor approximation. In this paper, we discuss what is presently known about the validity of form-factor approximations for predictions of elastic photon scattering by atoms. We quantify the uncertainty in form-factor theories for sample atoms of biomedical interest, including: carbon, oxygen, aluminum, calcium, iron, iodine and lead. The importance of effects that go beyond form-factor approximation is illustrated by demonstrating that errors can be introduced in using a simple form-factor-based scaling technique using scattering factors measured at one energy to predict scattering at another energy. These anomalous dispersion have been used extensively in recent years in studying structures of biological macromolecules, either in combination with or as an alternative to isomorphous replacement techniques. We present accurate, high precision anomalous scattering factors for a range of elements commonly used in macro-molecular structure studies, tabulated on a fixed grid interval in the energy range 1-100 keV.

Ibrahim et al (2000) determined total differential scattering cross-sections using the 59.54 keV gamma rays emitted by the radionuclide \(^{241}\)Am, for eleven moderate to high atomic number elements. Measurements were performed using a standard back-scattering geometry arranged to obtain scattering angles of 145°, 154° and 165° and associated photon momentum transfers, 4.58 \(\leq x \leq 4.76 \text{ Å}^{-1}\). High purity (>99.9%) foils of Cu, Zn, Zr, Nb, Mo, Ag, Cd, In, Sn, Ta and W were used as targets. Measurements have generally been found to be in accord with predictions to within a
conservative uncertainty of 10%, predicted values being obtained as total differential scattering cross-sections based upon the tabulations of modified form factors corrected for anomalous scattering (ACMFF) and non-relativistic wave functions for incoherent scattering.

Evans and Pettifer (2001) have used Fortran program CHOOCH, which derives experimental values of the anomalous-scattering factors $f''$ and $f'$ from X-ray fluorescence spectra, is described. The program assumes knowledge of theoretical values for the imaginary term, $f''$, of the anomalous-scattering factor away from the absorption edge to scale the experimental fluorescence spectrum and thus derive values of $f''$ near the absorption edge, where tabular data are inappropriate. The Kramers-Kronig relation is used to calculate the real part, $f'$, of the anomalous-scattering factor. The program aids the decision-making process in macromolecular crystallographic experiments where optimal wavelength selection is required. Magnitudes of $f'$ and $f''$ at selected wavelengths can later be used as starting values for heavy-atom refinement with crystallographic phasing programs.

Hugtenburg (2002) has studied ASF for dilute concentrations of the biomedically relevant element iodine in aqueous media including measurements with monochromatic synchrotron radiation in the vicinity of the iodine K-edge. The measurements agree with anomalous scatter-factor corrections to the form-factor approximation, which has been shown to have good agreement with higher precision S-matrix calculations for small angle scatter over a wide range of energies but has not been adequately tested at the edge. Monte Carlo modeling, including the modeling of polarized Compton and Rayleigh scattered x-rays, is used to determine the relative contributions of the scatter and fluorescent components at the detector as well as the modeling of self-absorption and relative dose in the determination of detection limits. A Rayleigh scatter minimum of 28 barns/sr was observed at an energy $10 \pm 5$ eV below the K-edge of iodine at a position predicted from an evaluation of the dispersion integral that includes bound-bound resonance contributions. Minimum detectable concentrations for observation of the anomalous Rayleigh scatter feature at an exposure of 10 mSv, predicted for iodine and iron, are 1 mg/ml-1 and 10 mg/ml-1, respectively. Upper limits to detection of the feature imposed by degradation of the signal by self-absorption are 0.021 g cm$^{-2}$ and 0.0029 g cm$^{-2}$ radiation lengths, respectively.
Hugtenburg and Bradley (2004) have examined the ASF correction to the relativistic form factor approximation for Rayleigh scattering in support of its utilization in radiographic imaging. ASF corrected total cross section data have been generated for a low resolution grid for the Monte Carlo code EGS4 for the biologically important elements, K, Ca, Mn, Fe, Cu and Zn. Points in the fixed energy grid used by EGS4 as well as 8 other points in the vicinity of the K-edge have been chosen to achieve an uncertainty in the ASF component of 20 per cent according to the Thomas Reich Kuhn sum rule and an energy resolution of 20eV. Such data are useful for analysis of imaging with a quasi-monoenergetic source. Correction to the sampled distribution of outgoing photons, due to ASF, are given and new total cross-section data including that of the photoelectric effect have been computed using the Slater exchange self-consistent potential with the latter tail. A measurement of Rayleigh scattering in a dilute aqueous solution of manganese (II) was performed, this system enabling determination of the absolute cross-section although background subtraction was remove K fluorescence and resonant Raman scattering occurring within several 100 eV of the edge. Measurements confirm the presence of below edge bound-bound structure and variation in the structure due to the ionic state that are not currently included in tabulations.

1.8 Motivation for the current work

Accurate data on X-ray attenuation coefficients and anomalous scattering factors (also called real and imaginary parts of (or dispersion corrections to) the forward Rayleigh scattering amplitude) find diverse applications in numerous fields like medicine, agriculture, technology and scientific research etc. In particular, knowledge of anomalous scattering factors is of great importance in condensed matter studies, X-ray diffraction analysis, X-ray optical designs and structural studies of macromolecules etc. The interferometer techniques have been widely used to measure the scattering factors. The main drawback of these techniques is that the range of X-ray wavelengths and atomic numbers that can be covered is limited. Also, there are problems associated with specimen dimensions and device stability. However, the attenuation coefficient technique does not suffer from the problems faced by the interferometer techniques. Also, the attenuation cross section measurements can be made for a larger range of elements over a wider range of energies as compared to the interferometric techniques and hence are expected to give a good quality of data after
the inclusion of a proper relativistic correction term. The inclusion of the relativistic correction term (high-energy limit) is necessitated because the $f'$ values based on attenuation coefficient method are systematically higher than those obtained using direct method. At incident photon energies very much larger than the absorption edges of a particular element, the value of the dispersion term is expected to approach this relativistic correction term. Thus it is possible to obtain the appropriate value of this relativistic correction term from the attenuation coefficient method. It is also expected that the inclusion of the relativistic corrections calculated using either S-matrix approach or higher order multipole approximation together with the retardation effects, can yield good agreement between the experiment and theory.

It is known from dispersion theory that there exists a relation between photoeffect cross sections of element and the real and imaginary parts of the forward Rayleigh scattering amplitude $f'$ and $f''$ through Optical theorem. The $f'$ and $f''$ values are themselves related mutually via the Kramer's-Kronig transform. Hence, it is clear that the photo effect cross sections of elements in the low energy region below 100 keV, can be made use of to numerically evaluate the $f'$ and $f''$ values around their absorption edges by the attenuation coefficient method. However from the survey detailed in the preceding sections it is evident that reports of such work particularly with radioisotopes are scarce in literature. This may be due to the fact that such a method requires high-resolution detectors for the measurement of the photo effect cross sections in the low energy region. Also, the data cover elements like C, Al, Cu, Zr, Ag, Sn, Ta, Au, Pb, Th and U which are available in pure elemental form in nature. Hence, in particular, data on rare earth elements, which are not available in pure elemental form, are either scarce or practically non-existent.

In view of all these, it was felt worthwhile to determine, the dispersion corrections for the rare earth elements La, Ce, Pr, Nd, Sm, Gd, Dy, Ho and Er as well as for some high atomic number elements Ta, Hg and Pb by using their photoeffect cross sections by adopting the attenuation coefficient method. In this method, we measured the total attenuation cross-sections of the simple oxides of rare earth elements La, Ce, Pr, Nd, Sm, Gd, Dy, Ho and Er in the energy range 5-85 keV and the total attenuation cross sections of the elements Ta, Hg, Pb in the energy range 6-136 keV in a narrow beam good geometry set up by employing a high-resolution hyper pure germanium detector. From the cross sections of the rare earth oxides, the
elemental cross sections were derived with the aid of mixture rule by suitably subtracting the oxygen cross sections. The oxygen cross sections were taken to be the difference between the cross sections of NaNO₃ and NaNO₂ measured at each energy of interest. From the total attenuation cross sections, the photo effect cross sections of the elements were derived by subtracting a small contribution of the sum of the coherent and incoherent scattering cross sections interpolated from the XCOM data (Berger and Hubbell 1987) for the energies of interest. The corresponding values of photoeffect cross sections of each element so obtained were further used to determine the real and imaginary parts of the dispersion corrections to the forward Rayleigh scattering amplitude by a numerical evaluation of the dispersion integral that relates them. The numerical evaluation of the dispersion integral was carried out by a new technique. Based on this method, the $f'$ and $f''$ values around the K-edges of the elements La, Ce, Pr, Nd, Sm, Gd, Dy, Ho, Er, Ta, Hg and Pb were determined. In the case of Ta and Pb the $f'$ and $f''$ values around their L-edges were also determined. The relativistic corrections $f'(\infty)$ suggested by different authors were separately included in the values of $f'$ so obtained. Three simple semi-empirical formulae have also been derived which yield the $f''$ values, below, above and at the K-edge of rare earth elements (La-Er) respectively.

The values of the dispersion corrections $f'$ and $f''$ obtained from the present investigation are compared with the other available theoretical and the experimental data and discussed. Details regarding this investigation are described in the subsequent chapters.
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