

Experimental measurement of effective atomic number of composite materials for Compton effect in the γ -ray region 280–1115 keV by a new method

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Abstract. In this paper, we report a new method to determine the effective atomic number, Z_{eff} , of composite materials for Compton effect in the γ -ray region 280–1115 keV based on the theoretically obtained Klein–Nishina scattering cross-sections in the angular range 50° – 100° as well as a method to experimentally measure differential incoherent (Compton) scattering cross-sections in this angular range. The method was employed to evaluate Z_{eff} for different inorganic compounds containing elements in the range $Z = 1$ –56, at three scattering angles 60° , 80° and 100° at three incident gamma energies 279.1 keV, 661.6 keV and 1115.5 keV and we have verified this method to be an appropriate method. Interestingly, the Z_{eff} values so obtained for the inorganic compounds were found to be equal to the total number of electrons present in the sample as given by the atomic number of the elements constituting the sample in accordance with the chemical formula of the sample. This was the case at all the three energies.

Keywords. Effective atomic number; new method; Compton effect; composite materials.

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1. Introduction

Recently [1], we have reported the effective atomic number, Z_{eff} , for Compton effect of some H-, C-, N- and O-based composite materials in the energy range 280–1200 keV. These values have been determined from a mathematical relation, which is based on the measured differential incoherent scattering cross-sections of elements of atomic number in the range 4–22. The drawback of this method is that it holds good only for H-, C-, N- and O-based samples and fails to yield accurate Z_{eff} values for samples which contain elements with Z more than 22. Also, this mathematical relation relies on the experimentally measured cross-sections of some selected low Z elements. However, in most of the applications of radiation such as dosimetry, shielding, industrial radiography etc., in the photon

energy regime 200 to 1500 keV, materials which essentially contain elements with $Z > 22$ are invariably employed. Also in this region, Compton scattering is a significant interaction process. Hence, we felt it worthwhile to evolve a new technique which is devoid of the limitations of the method reported earlier. For this purpose, we have first studied the variation of the theoretical Klein–Nishina (KN) cross-sections in the angular range 50° – 100° at three photon energies 279.1, 661.6 and 1115.5 keV. Based on this, we have derived a mathematical expression which yields KN cross-sections in millibarn per electron per steradian over this angular and energy range. Further, the differential incoherent (Compton) scattering cross-section of the sample of interest was measured in millibarn per atom per steradian at some angles and energies in this angular and energy range. The ratio of the measured scattering cross-section of the sample at a particular angle to the corresponding Klein–Nishina cross-section (obtained from the mathematical relation) was found to yield reasonably accurate Z_{eff} of the sample for Compton effect in the present energy and angular regime within the free electron approximation.

This method can be used to evaluate Z_{eff} for Compton effect of any material, for which the measured scattering cross-sections are available in a region so long as electron binding effect is ignored. To verify the efficacy of this method, in the present study, Z_{eff} of several inorganic compounds containing different constituent elements in the atomic number range 1–56 have been determined using this method. For this purpose, differential incoherent scattering cross-sections of these compounds were measured at three scattering angles 60° , 80° and 100° in a goniometer assembly that employs a high-purity Ge detector.

2. Theory

The incoherent scattering from free electrons is accurately described by the Klein–Nishina (KN) theory. Departures from KN theory occur in situations where the incident γ -ray energies are comparable with the binding energy of the inner-shell electrons of the atom. 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 $\sigma_{\text{KN}}(\theta)$ (per electron) as

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

where $\sigma_b(\theta)$ is in millibarn per atom per steradian, $\sigma_{\text{KN}}(\theta)$ is the Klein–Nishina cross-section in millibarn/electron/steradian, Z is the atomic number of the scatterer and $S(X, Z)$ is the incoherent scattering function whose value is a measure of the electron binding effects in the atom. (For the present calculation, we have used millibarn rather than barn for ease of calculations.) Here, $X = (\sin(\theta/2)/\lambda(\text{\AA}))$, where λ is the wavelength corresponding to the incident photon. When the scattering electron is completely free from atomic binding effects, $S(X, Z)$ will be equal to the atomic number Z . With binding effects it will be slightly less than Z . Thus, for larger scattering angles and energies (such as the ones used in the present study), since the electron binding effects are quite negligible, eq. (1) can be rewritten as

$$\sigma_b(\theta) = \sigma_{\text{KN}}(\theta)Z. \quad (2)$$

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

3. Procedure to evaluate Z_{eff}

In the present study, first, the Klein–Nishina formula [2] was used to calculate the theoretical differential free electron scattering cross-sections, $\sigma_{\text{KN}}(\theta)$, at six scattering angles, $\theta = 50^\circ, 60^\circ, 70^\circ, 80^\circ, 90^\circ$ and 100° for three γ -ray energies $E = 279.2, 661.6$ and 1115.5 keV. These values in millibarn per electron per steradian are shown in table 1. Further, \ln – \ln plot of values of $\sigma_{\text{KN}}(\theta)$ vs. energy E in keV were drawn at each scattering angle of interest. These plots are shown in figure 1. Based on these plots, by a proper regression analysis, a handy and convenient expression of the form

$$\sigma_{\text{KN}}(\theta) = 403.567E^{-k_\theta} \quad (3)$$

was obtained. The values of k_θ obtained at different angles are shown in table 2. The expression in eq. (3) could reproduce the values in table 1 satisfactorily. However, its only limitation was that it could yield the values of $\sigma_{\text{KN}}(\theta)$ only at specific angles $\theta = 50^\circ, 60^\circ, 70^\circ, 80^\circ, 90^\circ$ and 100° . We felt that it would be more beneficial if eq. (3) could be further modified suitably so that it can yield $\sigma_{\text{KN}}(\theta)$ values at any angle amenable for measurement in the range 50° – 100° . For this purpose, the k_θ values were once again plotted vs. the scattering angle θ . The resulting graph is shown in figure 2. It was found by a suitable curve fitting procedure that a second-order polynomial of the form

$$k_\theta = a + b\theta + c\theta^2 \quad (4)$$

could very well match the trend of variation in figure 2. The best-fit coefficients a , b and c so obtained are also listed below table 2. These values provide the values of k_θ at any angle in the range 50° – 100° . Thus with a , b and c , the expression in eq. (3) would yield KN cross-sections in millibarn per electron per steradian in the energy grid

Table 1. Differential free electron (Klein–Nishina) scattering cross-section^a, $\sigma_{\text{KN}}(\theta)$ (millibarn/electron/steradian).

Angle in degree	$\sigma_{\text{KN}}(\theta)$		
	279.1 keV	661.6 keV	1115.5 keV
50	40.151	28.931	21.982
60	32.038	21.996	16.506
70	26.026	17.458	13.128
80	22.053	14.664	11.058
90	19.806	13.044	9.783
100	18.878	12.173	8.987

^aCalculated using Klein–Nishina formula [2].

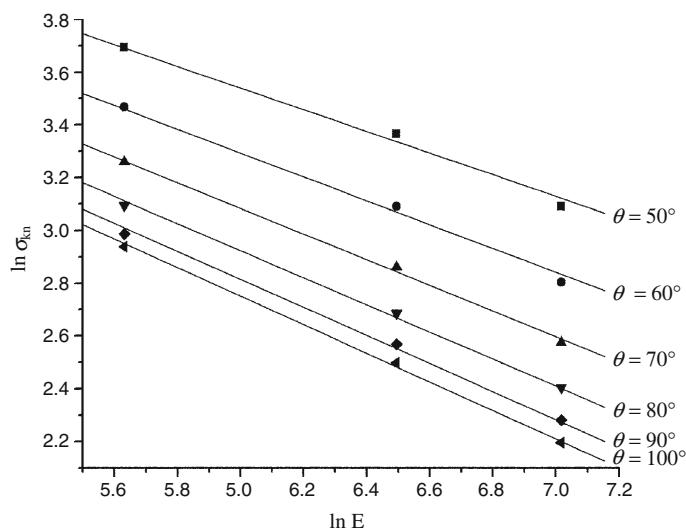


Figure 1. ln–ln plot of Klein–Nishina cross-sections (in mb/steradian/electron) vs. energy in keV.

Table 2. Best-fit values of k_θ and polynomial coefficients a , b and c .

Scattering angle	k_θ in eq. (3)
50	0.4102
60	0.4513
70	0.4862
80	0.5130
90	0.5310
100	0.5416

Note: a , b and c are the polynomial coefficients in eq. (4). They are energy- and angle-independent in the energy grid and angular grid of present interest. Their values are $a = -8.17\text{E-}2$, $b = -8.53\text{E-}3$, $c = 3.93\text{E-}5$.

279.1–1115.5 keV provided the energy value is substituted in keV. So, it is clear that if $\sigma_b(\theta)$ can be experimentally determined for the sample of interest at any angle θ in the range 50° – 100° in this energy grid, then Z_{eff} of the sample can be determined using eqs (1) and (2) via eqs (3) and (4).

4. Experimental details

In the present study, to verify the usefulness and efficacy of the method, the effective atomic number of some inorganic compounds has been determined from their differential

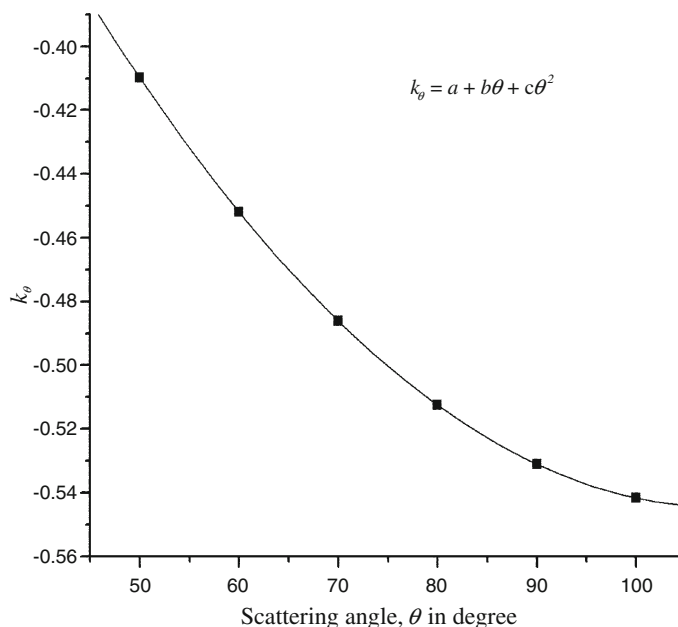


Figure 2. Plot of k_θ vs. scattering angle θ .

incoherent scattering cross-sections. A list of compounds used along with their purities and the names of the manufacturers is given in table 3.

The differential incoherent scattering cross-sections of the inorganic compounds were measured at the scattering angles 60° , 80° and 100° on a goniometer assembly for γ -rays emitted by ^{203}Hg , ^{137}Cs and ^{65}Zn sources. Detailed information about these sources is provided in table 4. A schematic diagram of the experimental set-up used is shown in figure 3. The well-collimated beam of photons from the source S was made to fall on the target T mounted on the target holder. The detector D received the scattered γ -rays. The distance from the detector to the target was 28 cm and the distance from the target

Table 3. Purities and molecular weights of the compounds.

Compound	Molecular weight	Percentage purity	Manufacturers
LiOH	23.95	99.00	Sarabhai-Merck Pvt., Ltd
MgO	40.31	99.00	E. Merck, Germany
NaCl	58.44	99.90	Sarabhai-Merck
KCl	74.56	99.80	British Drug Houses, Ltd.
CuCl	98.99	99.00	British Drug Houses, Ltd.
RbCl	120.92	99.99	Reidel, West Germany
KI	166.01	99.00	British Drug Houses, Ltd.
BaO	153.34	99.00	British Drug Houses, Ltd.

All samples were provided by our chemistry department.

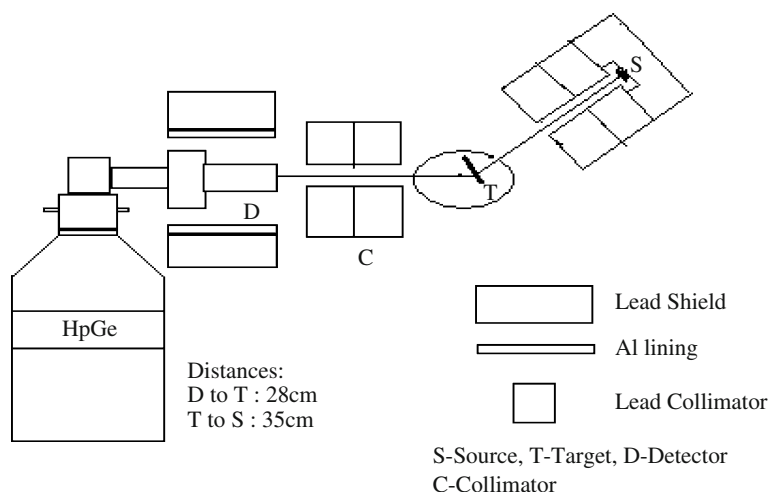
Table 4. Radioactive sources used, along with their half-lives and gamma energies.

Isotopes	Mode of decay	Half-life	Energy (keV)
^{203}Hg	β^- , γ	47 days	279.1
^{137}Cs	β^- , γ	31.1 years	661.6
^{65}Zn	β , γ , EC	245 days	1115.5

to the source was 35 cm. The γ -ray beam was properly shielded by lead throughout its journey from the source to the detector and care was taken to minimize the background radiation. An ORTEC model 23210 gamma-x high purity germanium detector has been used to record the data along with a personal computer-based multichannel analyser. The counts under the peak were determined accurately after subtracting the background counts by applying Gaussian fitting. The entire experiment was carried out in an air-conditioned room wherein the mains' voltage was stabilized to minimize the channel drift.

The thickness of the composite materials ranged from 32 to 52 g/cm², while the purity of the samples was better than 99.9% as mentioned by the suppliers. The experiment was then repeated with the ^{203}Hg and ^{65}Zn sources, which emitted 279.1 and 1115.5 keV γ -rays respectively. These two sources were procured in the form of radiographic capsules from the Bhabha Atomic Research Centre, Mumbai, India.

The ^{137}Cs source was procured in the form of a radiographic capsule from Radiochemical Centre, Amersham, UK. An ORTEC model 23210 gamma-x high-purity germanium detector has been used to record the data along with a personal computer-based multichannel analyser. The solid inorganic compounds were ground into a fine powder form and confined in cylindrical plastic containers. The thickness of the samples so prepared ranged

**Figure 3.** Schematic diagram of the experimental set-up.

from 32 to 52 g/cm². The purity of the samples was 99% and above as specified by the suppliers.

5. Results and discussion

The differential incoherent scattering cross-sections of the inorganic compounds of interest in the present work were obtained using the scattered intensity, source strength and the geometry factor by adopting a procedure similar to an earlier work carried out in our laboratory [1,3].

The measured cross-sections of the inorganic compounds so obtained at the three scattering angles and the three energies 279.1, 661.6 and 1115.5 keV are listed in table 5 along with the experimental errors and compared with other available data [4,5]. A good agreement was noticed among the present values and the other available experimental values within the range of experimental errors.

The errors in the present measurements were mainly a result of the counting statistics. The error due to the counting statistics was kept below 0.3% by accumulating 10⁵–10⁶ counts within the photopeak of the scattered spectrum.

Table 5. Differential incoherent scattering cross-sections (millibarn/atom/steradian) and effective atomic numbers of samples (experimental errors are to the extent of 2–3%).

Composite material	279.1 keV			661.6 keV			1115.5 keV			Mean Z_{eff}
	60°	80°	100°	60°	80°	100°	60°	80°	100°	
LiOH	384.4 ^a 12.1 ^b	264.6 ^a 11.8 ^b	226.5 ^a 11.9 ^b	263.9 ^a 12.3 ^b	175.9 ^a 12.1 ^b	146.1 ^a 12.2 ^b	198.0 ^a 11.7 ^b	132.7 ^a 12.0 ^b	107.8 ^a 11.9 ^b	12.0
MgO	640.7 ^a 20.2 ^b	441.0 ^a 19.6 ^b	377.5 ^a 19.8 ^b	439.9 ^a 20.5 ^b	293.2 ^a 20.2 ^b	243.4 ^a 20.3 ^b	330.1 ^a 19.5 ^b	221.1 ^a 20.0 ^b	179.7 ^a 19.9 ^b	20.0
NaCl	896.9 ^a 28.3 ^b	617.4 ^a 27.4 ^b	528.6 ^a 27.6 ^b	615.8 ^a 28.2 ^b	410.5 ^a 28.3 ^b	340.8 ^a 28.4 ^b	462.1 ^a 27.3 ^b	309.6 ^a 27.9 ^b	251.6 ^a 27.9 ^b	27.9
KCl	1153.0 ^a 36.4 ^b	793.8 ^a 35.2 ^b	679.6 ^a 35.6 ^b	791.8 ^a 36.9 ^b	527.9 ^a 36.5 ^b	438.2 ^a 36.5 ^b	594.2 ^a 35.2 ^b	398.0 ^a 35.9 ^b	323.5 ^a 35.8 ^b	36.0
CuCl	1471.4 ^a 46.5 ^b	1014.0 ^a 45.1 ^b	868.2 ^a 45.5 ^b	830.0 ± 80 ^d 1011.7 ^a 46.2 ^b	674.5 ^a 46.6 ^b	559.9 ^a 46.7 ^b	759.2 ^a 44.9 ^b	508.6 ^a 45.9 ^b	413.4 ^a 45.8 ^b	45.9
RbCl	1723.4 ^a 54.4 ^b	1189.4 ^a 52.8 ^b	1018.9 ^a 53.3 ^b	1030 ± 100 ^d 1187.6 ^a 55.4 ^b	791.7 ^a 54.7 ^b	657.3 ^a 54.9 ^b	891.3 ^a 52.7 ^b	597.1 ^a 54.0 ^b	485.2 ^a 53.8 ^b	54.0
KI	2284.7 ^a 72.1 ^b	1581.2 ^a 70.3 ^b	1356.2 ^a 71.0 ^b	1582.6 ^a 73.8 ^b	1055.3 ^a 72.9 ^b	876.2 ^a 73.2 ^b	1188.2 ^a 70.2 ^b	796.1 ^a 71.9 ^b	647.0 ^a 71.7 ^b	71.9
BaO	2025.0 ^a 63.9 ^b	1403.4 ^a 62.4 ^b	1204.5 ^a 63.1 ^b	1670 ± 100 ^d 1406.3 ^a 65.6 ^b	937.8 ^a 64.8 ^b	929.0 ± 56 ^d 778.7 ^a 65.0 ^b	1056.1 ^a 62.4 ^b	707.7 ^a 63.9 ^b	575.2 ^a 63.7 ^b	63.9

^aDifferential incoherent scattering cross-section.

^b Z_{eff} (present values).

^cShivananda *et al* [5].

^dShivananda *et al* [4].

The other sources of errors are also described below:

The error associated in evaluating the area of the scattered peak by the peak fitting routine was less than 1%.

Each compound under investigation was taken in fine powder form and confined in a cylindrical plastic container. The sample thus prepared was weighed in an electrical balance to the third decimal place. The weighings were repeated a number of times to get concordant values of the mass. A mean of this set of concordant values was taken to be the mass of the sample.

The inner diameter of each plastic container was determined with the help of travelling microscope. Using the mean value of the mass of the compound and the inner diameter of the corresponding container, the mass per unit area of the sample was determined. The uncertainty in the mass per unit area (sample thickness) was less than 0.05%.

The error in the determination of the number of atoms in the scatterer was negligible.

In the present measurements, although the mass per unit area (thickness) of the inorganic samples was high, care was taken to maintain the same diameter for all the cylindrical sample containers. They differed only in their heights. Therefore, the angle of acceptance was almost the same in each measurement.

It may be argued that the multiple scattering of photons occurs whenever thick samples are used because such samples offer a larger mean free path for the incident photons to scatter and rescatter inside the target material. Thus the multiple scattering can result in energy degraded photons which may contribute to the lower energy side of the photopeak thus leading to an overestimation of the scattered intensity. However, in the present study, the intensity under the scattered peak was determined from the background subtracted scattered photopeak by a suitable peak fitting routine. A high-resolution detector as well as targets of optimum thickness were also employed. So, the multiple scattering effects were negligible during the present study.

The uncertainty in calculating the transmission factors using the transmitted intensities was less than 1%.

The error due to the sample impurity could be significant only when large percentages of high-Z impurities are present in the sample. In the present case, the percentage of high-Z impurities was less than 0.02%. Hence sample impurity corrections were not applied to the measured data.

The error due to non-uniformity of the sample was estimated according to Carter *et al* [6]. It was found that this error was less than 0.05% for all samples.

The dead time of the multichannel analyser was a combination of the rise time of the pulse, the conversion time in the analog-to-digital converter and the data processing time. In the multichannel analyser used in the present study, there was a built-in provision for dead time correction. The percentage dead time correction was always less than 2% in the present study. Thus the overall error in the present measurement was to the extent of 2 to 3% of the measured values.

The $\sigma_b(\theta)$ values of the inorganic compounds listed in table 5 were used in eq. (2), via eqs (3) and (4) to calculate the Z_{eff} values at all angles and energies of present interest. These values are also shown in table 5.

In the present method, it was also essential to assess the extent of approximation on Z_{eff} rendered as a result of using eq. (2) in place of eq. (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 $9.5\text{--}68.9\text{ \AA}^{-1}$ for the angles in the range $50^\circ\text{--}100^\circ$ and energies in the grid $279.1\text{--}1115.5\text{ keV}$ respectively. From the tabulated data of Hubbell *et al* [2] (please refer figures 45 and 47 of this reference), it was observed that the quantity $(S(X, Z)/Z)$ remains almost a constant (≈ 1) beyond $X = 9.5\text{ \AA}^{-1}$. However, at $X = 9.5\text{ \AA}^{-1}$, the error due to this free electron approximation on Z_{eff} was estimated by using the Hubbell *et al* [2] tables to be about 0.8% for $Z = 40$ 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.

From table 5, it is interesting to note that Z_{eff} for a given sample is almost a constant at all angles and energies of present interest. This means that a unique Z_{eff} , which remains a constant across the angular and energy grid of present interest, can signify the Compton scattering characteristics of such inorganic compounds. Keeping this in mind, the mean Z_{eff} was calculated from the arithmetic average of all the Z_{eff} values of each sample at all the angles and energies of present interest. These values have also been tabulated in table 5. It can also be observed that among the various inorganic samples studied, LiOH possesses the lowest Z_{eff} of 12 and KI exhibits the highest Z_{eff} of 71.9 for Compton effect.

From table 5, we can also observe that the mean Z_{eff} for a given sample is numerically equal to the sum of all the electrons (in terms of atomic number) present in it as given by the chemical formula for the sample.

To illustrate this point, consider Z_{eff} of NaCl compound. From table 5 we note that it is 27.9. The number of electrons based on its chemical formula is $11(Z_{\text{Na}}) + 17(Z_{\text{Cl}}) = 28$.

6. Conclusions

Thus in the present work, it has been possible to evolve a new handy and easy technique to evaluate the effective atomic number for Compton effect of any composite materials in the γ -ray energy region $280\text{--}1115\text{ keV}$ by deducing an expression for Klein–Nishina cross-sections over a chosen range of angle and energy. This eliminates the dependence of the Z_{eff} calculations on the accuracy of the elemental cross-section measurements as in our earlier work. The method used earlier could be used only for samples with elements of $Z \leq 22$. The present method is an improvement over the work reported earlier [1] because it has no such limitation over Z of the constituent elements of the samples. In this investigation, we have verified the advantage of this method by employing it to determine Z_{eff} of compounds containing elements in the range $Z = 1\text{--}56$ within the free electron approximation. Another interesting finding is that for Compton effect in the energy region $279.1\text{--}1115.5\text{ keV}$, samples such as the inorganic compounds could be characterized by a mean Z_{eff} . This behaviour resembled that of an elemental sample (which is identified by an angle-independent, energy-independent and single atomic number, Z). This concurred with the inference of the previous works [1,7,8] that in the energy region wherein the Compton scattering is a dominant mode of photon interaction, Z_{eff} of any composite material can be represented by a mean atomic number. The results of the present work suggest that the effective atomic number of any inorganic sample containing constituent elements in the atomic number range $1\text{--}56$ for Compton effect in the range $280\text{--}1115.5\text{ keV}$ can be obtained by simply adding the Z -values of the constituent elements as per the chemical

formula of the compound. However, it is interesting to note that this rule cannot be applicable for H-, C-, N- and O-based composite materials. Hence more investigation is needed in this direction before this rule may be generalized.

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