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# Determination of effective atomic number and effective electron densities of some inorganic compounds for compton effect in the gamma energy range 280KEV to 1115KEV

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# ABSTRACT

In this paper, we report the effective atomic number and effective electron densities of some inorganic compounds at three scattering angles  $60^{\circ}$ ,  $80^{\circ}$  and  $100^{\circ}$  on a goniometer assembly for Compton Effect in the gamma energy range 280keV to 1115keV. An ORTEC model 23210 gamma-x high purity germanium detector (HpGe) has been used to record the data along with a personal computer based MCA in the angular region  $50^{\circ}$ - $110^{\circ}$ . It is observed that the effective atomic numbers can be obtained by simply adding the Z-values of the constituent elements as per the chemical formula of the compound in accordance with the literature [5]. The results so obtained with respect to the inorganic samples of interest that the effective atomic number and effective electron densities are first of their kind at these energy ranges and are expected to be important in a variety of applications of Radiation Physics and Chemistry.

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# Introduction

Increased use of radioactive isotopes in various fields of science and technology warrants a need for a detailed knowledge of the processes involved in the interaction of gamma rays with matter. In the energy region 200keV to 1500keV, the most dominant mode of interaction of gamma rays with matter is the incoherent (Compton) scattering by atomic electrons.

The interaction of gamma rays with elements and other materials is usually understood in terms of quantities such as mass attenuation coefficient, the differential incoherent scattering cross sections, mass energy absorption coefficient, effective atomic number  $Z_{eff}$ , electron density  $N_{eff}$  and Compton profiles etc.

In the energy region 2MeV down to about 200keV, Compton scattering process is known to be a significant contributor to gamma ray interaction with materials.

The effective atomic number  $Z_{eff}$ , indicates on an average, the number of electrons of the material that actively participate in the photon- atom interaction. It depends on the incident energy as well as the atomic number of the constituent elements. The value of  $Z_{eff}$  also finds its use in the computation of other useful quantities like the absorbed dose and built up factor.

The electron density  $N_{eff}$  is the measure of the probability of an electron being present at a specific location.

The precise knowledge of effective atomic number and electron density are used in radiation dosimetry and medical imaging, when the cross sectional anatomy is generated by computer tomography (CT) scan. The knowledge of effective atomic number and electron density of the biologically important compounds is necessary in the energy range of medical interest [4]. Hence, a good knowledge of these parameters of the materials in this energy region will be quite useful. A literature survey reveals the fact that, the measurement of the effective atomic numbers and electron densities of inorganic compounds of present interest are relatively scarce. Hence we felt that, it is worthwhile to determine the effective atomic numbers and electron densities of some inorganic compounds such as LiOH, NaF, NaCl, NiO, CuCl, KBr and AgCl at three incident gamma ray energies 279.1keV, 661.6keV and 1115.5keV and three scattering angles of 60<sup>0</sup>, 80<sup>0</sup> and 100<sup>0</sup>. **Theory** 

# In the impulse approximation, the observed differential bound electron incoherent scattering cross section $\sigma_b(\theta)$ per atom can be expressed in terms of the KN cross-sections $\sigma_{KN}(\theta)$ per electron and the incoherent scattering function S(X,Z); whose

value is a measure of the electron binding effects in the atom as  

$$\sigma_b(\theta) = \sigma_{KN}(\theta) S(X,Z)$$
 (1)

Here,  $X = (Sin (\theta/2)/\lambda (\mathring{A}))$ , where  $\lambda$  is the wavelength corresponding to the incident photon.

When the scattering electron is completely free from atomic binding effects, S(X, Z) = Z. With binding effects it will be slightly less than Z. Thus for larger scattering angles and energies in the present study, since the electron binding effects are quite negligible, (1) can be rewritten as

$$\sigma_b(\theta) = \sigma_{KN}(\theta)Z \tag{2}$$

In eq.(2), if the scatterer is a pure element, then Z is its atomic number, If the scatterer is a composite material such as a chemical compound or a mixture then Z is its effective atomic number,  $Z_{eff}$ .

# Procedure to evaluate effective atomic number, $~~\mathbf{Z}_{eff}$

In the present study, first, the Klein-Nishina formula [1] was used to calculate the theoretical differential free electron scattering cross sections,  $\sigma_{KN}(\theta)$ , at six scattering angles,  $\theta = 50^{\circ}$ ,  $60^{\circ}$ ,  $70^{\circ}$ ,  $80^{\circ}$ ,  $90^{\circ}$  and  $100^{\circ}$  for three gamma ray energies E= 279.2keV, 661.6keV and 1115.5keV. Further, ln-ln plot of

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values of  $\sigma_{KN}(\theta)$  versus energy E in keV produces straight lines with the slope  $k_{\theta}$  (table 1) at each scattering angle of interest (figure 1). Based on these plots, by a proper regression analysis, a handy and convenient expression of the form was obtained.

$$\sigma_{KN}(\theta) = 403.567 E^{-\kappa_{\theta}} \tag{3}$$



However, its only limitation was that it could yield the

values of  $\sigma_{KN}(\theta)$  only at specific angles  $\theta = 50^{\circ}$ ,  $60^{\circ}$ ,  $70^{\circ}$ ,  $80^{\circ}$ ,  $90^{\circ}$  and  $100^{\circ}$ . It would be more beneficial if eq (3) could be further modified suitably so that it can yield  $\sigma_{KN}(\theta)$  values at any angle amenable for measurement in the range  $50^{\circ}$ - $100^{\circ}$ . For this purpose, the  $k_{\theta}$  values were once again plotted versus the scattering angle  $\theta$ . (figure 2). It was found by a suitable curve fitting procedure a second order polynomial of the form

$$k_{\theta} = a + b\theta + c\theta^2 \tag{4}$$

Table 1 . Scattering angle  $\theta$ , and values of  $k_{\theta}$ 



If  $\sigma_b(\theta)$  can be experimentally determined for the sample of interest at any angle  $\theta$  in the range 50<sup>0</sup> - 100<sup>0</sup> in this energy grid [2, 3], then the  $Z_{eff}$  of the sample can be determined by using equations 1 and 2 via equations (3) and (4).

# Procedure to evaluate Effective electron density, $N_{\text{eff}}$

The electron densities  $N_{eff}$ , have been calculated based on the expression [4] for effective electron density as  $N_{eff} = (N_A Z_{eff}) / A_{eff}$ , Where  $N_A$  is the Avogadro number in and  $A_{eff}$  is the effective atomic weight, which is the molecular weight of the sample divided by the total number of all kind of the atoms present [4]. **Experimental details:** 

In the present investigation, the effective atomic number and effective electron densities are determined on a goniometer assembly by making use of the <sup>137</sup>Cs radioactive source emitted gamma radiations of 661.6keV. It was procured in the form of a radiographic capsule from Radiochemical Centre, Amersham, U.K. The experimental setup was as shown in figure 3. The experiment was repeated with the other sources <sup>203</sup>Hg and <sup>65</sup>Zn which emit 279.1keV and 1115.5keV gamma rays respectively which were procured in the form of radiographic capsules from the Bhabha Atomic Research Centre, Mumbai, India.



Figure 3: The experimental setup used

An ORTEC model 23210 gamma-x high purity germanium detector has been used to record the data along with a personal computer based multi channel analyzer. The solid inorganic compounds were ground into a fine powder form and molded in the form of pellets of equal dimensions. The thickness of the samples so prepared ranged from 32 to 52 g /cm<sup>2</sup>. The purity of the samples was 99.0% and above as quoted by the suppliers.

In the present study, the effective atomic numbers  $Z_{\rm eff}$  were determined by using the measured values of differential incoherent scattering cross sections as per references [2,3] for some inorganic samples. The list of the inorganic samples used, their molecular formula, molecular weight, percentage purity and the manufacturers are listed in the table 2. The effective atomic numbers were further used to determine the effective electron densities  $N_{\rm eff}$  of the same samples.

Table 2 . Purities and molecular weights of the compounds

Sl	Compound	Molecular	Percentage	Manufacturers		
No		weight	purity			
1	LiOH	23.95	99.00	Sarabhai-Merck		
				Pvt., Ltd		
2	NaF	41.99	99.00	E.Merck,		
				Germany		
3	NaCl	58.44	99.00	Sarabhai-Merck		
				Pvt., Ltd		
4	NiO	74.69	99.80	British Drug		
				Houses, Ltd		
5	CuCl	99.00	99.00	British Drug		
				Houses, Ltd		
6	KBr	119.00	99.99	Reidel, West		
				Germany		
7	AgCl	143.32	99.00	British Drug		
	~			Houses, Ltd		

In the calculation, first, we have measured the differential incoherent scattering cross sections of the inorganic compounds at the scattering angles  $60^{\circ}$ ,  $80^{\circ}$  and  $100^{\circ}$  on a goniometer assembly [2, 3] for gamma rays of radiation energy 279.1keV, 661.6keV and 1115.5keV emitted by  $^{203}$ Hg,  $^{137}$ Cs and  $^{65}$ Zn sources and the results so obtained are used in the equation (1)

and (2) via equations (3) awed (4) to determine  $Z_{\rm eff}.$  In the second part of the calculation, the same  $Z_{\rm eff}$  were used to get their Effective electron densities (electrons/gram)  $N_{\rm eff}.$ 

## **Results and Discussion:**

In the present work, it was essential to assess the extent of approximation on Z<sub>eff</sub> rendered as a result of using equation (2) in place of equation(1) (treating the electron binding effects as negligible). This was done by determining the value of S(X, Z) at each X value corresponding to the scattering angle and incident energy. In the present study, the value of X was in the range 9.5  $\mathring{A}^{-1}$ - 68.9  $\mathring{A}^{-1}$  for the angles in the range 50<sup>°</sup>- 100<sup>°</sup> and energies in the grid 279.1keV- 1115.5 keV respectively. From the tabulated data of Hubbell et al [1] (please refer figures 45 and 47 of this reference) it was observed that the quantity (S(X, Z)/Z)remains almost a constant ( $\approx$  1) beyond X=9.5 Å<sup>-1</sup>. However at X=9.5 Å<sup>-1</sup> the error due to this free electron approximation on Z<sub>eff</sub> was estimated by using the Hubbell et al [2] tables to be about 0.8% for Z=26 and it increased to about 2% for Z=82. However for other X values of the present work, this error was negligible for all Z in this range.

Table 3: Effective atomic number of samples and Effective electron density (electrons/gram) (Experimental errors are to the extent of 2–3%).

Inorganic	279.1 keV		661.6 keV		1115.5 keV			Mean	N <sub>eff</sub> *E24		
compound	<b>60</b> <sup>0</sup>	80 <sup>0</sup>	<b>100<sup>0</sup></b>	60 <sup>0</sup>	80 <sup>0</sup>	100 <sup>0</sup>	60 <sup>0</sup>	80 <sup>0</sup>	<b>100<sup>0</sup></b>	Z <sub>eff</sub>	
LiOH	12.1	11.8	11.9	12.3	12.1	12.2	11.7	12.0	11.9	12.0	0.906
NaF	20.2	19.6	19.8	20.5	20.2	20.3	19.5	20.0	19.9	20.0	0.574
NaCl	28.3	27.4	27.6	28.2	28.3	28.4	27.3	27.9	27.9	27.9	0.575
NiO	36.4	35.2	35.6	36.9	36.5	36.5	35.2	35.9	35.8	36.0	0.581
CuCl	46.5	45.0	45.5	46.2	46.6	46.7	44.8	45.9	45.8	45.8	0.559
KBr	54.4	52.8	53.3	55.4	54.7	54.9	52.7	54.0	53.8	54.0	0.547
AgCl	63.9	62.4	63.1	65.6	64.8	65.0	62.4	63.9	63.7	63.9	0.537

From table 3, it was interesting to note that the  $Z_{eff}$  for a given sample was almost a constant at all angles and energies of present interest. The arithmetic average of all the  $Z_{eff}$  values of each sample at all the angles and energies of present interest have been tabulated in table 3. It can also be observed that among the various inorganic samples studied while LiOH

possessed the lowest  $Z_{eff}$  of 12, AgCl exhibited the highest  $Z_{eff}$  of 63.9 for Compton effect. It is also observed that for Compton effect in the present energy region of interest, the effective atomic number of the samples used can be obtained by simply adding the Z-values of the constituent elements as per the chemical formula of the compound [5].

The effective electron densities of the samples ranged from minimum  $0.537 * 10^{24}$  electrons/gram for AgCl to maximum of  $0.906 * 10^{24}$  electrons/gram for LiOH.

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