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Establishment of a Photon Data Section of the

BNL National Nuclear Data Center:

a Preliminary Proposal

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## Acronyms

| | |
|---|---|
| BNL | Brookhaven National Laboratory |
| IAEA | International Atomic Energy Agency |
| LBL | Lawrence Berkeley Laboratory |
| NIST | National Institute of Science and Technology |
| NNDC | National Nuclear Data Center |
| ORNL | Oak Ridge National Laboratory |
| PDS | Photon Data Section |
| EXAFS | extended x-ray absorption fine structure |
| PIXE | particle induced x-ray emission |
| XANES | x-ray absorption near edge structure |
| XAS | X-ray Absorption Spectroscopy (a generic grouping of the absorption techniques) |
| XRF | x-ray fluorescence |
| aC | atomic Compton |
| AFF | atomic form factor |
| MFF | modified form factor |
| ISF | incoherent scattering function |
| IA | impulse approximation |
| PE | photoelectric |
| XRRS | X-Ray Resonant Raman Scattering |
| XRS | X-Ray Raman Scattering |
| ENDF/B | Evaluated Nuclear Data File/B |
| ENSDF | Evaluated Nuclear Structure Data File |
| NDS | Nuclear Data Sheets |
| CSEWG | Cross Section Evaluation Working Group |
| MENDWG | Medium Energy Nuclear Data Working Group |

## Symbols

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|---|---|
| $E_o$ | Energy of the incident photon |
| $E$ | energy of the scattered photon |
| $E'$ | the incremental energy of the Compton scattered photons |
| $E_b$ | binding energy of a particular electron |
| $\gamma$ | normalized photon energy $\gamma = \frac{E_o}{mc^2}$ |
| $\epsilon$ | the kinetic energy of the ejected electron |
| $\hbar \vec{q}$ | the momentum transfer from the incident photon to the target electron $\hbar \vec{q} = \vec{k}_o - \vec{k}$. |
| $\hbar q_{coh}$ | momentum transfer in a coherent scattering event $\hbar q_{coh} = 2k \sin \frac{\theta}{2}$ |
| $\hbar q_{incoh}$ | momentum transfer in a incoherent scattering event $\hbar q_{incoh} = 2k \sin(\frac{\theta}{2}) \frac{(1+(k^2+2k)\sin^2(\frac{\theta}{2}))^{\frac{1}{2}}}{(1+2k\sin^2\frac{\theta}{2})}$ |
| $x$ | a parameter commonly used for momentum transfer, in $\text{Å}^{-1}$, $x = \frac{\sin\frac{\theta}{2}}{\lambda} = 20.60744q$ |
| $f(q, Z)$ | Atomic form factor |
| $f(q, E_o, Z)$ | the atomic form factor including anomalous corrections |
| $f'(q, E_o, Z)$ | the real component of the anomalous correction |
| $f''(q, E_o, Z)$ | the imaginary component if the anomalous correction |
| $F_{hkl}$ | the geometrical structure factor |
| $S(q, Z)$ | incoherent scattering functuib |
| $U(r)dr$ | the probability of finding an electron between $r$ and $r + dr$ from the nucleus |
| $\rho(r)dr$ | , the electron density as a function of r from the nucleus |
| $V(r)$ | is the central potential of the atom |
| $\theta$ | is the scattering angle; $\theta = \vec{k} \cdot \vec{k}_o$. |
| $|\vec{k}_o|$ | propagation vector of the incident photon |
| $|\vec{k}|$ | propagation vector of the scattered photon |
| $r_o^2$ | , classical electron radius, |
| $m_o$ | the rest mass of the electron |
| $\vec{e}_o$ | is the electric field vector of the incident photon |
| $\vec{e}$ | is the electric field vector of the scattered photon. |
| $(\frac{d\sigma}{d\Omega})_{Th}$ | The differential Thomson scattering cross section $(\frac{d\sigma}{d\Omega})_{Th} = r_o^2 \cos\alpha = r_o^2 \vec{e} \cdot \vec{e}_o$. |
| $(\frac{d\sigma}{d\Omega})_R$ | The differential Rayleigh scattering cross section |

$$\left(\tfrac{d\sigma}{d\Omega}\right)_R = f^2(q, Z)\left(\tfrac{d\sigma}{d\Omega}\right)_{Th}$$

$\left(\tfrac{d\sigma}{d\Omega}\right)_C$   the differential Compton scattering cross section, usually in the form of the Klein-Nishina cross section.

$\left(\tfrac{d\sigma}{d\Omega}\right)_{aC}$   the differential atomic Compton scattering cross section
$$\left(\tfrac{d\sigma}{d\Omega}\right)_{aC} = S(q, Z)\tfrac{d\sigma}{d\Omega}\right)_C$$

$\left(\tfrac{d^2\sigma}{dE'd\Omega}\right)_{IA}$   the double differential atomic Compton scattering cross section.

$n$   indice for the initial electron state.

$m$   indice the final electron state.

$Z$   the atomic number of the element

$\vec{A}$   is the vector potential of the perturbing electromagnetic field

$\Gamma$   the level width of the electron state.

$\omega$   is the frequency of the incident photons

$\omega_\kappa$   is the frequency of the absorption edge of the $\kappa^{th}$ shell.

$\left(\tfrac{dg}{d\omega}\right)_\kappa$   is the oscillator density of states for the $\kappa^{th}$ shell.

$\mu(E)_i$   mass attenuation coefficient

$g_n$   the oscillator strength

$\omega_n$   the fluorescence yield

$\vec{p}$   the momentum of the electron

$p_z$   the projection of the electron's momentum onto the Z axis, with $z$ representing the direction of the scattered x ray

$J(p_z)$   the Compton profile (the electron momentum distribution).

## Abstract

It is proposed to establish a Photon Data Section (PDS) of the BNL National Nuclear Data Center (NNDC). This would be a total program encompassing both photon-atom and photon-nucleus interactions. By utilizing the existing NNDC data base management expertise and on-line access capabilities, the implementation of photon interaction data activities within the existing NNDC nuclear structure and nuclear-reaction activities can reestablish a viable photon interaction data program at minimum cost. By taking advantage of the on-line capabilities, the x-ray users' community will have access to a dynamic, state-of-the-art data base of interaction information.

The proposed information base would include data that presently are scattered throughout the literature usually in tabulated form. It is expected that the data bases would include at least the most precise data available in photoelectric cross sections, atomic form factors and incoherent scattering functions, anomalous scattering factors, oscillator strengths and oscillator densities, fluorescence yields, Auger electron yields, etc. It could also include information not presently available in tabulations or in existing data bases such as EXAFS (extended x-ray absorption fine structure) reference spectra, chemical bonding induced shifts in the photoelectric absorption edge (XANES or x-ray absorption near edge structure), matrix corrections, x-ray Raman, and x-ray resonant Raman cross sections. The data base will also include the best estimates of the accuracy of the interaction data as it exists in the data base. It is proposed that the PDS would support computer programs written for calculating scattering cross sections for given solid angles, sample geometries, and polarization of the incident x rays, for calculating Compton profiles, and for analyzing data as in EXAFS and x-ray fluorescence.

The program will also work on development of parameterization and scaling techniques for the data where it is reasonable and consistent with theory. In order to maintain the highest quality information in the data bases and in order to properly

incorporate new information as it becomes available, leading scientists in the field of photon interactions will be encouraged to spend time working with the PDS staff. In order to bring the PDS on line as rapidly as possible, presently available data bases and tabulations will be incorporated into the on-line system. After this the PDS will develop an active effort in evaluation and tabulation of new experimental and theoretical data as they become available. With this the proposed program will become an integral part of the quality assurance of many experimental and theoretical endeavors not only at BNL but at institutions of users of the data base.

## A. Introduction

The purpose of this report/pre-proposal is to present arguments and request comments concerning the establishment of the proposed Photon Data Section (PDS) of the Brookhaven National Laboratory (BNL) National Nuclear Data Center (NNDC). The activities of this proposed PDS is to maintain data bases of basic photon interactions that would be oriented to the research community. In addition a fully operational PDS would also support distribution of computer programs, bibliography, and a library of interaction publications. The information would be made available through the existing NNDC networked, on-line data base system, publications, and distribution of printed tables and, if possible, diskettes for personal computers. The only program that was similar to the proposed PDS, for the independent collection and evaluation of data from photon-atom interactions (i.e. photoelectric effect cross sections, fluorescence yields, scattering cross sections, etc.), was handled by Mr. J.H. Hubbell at the National Institute of Science and Technology (NIST). However, Mr. Hubbell has recently retired, the program scaled back, leaving Mr. Hubbell to continue the work solo on a consulting basis. There are currently no plans within NIST to continue this program after Mr. Hubbell terminates his efforts. Likewise, compilation of photon-nuclear interactions and indexes to the bibliography were at one time handled by E.G. Fuller at the former National Bureau of Standards (now NIST), but that effort was likewise terminated leaving a major gap in that field that has yet to be filled.

Accurate photon-atom interaction cross section data are important in all photon energy ranges. The proposed PDS would cover vacuum ultraviolet and soft x rays (tens of eV) on to low energy end up through the multi-GeV range. Interactions in these energy regions are important not only in research in basic physical sciences but also in industry, medicine and astrophysics to name a few. The need for and utilization of this work is apparent from the number of citations of several previously

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published compilations. The Jan. 9, 1989 Current Contents featured an evaluation and compilation of x-ray scattering data by Hubbell, et al., [Hu75] as a "Citation Classic" stating it had been cited in over 330 publications. The more general photon interaction data reviews and compilations, which include attenuation coefficients, by Hubbell [Hu69, Hu82], have also been featured as citation classics (Current Contents, Feb. 22, 1982 for Hu69 and in press for Hu82). As of Jan., 1989 [Hu69] had been cited over 400 times and as of May 21, 1990, [Hu82] had been cited over 175 times. The Cromer and Mann [Cr68] x-ray scattering factors have been cited over 5500 times; the Veigele [Ve73] cross sections between 0.1 keV and 1.0MeV have been cited 275 times; the Hubbell et al., [Hu80] work on pair, triplet, and total atomic cross sections for 1 MeV - 100 GeV has been cited 40 times; and the Schaupp, et al., [Sc83] work on small-angle Rayleigh scattering of photons at high energies has been cited 20 times. These tabulations do have significant discrepancies between them. Therefore, the need for continued work in evaluation is that the present data are often not as accurate as is needed. The shortcomings in accuracy is many times not appreciated by the end users and the end users need assistance in determining the most appropriate reference data. Improving the knowledge of the basic interactions that could be incorporated into the PDS data bases is presently an active pursuit of both experimentalists and theoreticians.

Throughout this proposal we will discuss areas where photon interaction data inaccuracies are known to exist. These are representative and not meant to be totally inclusive of all problems. Therefore these problems will be discussed in the realm of justifying the creation of a center (within the existing NNDC) for the independent evaluation and tabulation of photon interaction data. We will also discuss types of information that we feel should be included in a managed data base. The ultimate level of support that we will be able to give to the data bases and end users will depend on the level of funding and staffing that we are able to raise. Final selection ·

of the PDS efforts would be made with consultation and under the direction of an outside program committee. Short comings of data bases that we may not be able to actively support could be handled through including tabulations that the PDS does not actively support and through the establishment of other complementary data centers throughout the world, such as exists in the nuclear physics community.

The establishment of such a data section within the BNL NNDC is reasonable since BNL has personnel (permanent, temporary, and visiting) at the forefront of the physics of x rays in the VUV to 100+ keV range and in the 300 MeV range and since the NNDC has, in nuclear physics, extensive experience in on-line data base development, management, and information distribution along with evaluation of theoretical and experimental data. Therefore interactions between the Center staff and end users will be relatively easy.

The basic information that would be included is critical for most experimental and theoretical research programs dealing with interactions between x rays and/or gamma rays and atoms. With the growing use of synchrotron radiation for experimental work, the need for accurate interaction data is imperative since the x-ray energy regions that are available with synchrotron radiation, and the energy resolutions frequently used, coincide with energy regimes where much of the data is least accurate.

## A.1 Photon-Atom Interactions

The uses of x-ray beams in pure and applied sciences have flourished and have greatly expanded in the past few years due in part to the development of efficient, "medium" energy resolution solid state detectors (resolution of about 150 eV at 5.9 keV) and to the development of high intensity, versatile sources of x rays. In the early part of this century the main uses of x rays as probes of matter were dominated by x-ray diffraction, for solid state physics, metallurgy, protein structure, etc.; and by radiography. The development of crystal spectrometers opened the path for

quantitative elemental analysis by x-ray fluorescence (XRF) and also allowed for the elemental characterization of materials with electron microscopes by electron impact induced fluorescence. This led to the development of the electron microprobe, a system optimized for the characterization of elements by electron-induced fluorescence with the electron beam without providing imaging capabilities.

Major progress has been made in the past 25 years in the development of x-ray and γ-ray based analytical techniques for materials. We have witnessed the development of energy dispersive x-ray fluorescence (with solid state detectors for multi-elemental capabilities, for reviews see [Ma84a, Ma86, Ma88, Ma90]), Compton profile spectroscopy (for the measurement of bound electron momentum distributions [Co85, Ko81]); extended x-ray absorption fine structure (EXAFS, for the determination of interatomic distances in solids along with coordination numbers [Bo89, Fa88]); x-ray absorption near edge structure (XANES) and chemical speciation (determination of chemical states of elements [Go87, Pe87]); tomography and other imaging techniques; topography [Du87]; characterization of materials by x-ray scattering (Rayleigh, atomic Compton, anomalous coherent, x-ray Raman scattering, x-ray resonant Raman, and combinations thereof [Gi85, Ha86, Ho87, Ho88, Ma84b, Mo87, Po90, Sc86]); along with other analytical techniques. In all of these probes, accurate interaction data is essential for proper analysis of the experimental data. Reliable interaction data is also important for basic physics, such as atomic physics, where normalization to fluorescence, ejected electrons, or scattered radiation is needed.

A mistake that is all too commonly made is to assume that the tabulated numbers are exact. As will be discussed in the introduction and in more depth in the appendix, there are many areas where the existing data should not be considered to be very accurate. An interesting illustration of this point is to note that if we consider the transmission of photons through a sample, or when one determines an effective

depth, a 2-5% uncertainty in the absorption coefficient, depending on the thickness of the sample, can lead to a 10% uncertainty in the transmission [IC89]. Because of the problems with accuracy in the attenuation data, the International Union of Crystallography sponsored a "round robin" analyses of x ray attenuation in silicon using 8 techniques in order to obtain an assessment of the problem [Cr87a]. In general the error estimates for the separate analyses were on the order 1%, but deviations between the analyses were as much as 5-10%. These two illustrations emphasize the need for end users to be aware of the accuracy of the data, be confident of the quality of the data, be informed as to the limitations, and be knowledgeable of the sources of the data being used. The sources of the data that would be incorporated would be theoretical, experimental or both. However, data for all elements, and energy-angle regimes are not always available and sometimes interpolations and extrapolations need to be included in the data base.

A data base of "best value" experimental measurements is important to theoreticians to bench mark different models of the atomic system as they are developed. Because of the complexity of the atomic system, many of the models are developed in a "simplified" manner and later corrections to the calculations are included. Even then the theoretician has several atomic potentials from which to choose and the experimental measurements will help determine the most appropriate potentials to use.

In addition to the above mentioned analytical techniques, medical physics has witnessed, in the past few years, major advances in radiation therapy. Some of the advances have resulted from perfecting "focussed", multi-beam sources and others in understanding how to use these focussed beams. The ultimate success of the therapy depends on optimization procedures to maximize dose to the tumor and to minimize the dose to the surrounding tissues. This dose is mostly deposited by the electrons ejected from the atom during the interaction. Many variables such as energy spectrum

of the x-ray beam, which depends on the absorption characteristics of the target, are at the disposal of the therapist. The optimization procedures require accurate interaction data for determining absorbed dose. A second aspect that is extremely important to the therapist is the need for accurate calibration of the instrumentation so the therapy can be reproduced and properly documented [Lo81]. There have also been recent developments in medical applications to use scattered radiation for the determination of fat content of patients [Ko87].

In the areas of radiography and radiometric gauging, surveillance and inspection of air cargo by x-ray techniques require accurate and reliable information concerning x-ray interactions in the 0.14-10MeV range in order to maximize sensitivity of the techniques and to minimize the time for analysis. This maximizes throughput, and minimizes the absorbed dose, which is important especially for examination of foodstuffs [Hu89b]. In surveillance and inspection (of large items with high energy, MeV+, photons) technology accurate photonuclear cross sections are needed in order to avoid activation of the materials being inspected.

The basic interactions of photons with atoms depend on the energies of the incident photons and, depending on the interactions, the angles between the direction of the incident photons and the direction of observation. The interactions can involve both the atomic electrons and the nuclei, depending on the energy and angle. The basic interactions with atomic electrons are usually mathematically described as separate interactions: A. the photoelectric effect where the entire energy of the photon is absorbed in the interaction and an electron is ejected; B. coherent scattering where momentum of the photon is changed but there no change in the energy or phase of the photon; and C. incoherent scattering where some of the energy of the incident photon is imparted to an atomic electron. If the energy of the photon is above 100 keV, depending on the angle of observation, nuclear effects start to be observable (that is with the exception of a few low energy states used in Mössbauer

spectroscopy). These effects include (a) Nuclear Thomson (>100 keV), where there is coherent scattering by the nuclear charge, (b) Nuclear Resonance (>1MeV), where nuclear states are resonantly excited, and (c) Delbrück scattering, where the photons are scattered by virtual electron-positron pairs.

Tabulations presently exist that include information on photoelectric (PE) cross sections, pair and triplet production cross sections, and the scattering factors that are used to calculate the scattering cross sections. There are other tables that provide strictly the attenuation of radiation through matter. Some tabulations have been created that include corrections to the scattering factors that are necessary to try to handle effects like anomalous scattering. All of these tabulations are deficient in one form or another and hence not only do they need to be reassessed on a periodic basis, but more sophisticated and more complicated data bases need to be established that can more accurately handle the data.

The understanding of the PE cross sections are frequently considered to be in "good shape". However, there are a few areas where inaccuracies still exist and at least one where no consistent tabulations exist at all. One area where there is still confusion is in the fluorescence yields, or the ratio of fluorescence x rays to total number of photoelectric interactions. A second area is in the jump ratios, which are the ratios of the PE cross section below and above the absorption edge. A third area is in the shift of the absorption energy due to chemical bonding. Fourth, the shape of the low energy PE cross sections around the absorption edge is not correctly predicted by existing theory and corrections need to be determined [Gr87]. In the past few years the Nuclear Data group at Livermore National Laboratory [Pl81, Cu89] has been working on including photon interaction data into the ENDF library, a library developed mainly for the nuclear industry. The 1981 version of the library relied on the original version of the McMaster tables [Mc69] for the photoelectric cross sections between 1keV and 1MeV and on Hubbell and Berman [Hu66] for the cross sections

when $E_o > 1\text{MeV}$. The values from these tables do not agree at 1MeV, so the Hubbell data was normalized to the McMaster data at this energy. The correction for argon was 18%; for iron, 20%; for tin, 12%; and for lead, 6%. The 1989 version [Cu89] relies on the calculated Scofield data [Sc73] for the cross sections below 1 MeV along with a combination of the various Hubbell tables for energies greater than 1 MeV. For this particular library, the per shell photoelectric cross section information was desired, so they assumed the fractions per shell from the Scofield data to be valid from 1 MeV up to 100 GeV.

The scattering of photons by bound electrons is generally divided into two main categories, Rayleigh, for the coherent scattering, and atomic Compton, for the incoherent scattering. Under specific conditions, anomalous effects can be significant and can even used as a probe since they usually contain information that is matrix dependent. The most widely used approximations for the Rayleigh and atomic Compton scattering cross sections are the atomic form factor and incoherent scattering function approximations, respectively. While the atomic form factor (AFF) and incoherent scattering function (ISF) approximations are not the most accurate methods of calculating the Rayleigh and atomic Compton cross sections, they are by far the simplest and most widely used, albeit poorly understood approximations. Therefore, by default, they are the most important approximations in use today. The assumptions that go into the approximations include:

1.    The Rayleigh (coherent) scattering cross section can be described as a product of the Thomson cross section and the square of the atomic form factor, $f(q, Z)$.

2.    The atomic Compton (incoherent) scattering cross section can be described as a product of the Compton (free electron) cross section and the incoherent scattering function, $S(q, Z)$.

3.    For each element the value of $f$ and $S$ is dependent only on the magnitude of the

momentum transfer between the photon and the target electron, in terms of the normalized photon energy $\gamma = \frac{E_0}{mc^2}$. For coherent scattering, $\hbar q_{coh} = 2\gamma \sin\frac{\theta}{2}$ and, for incoherent scattering, $\hbar q_{incoh} = 2\gamma \sin(\frac{\theta}{2})\frac{(1+(\gamma^2+2\gamma)\sin^2(\frac{\theta}{2}))^{\frac{1}{2}}}{(1+2\gamma \sin^2\frac{\theta}{2})}$

4. $f$ decreases monotonically with the momentum transfer from $Z$ to 0.

5. $S$ increases monotonically with the momentum transfer from 0 to $Z$.

6. Matrix effects, such as crystalline structure (as in Bragg diffraction), and temperature effects, such as thermal diffuse scattering, can be accounted for independently of the approximations.

7. The cross sections for scattering can be determined by a linear superposition of the "parallel" and "perpendicular" components (of polarization) weighted by their respective fractions. Therefore the unpolarized x rays can be treated as a superposition of polarized waves.

8. The interactions do not change the polarization of the x rays other than as described by the Thomson and Compton cross sections for the scattering of photons by free electrons.

9. The interactions are high enough in energy, from the absorption edge, that the anomalous scattering effects are not significant (generally $E_0 > 5E_b$).

10. The energy of the incident photon is less than 500keV.

From this list of assumptions it should be apparent that one needs to be careful in the use of these approximations. Tabulations of $f$ and $S$ exist, some of the most widely used being Hubbell, et al., [Hu75].

The values of $f$ and $S$ are calculated from first-order perturbation theory by iteratively calculating (self-consistent) the electron wave functions, as a function of distance from the nucleus, in the presence of the perturbing electric field of a photon.

When the energy of the incident photon is near an absorption edge the electron can be resonantly excited so the first-order perturbation theory cannot be used to calculate the cross section. This is known as anomalous scattering and the anomalous scattering corrections can be significant. If the photon energy is below the absorption edge, the electron is not free to scatter the photon as described before. Neither of these two effects can be handled in the single parameter ($q$ dependence) approach of calculating the atomic form factors.

In addition to the problems of edge effects, the incoherent scattering is further complicated by the fact that not only is there momentum transfer, but there is also an energy transfer between the photon (initial energy of $E_o$) and the electron. If the electron is stationary, the scattered photon energy $E$ is:

$$\frac{E}{E_o} = \frac{1}{1 + \gamma(1 - \cos\theta)} \tag{1}$$

where $\gamma = \frac{E_o}{m_o c^2}$ and $\theta$ is the scattering angle. There is an additional problem that the target electrons themselves appear to the photons to have a momentum distribution, known as the Compton profile. The momentum distribution results in an energy distribution of the scattered photons. This energy distribution is inherently broad and the distribution from an atom is actually a sum of many components, each component from interactions with the individual orbitals of the atom. These individual distribution components are centered about the same mean $\frac{E}{E_o}$ but have different widths.

The values of cross sections can be used to study the specific interactions, whether they are scattering or photoelectric interactions. These values are also needed in order to construct attenuation coefficients that are used to determine the transmission of radiation through matter. Several tables have been developed over the years. One of the most widely used though are the tables found in the *International Tables for X-Ray Crystallography* [Hu74]. These tables have been reassessed and a

new version is in press [Cr90b]. Some of the changes in attenuation coefficients are as much as 10% from the values of [Hu74].

## A.2 Photon-Nucleus Interactions

Evaluated photonuclear data are needed for a number of applications that include photoneutron sources, isotope production, radiation damage studies, gamma ray processing and surveillance. The latter two need the information since there are trade offs between high penetration and activation of the material. The compilation of photonuclear experimental data and the indexes to the bibliography were at one time handled by E.G. Fuller at NIST, but that effort was likewise terminated leaving a major gap in that field that needs to be filled. The NNDC, which DOE has designated to coordinate the development of evaluated data files and also has the appropriate computer hardware and software for data exchange can provide an effective coordination point for the organization of photonuclear data. This is a useful adjunct to the NNDC coordination of neutron and charged particle reaction data files. In addition to the experience still resident or loosely associated with NIST, there is strong interest on the part of a data group at the Lawrence Livermore National Laboratory and the CDFE, the photonuclear data center at the Institute of Nuclear Physics, Moscow State University, USSR, in collaborating to improve the exchange of bibliography experimental data and other information leading to evaluated nuclear data files. Initially, the head of CDFE has offered to be resident at the NNDC for an extended period with USSR paid travel to help implement the collaborative arrangement.

The starting point for the NNDC photonuclear data activity would focus on the following:

1.    Photon energy range: Threshold to GeV (to include the BNL LEGGS facility).

2.    Photon source type: Monoenergetic. Techniques using single gamma line emit-

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ters, tagged or annihilation photons, or narrow bremsstrahlung tips are included.

3. Data types: Total absorption cross sections, yield cross sections, angular integrated cross sections, and angular differential polarized or unpolarized cross sections.

In November, 1989, the Charged Particle and Photonuclear Data Subcommittee of the Cross Section Evaluation Working Group, a DOE sponsored cooperative effort coordinated by the NNDC, endorsed a NIST-NNDC-LLNL-CDFE collaborative effort to evaluate photonuclear data.

## B. The National Nuclear Data Center

The National Nuclear Data Center (NNDC) is the result of over 40 years of activity at BNL in the area of low energy neutron physics. The work started with experimental neutron data compilation including the publication of a neutron data atlas, BNL-325. In 1964, the neutron data evaluation activity was merged with the compilation activity.

Also that year, at the request of the Atomic Energy Commission's Division of Reactor Development and Technology, the Center began coordinating the work of other laboratories to provide a unified system of evaluated nuclear data and associated computer codes for use in federal and private nuclear power programs.

In April, 1975, the NNDC was requested by the DOE Division of Physical Research to investigate national and international coordination of nuclear structure and charged particle reaction data. Increased coordination of U.S. and non-U.S. activities was recommended to eliminate wasteful duplication of effort and to improve utilization of manpower.

In September, 1979, NNDC was requested to assume the data base and publication activities of the Oak Ridge National Laboratory (ORNL) Nuclear Data Project.

The NNDC is responsible for data compilation, evaluation and information services for neutron, charged particle and nuclear structure physics. The NNDC maintains bibliographic, experimental and evaluated data files for these three areas of physics and provides data services to basic applied scientists in the United States and Canada and is the focal point for data exchange with other countries. In particular, the NNDC is responsible for the development, maintenance, coordination, promotion and distribution of the reference nuclear data base, the Evaluated Nuclear Data File/B (ENDF/B) and the Evaluated Nuclear Structure Data File (ENSDF).

The NNDC assists applied and basic research scientists by coordination of interlaboratory groups of experts to provide recommended values for nuclear data. There are two major efforts coordinated by the NNDC: (1) the Cross Section Evaluation Working Group (CSEWG) consisting of representatives from over 20 U.S. laboratories, meeting annually to develop an internationally recognized data base for nuclear energy applications; and (2) the U.S. Nuclear Data Network, consisting of low energy nuclear physics information centers, meeting annually to develop an internationally recognized data base for nuclear energy research. These coordinated efforts unite and integrate data compilation and evaluation efforts to achieve maximum utilization of manpower. The NNDC also coordinated the Medium Energy Nuclear Data Working Group (MENDWG) to discuss the overlapping interlaboratory, interagency and international interest in medium energy nuclear data.

The NNDC exchanges experimental data freely with other nuclear data centers throughout the world. The principal centers in the world, in addition to the NNDC, are the Nuclear Energy Agency Center near Saclay, France, the International Atomic Energy Agency (IAEA) Center in Vienna, Austria, and the U.S.S.R. Centers at Obninsk and Kurchatov. The data files are used extensively in support of the ENDF effort.

International nuclear structure and decay evaluations are coordinated by the

NNDC under the auspices of the IAEA. Mass-chain evaluations are performed by the ORNL Nuclear Data Project, the Lawrence Berkeley Laboratory (LBL) Table of Isotopes project, the University of Pennsylvania, and the Idaho Nuclear Engineering Laboratory, as well as the NNDC and at laboratories in Belgium, France, Canada, U.S.S.R., Japan, Sweden, the Netherlands, the People's Republic of China, Taiwan, and Kuwait. The result of this coordinated effort is the international file of reference data for nuclear structure and radioactive decay, ENSDF.

Periodically, the Center prepares publications from its computerized data bases to aid basic research and technology development activities in the United States. The Center prepares the monthly issues of Nuclear Data Sheets (NDS) journal published by the Academic Press.

The NNDC is supported mainly by the Office of High Energy and Nuclear Physics of the DOE. It also receives support from the Office of Fusion Energy Component of DOE.

## C. Proposed Efforts of the Photon Data Section and Initial Program

The purpose of this proposed center is to provide scientists and engineers with data bases of state-of-the-art evaluated photon-interaction information. Presently there is no coordinated effort to provide a comprehensive set of data in photon-interaction physics (for 0.01 keV to GeV energies). One of the purposes of this proposal is to establish a coordination effort similar to the effort in the nuclear physics community. We feel this is imperative for continued strength in the sciences and engineering dealing with photon-atom interactions. The purpose of this program would not be to displace or absorb existing efforts to calculate, measure, or parameterize data that may be included in this data base. On the contrary, due to the enormity of the data that should be included in a complete data base, we would encourage outside development, refinement, and verification of information that could be incorporated in the proposed data bases.

The establishment of the proposed Photon Data Section (PDS) of the BNL, National Nuclear Data Center (NNDC) will provide scientists with a dynamic on-line data bases of state-of-the-art photon-atom interaction data. These data bases would utilize the already existing on-line capabilities of the NNDC that have been developed and implemented for their on-going efforts in nuclear structure and nuclear-reaction data. The proposed program would endeavor to provide, for each energy-angle-atom (and/or compounds) combination, standard reference data such as: attenuation coefficients (including EXAFS); photoelectric cross sections (including EXAFS); absorption edge jump ratios; photoelectric fluorescence yields; atomic form factors; incoherent scattering functions; coherent anomalous scattering factor corrections; oscillator strengths; oscillator densities; Auger electron yields; x-ray Raman scattering cross sections; x-ray resonant Raman scattering cross sections; Compton profiles; and absorption edge energy shifts due to matrix effects. If needed, the program would also support storage and distribution of reference spectra, as has been identified by the

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EXAFS community. Computer programs would also exist that could calculate cross sections for the interactions given the experimental geometry and polarization of the incident photons [Ha90]. A library of computer programs could also be maintained for analyzing and predicting spectra. This latter aspect is particularly important in cases such as Compton profile measurements where there are several different methods of calculating distributions none of which is simple. In EXAFS this is important since the development of computer codes is in its early stages. There is also a need for standardizing analyses. An important aspect of the program would be an effort to provide estimates of the accuracy of all of the data in the data bases and a means to provide information as to the sources of the data. One aspect of the present NNDC program that has been successful is the maintenance of an annotated bibliography of references on which the data is based.

The efforts of the PDS will need to include not only the data base management; but also evaluation of the data contained in the data base; computation of theoretical data; development of scaling techniques; development of techniques to properly utilize the data; assessment of accuracy of the data; working with end users to properly utilize the data bases; identification of areas where data are insufficient or conflicting; and maintenance of a photon interaction library. Depending on the needs and demands of the user community the PDS would also act as a depository of reference spectra so that scientists will be able to directly compare experimental results with results of other scientists. As in the case of EXAFS, these reference spectra would also be used in the analysis of other data. Presently the NNDC acts as a depository of spectra for the nuclear physics community as an alternative to journal publication of the spectra. This system has been well accepted by scientific journals.

The main advantage of on-line data base approach is that the available information can be maintained as state-of-the-art data bases. There are presently several programs within the U.S.A. and around the world to re-measure interaction data

[Cr87a, Gr90] and to develop better methods for calculating many of the interactions. With the on-line system the improvements can be incorporated and made available as the data are released, and errors that may have been included in the data can be corrected as they become known. The success of the PDS requires that the staff not work in isolation from the user community. The staff will be encouraged to work with both end users and scientists providing the data for inclusion in the data base. This will assure that the information is in forms that are most useable to the community and that the data is inputted correctly. Effort will also be required in order to deal with, not only free-atom information, but also, as best as possible changes in the basic data arising from matrix effects. With the growing use of synchrotron radiation other effects such as polarization of the incident beam must also be incorporated into the system.

It is proposed that the initial efforts of the PDS program will be directed towards the needs of the EXAFS community (which is not exclusive of the needs of other disciplines). This is because of the large number of users and their articulation of their needs of the EXAFS Standards Data Base as described in the Report of the International Workshop on Standards and Criteria in X-Ray Absorption Spectroscopy held at BNL, March 7-9, 1988 [Ly89]. If approved the following approach will be taken:

1. Compile measured spectra for reference compounds and spectra appearing in publications. The compilations will have a standard format and contain documentation that describes the experimental conditions and analysis. Clerical and physical checking of the data will be performed to ensure accuracy.

2. Store data from state-of-the-art calculations.

3. Store evaluated data that comprise the experts' best estimate of the result of several independent measurements of the same quantity.

4.     Availability of tested software packages for distributed use or centralized access.

5.     If demanded, the bibliography to photon-interaction data, on both measurements and theory will be indexed for current awareness and keyword searching.

6.     On-line access to data and computer codes. Proprietary interests can be protected by tailoring access privileges to authorization codes.

7.     A Review Committee for EXAFS data will be established to recommend priorities for the PDS and to monitor progress.

One of the principal investigators (S.P.) is head of the Division of the NNDC within the BNL Department of Nuclear Energy. He has 26 years of experience with the NNDC (23 years as division head). Because of this he has accumulated considerable expertise in operations of the Center, data base management, theoretical and experimental data evaluation, and national and international coordination efforts. The other principal investigator (A.L.H.) has more than 8 years professional experience with x-ray physics. This experience has included developing analytical techniques (experimental) using synchrotron radiation and developing mathematical techniques for calculating cross sections for the scattering of highly polarized x rays from beams into finite solid angles.

## D. Budget

The proposed startup staffing is:

| FTE* | Function |
|---|---|
| | Data Compilation |
| $\frac{1}{2}$P | Current |
| $\frac{1}{2}$P | Retrospective |
| 1S | Theory, evaluations and reference spectra |
| $\frac{1}{2}$S | System Design and Development |
| 1P | Programmer |
| 1S | Bibliographic File |
| $\frac{1}{4}$S | Users Services |
| $\frac{1}{2}$P | Users Services |
| 1O | Data Services Assistant |
| $\frac{1}{4}$S | Consultants |
| | Travel |
| | Materials |
| | Computer |
| | |
| | Total |

*S: Scientist, P: Professional. O: Other

It is expected that we will be able to hire Mr. J. Hubbell. NIST, Ret., in the first year as a part time consultant to expedite incorporation of the former NIST program into the PDS.

The program outlined is ambitious and would require additional staffing. In the second year at least 1 FTE scientist will be added along with visiting scientists and post-graduates resident at the PDS.

At the present time no funds are requested for an experimental program. The desirability and scale of such a program will be assessed in the future. If an experimental program is deemed necessary for adequate progression of the program, funds will be requested at that time.

# Appendix

In this section we will provide a short review of some of the interactions of eV to GeV photons with atoms. A major part of this discussion is to emphasize the shortcomings of the present data and some sources of error in the interaction data. This appendix is to emphasize that the level of accuracy and present level of knowledge of information is not at a level that many scientists and engineers require.

## A. Elastic Interactions

### A.1. Rayleigh (Coherent) Scattering

Rayleigh scattering, being coherent, requires a momentum transfer with no energy transfer. That is, only the direction of the photon propagation is changed as a result of the interaction. There are numerous approaches for calculating the Rayleigh scattering cross sections for atoms. As it stands to date, even the most rigorous methods do not fully account for the effects of matrices on the atoms.

### A.1.a. Atomic Form Factor Approximation

The atomic form factor (AFF) approximation to the Rayleigh scattering of photons by atoms is the simplest and most widely used approximation today. It assumes that the Rayleigh scattering cross section can be described as a product of the Thomson cross section and the square of the AFF, $f(q, Z)$:

$$(\frac{d\sigma}{d\Omega})_R = f^2(q, Z)(\frac{d\sigma}{d\Omega})_{Th} \tag{2}$$

where q is the magnitude of the momentum transfer between the initial photon and the electron. It can be written then as the difference between the momenta of the incident and scattered photons: $\hbar\vec{q} = \vec{k}_o - \vec{k}$. Since in coherent scattering there can be no energy transfer, $|\vec{k}_o| = |\vec{k}|$, and $q$ can depend only on the change of angle. The magnitude of $q$ for coherent scattering is written in terms of the incident photon energy $E_o$: $q = \frac{2E_o \sin\frac{\theta}{2}}{m_o c^2}$. (This should not be confused with the "x" parameter that many

of the form factor tables use where $x = \frac{\sin\frac{\theta}{2}}{\lambda} = 20.60744q$.) Even though the form factor, $f$, for each element relies on only a single parameter, $q$, this approximation gives reasonable results over a moderately large dynamic range of momentum transfer values. However, as will be discussed later there are significant energy-angle regimes where this approximation does not work well at all, especially when using x-ray tubes, synchrotron radiation, and other "low" energy photon sources. These sources are singled out since the energies of the photons can easily be near absorption edges of elements in the sample.

The Thomson cross section describes the simple classical dipole interaction between a free electron and the electric field of a photon. The Thomson cross section is the square of the classical electron radius, $r_o^2$, weighted by the probability of the photon to change the direction of it's electric field vector: $\cos\alpha = \vec{e}\cdot\vec{e}_o$. Here $\vec{e}_o$ is the electric field vector of the incident photon and $\vec{e}$ is the electric field vector of the scattered photon. The Thomson cross section is:

$$(\frac{d\sigma}{d\Omega})Th = r_o^2 \cos^2\alpha \tag{3}$$

If we start with a beam of polarized photons that has 100% of the electric field vectors $\vec{e}_o$ pointing in the same direction then the "parallel" cross section (scattering measured in the $\vec{e}_o$ plane) is:

$$(\frac{d\sigma}{d\Omega})Th,\| = r_o^2(\cos^2\theta) \tag{4}$$

and in the "perpendicular" direction:

$$(\frac{d\sigma}{d\Omega})Th,\perp = r_o^2 \tag{5}$$

Here $\theta$ is the traditionally defined scattering angle, the angle between the propagation vectors of the incident and scattered x rays ($\cos\theta = \vec{k}\cdot\vec{k}_o$). If the fraction of photons with parallel polarization is $P_\|$, the fraction of photons that have perpendicular

polarization is $P_\perp = 1 - P_\parallel$ and the cross section is:

$$\left(\frac{d\sigma}{d\Omega}\right)_{Th} = P_\parallel \left(\frac{d\sigma}{d\Omega}\right)_{Th,\parallel} + P_\perp \left(\frac{d\sigma}{d\Omega}\right)_{Th,\perp} \tag{6}$$

With this definition (not to be confused with the "traditional" definition of polarization $P = \frac{P_\parallel - P_\perp}{P_\parallel + P_\perp}$) incident photons are completely unpolarized when $P_\parallel = P_\perp = 0.5$ (or when $P = 0$):

$$\left(\frac{d\sigma}{d\Omega}\right)_{Th} = \frac{r_o^2}{2}(1 + \cos^2\theta) \tag{7}$$

The AFF approximation assumes that for a given element, the interactions are dependent only on the momentum transfer, $q$. In this approximation it is assumed that matrix effects such as diffraction can be calculated independently. In this approximation it is also assumed that the incident photons are high enough in energy that anomalous (near edge) effects are not significant.

Since the AFF approximation is so widely used, considerable effort has been made to calculate $f(q, Z)$ as accurately as possible. To fully understand the limitations and potential problems of this approach, we should note that the true definition of $f$ is not a description of electron densities, but is a fudge factor defined as the ratio of the Rayleigh to Thomson cross section:

$$f^2(q, Z) = \frac{\left(\frac{d\sigma}{d\Omega}\right)_R}{\left(\frac{d\sigma}{d\Omega}\right)_{Th}} \tag{8}$$

It is claimed that $f(q, Z)$ can be calculated by integrating the probability ($U(r)dr$) of finding an electron between $r$ and $r + dr$ over all $r$. This calculation is made for each state, $n$, using a first-order perturbation theory, usually a Hartree-Fock approach with some assumed atomic potential. This is a variational approach where the perturbation is the electric field potential of the photon. For a charged particle in a perturbing electromagnetic field, the contribution to the Hamiltonian for the perturbation [He47] is:

$$H' = \sum_k \frac{e}{m_o c^2}(\vec{p} \cdot \vec{A}) - \frac{e^2}{m_o c^2}A^2 \tag{9}$$

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where $\vec{p}$ is the momentum of the electron and $\vec{A}$ is the vector potential of the perturbing electromagnetic field. The wave functions are calculated for each electron starting from state $n$ and ending in state $m$. For Rayleigh scattering $n$ must be equal to $m$, otherwise there is energy transfer and the scattering cannot be coherent. This is usually denoted with a subscript $n, n$. The form factor for the entire atom is then summed over all states. Since the probability function, $U(r)dr$, is the probability of finding the electron between $r$ and $r + dr$ it is related to the electron density function, $\rho(r)dr$, as:

$$U(r)dr = 4\pi r^2 \rho(r)dr \tag{10}$$

The normalization is set up so that after summing over all states:

$$4\pi \int_0^\infty r^2 \rho(r)dr = Z \tag{11}$$

The form factor is then the Fourier transform of the electron density function for each state $n$:

$$f_{n,n}(q, Z) = \int_0^\infty \rho_{n,n}(\vec{r}, Z)e^{i\vec{q}\cdot\vec{r}}d\vec{r} \tag{12}$$

For the case where atom's electron charge density has spherical symmetry:

$$f_{n,n}(q, Z) = 4\pi \int_0^\infty r^2 \rho_{n,n}(r, Z)\frac{\sin(qr)}{qr}dr \tag{13}$$

The form factor for the entire atom is summed over all states:

$$f(q, Z) = \sum_n f_{n,n} \tag{14}$$

With this method the value of $f(q, Z)$ is always real and positive with values varying from $f(0, Z) = Z$ to $f(\infty, Z) = 0$. This approach was used to generate the most commonly used tabulations of $f$ [Cr68, Hu75].

Even though the AFF approximation requires $E_o >> E_b$, where $E_b$ is the binding energy of the electron, it has been shown not to be valid when $E_o > 500$ keV [Go68]. In order to deal with this problem, the modified form factor (MFF)

was developed in which the wave function is weighted with $\frac{mc^2}{E-V(r)}$ where E is the relativistic total energy of the bound electron ($E \approx m_0c^2 + E_b$) and $V(r)$ is the central potential. Schaupp, et. al., [Sc83] presented calculated values for MFF's for all of the elements. They noted this MFF is still limited to forward angles. As an example, for outer shell electrons $\theta < 77°$ for 1 MeV photons, 36.1° for 2 MeV photons, 14.2° for 5 MeV photons, 7.1° for 10 MeV photons, and 3.6° for 20 MeV photons. Because of the severe limitations of the MFF approximation, the Schaupp tables provided form factors with the K shell electrons removed so that more accurate models of the interactions with the K shell electrons can be included as these models are developed. In the Schaupp tables, they also presented differences between the MFF and the AFF values by Hubbell, et al., [Hu75, Hu79] for 10 elements. When $x = (\frac{\sin\frac{\theta}{2}}{\lambda} =)50\overset{\circ}{A}^{-1}$ the differences were at least 100% and for the case of aluminum the difference was 2000%.

A more rigorous, but of course much harder and computationally more time consuming, approach to calculating the Rayleigh scattering cross sections is the S-matrix approximation. This was originally worked on by Brown, et al., [Br55] and Johnson, and co-workers [Jo68, Fe69, Li75]. The most rigorous version was put forth by Kissel, et al., [Ki80]. In [Ki80] it was stated that one of the reasons for working on this approach was the lack of accuracy of the AFF approximation noted by experimentalists. This method is computationally time consuming enough that Kissel et al., presented calculations for only selected elements and for only the K and L shells. Their results are very promising and would provide bench marks for a modern version of scattering function tabulations.

One of the aims of the PDS is to maintain a dynamic data base so that real improvements in the libraries can be made available as the data become available. One approach to developing a modern version of the AFF and MFF tables is to utilize results from all three methods where it can be determined to be valid. The AFF or

MFF values would probably be used for the outer shell electrons and the S-matrix values would be used for the inner shell electrons. This is possible since the total atom form factor is the summation of form factors for all electrons. The dynamic nature of the proposed data base would allow the community to aid in the determination of which approach appears to provide the most accurate data. Sometimes in the efforts to develop new computational methods, the "improved" data may not be as accurate as the prior data. One classic example was the effort by Hubbell and Øverbø [Hu79] recalculate the form factors with relativistic corrections. Six years later it was shown that these corrections actually made the values of the form factors less accurate since according to Kissel and Pratt [Ki85] the magnitude of the relativistic corrections are "canceled" by other neglected corrections. Since the data in the data base will contain a certain level of errors, we would emphasize to the end-user the expected level of accuracy of the data in the library and would also note sources of the numbers and if the data has been bench marked by other methods.

According to the AFF approximation all of the polarization information is contained in the $\cos^2 \alpha$ term of equation (6). This approximation predicts that if the photons are 100% polarized, then the scattering in the plane of polarization is 0 directly into $90°$. Kissel, et al, [Ki80] showed, using the S-matrix approximation, that this differential cross section is not necessarily zero for the scattering directly into $90°$ so the polarization effects are not well understood. Further work along this line has been carried out by Roy et al, [Ro86] but there is little information in this field as of today. This aspect is very important with the ever increasing use of the inherently polarized synchrotron radiation for probes of matter.

## A.1.b. Anomalous (Near Edge) Scattering

If we return to the form factor approximation, we remember that a photon induces the target electron to oscillate. If the energy of the photon (or in this case probably better to think in terms of photon's frequency) is of the order of the fre-

quency of an absorption edge, a natural vibration state is matched. In this case first-order perturbation theory is not valid. In the manner of calculating $f$ described above the results are always real and positive. However as in any wave propagation and in oscillating systems, $f$ is in reality a complex number. The relative magnitude of the complex component depends on the proximity of the incident frequency to the oscillator (the electron). In general, when the energy is far above the energy of the absorption edge, the relative magnitude of the anomalous correction is small. One method of accounting for the anomalous scattering is to write the form factor as:

$$f(q, E_o, Z) = f_o(q, z) + f'(q, E_o, Z) + if''(q, E_o, Z) \qquad (15)$$

where $f_o(q, Z)$ is the form factor as calculated above. Equation 15 is written in a manner that illustrates the energy dependence of the coherent scattering factor when anomalous corrections are included. This is important since the single parameter, $q$, dependence cannot describe the anomalous corrections. This approximation is based on the per electron form factor near an edge, $n$ [Ja62]:

$$f_e = \frac{\omega^2}{\omega^2 - \omega_n^2 - ik\omega} \qquad (16)$$

This is strictly for a dipole oscillator whose natural frequency is $\omega_n^2$ with a damping factor $k$. For a bound state $k$ is related to the level width, $\Gamma$.

Since $f$ is a complex number, the effects from scattering around an absorption edge can be utilized in crystallography for studying specific atoms in a matrix. The traditionally defined geometrical structure factor is a measure of particular atoms located in a cell in a manner to cause diffraction. If $h$, $k$, and $l$ are the Miller indices of the crystal cell and $u_n, v_n$ and $w_n$ represents the location of a specific atomic specie in the cell, then the geometrical structure factor is:

$$F_{hkl} = \sum_n f_n(q, Z) e^{[2\pi i(hu_n + kv_n + lw_n)]} \qquad (17)$$

Now both the geometrical structure factor and the modified AFF are imaginary so effects of atomic specie can be preferentially enhanced by tuning the radiation to an absorption edge of element $n$.

In his review article Helliwell [He84] discussed how the enhancement, or suppression, from the complex components can be utilized to study small amounts of a specific element in a large organic matrix. This is effected by tuning the incident radiation energy to match the absorption edge of the element being studied. Helliwell points out that there are tabulations of theoretical $f'$ and $f''$, but these values are not applicable near the absorption edge. As an example he mentions that Pt in $K_2Pt(CN)_4$, has a $f''$ of 19 electrons by experiment and only 9 electrons by theory. This illustrates a need for a data base containing experimental and theoretical values of $f'$ and $f''$ as they are investigated. Accurate values of $f'$ and $f''$ are required for normalization of experimental data.

As with the other aspects of photon interactions, there are several approaches to calculating $f'$ and $f''$. One such approach uses the dipole approximation [Ka86, Cr87b]:

$$f'' = \frac{\pi}{2}\omega \sum_k (\frac{dg}{d\omega})_k \tag{18}$$

$$f'(\omega) = \frac{2}{\pi} \int_0^\infty \frac{\omega' f''(\omega')}{\omega'^2 - \omega^2} d\omega' \tag{19}$$

where $\omega$ is the frequency of the incident photons and $\omega_\kappa$ is the frequency of the absorption edge of the $\kappa^{th}$ shell. Again frequency is used to emphasize the concept of matching natural frequencies of the system. Note that this approximation does not show the damping term of equation 16. Close to the absorption edge, this damping cannot be ignored. For a review of other theories for determining $f'$ and $f''$, see [Cr87b].

The term $(\frac{dg}{d\omega})_\kappa$ is the oscillator density of states for the $\kappa^{th}$ shell. As will be discussed later, the PE effect is also proportional to $(\frac{dg}{d\omega})_\kappa$, so $f''$ is directly propor-

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tional to the PE energy absorption coefficient:

$$f'' \propto \mu(E)_i E_i \qquad (20)$$

or in terms of photon frequency:

$$f'' \propto \mu(\omega)_i \omega_i \qquad (21)$$

It is also interesting to define $f_A = f' + if''$, then

$$|f_A| = \sqrt{f'^2 + f''^2} \qquad (22)$$

$$f'^2 + if''^2 = |f_A|(\cos \delta + i \sin \delta) = |f_A|e^{i\delta} \qquad (23)$$

With this $\delta$ is the phase shift from this scattering:

$$\delta = \frac{f''}{f'} \qquad (24)$$

There are two parameters of the anomalous contributions that need to be understood before they can be properly utilized. The first is the obvious magnitude of the corrections and the other is the width of effects.

Tabulations of $f'$ and $f''$ were generated by Cromer and Liberman [Cr70] using the optical theorem [Ja62]. Values of the corrections were calculated for specific energies of commonly used x-ray tube anodes. Being a dipole approximation these values increasingly suffer in accuracy as the energy of the photon approaches the energy of the absorption edge. Cromer and Liberman [Cr81] recalculated some of the terms on the low energy side of the edges to account for some of the short comings of the dipole approximation. These tables are the "most extensive" to date and have been deemed to be valid only when $E_o$ is not too close to $E_b$. Cromer has also provided a computer program to calculate the anomalous corrections [Cr83]. These tables indicate no angle dependence and the values were calculated for $\theta = 0°$. Kissel and Pratt [Ki85] state that the "traditional" approach to correct for the angle

dependence is to assume that $f'$ and $f''$ follow the angular dependence of $f_0$. Parker and Pratt [Pa84] showed that for low angles a better approximation is to assume $f'$ and $f''$ are independent of angle in the forward angles followed by a drop off only in the backwards angles. The latter statement was supported by Suortti, et al [Su85] who measured $f'$ for nickel at $43°$, $89°$, and $134°$ for 9 energies whose $\Delta E (= E_b - E_0)$ was between 2.7 and 289 eV. They measured no significant angle dependence of $f'$. For the lower energy photons ($30 < E_0 < 10,000 eV$) values of the anomalous corrections (which are defined slightly differently) have been given in Henke [He82].

Wang and Chia [Wa88a and Wa88b] have tested different atomic potentials to determine which provide the "most accurate" values of $f'$. Table 1 shows an illustration of three different calculations. The first calculation was by Wang and Chia using Dirac-Slater potentials, the second by Wang and Chia using Dirac-Kohn-Sham potentials, and the third by Cromer-Liberman [Cr70]. They also included values from experimental measurements. It should be understood that it is generally accepted that the Cromer-Liberman values deviate more from true values as $E_0 \rightarrow E_b$.

Table 1 Values of $f'$ for Si for Two X-Ray Energies

| | $f'_{DS}$ | $f'_{DKS}$ | $f'_{CL}$ | $f'$ (exp) |
|---|---|---|---|---|
| Ag $K_\alpha$ | 0.0535 | 0.0518 | 0.042 | 0.0560± 0.0015 |
| Mo $K_\alpha$ | 0.0834 | 0.0810 | 0.072 | 0.0858± 0.0012 |

A second illustration of the variations is presented in table 2, which shows differences between the Wang and Chia [Wa88a] calculated $f'$ values for some light elements compared to Cromer and Liberman [Cr70]. It should be noted that these values are for energies "far" in energy from the absorption edges.

The data base that needs to be established then would include the magnitude of the correction factors along with the widths of the effects; for each element and

Table 2 Values of $f'$ for Different Energies and Atoms

The first number is [Wa88a] and the second is [Cr70]

|    | Ag K$_{\alpha 1}$ | | Mo K$_{\alpha 1}$ | | Cu K$_{\alpha 1}$ | | Fe K$_{\alpha 1}$ | | Cr K$_{\alpha 1}$ | |
|----|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| F  | 0.0106 | 0.006 | 0.0183 | 0.014 | 0.0756 | 0.069 | 0.108 | 0.100 | 0.138 | 0.129 |
| Na | 0.0221 | 0.0126 | 0.0367 | 0.030 | 0.137 | 0.0129 | 0.188 | 0.180 | 0.231 | 0.223 |
| Si | 0.0532 | 0.042 | 0.0830 | 0.072 | 0.256 | 0.244 | 0.323 | 0.311 | 0.365 | 0.355 |
| Cl | 0.100 | 0.084 | 0.148 | 0.132 | 0.358 | 0.348 | 0.380 | 0.375 | 0.333 | 0.335 |
| K  | 0.139 | 0.118 | 0.200 | 0.179 | 0.380 | 0.365 | 0.298 | 0.286 | 0.0831 | 0.070 |
| Ca | 0.161 | 0.137 | 0.227 | 0.203 | 0.372 | 0.341 | 0.186 | 0.163 | -0.191 | -0.221 |

its associated ionic and chemical states. As information concerning the magnitude of the effects are honed down, we can then work on parameterizing and scaling these magnitudes so that they can be used for analyses of experimental data.

Equations 20 and 21 illustrate that the anomalous scattering is related to the photoelectric cross sections. Since above the absorption edge the cross section is modulated with fine structure (EXAFS) the anomalous corrections also exhibit this fine structure. As in EXAFS the anomalous scattering can be used to determine the interatomic distances and coordination numbers for specific elements in a matrix. However, the information that can be extracted by studying the anomalous scattering is not limited to crystalline materials and has been used to extract structural information on disordered and amorphous systems [Dr84, Fu81, La87, Lu87, Sh77, Te82, Te88].

The use of anomalous scattering factors to study atomic distances is beginning to be used also in the study of enzymes and proteins [Po90], along with X-ray absorption spectroscopy (XAS). The inter-atomic distances in enzymes and proteins can include distances that are well beyond the few angstrom limit ($<10$Å) of the XAS techniques. The anomalous scattering can be used from the XAS limit to approximately 1500Å.

## B. Inelastic Interactions

### B.1. Photoelectric Effect

The photoelectric (PE) effect is probably the most studied and well understood of the photon-atom interactions. For elements with Z>20 [Mc69] the PE effect is in general the dominant interaction for all but the most forward angles and for most photon energies less than 50 keV. It then becomes less dominant as $Z \rightarrow 1$. The PE effect occurs when the energy of a photon is completely absorbed by a bound electron. This electron is ejected to the continuum and is "lost" to the atom. This of course leaves an ion in an excited state, i.e. with an inner shell vacancy. The ion then de-excites by an outer electron filling the vacancy. The energy released by this transition is carried off by one or more outer shell electrons or by emitting a characteristic x ray. The characteristic x ray has an energy equal to the difference between the initial electron's energy state and the energy state of the vacancy.

The general form of the PE cross section for each shell, $n$, with a binding energy of $E_{b,n}$ follows, to a first-order approximation: $\sigma_n = (\frac{E_{b,n}}{E})^s \sigma(E_{b,n})$ when $E_o > E_{b,n}$ and $\sigma_n = 0$ when $E_o < E_{b,n}$. The value of $s$ ranges between 2.75 and 3 [Ja81]. As was discussed in the review by Jackson and Hawkes, [Ja81] there are several lengthy approximations for calculating the photoelectric cross section. The simplest form is to write the cross section in terms of the oscillator density, $(\frac{dg}{d\omega})_n$, which is a representation of the transition probability from state $n$ into the continuum.

$$\sigma_n = \frac{2\pi^2 e^2}{mc} (\frac{dg}{d\omega})_n \tag{25}$$

The oscillator density is related to the oscillator strength $g_n$ which describes the number of oscillators free to absorb the radiation of frequency $\omega$. The oscillator strength is normalized such that:

$$Z = \sum_n g_n \tag{26}$$

One of the "standard" references for photoelectric effect cross sections was a table generated by J.H. Scofield [Sc73]. In this table Scofield calculated the cross

sections using the relativistic Hartree-Slater model. This model assumes there are no interactions between the electrons in the atom. The electrons are dependent only on the central potential of the atom. Scofield later stated that this is a major source of errors [Sc87].

The probability of an electron leaving the atom is modulated by the potential fields of neighboring atoms. This modifies the oscillator densities and cross sections. This modulation is known as the EXAFS (extended x-ray absorption fine structure) and occurs in the hundreds of eV above the absorption edge. Closer to the edge, within tens of eV, the probability of ejecting the electron can be modified by the shifts due to chemical bonding (known as XANES). From this, the oscillator strengths and oscillator densities are themselves important numbers and will be seen again in the next few sections. Good tabulations of recommended values for free elements and compounds need to be established.

Another area where the "best" information for the PE effects needs to be tabulated and constantly updated is in the energy shifts of the absorption edge due to chemical bonding. This information is critical in the experimental fields of EX-AFS, XANES, and chemical speciation (determination of the chemical states of the elements). It is also important for testing theoretical models of the atomic system [De86]. When one scans the energy of a monochromatic beam of photons over an absorption edge of an atom, theory tells us there is no contribution to the absorption below the edge of the particular state and above the edge the electrons are resonantly excited. Chemical bonds of the elements in a matrix can cause shifts in the absorption energy as much as 20eV. By measuring the changes of absorption edges one can determine the chemical states of the elements in the matrix. Using a fluorescence probe these states can be determined even at the "high" trace level.

The fluorescence yield is a parameter that is itself interesting. It is defined the ratio of the number of fluorescent x rays from the decay of the excited states, $f_n$

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to the number of vacancies, $v_n$, created in state $n$. The fluorescence yield is defined as $\omega_n = \frac{f_n}{v_n}$. Recently Hubbell [Hu89a] published a new compilation of $\omega_i$ for each element for the K, L, and M shells. In this review he suggested no improvements over the values for the fluorescence yield over the previous values of Bambynek [Ba84] for the K shells for the elements $1 \leq Z \leq 110$. The recommended fit for this parameter is:

$$\omega_K = \frac{A}{1 + A} \tag{27}$$

$$A = [\sum_{i=0}^{3} (C_i Z^i)]^4 \tag{28}$$

For the L shells, when $Z \geq 37$, Hubbell again suggested no improvements over the fits worked out by Cohen [Co87]. For $Z \leq 36$ Hubbell suggested values for $\omega_L$ to be $1.939x10^{-8}Z^{3.8874}$. He also provided a fit to determine values of $\omega_M$. This fit is $\omega_M = 1.29x10^{-9}(Z - 13)^4$. For both L and M shells, Hubbell suggested that the fits should be considered "provisional", because of the relative uncertainty in the experimental values he had to work from. The review work of Hubbell [Hu89a], provided an annotated bibliography for work done between 1978 and 1988 (prior to 1978 are reviews by Krause [Kr79a], Bambynek, et al., [Ba72], and Fink, et al., [Fi66]). Hubbell cited a total of 89 publications of newly measured data. The conclusion is that the recommended values for fluorescence yields are still not completely worked out and need to be periodically re-evaluated. One practical application of the fluorescence yield is in "standardless" x-ray fluorescence and particle induced x-ray emission (PIXE). The purpose of the standardless analysis is to provide an analysis of the data from first principles. If the samples are geological in nature the accuracy of this method has been reported to be on the order of 20% [Su90] for the analysis of K x rays. However for the analysis of L x rays the analysis is no better than 30%.

The value of $\omega$ along with the total number of Auger electrons is essential in health physics and radiation therapy since the damage to the tumor is determined by

the number and energy spectrum of the electrons, which are the major mechanism for ionization, ejected from the atoms during the therapy. This is extremely important for the dosimetry so the dose to the tumor can be maximized (or at least well understood) while minimizing the dose to the surrounding tissue. The same is true for the radiation processing industry.

The actual value of the "jump ratio", the ratio of the cross section above and below the absorption edge, is an additional area of interest. The jump ratio is used for normalization in EXAFS, selective and difference x-ray fluorescence, x-ray absorption imaging for contrast enhancement [Ce88, Bo86], and bench marking theoretical developments. Table 3, most of which was copied from [De86], illustrates the problem in the status of the K-edge jump ratios. They reported K-edge jump ratios of argon and krypton as determined by several theories and two experiments. Added to this table are calculated values from Scofield [Sc74], and Storm and Israel [St70] and values from Veigele [Ve73], which are based on experimental data. Argon and Krypton are used since they are free monatomic atoms so they exhibit no chemical effects and no matrix induced fine structure. Most other atoms have some matrix problems and the jump ratio is much harder to define. Clearly from this table, the situation needs to be improved.

In the soft x-ray range ($< 2$keV), the photoelectric effect is in general the dominant interaction. However in this region the photoelectric absorption cross section is not well known. The first comprehensive compilation of cross sections, based on experimental data, in the 30 to 300eV region was only recently published by Henke [He82]. It has been established that this compilation which is based on experimental results has many conflicts with theoretical predictions [Sa88]. In many of the light elements there is structure just above and below the absorption edges that are not predicted by theory. This fact has prompted a comprehensive program at Lawrence Livermore National Laboratory [Gr87, Gr90] to remeasure with high precision and

Table 3. Values of K-Edge Jump Ratios for Ar and Kr. [table from De86]

|                | Ar    | Kr    |
|----------------|-------|-------|
| Sl30 (calc)    | 14.97 | 8.59  |
| Cl63 (calc)    | 17.65 | 10.99 |
| HF (calc)      | 13.40 | 8.74  |
| DF (calc)      | 13.38 | 8.64  |
| Ja81 (calc)    | 7.15  | 7.15  |
| Mc69 (calc)    | 9.91  | 7.04  |
| De83 (exp)     | 11.2  |       |
| De86 (exp)     |       | 8.6   |
|                |       |       |
| Sc73 (calc)    | 8.87  | 6.91  |
| St70 (calc)    | 9.57  | 7.19  |
| Ve73 (exp)     | 10.3  | 6.92  |

high resolution the photoelectric cross sections for low energy x rays. The expressed purpose of this work [Gr90] is to provide a base of experimental data "to prompt refinement and testing of theoretical methodologies". In the earlier paper, [Gr87], detailed absorption cross sections around the K-absorption edge of carbon were presented and it showed an enhancement of 30% in the cross section just above the edge, when compared to theoretical data. The data presented in the Saloman and Hubbell compilation [Sa88] for carbon would indicate that this is a real effect. The results presented in [Gr90] for the L-edges in the 3d transition metals, Ti, V, Cr, Fe, Ni and Cu likewise show discrepancies with theory as much as 50%. The 3d metals are problematic in that there is a 2p-3d autoionizing resonance that does not end up with a fluorescence x ray, only Auger electrons. In this paper it is emphasized that for many of these elements the measured cross sections are "consistently about 60% lower than predictions of theory which is based on a relativistic version of the Hartree-Slater model".

In this section we established that there are many sources of inaccuracies in present data tabulations. Other areas of tabulated data are not necessarily accurate to the level desired by many scientists. There are even a few areas where no tabulations

exist at all.

## B.2. Incoherent Scattering

### B.2.a. Incoherent Scattering Function Approximation

The atomic Compton (aC) scattering is more complicated than the Rayleigh scattering, hence the aC scattering cross section is harder to calculate. This is in part due to the fact that the Rayleigh scattering is characterized with momentum transfer without energy transfer and the atomic Compton scattering exhibits not only momentum transfer, but also an energy transfer from the photon to the electron, removing the electron from its bound state. The most commonly used method for calculating the overall atomic Compton scattering cross section is the incoherent scattering function (ISF) approximation, which has a direct analogy with the AFF approximation in that it assumes the differential cross section can be described as a product of the free electron Compton cross section and a function ($S(q, Z)$) describing the number of electrons that are free to incoherently scatter the photon:

$$(\frac{d\sigma}{d\Omega})_{aC} = S(q, Z)(\frac{d\sigma}{d\Omega})_C \qquad (29)$$

As with the AFF approximation, it is claimed that the ISF, $S(q, Z)$ can be calculated from wave functions of the bound electron in an atomic field perturbed by the electric field of the incident photon. One of the most commonly used methods for calculating $S(q, Z)$ is the Waller-Hartree approach, which is similar to the AFF:

$$S(q, Z) = Z - \sum_i \sum_j | < i|exp(i\vec{k} \cdot \vec{r})|j > |^2 (\frac{E}{E_o})^2 \qquad (30)$$

As in the Hartree-Fock approach, the wave functions are usually calculated with a first-order variational approach invoking some assumed atomic potential. Therefore the Rayleigh and atomic Compton scattering can be thought of as competing processes. It should be pointed out that the AFF can be written as:

$$f^2(q, Z) = \sum_i | < i|exp(i\vec{k} \cdot \vec{r})|i > |^2 \qquad (31)$$

The $(\frac{E}{E_o})^2$ term in equation 30 is not an inconsistency since $E$ is the energy of the scattered photon, and with coherent scattering (equation 31) $E = E_o$.

All of the problems with sources of error associated with the calculation of $f(q, Z)$ exist with this method of calculating $S(q, Z)$. Additional errors now creep into the calculations. The most glaring problem is that first-order perturbation theory is used to calculate the interaction probability for the removal of an electron from the system. The second is that the (free electron) Compton cross section was derived for elastic scattering but is then multiplied by the ISF, S, to describe an inelastic event. Third, the description of the scattering process depends only on the energy of the incident photon so the energy transferred to the electron and the removal of the electron is assumed to play no part in the scattering.

There is experimental evidence that the per electron scattering factor, $S_e$, is not bounded between 0 and 1, indicating flaws in the ISF approximation. Shimizu, et al., [Sh65] presented experimental values along with a theoretical model for the atomic Compton scattering of 662 keV gamma rays by the K-shell electrons of three elements, Tin, Tantalum, and Lead for 5 angles. This work illustrated that the value of $S_e$ can be substantially greater than 1, which is in direct conflict with the ISF approximation. The largest measured value of $S_e$ for scattering by lead into $100^o$ was reported to be 1.4. Kane and Prasad [Ka77] likewise presented experimental results for the scattering of 1.12MeV gamma rays by K-shell electrons of several elements. They compared their results to impulse approximation calculations of Prasad and Kane [Pr74], integrated over all available momenta, and to values of $S_{k,e}$ calculated with the formalism presented in Shimizu, et al., [Sh65]. The results are shown in table 4. The experimental values of Kane and Prasad are interesting for two reasons: First, the measured values of $S_{k,e}$ do not agree with the theoretical values. Second, the value of $S_{k,e}$ is not necessarily a consistently increasing function of $q$. Similar conflicts with the ISF approximation have been reported by other authors (for example see Ra89,

Wo89, and references therein). From the results presented in Table 4, it is apparent that considerable work is needed in order to resolve the discrepancies and to provide accurate data. These conflicting results should not be too surprising since an inherent assumption in the ISF approximation is that the energy of the incident photon is greater than the binding energy of the electron but less than 500keV. Therefore the ISF approximation needs considerable work in order for accurate data to be available to the scientific community.

Table 4. Comparison of S per K-Shell Electron as Described in Ka77

| element | $\theta$ | q | Exp: $S_{k,e} = \frac{d\sigma}{d\sigma_{KN}}$ | IA | $S_{k,e}$ (Sh65) |
|---|---|---|---|---|---|
| Sn | 25 | 0.94 | 0.71 ±0.07 | 0.97 | 1.49 |
| | 60 | 1.11 | 0.86 ±0.08 | 0.98 | 4.41 |
| | 90 | 2.30 | 0.94 ±0.08 | 0.99 | 5.77 |
| Ta | 120 | 2.49 | 0.91 ±0.26 | 0.91 | 2.74 |
| Au | 25 | 0.94 | 0.63 ±0.09 | 0.93 | 0.56 |
| | 60 | 1.11 | 0.81 ±0.09 | 0.94 | 1.58 |
| | 90 | 2.30 | 1.33 ±0.12 | 0.95 | 2.05 |
| | 100 | 2.38 | 1.44 ±0.15 | 0.94 | 2.09 |
| | 120 | 2.49 | 0.981 ±0.15 | 0.90 | 2.28 |
| Pb | 60 | 1.11 | 0.86 ±0.10 | - | 1.45 |
| Th | 25 | 0.94 | 0.40 ±0.13 | 0.90 | 0.42 |
| | 60 | 1.11 | 0.91 ±0.11 | 0.92 | 1.15 |
| | 90 | 2.30 | 1.36 ±0.12 | 0.93 | 1.49 |
| | 100 | 2.38 | 1.20 ±0.39 | 0.91 | 1.56 |

## B.2.b. Compton Profile

Atomic Compton scattering is a rather complicated process since the atomic Compton scatter distribution is not measured as a well defined "peak" but as a broad distribution. Understanding this distribution is important when the number and distribution of Compton scattered photons needs to be extracted from a spectrum. As will be discussed, the width of the distribution results from the apparent electron momentum distribution so it has become an important technique in materials science for extracting information contained in the electron momentum distribution (Compton

profile) [Co76, Co85, Ko81, Ko84, Re74].

In atomic Compton scattering, the energy transfer to the electron has the result that the energy of the scattered photon, E, is smaller than the energy of the incident photon $E_o$:

$$E = \frac{E_o}{1 + \gamma(1 - \cos\theta)} \qquad (32)$$

where $\gamma = \frac{E_o}{m_o c^2}$, $m_o$ is the rest mass of the electron and $\theta$ is the scattering angle. The spectra of Compton scattered photons is complicated because the scattering results in a broad distribution centered, but not necessarily symmetric about $E$. As mentioned before, the measured energy distribution from atomic Compton scattered photons is in part due to the electron momentum distribution (commonly known as the Compton profile) and in part due to geometrical broadening. Every detector subtends a $\Delta\theta$ which results from the detector subtending a finite solid angle and hence a $\Delta\theta$ about $\theta$ [Ha89]. Equation 32 tells us that there will be a geometrical $\Delta E$ due to the subtended $\Delta\theta$.

The simplest and most widely used method for calculating the spread in energy is the impulse approximation for the double differential scattering cross section, a simple form of which can be written as [Ca82]:

$$\left(\frac{d^2\sigma}{dE'd\Omega}\right)_{IA} = \frac{m_o r_o^2}{2|\vec{k}_o - \vec{k}'|}\left(\frac{E_o}{E'}\right)\left(\frac{E_o}{E'} + \frac{E'}{E_o} - \sin^2\theta\right)J(p_z) \qquad (33)$$

where $E_o$ is the energy of the incident photon, $E'$ is the incremental energy of the Compton scattered photons, $r_o$ is the classical radius of the electron ($r_o^2 = 0.079929b$), $p_z$ is the projection of the electron's momentum onto the Z axis, and $J(p_z)$ is the Compton profile (the electron momentum distribution).

$$p_z(a.u.) = \frac{\frac{137}{m_o}[E_o E'(1 - \cos\theta) - m_o(E_o - E')]}{|\vec{k}_o - \vec{k}'|} \qquad (34)$$

$$|\vec{k}_o - \vec{k}'| = (E_o^2 + E'^2 - 2E_o E' \cos\theta) \qquad (35)$$

This approximation requires that the energy transferred to the electron be large with respect to the binding energy of the electron. As was pointed out before (equation

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32), this criterion is angle dependent. Meeting this criteria becomes harder in the forward angles.

The Compton profile $(J(p_z))$ for the entire atom is the probability of finding an electron with the momentum $p_z$, with $z$ representing the direction of the scattered x ray, so $J(p_z)$ is the projection of the Compton profile onto the scattered photon [Ri82]:

$$p_z = \frac{\vec{p} \cdot \vec{q}}{|\vec{q}|} \tag{36}$$

$$\vec{q} = \vec{k} - \vec{k}_o \tag{37}$$

Cooper [Co76] writes this as:

$$J(p_z) = \int_{p_z} \int_{p_y} \chi^*(p_x, p_y, p_z) \chi(p_x, p_y, p_z) dp_x dp_y \tag{38}$$

where $\chi(p_x, p_y, p_z)$ is the electron wave function Fourier transformed from coordinate space into momentum space. Tables of $J_i(p_z)$ per electron for each orbital have been computed, an example of which is Biggs, et al., [Bi75] using Hartree-Fock and Dirac-Hartree-Fock wave functions calculated by Mann and Waber [Ma73a] and Mann [Ma73b]. The profile for each atom is then the sum over each electron $(n_i)$ in the atom:

$$J(p_z) = \sum_i^Z J_i(p_z) \tag{39}$$

The normalization is such that:

$$\int_{-\infty}^{+\infty} J(p_z) dp_z = Z \tag{40}$$

The contribution to the scattered photon distribution from each electron (or orbital) $J_i(p_z)$ is quasi-gaussian in shape. By summing over all states (as opposed to convoluting the distributions) we end up with a rather unique and broad distribution. The widths of each orbital's Compton profile depends strongly on the binding energy of the orbital. The more tightly bound (inner shell) electrons exhibit broad profiles. The least tightly bound (outer shell or valence) electrons exhibit narrow

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profiles. Therefore the central portion of the distribution contains the information on the valence electrons. The utilization of this information has led to a field known as Compton profile measurements where the measured photon distribution is used to ascertain information concerning the electron momentum distribution. The central portion of the distribution, being determined by the valence electrons, changes significantly with matrix, chemical, and crystalline effects.

The ready-to-use tables, tables concise enough to print, are adequate for many applications but in general are not applicable for quantitative determination of electron momentum distributions. This is because the matrix, chemical, and crystalline effects (which frequently are studied) change the distribution. These tables are usually valid only for free atoms. Because of the widespread use of Compton profile measurements, many methods of calculating the distributions, using the many and varied atomic potentials, have been developed. In order to include the chemical bonding and matrix effects in the calculated distribution, the atomic Compton scattering cross sections need to be calculated for each specific case. Most of the computational techniques use the impulse approximation (IA). There are two basic assumptions in the IA: (1) the target electron is assumed to be unbound, when compared to the photon energy, but is in motion; (2) the atomic potential does not change during the interaction because it is assumed that the electron is ejected quickly enough that the atom does not respond until the electron has left the atom.

Many papers have been written discussing the Compton profiles that have been calculated for specific materials [Ba83, Ko81, Ba85, Be75, La74, Pa86]. Many utilize a "self-consistent" approach [Ho64, Ko81, Ko65] in order to handle the differences resulting from matrix effects. In the self-consistent approach one: (1) starts with an assumed potential, V; (2) solves for the eigenvalues and then specific values of the wave functions as a function of distance from the nucleus (band structure calculations); (3) squares the wave functions to determine the electron density; (4) calculates a new

potential, V, and iterates this process until convergence.

One interesting application of Compton profile measurements has been the study of crystalline orientation (for single crystals). In this method the crystallographic orientation results in anisotropies of the measured photon distributions. The measurements are made along two directions, such as $< jkl >$ and $< j'k'l' >$. These two measured distributions are then subtracted to yield the difference profile:

$$\delta J(p) = J_{<jkl>}(p) - J_{<j'k'l'>}(p) \qquad (41)$$

The value of $\delta J(p)$ is typically on the order of a few percent [Ro87]. Measurements such as this are important for determining the quality of the calculational methods.

Bauer and Schneider [Ba85] measured Compton profiles for 412 keV x rays scattered by $< 110 >$ copper and compared the measurements to the results of three computational methods with five potential models. None of the calculations showed good agreement with heights of oscillations in the difference profiles, but all showed very good agreement with the energies of the structure, which is consistent with variational techniques. Difference profiles are usually used instead of absolute numbers since there are apparently many distinct problems associated with Compton profile measurements. Benesch and Smith [Be75] reported 25% difference between two profiles computed with a different modification to the Hartree-Fock calculation.

A second illustration of the technique was reported by Boulakis [Bo86]. In this paper he presented experimental measurements of Compton profiles from hydrogen dissolved in titanium to form $TiH_{1.98}$. These experimental results were compared to 3 calculated profiles in which the hydrogen was dissolved as a proton, neutral atom and a negative ion. There were substantial differences between the three calculations, but the results of the comparison indicated that the hydrogen behavior closer to that of the proton model than that of the other two models.

## B.2.c. Anomalous Scattering (X-Ray Resonant Raman)

The resonant inelastic scattering of x rays near to but below an absorption edge is sometimes referred to Anomalous Incoherent or X-Ray Resonant Raman Scattering (XRRS). This process is unlike coherent anomalous scattering in that there is no theoretical symmetry about the absorption edge. It only occurs on the low energy side of the resonance, for on the high energy side the excitation becomes the photoelectric effect. In short this scattering is a resonant process where the energy of the photon is not great enough to remove the electron from the atom but excitation of the atom is permitted. This is then followed by an electronic transition (to the vacancy $n$ from a higher state $n + 1$, $n + 2$, ...), with the associated x ray. For the promotion of a K shell electron, a virtual state in the K shell is created and an electron from the L or M shell fills the vacancy. For formal scattering theory, this L or M electron is considered to be the electron that scatters the photon [Ma85]. Suortti [Su87] describes the process as "There is a virtual K-shell hole in the intermediate state, and the final state is that of an L-shell hole, an electron in the continuum and an emitted photon".

This process is similar to the photoelectric effect except that the atom is not ionized. When the energy of the photon is greater than the binding energy of the electron, $E_o > E_{b,n}$, the photoelectric effect occurs and then the energy of the incident photon is less than the binding energy $E_o < E_{b,n}$, XRRS can occur. In the PE effect the energy of the photon is shared between the kinetic energy of the ejected electron, $\epsilon$ and the ionization of the atom $E_o = E_{b,n} + \epsilon$. The energy of, for example, the $K_\alpha$ radiation is then: $K_\alpha = E_{b,K} - E_{b,L} = (E_o - \epsilon) - E_{b,L}$. Since XRRS occurs when $E_o < E_{b,n}$, there is promotion of the electron (excitation of the atom), but the electron is not ejected from the atom (no ionization). The maximum energy of the scattered photon, $E_{XRRS} = (E_o) - E_{b,L}$, is then the difference between the incident photon energy and the binding energy of the electron that fills the virtual vacancy, since $\epsilon$ must be zero. This is a maximum energy since some of the energy can be shared with an Auger

electron. The scattered x-ray spectra is further complicated since the energy of this ejected electron is modulated as in EXAFS. However, this means that XRRS can provide the same type of matrix information as EXAFS provides. The methodology for an XRRS measurement would require a fluorescence type measurement, where the scattered radiation is measured.

Returning to perturbation theory, the contribution to the Hamiltonian from the perturbing electric field is [He47]:

$$H' = \sum_k \frac{e}{m_o c^2}(\vec{p}_k \cdot \vec{A}(k)) - \frac{e^2}{m_o c^2} A(k)^2 \qquad (42)$$

where $\vec{A}$ is the vector potential field of the incident photon and $\vec{p}$ is the electron momentum. The atomic Compton scattering cross section is usually calculated by using first-order perturbation theory in which only the $A^2$ term contributes. For the case of XRRS it is the $(\vec{p}_k \cdot \vec{A}(k))$ term that needs to be evaluated, but the analysis of this term requires second-order perturbation theory [Br81]. Because of the complexity of the theory, it was not predicted until 1974-1975 [Ga75]. At the same time it was measured by Sparks [Sp74] who reported a large amount of inelastic scattering of x rays when the metal targets Ni, Cu, Zn, Ge, Ta were irradiated with Cu $K_\alpha$ x rays. The energies of the Cu $K_\alpha$ x rays are just below the K absorption edges of Ni, Cu, Zn, Ge, and just below the L absorption edge of Ta. He measured cross sections as large as $7r_o^2$ and unlike atomic Compton scattering he measured no apparent angular dependence. The Sparks work prompted the theoretical analysis by Bannet and Freund [Ba75].

There are several methods that have been reported for calculating the XRRS cross sections. For metals, it is common to use $\hbar\Omega_n$ as the energy difference between the initial energy state and the Fermi energy, $E_F$, so the binding energy is $E_{b,n} = \hbar\Omega_n + E_F$. The more commonly used methods use the single electron central field approximation to describe all electronic states. One such method was presented by

Åberg and Tulkki [Ab85] who derived the expression for the double differential cross section:

$$\frac{d^2\sigma}{dE_2 d\Omega} = 2\pi r_o^2 \int_0^\infty (\frac{E_2}{E_o}) \frac{(\Omega_{1s} - \Omega_{np_j})g_{np_j 1s}(\Omega_{1s} + \epsilon)}{(\Omega_{1s} + \epsilon - E_o)^2 + (\frac{\Gamma_{1s}}{4\hbar^2})^2}(\frac{dg}{d\omega})_{1s}\delta(E_o - \Omega_{np_j} - \epsilon - E_2)dE'$$

(43)

where as with the PE cross section, $g_{np_j 1s}$ is the oscillator strength for the 1s to $np_j$ transition, $(\frac{dg}{d\omega})_{1s}$ is the oscillator density, which is proportional to the density of states, $\epsilon$ is the kinetic energy of the ejected electron, and $\Gamma_{np_j}$ is the level width (for example see [Kr79b]). In these equations $\hbar$ has been set to 1. However, Åberg and Tulkki [Ab85] point out that the one-electron approximation is not adequate to handle the problem. Suortti showed that equation 42 can be integrated to [Su87]:

$$\frac{d^2\sigma}{dE_2 d\Omega} = \frac{1}{2}r_o^2(\frac{E_2}{E_o})\frac{(\Omega_{1s} - \Omega_{2p_j})g_{1p_j,1s}(\Omega_{1s} + \epsilon)}{(\Omega_{1s} - \Omega_{2p_j} - E_2)^2 + (\frac{\Gamma_{1s}}{2\hbar})^2}(\frac{dg_{1s}}{d\omega})_{\Omega_{1s}+\epsilon}$$

(44)

The XRRS cross section contains terms that are very similar to the photoelectric cross section, so if we integrate with respect to $E_2$, the differential cross section for the K-shell excitation becomes:

$$\frac{d\sigma}{d\Omega} \approx \frac{\Gamma_{K_\alpha}}{4\pi^2(\Omega_K + E_F - E_o)}\sigma_{aK(\Omega_I + \bar{\epsilon})}$$

(45)

If we define $\Delta E = (\Omega_k - E_o)$ when $\Delta E > \Gamma_{1s}$ [Ma87],

$$\frac{d\sigma}{d\Omega} \approx \frac{\Gamma_{K_\alpha}(\Omega_{1s} + \omega)}{8\pi^2(\Delta E \omega_{1s})}\sigma_{1s}(\Omega_{1s} + \omega)$$

(46)

The properties of XRRS include: (1) It is a resonance phenomenon which occurs when the energy of the incident x rays are just below the energy of the absorption edge. (2) The cross section is related to the oscillator strength and the density of states. (3) An electron can be ejected which shares energy with the scattered photon. The energy of this electron is modulated as in EXAFS which can be measured as a modulation of the scattered photon. (4) The XRRS cross section will approximately be a mirror image of the PE cross section.

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The first high resolution (in energy) study of the effect was made with monochromatic synchrotron radiation by Eisenberger, et al., [Ei76]. Jaklevic et al., [Ja88] investigated the effect with tuned synchrotron radiation and showed that in a typical synchrotron radiation x-ray fluorescence spectra (using monochromatic radiation as opposed to "white" radiation) XRRS scattering can be the dominant feature of the spectra.

A substantial study of XRRS on xenon was made by Czerwinski, et al., [Cz85]. Xenon was chosen since it is a free, symmetric atom and is free of chemical, matrix and shape effects. Their measurements were within 5% of the cross sections calculated with the method of Tulkki and Åberg [Tu80] when relativistic and interference corrections were included. Tulkki and Åberg predicted that, to a first-order approximation, spherically symmetric atoms will resonantly scatter photons in a manner that is free of angular and polarization effects. The measurements of Czerwinski, et al., at $60°$, $90°$, and $120°$, indicated that within the 5% precision of their measurements, this is true. Schaupp, et al., [Sc84] also tested the angular dependence of x rays XRR scattered by Nd at two angles, 80 and $110°$. They likewise measured no angle dependence within the estimated 5% accuracy of their measurements.

Another recent study was made by Udagawa and Tohji [Ud88] who measured XRRS spectra Cu, CuO, and $Cu_2O$. These measurements illustrated substantial differences between the 3 compounds and showed how the spectra are dependent on the chemical form of the targets. These measurements also illustrated the evolution of the spectra as a function of incident energy.

## B.2.d. X-ray Raman Scattering

The scattering that is known as X-Ray Raman Scattering (XRS) is similar to XRRS in that an electron is promoted from an inner shell to the continuum followed by an inner shell transition. The difference is that XRS is not a resonance phenomenon and occurs when only part of the photon's energy is imparted to the electron in

promoting it. Secondly, XRS occurs when the energy of the photon is above the absorption edge. The energy of the scattered photon has a sharp rise at $E = E_o - E_{b,n}$ and the energy of the scattered photon is modulated since it can be shared with an Auger electron. The signal from this scattering process is weak but has been used to measure correlation lengths for light elements such as carbon that cannot be determined with EXAFS using keV x rays.

Theory predicts that the XRS cross section should be proportional to the photoelectric cross section and exhibit an angular correlation as [Mi67]:

$$\frac{d^2\sigma}{d\Omega d\omega} \propto (1 + \cos^2 \phi) \sin^2(\frac{\phi}{2}) \qquad (47)$$

So far most of the experiments have shown no dependence on angle [Su75, Ko80, Ka83]. Tohji and Udagawa [To87] demonstrated that XRS can be used successfully to measure the atomic distances in carbon. They measured 1.43 and 2.48 Å, which is very close to other analyses of 1.42, 2.46, and 2.84 Å. Koumelis and Londos [Ko80] also studied graphite. They measured the shift between the incident photons and the XRS distribution to be 288.3±0.6 eV for amorphous graphite and 284.9±0.5 eV for polycrystalline graphite.

## C. Nuclear Reactions

The photoelectric effect, Rayleigh scattering, and atomic Compton scattering are not the only photon-atom interactions that occur so the other interactions need to be included in the proposed on-line system. Other interactions include pair production, triplet production, nuclear Thomson scattering, nuclear resonance scattering, Delbrück scattering, and photon induced nuclear reactions. These interactions in general only occur above 100keV. Likewise, most of these interactions have small contributions to the total interaction cross sections. In the "low" energies (the transition being Z dependent) the largest contribution to the total attenuation is the photoelectric effect. In the high energy region it is pair production, and in the intermediate

region is the atomic Compton scattering.

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