Available online at www.sciencedirect.com
ScienceDirect
Nuclear Instruments and Methods in Physics Research B 261 (2007) 193–196
NIM B
Beam Interactions with Materials & Atoms
www.elsevier.com/locate/nimb

Whole-atom Compton scattering cross-sections and individual shell cross-sections for the biological elements in the energy region from 1 to 4 keV

D.V. Rao [a,*], T. Yuasa [b], T. Akatsuka [b], G. Tromba [c], T. Takeda [d], R. Cesareo [e], A. Brunetti [e], G.E. Gigante [f]

[a] Department of Physics, Sir C.R.R. College, Industrial Estate, Eluru 534007, Andhra Pradesh, India
[b] Department of Bio-Systems Engineering, Faculty of Engineering, Yamagata University, 4-3-16 Jonan, Yonezawa, Yamagaa 992-8510, Japan
[c] Synchrotron Radiation for Medical Physics, Elettra, Basoviza, Trieste 34012, Italy
[d] Institute of Clinical Medicine, University of Tsukuba, Tsukuba, Ibaraki 305-8575, Japan
[e] Instituto di Fisica e Mathematica, Universita di Sassari, Sassari, Via Vienna, Sassari 2-07100, Italy
[f] Dipartimento di Fisica, Universita di Roma "La Sapienza", Ple A. Moro 2, Rome 00185, Italy

Available online 22 April 2007

Abstract

Whole-atom Compton scattering cross-sections are evaluated for selected biological elements in the energy region from 1 to 4 keV and from 5 keV to 10 MeV, for the other elements. These cross-sections were calculated within the non-relativistic impulse approximation. The Compton profiles utilized here were taken from the tables of Biggs et al. Total cross-section for fixed incident photon energy were obtained by summing the sub-shell contributions.

PACS: 32; 32.80.Cy; 32.90.+a; 33.90.+h

Keywords: Whole-atom; Compton; Biological elements; Double differential scattering cross-section; Impulse approximation; Compton profile

1. Introduction

Of all the possible types of keV photons with matter, photoelectric effect, Rayleigh and Compton scattering are important in the X-ray region for medical and biological applications. In all these cases, the photons interacting with the sample and reaching the detector contribute to background. Among these interactions the Compton scattering is usually the most significant one.

Compton scattering is produced by the interaction of a photon with a electron usually assumed to be initially at rest and free. The probability of a Compton interaction is described by the Klein–Nishina formula [1]. The Compton scattered photon energy is Doppler broadened by the pre-collision motion of the bound electron. It is necessary to take this binding effect into account when carrying out a precise simulation of low energy transport. Due to the electron binding effect, a part of the broadened spectrum is suppressed and results in a reduction in the total Compton scattering cross-section. A modification of the angular distribution is obtained by integrating the broadened spectrum of the scattered photon energy; the reduced total Compton scattering cross-section is obtained by integrating the modified angular distribution of the Compton scattered photon. Compton scattering of X-ray photons is a potential tool for the determination of bone mineral content or tissue density for dose planning purposes and requires knowledge of the energy distribution of the X-rays scattered through various biological materials of medical interest in the X-ray region. Compton scattering causes

* Corresponding author. Tel.: +91 8812 230084; fax: +91 8812 233471.
E-mail address: donepudi_venkateswararao@rediffmail.com (D.V. Rao).

0168-583X/$ - see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.nimb.2007.04.194

inner shell ionization similar to photoelectric absorption. This type of scattering cross-section will also be used in other branches of physics, in which the momentum distribution of electrons in atoms, molecules and condensed matter are studied. For example, close to excitation thresholds and in situations of small scattering angles one should

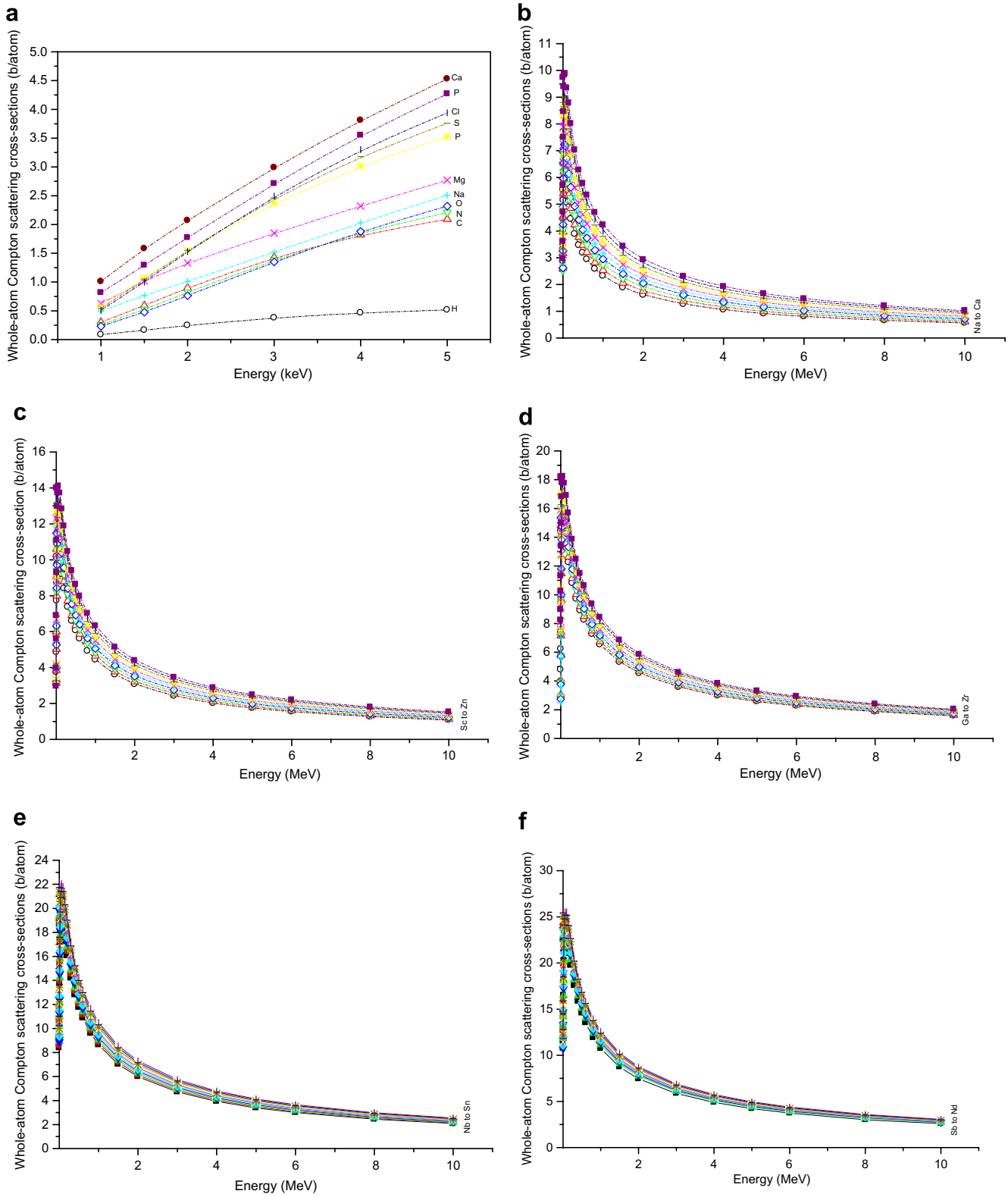

Fig. 1. (a)–(i). Variation of the whole-atom Compton scattering cross-section with energy, for few biological elements in the energy region from 1 to 4 keV and from 5 keV to 10 MeV for the other elements up to U.

expect deviations from simple impulse approximation in the form of many-body effects and final state effects such as in extended X-ray absorption fine structure.

In view of above, we evaluated the whole-atom Compton scattering cross-sections for selected biological elements in the energy region from 1 keV to 4 keV and from 5 keV to 10 MeV, up to U. These cross-sections are calculated within the non-relativistic impulse approximation, utilizing the tabulated values of the Compton profile [2]. The shape of the profile is sensitive to the valencies of the electrons in the atoms and can also give some information about molecular structure. Although it is used to determine the electron momentum distributions in condensed matter physics, little attention is focused for its use in medical applications. For example, most biological and phantom materials of medical interest contain varying proportions of the biological elements. It is an attempt to know the effect of Doppler broadening for single atoms, many of which constitute the biological materials. One particular area of interest for these values is in Monte Carlo simulation of photon transport in applications of medical physics. Further, to generate the tables of whole-atom Compton scattering cross-sections and cross-sections for the individual shells for the elements covering a wide range of energies. X-ray absorption coefficients of light elements (H, C, N and O and many of these constitute the soft-tissue) are extremely small. This type of new table is not available in the literature and will be useful for comparison, compilation and simulation purposes for medical and biological applications [3,4].

2. Theoretical methods

The Compton equation assumes that the collision electron is initially unbound and at rest. However, in a real material, the momenta of the bound electrons give rise to a range of possible

$$\begin{aligned} d^2\sigma/d\Omega'\, d\omega_2 = (r_0^2/2)m(\omega_2/\omega_1)((\omega_1^2+\omega_2^2-2\omega_1\omega_2 \\ \times \cos(\theta))^{0.5})^{-1}X(\omega_1/\omega_2+\omega_2/\omega_1 \\ -\sin^2(\theta))J_i(p_z) \end{aligned} \quad (1)$$

energies ω_2 for fixed ω_1 and angle θ, which is refered to as Doppler broadening. The impulse approximation gives

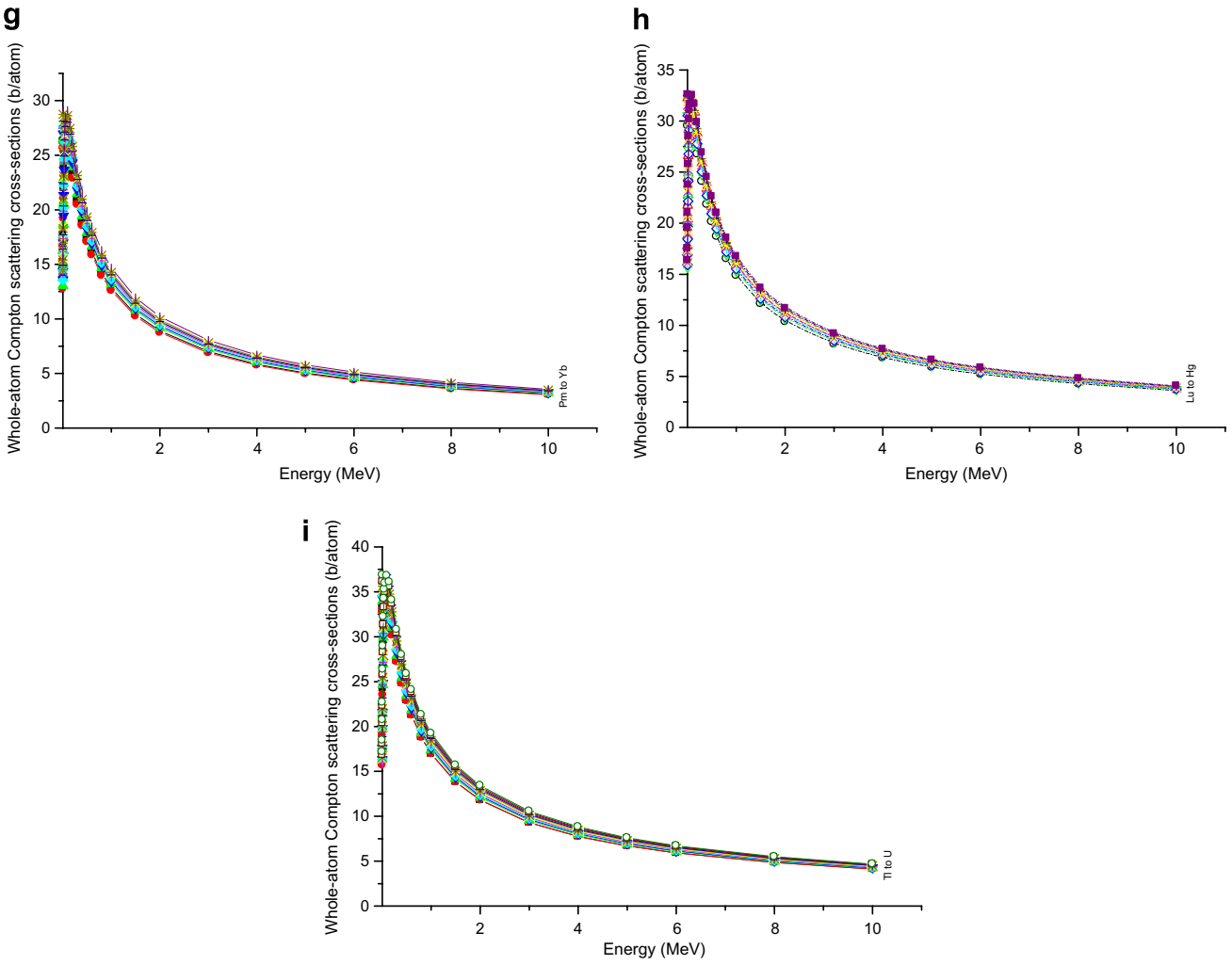

Fig. 1 *(continued)*

double differential scattering cross-section for scattering at an angle θ per solid angle $d\Omega'$ and $d\omega_2$. In this equation, r_0 is the classical electron radius, ω_1 and ω_2 are incident and the scattered photon energies for an electron at rest in keV, θ is the scattering angle, $J_i(p_z)$ is the Compton profile of an electron in the ith shell and p_z is the projection of the recoil electron momentum on the scattering vector, which bisects the incident and scattered photon vectors. The value of p_z and ω_2 are evaluated using the following expressions.

$$P_z = \omega_1\omega_2(1-\cos(\theta)) - m(\omega_1-\omega_2) \left[(\omega_1^2+\omega_2^2-2\omega_1\omega_2\cos(\theta))^{0.5}\right]^{-1} \quad (2)$$

$$\omega_2^c = \omega_1[1+(\omega_1/m_0c^2)(1-\cos(\theta))]^{-1} \quad (3)$$

The whole-atom differential scattering cross-sections including the number of electrons in the individual shells is evaluated using the following relation

$$d^2\sigma/d\Omega'\,d\omega' = \sum N_i(d^2\sigma/d\Omega'\,d\omega')_i \quad (4)$$

where N_i is the number of electrons in the $i$sth shell.

3. Results

Theoretical scattering cross-sections estimated with the use of Eqs. (1)–(4) are displayed in Fig. 1. Whole-atom Compton scattering cross-sections for selected biological elements in the energy region from 1 to 4 keV are presented in Fig. 1(a) and for the other elements, up to U, in the energy region 5–10 MeV are presented in Figs. 1(b)–(i).

Acknowledgements

One of the authors (D.V.R.) under took part of this work with a financial assistance from ICTP, Trieste, Italy and Department of Bio-System Engineering, Yamagata University, Yonezawa 992-8510, Japan. In addition, the potential author (DVR) would be very grateful to Prof. Dr. G. Furlan, ICTP, Trieste, Italy, for continuous encouragement and help throughout the study.

References

[1] O. Klein, Y. Nishina, Z. Phys. 52 (1929) 853.
[2] F. Biggs, L.B. Mendelsohn, J.B. Mann, Atom. Data Nucl. Data 16 (1975) 201.
[3] D.V. Rao, T. Takeda, Y. Itai, T. Akatsuka, R. Cesareo, A. Brunetti, G.E. Gigante, J. Phys. Chem. Ref. Data 31 (3) (2002) 769.
[4] D.V. Rao, T. Takeda, Y. Itai, T. Akatsuka, R. Cesareo, A. Brunetti, G.E. Gigante, J. Phys. Chem. Ref. Data 33 (2004) 627.