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The Energy Dependence of the Photoelectric Attenuation Coefficient of Substances

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Abstract

Introduction: The photoelectric attenuation coefficient of substances is known to depend upon the energy E of the photon and the effective atomic number of substances (Z_{eff}) as (Z_{eff}^{x}/E_{y}). No definitive values about these indices x, y are given in the literature. The index x is said to lie between, 3.0 and 4.0, while for 'y' different values have been assigned, between 3.0 and 4.0.

Methodology: We followed a methodology to find both the exponent y explicitly, from a formula which does not contain x. Through this way, the risk of one parameter leading to an estimation error for the other is automatically eliminated. With the value of y being unmistakably established, we determined the exponent x for different elements.

Results: It was found from the NIST data that 'y' = 3.0669 for most substances with low atomic number but no single value can be assigned for the exponent 'x'.

Conclusions: These results help us to perform model calculations for the attenuation coefficients of different substances. They can also provide important inputs for the diagnostic purposes in the DECT method.

Keywords

X-ray, Photoelectric effect, Attenuation coefficient, Photon energy

Introduction

The principle of Dual Energy Computed Tomography (DECT) which is now emerging as a very important tool for non invasive diagnosis, is based on the determination of mass attenuation coefficient of substances, at different energies [1-4]. The mass attenuation coefficient of any substance consists of the contributions from the Compton scattering part and from photoelectric effect. The Compton scattering is dependent linearly on the electron density ρ_e. The photoelectric part, on the other hand, depends on the product $\{\rho_e (Z_{eff}^{x})/E^{y}\}$, where the effective atomic number Z_{eff} and the exponents 'x' and 'y' are to be precisely defined. The importance of these quantities will be understood from what follows.

For hydrogen, it can be shown theoretically, that, y=7/2 and x=4.0. But the literature of medical physics is replete with various choices, $3.0 \leq y \leq 3.5$ and $3.0 \leq x \leq 4.0$. With such wide choice of the two parameters 'x' and 'y', various data can be "satisfactorily fitted". However, it also leaves wide gaps in our understanding and thus may act as a serious impediment for the design of effective and accurate inversion procedures.

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We describe here a strategy for accurately finding 'x' and 'y'. We begin by first defining some important physical quantities.

Theoretical Background

Let us consider an atom A_i, with atomic number Z_i, then the total scattering cross section for a photon of energy E is given by [5,6],

$$\sigma_i(E) = \frac{8\pi}{3} r_e^2 f_{KN}(E)\, Z_i + \left(\frac{256\,\pi}{3}\right)\left(\frac{1}{137}\right) a_0^2 \left(\frac{I_0}{E}\right)^y (Z_i)^{[x(i)+1]} \quad (1)$$

where the first term gives the contribution from Compton scattering, with $f_{KN}(E)$ as the Klein-Nishina factor and the second term denotes the contribution from the photoelectric effect. In the second term we have I_0 (= 13.5 eV) denoting the ionization energy of hydrogen from the first Bohr orbit, r_e (= 2.82×10^{-13} cm) the classical electron radius, a_0 (= 5.29×10^{-9} cm) denoting the first Bohr radius of hydrogen and $x(i)$ an exponent, which is characteristic of the atom[5,6]. The Klein Nishina factor is given by [5-7],

$$f_{KN}(E) = \left(\frac{3}{4}\right)\left\{\left(\frac{1+\gamma}{\gamma^3}\right)\left(\frac{2\gamma(1+\gamma)}{1+2\gamma} - \ln(1+2\gamma)\right) + \frac{1}{2\gamma}\ln(1+2\gamma) - \frac{1+3\gamma}{(1+2\gamma)^2}\right\} \quad (2)$$

with $\gamma = E / mc^2$, m being the mass of the electron and c the velocity of light in vacuum, with mc^2 = 511.8 keV.

Now, suppose we have a collection of molecules, designated by j, with the formula, $\sum n(j,i)\, A_i$, where A_i denotes different types of atoms in the molecule and let there be $v(j)$ molecules of type j per unit volume of the substance. Then the linear attenuation coefficient of the substance, for x-rays is obtained by adding the contributions from the different chemical constituents. This is given by,

$$\mu(E) = \sum_j v(j) \sum_i n(j,i)\, \sigma_i(E) = \mu_{Compton}(E) + \mu_{Photo}(E) \quad (3)$$

where, in terms of the electron density (ρ_e = number of electrons per unit volume), we can write,

$$\mu_{Compton}(E) = \left(\frac{8\pi}{3}\right) r_e^2\ f_{KN}\ (E)\ \rho_e \quad (4)$$

and the photoelectric part is given by,

$$\mu_{Photo}(E) = \left(\frac{256\,\pi}{3}\right)\frac{1}{137} a_0^2 \left(\frac{I_0}{E}\right)^y F \quad (5)$$

with

$$F = \sum_j v(j) \sum_i n(j,i) Z_i^{x(i)+1} \quad (6)$$

We now give below, a method to estimate the electron density from the density (mass per unit volume of the substance). Consider $c(j)$ as the concentration of the component j in the mixture (number of molecules of j/the total number of molecules), then in terms of the density ρ of the system (mass per unit volume) we can write,

$$\rho_e = \frac{\rho}{m_p} \frac{\sum_j \sum_i c(j) n(j,i) Z_i}{\sum_j \sum_i c(j) n(j,i) A_i} \quad (7)$$

where Z_i is the atomic number and A_i is the atomic weight of the i^{th} atom and m_p is the mass of the proton. It is clear that in terms of the $w(j)$, i.e. the weight/weight concentration of the j^{th} component, we have, $c(j) = w(j) / M(j)$, where $M(j)$ is the molecular weight of the j^{th} component. We further define an effective atomic number Z_{eff} as,

$$Z_{eff}^p = \frac{\sum_j \sum_i c(j) n(j,i) Z_i^{p+1}}{\sum_j \sum_i c(j) n(j,i) Z_i} \quad (8)$$

where $p \geq 1$. The quantity Z_{eff} is thus a weighted average of the atomic number, giving a higher weightage on atoms with higher Z. Having thus defined Z_{eff}, the next question to be asked is: "What power of Z_{eff} does the photoelectric attenuation coefficient follow?" In order to describe this power law dependence, we define an exponent x, so that,

$$F = \rho_e Z_{eff}^x \quad (9)$$

Thus, we obtain Z_{eff}^{x} from Eqs. (8) and (9),

$$Z_{eff}^{x} = \frac{\sum_j c(j) \sum_i n(j,i) Z_i^{x(i)+1}}{\sum_j c(j) \sum_i n(j,i) Z_i} \quad (10)$$

The quantity Z_{eff} is defined by Eq. (8) (by assuming a value for p), the value of the exponent 'x' then automatically follows, so as to satisfy Eqs. (9) and (10). Alternatively, one can assign a fixed value for x, and then the value of Z_{eff} follows from Eqs. (9) and (10) (again assuming a value for p). In our paper, we shall follow the former approach, i.e., define Z_{eff} using Eq. (8), and then allow 'x' to follow Eq. (9). It is clear from the above definition that for a compound or for mixtures of compounds, the value of Z_{eff} changes for different choices of p. Various authors have used different values for p and hence different values appear in the literature for the Z_{eff} of a given compound [7,8]. This is so even for water, which is accepted as a standard. In the present paper, we shall use p = 4.0. This choice, though ad hoc, has been made in view of the fact that for a hydrogen-like atom, the theoretical prediction for the photoelectric attenuation coefficient goes as ($\rho_e Z^4$) [5,7]. It is thus clear from the above discussions, that we can write the linear attenuation coefficient of substances to be,

$$\mu(E) = \sum_j \nu(j) \sum_i n(j,i) \sigma_i(E)$$
$$= \left(\frac{8\pi}{3}\right) r_e^2 f_{KN}(E)\, \rho_e + \left(\frac{256\pi}{3}\right) \frac{1}{137} a_0^2 \left(\frac{I_0}{E}\right)^y \rho_e\, Z_{eff}^{x} \quad (11)$$

This will be used in the analysis of the problem of the photoelectric part of the attenuation coefficient of mixtures.

Estimate for the exponent y

As can be seen, the photoelectric part of the attenuation coefficient depends strongly upon the values of x and y. Simultaneous determination of both the unknown exponents x and y from the experimental data may give rise to cross interference. It is hence advisable to derive an equation, in which one of the parameters (say x) has been eliminated. We are then left with an equation with a single unknown, i.e. y. We then use the data in this single parameter equation to find the parameter y. Once the value of y is fixed, the value of x can then be calculated subsequently [9].

Equation (11) suggests that at any given energy, the contribution from the photoelectric part can be estimated by subtracting the Compton part from the known total linear attenuation coefficient of the substance. As can be seen, the contribution from the Compton scattering can be accurately calculated from the first term of Eq. (11), by knowing the density and the chemical formula of the substance. This would give, at any given energy,

$$\Delta\chi(E, Z_{eff}) \equiv \left[\frac{\mu}{\rho}\right] - \left[\frac{\mu}{\rho}\right]_{compton} = \left(\frac{\rho_e}{\rho}\right)\left(\frac{256\,\pi}{3}\right)\left(\frac{1}{137}\right) a_0^2 \left(\frac{I_0}{E}\right)^y Z_{eff}^{x} \quad (12)$$

We now define the ratio $R(E, E_0 : Z_{eff})$ to be as given below.

$$R(E, E_0 : Z_{eff}) = \frac{\Delta\chi(E, Z_{eff})}{\Delta\chi(E_0, Z_{eff})} = \left(\frac{E_0}{E}\right)^y \quad (13)$$

Hence, on taking the log of both sides of Eq.(13), we have,

$$\log\left[R(E, E_0 : Z_{eff})\right] = y \log(E_0) - y \log(E) \quad (14)$$

We note that the operations, given above allow us to arrive at Eqs(13,14) in which the exponent x has been eliminated. This equation contains only one unknown, i.e. y. By calculating $\Delta\chi(E, Z_{eff})$ and $R(E,E_0: Z_{eff})$ for different substances (of low effective atomic number, $6 \leq Z_{eff} \leq 8$), we find the unmistakable feature that for any given energy, the ratio $R(E,E_0 :Z_{eff})$ is independent of the substance (i.e. independent of Z_{eff}). The plot of log [$R(E, E_0: Z_{eff})$] versus log (E) would then give us the value of y. We also thus see that equation (13) and (14) are independent of Z_{eff} and hence of the mate-

rial. A least square fit of the data with Eq(14) will give us the value of the exponent y.

It is also to be emphasized that to obtain the calculated values of the mass attenuation coefficient for substances, the Compton scattering part of Eq. (11) has been evaluated by using the Klein-Nishina formula as in Eq. (2). The importance of this complete expression for the Klein-Nishina formula can be seen from Fig. 1. In conventional calculations one uses $f_{KN}(E) = 1.0$ identically for all energies. As can be seen from Fig. 1, these will give rise to large errors when we work with higher energies, as many CT machines do.

Determination of 'x'

It is easy to see that, for any substance with molecular weight M and total number of electrons being Z_{tot} we can write, $(\rho_e/\rho) = (1/m_p)(Z_{tot}/M)$. It then follows from (12), that

$$\Delta\chi(E, Z_{eff}) = \frac{1}{m_p}\frac{256\pi}{3}\frac{a_0^2}{137}\left(\frac{I_0}{E}\right)^y \left[Z_{eff}(j)\right]^x \quad (15)$$

with the uncertainty in the value of y being removed, it would be possible to unmistakably establish the dependence on Z_{eff}. This is achieved as follows. Having determined 'y' to be y=3.0669, we use this value in Eq. 15, to find the value of 'x' for different substances. The "data", as before, should be taken from the NIST tables.

Results and Discussions

The standard results given in the NIST tables allow us to calculate the values of the exponents 'y' and 'x', which are used to describe the photoelectric attenuation coefficient of substances. From a least square fit of the values tabulated from the NIST data, with Eq. 14, it is found that the quantity 'y' is remarkably independent of the substance under study and can be assigned a value y=3.0669 for substances when Z is less than 8.0. This is shown in Fig. 2. For substances with higher Z, there may be a marginal increase in the value of this exponent but this has a small effect on biological substances, which are generally made up of substances with low atomic number.

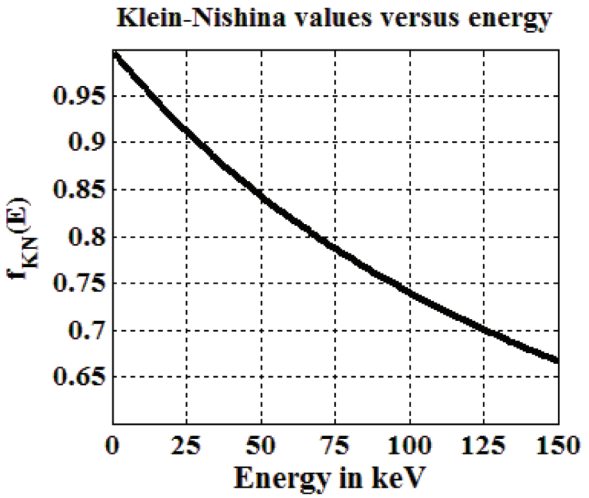

FIG 1: The Klein-Nishina coefficient fKN (E) versus Energy

Once the value of y is found, the value of x can be found using Eq. (15). The value of the exponent 'x' is, however, not a universal constant for different substances. It is seen that for a given substance, 'x' has a slight change with energy but different substances can have different values of 'x' and the exponent x is higher for higher Z values. What is clear, however, from the analyses, is that the value of x is much less than the values quoted in the literature. These results are shown in Table 1.

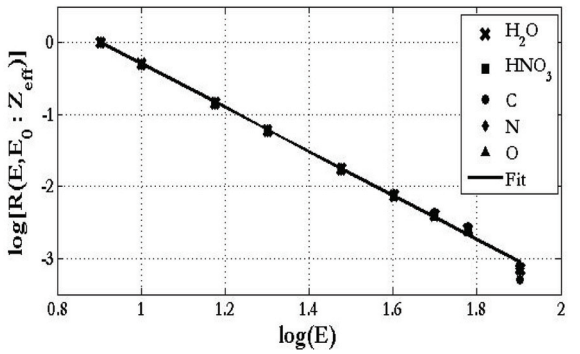

FIG 2: The log[R(E, E0 : Zeff)] versus log(E) plot, where E is in keV and E0 = 8 keV. The mass attenuation coefficient data from the NIST tables are correct up to 4 significant digits. This gives an error of only 0.1% in the values of log[R(E, E0 : Zeff)], which are plotted in the curve but cannot be seen.

TABLE 1: The values of the photoelectric exponent '*x*' for different elements at different energies are shown in this table. The value of the mass attenuation coefficient has been calculated by using y=3.0669 and $x = x_{average}$

Substance	Carbon	Nitrogen	Oxygen	Sodium	Phosphorous	Potassium	Calcium
Calculated $\mu(8)/\rho$	5.0788	8.1099	12.3127	32.3828	86.9416	179.7992	215.4145
Standard $\mu(8)/\rho$	4.5760	7.5620	11.6300	30.1800	76.5999	146.9000	172.6000
x_{match}	2.4823	2.5526	2.6001	2.6754	2.7100	2.7117	2.7104
Calculated $\mu(10)/\rho$	2.6561	4.1850	6.3050	16.4245	43.9458	90.7849	108.7523
Standard $\mu(10)/\rho$	2.3730	3.8790	5.9520	15.5700	40.3500	79.0700	93.4100
x_{match}	2.4748	2.5485	2.5994	2.6825	2.7252	2.7334	2.7336
Calculated $\mu(15)/\rho$	0.8989	1.3398	1.9511	4.8635	12.8012	26.3090	31.4936
Standard $\mu(15)/\rho$	0.8071	1.2360	1.8360	4.6940	12.3900	25.0300	29.7900
x_{match}	2.4657	2.5409	2.5955	2.6896	2.7447	2.7634	2.7658
Calculated $\mu(20)/\rho$	0.4791	0.6615	0.9145	2.1151	5.4012	10.9919	13.1402
Standard $\mu(20)/\rho$	0.4420	0.6178	0.8651	2.0570	5.3520	10.9300	13.0600
x_{match}	2.4677	2.5400	2.5942	2.6923	2.7534	2.7785	2.7824
Calculated $\mu(30)/\rho$	0.2637	0.3163	0.3892	0.7300	1.6790	3.2920	3.9147
Standard $\mu(30)/\rho$	0.2562	0.3066	0.3779	0.7197	1.7000	3.4130	4.0800
x_{match}	2.4915	2.5520	2.6014	2.6973	2.7620	2.7933	2.7990
Calculated $\mu(40)/\rho$	0.2083	0.2301	0.2603	0.3970	0.7909	1.4590	1.7193
Standard $\mu(40)/\rho$	0.2076	0.2288	0.2585	0.3969	0.8096	1.5410	1.8300
x_{match}	2.5309	2.5774	2.6179	2.7048	2.7678	2.8013	2.8076
Calculated $\mu(50)/\rho$	0.1858	0.1968	0.2120	0.2775	0.4770	0.8146	0.9479
Standard $\mu(50)/\rho$	0.1871	0.1980	0.2131	0.2804	0.4916	0.8679	1.0190
x_{match}	2.5824	2.6108	2.6408	2.7154	2.7736	2.8071	2.8136
Calculated $\mu(60)/\rho$	0.1735	0.1797	0.1885	0.2229	0.3378	0.5312	0.6092
Standard $\mu(60)/\rho$	0.1753	0.1817	0.1907	0.2268	0.3494	0.5678	0.6578
x_{match}	2.6357	2.6473	2.6692	2.7284	2.7800	2.8123	2.8191
Calculated $\mu(80)/\rho$	0.1591	0.1617	0.1653	0.1757	0.2242	0.3049	0.3394
Standard $\mu(80)/\rho$	0.1610	0.1639	0.1678	0.1796	0.2324	0.3251	0.3656
x_{match}	2.7552	2.7361	2.7331	2.7596	2.7953	2.8223	2.8289
$x_{average}$	2.5429	2.5895	2.6280	2.7050	2.7569	2.7804	2.7845

Conclusion

The paper has addressed the problem of attenuation coefficient of substances and separately analyzed the contributions arising from the Compton scattering and photoelectric effect. It has been pointed out that in order to estimate the Compton scattering part, the entire Klein Nishina formula has to be considered. It is clear that by using the low energy approximation, $f_{KN}(E) = 1.0$, as is usually done in the literature, the Compton scattering part is grossly overestimated. This paper, in section I, also gives an unambiguous method by which the effective atomic number has to be

estimated. These steps lead to the important identification that for most substances the energy dependence of the photoelectric part goes as $E^{-3.0669}$, the exponent given above being a universal quantity. Assuming that the photoelectric contribution has a dependence, $f_{photo}(E, Z_{eff}) \sim E^{-y} Z_{eff}^{x}$, we find that the exponent 'x' is dependent on the energy and is also different for different substances. These considerations enable us to perform model calculations for various substances of interest and their importance in inversion of DECT data will be demonstrated in future contributions.

Acknowledgements

Ms. Rezvan Ravanfar Haghighi would like to thank Shiraz University of Medical Sciences for granting study leave and constant encouragement in the present work. The authors would like to acknowledge the help that she received from the Indian Institute of Astrophysics during her recent visit to the institute. The Indian Council of Medical Research is thanked for financing the project.

References

1. Rutherford RA, Pullan BR, Isherwood I. Measurement of effective atomic number and electron density using an EMI scanner. Neuroradiology. 1976;11(1):15-21.
2. Heismann BJ, Leppert J, Stierstorfer K. Density and atomic number measurements with spectral x-ray attenuation method. J Appl Phys. 2003;94(3), 3, 2073-79.
3. Bazalova M, Carrier JF, Beaulieu L, Verhaegen F. Dual-energy CT-based material extraction for tissue segmentation in Monte Carlo dose calculations. Phys Med Biol. 2008;53(9), 2439-2456.
4. Ying Z, Naidu R, Crawford CR. Dual energy computed tomography for explosive detection. J Xray Sci Technol. 2006;14:235-256.
5. Agarwal BK, X-Ray Spectroscopy, An Introduction, Springer-Verlag, Heidelberg, 1991.
6. Jackson DF, Hawkes DJ. X-ray attenuation coefficient of elements and mixtures Phys Rep. 1981;70(3):169-233.
7. Johns HE, Cunningham JR. Physics of radiology, Charles C. Thomas Publisher, Springfield, 1983.
8. Khan FM, The physics of radiation therapy, Baltimore: Williams and Wilkins, 1994.
9. Bevington PR. Data reduction and error analysis for the physical sciences. McGraw and Hill, New York, 1969.
10. Hubbell JH, Seltzer SM. Table of X-ray mass attenuation coefficients from 1keV to 20MeV for elements Z=1 to 92 and 48 additional substances of dosimetric interest. available at http://physics.nist.gov/PhysRefData/Xcom/html/xcom1.html. accessed on:?