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Research Article

Effective atomic numbers and electron densities for some lanthanide oxide compounds using direct method in the energy region of 1 keV - 20 MeV

Mehmet Büyükyıldız [1] *

[1] *Yalova University, Faculty of Engineering, Department of Electronics and Communications, 77100 Yalova, Turkey*

* *Corresponding author: mehmet.buyukyildiz@yalova.edu.tr*

Abstract

In this paper, the effective atomic numbers (Z_{eff}) and electron densities (N_{eff}) representing interaction of gamma rays with oxides of lanthanides were studied. The effective atomic numbers for photon energy-absorption (Z_{PEAeff}), photon interaction (Z_{PIeff}), relative to air Z_{Reff}, the effective electron densities for photon energy-absorption (N_{PEAeff}) and photon interaction (N_{PIeff}) were calculated using the values of the mass attenuation and energy absorption coefficients. In the continuous energy region, agreements and disagreements were observed between photon interaction and photon energy-absorption for Z_{eff}s and N_{eff}s of compounds in different energy regions. In addition, absorption edge effects on Z_{eff}s leading more than a single value of Z_{eff} at a specific energy have been discussed for the given compounds. Comparisons with experiments wherever possible have been carried out for calculated values of Z_{eff} and N_{eff}.

Keywords: Lanthanides, Effective atomic number, Effective electron density, Radiation interaction.

1. Introduction

Radiation interaction with matter has become an important subject with the extensive use of X and/or gamma rays in various fields such as reactors, nuclear power plants, nuclear engineering and space technology, nuclear diagnostics, nuclear medicine, radiation dosimetry and radiation biophysics. Rapidly increasing use of radioactive materials in reactors, nuclear power plants, nuclear engineering leads to study of interaction parameters like attenuation coefficient, photon interaction cross-section, Z_{eff} and N_{eff}. Thus precise knowledge of these parameters should be known before their application (Kaewkhao et al. 2008; Kirdsiri et al. 2009; Demir and Han 2009).

The pure metals of the lanthanides have little use. Whereas, the alloys or compounds of the metals can be very useful. For example, the alloys of Cerium have been used for metallurgical applications due to their strong reducing abilities. In addition, the lanthanides can be used for nuclear purposes; oxides of lanthanides can be used as diluents in nuclear fields, can also be used for structural-alloy-modifying components of reactors. Thus, increasing usage of the radiations, it should be determined radiation matter interaction parameters of compounds such as total mass attenuation coefficient, Z_{eff} and N_{eff} (Petrucci et al. 2007).

The Z_{eff}s and N_{eff}s are employed in radiation studies, especially for the characterization of interaction processes in various multi-element materials. There are a lot studies in literature about Z_{eff}s and N_{eff}s for different materials, in different categories such as in different type of compounds (Shivaramu and V. Ramprasath 2000; Tengku Kamarul Bahr et al. 2014; Kurudirek 2014a, 2014b; Gowda et al. 2004; Önder et al. 2012; Kurudirek and Kurudirek 2015), in alloys (Kurudirek et al. 2010; Kaewkhao et al. 2008; İçelli et al. 2005; Murty 2004; El-Kateb et al. 2000), in glass and minerals (Kaewkhao and Limsuwan 2010; Manohara et al. 2009; Kirdsiri et al. 2009; Singh et al. 2002, 2005) in biological materials (Manohara et al. 2008; Manohara and Hanagodimath 2007; Gowda et al. 2005). However, studies about lanthanides on Z_{eff} and N_{eff} are very scarce (İçelli 2006; Singh et al. 2015). This motivated us to carry out the present study.

Niranjan et al. (2012) calculated Z_{eff} and N_{eff} (for total photon interaction) of these compounds using total and electronic cross-sections. But in the present work, the comparison between photon energy-absorption and photon interaction, and Z_{Reff} (relative to air) has been made in addition to the calculation of electron densities for photon interaction and photon energy absorption.

In the present work, the effective atomic numbers for photon energy-absorption (Z_{PEAeff}), for photon interaction (Z_{PIeff}), the effective electron densities for photon energy-absorption (N_{PEAeff}) and for photon interaction (N_{PIeff}) of La_2O_3, Ce_2O_3, Pr_2O_3, Nd_2O_3, Sm_2O_3, Eu_2O_3, Gd_2O_3, Tb_2O_3, Dy_2O_3, Ho_2O_3, Er_2O_3, Tm_2O_3, Yb_2O_3 and Lu_2O_3 have been calculated by using direct method. Wherever possible the results were compared with the experimental results available in the literature.

2. Calculation

The total mass attenuation coefficients of elements present in the compounds were obtained from the WinXCom computer program (Gerward et. al. 2001, 2004). The total mass attenuation coefficients (μ/ρ) for any compound or composite of elements is given by mixture rule:

$$(\mu/\rho) = \sum_i w_i (\mu/\rho)_i \quad (1)$$

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where, w_i and $(\mu/\rho)_i$ are the wight fraction and mass attenuation coefficient of *i*th constituent element, respectively (Jackson and Hawkes, 1981). These coefficients were then used to calculate the Z_{eff} of compounds for photon interaction with the help of the following practical formula (Manohara et al. 2008):

$$Z_{eff} = \frac{\sum_i f_i A_i \left(\frac{\mu}{\rho}\right)_i}{\sum_j f_j \frac{A_j}{Z_j}\left(\frac{\mu}{\rho}\right)_j} \quad (2)$$

where f_i is the fraction by mole of each constituent element provided $\sum_i f_i = 1$, Ai is the atomic weight (IUPAC 2007), Z_j is the atomic number and $(\mu/\rho)_i$is the mass attenuation coefficient. This formula is known as "Direct method". And Z_{Reff} is given Z_{eff}/ Z_{air}.

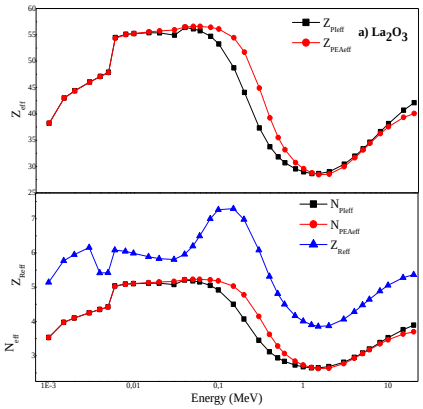
The effective atomic number, Z_{eff}, is closely related to the electron density, N_{eff}, which is expressed in number of electrons per unit mass. Also, the N_{eff} is expressed by the following relation (Manohara et al. 2008):

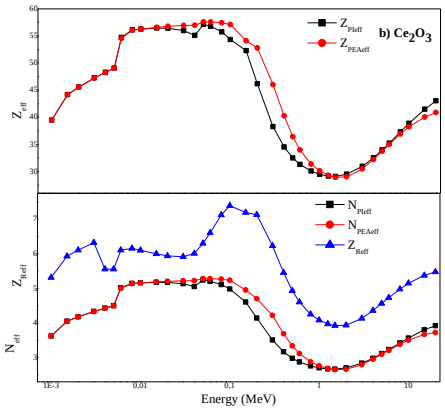
$$N_{eff} = N_A \frac{nZ_{eff}}{\sum_i n_i A_i} = N_A \frac{Z_{eff}}{<A>} \ (electrons/g) \quad (3)$$

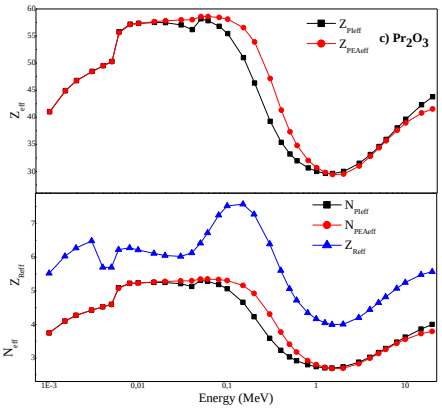
where $< A >$ is the average atomic mass of the compound.

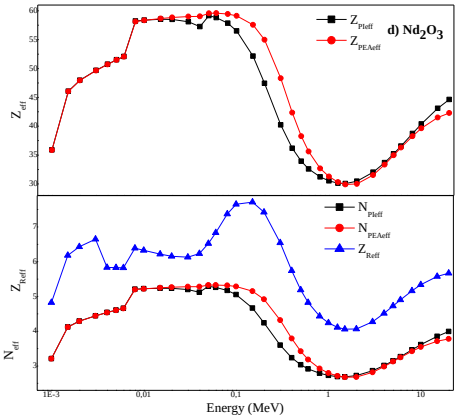
3. Results and Discussion

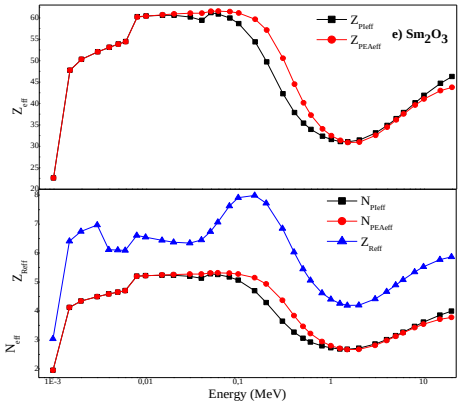
The variations of Z_{PEAeff}, Z_{PIeff}, Z_{Reff}, N_{PEAeff} and N_{PIeff} with photon energies are shown in Fig. 1 for all compounds.

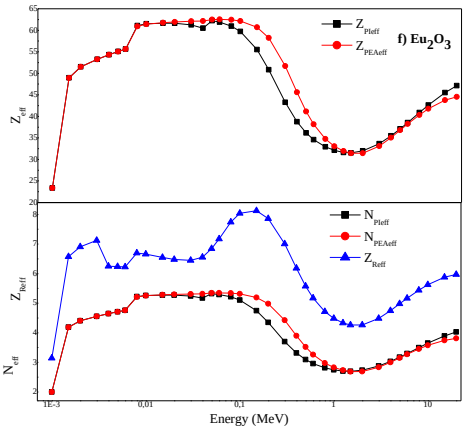












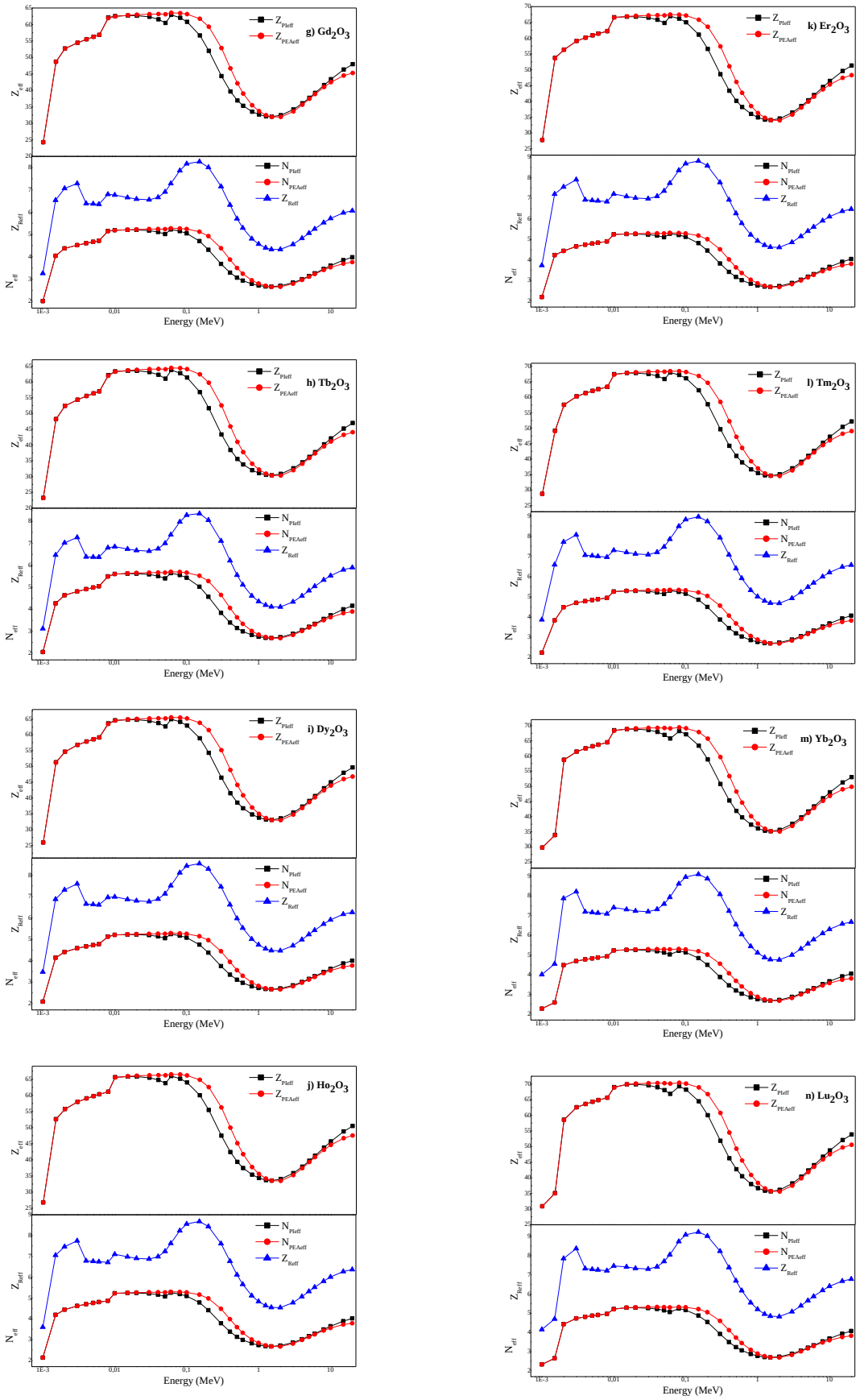


Figure 1. (a), (b), (c), (d), (e), (f), (g), (h), (i), (j), (k), (l), (m), (n) Z_{PEIeff}, Z_{PIeff}, Z_{Reff}, N_{PEIeff} and N_{PIeff} for the given compounds in the energy range of 1 keV–20 MeV.

From the results, it can be clearly seen that the Z_{eff} varies with energy. In the continuous energy range 1 keV-20 MeV, the variation of Z_{eff} with energy is mainly dominated by different partial photon interaction processes namely photoelectric absorption, Compton scattering and pair production.

It can be seen clearly from Fig. 1 that the variation of Z_{PEAeff} and Z_{Pleff} with energy is almost similar for all of compounds. In the energy region $E < 100$ keV (the first region), Z_{eff} and Z_{Reff} of compounds increase as energy increases. In this region photoelectric process dominates for Z_{eff}, and maximum variation observed in Z_{eff} due to variation of (μ/ρ) and μ_{en}/ρ, and since attenuation cross section proportional to Z^{4-5}. The Z_{eff} decreases rapidly with increasing energy in the energy region from 100 keV to 2 MeV where the importance of photoelectric absorption decreases and Compton scattering gradually becomes the main interaction process and Z_{eff}s depend on Z (the second region). In the immediate aftermath, the Z_{eff} increases with increasing energy as pair production gradually becomes the main interaction process to 20 MeV (the third region). So in the energy region $0.1 < E < 20$ MeV there is no energy region where Compton scattering is totally dominating as mentioned before Manohara et al. (2008).

Generally, (μ/ρ) and μ_{en}/ρ take values close to each other, hence Z_{PEAeff} and Z_{Pleff} take almost same values in the first energy region. Therefore, either Z_{PEAeff} or Z_{Pleff} can be used in this energy region. While in the second region, Z_{PEAeff} values are higher than the values of Z_{Pleff}, in the third energy region the values of Z_{Pleff} were found to be higher than the values of Z_{PEAeff}.

One can see clearly from Fig. 1, Z_{eff} has several discontinuous jumps in the low-energy range because of absorption edge effects of high elements. The values of M_5, M_4, M_3, M_2, M_1, L_3, L_2, L_1 and K absorption edge energies are shown in Table 1 (the absorption edge of the low-Z element oxygen occurs at energies <1 keV and is therefore of no importance in the present work). These discontinuities make the concept of the Z_{eff} somewhat problematic in the low-energy range.

The N_{eff} values for the present compounds were calculated using $< A >$ and Z_{eff}, and are given in Fig. 1. It is seen from this figure that N_{eff} varies with photon energy. N_{eff} is closely related to Z_{eff} and has the same qualitative energy dependence as Z_{eff}. Thus, N_{eff} values are proportional to Z_{eff} values for the present compounds in the continuous energy range 1 keV - 20 MeV.

There is no experimental data on μ_{en}/ρ for comparison since it is not possible to measure μ_{en}/ρ experimentally, unlike (μ/ρ) which can be easily measured using the conventional gamma spectrometry system (Manohara et al. 2008). Thus, comparison was carried out for photon interaction only. The experimental results for Z_{eff}s and N_{eff}s (for photon interaction) of the given materials are given in Table 2.

Table 1. K, L and M X-Ray absorption energies of lanthanides in keV.

Elements	K_{ab}	L_{1ab}	L_{2ab}	L_{3ab}	M_{1ab}	M_{2ab}	M_{3ab}	M_{4ab}	M_{5ab}
La	38.941	6.283	5.894	5.489	1.361	1.204	1.123		
Ce	40.449	6.561	6.165	5.739	1.437	1.273	1.185		
Pr	41.998	6.846	6.443	5.968	1.511	1.337	1.242		
Nd	43.571	7.144	6.727	6.215	1.575	1.403	1.297	1.005	
Sm	46.846	7.754	7.281	6.721	1.723	1.541	1.420	1.106	1.080
Eu	48.515	8.069	7.624	6.983	1.800	1.614	1.481	1.161	1.131
Gd	50.229	8.393	7.940	7.252	1.881	1.688	1.544	1.217	1.185
Tb	51.998	8.724	8.258	7.519	1.968	1.768	1.611	1.275	1.241
Dy	53.789	9.083	8.621	7.850	2.047	1.842	1.676	1.332	1.295
Ho	55.615	9.411	8.920	8.074	2.128	1.923	1.741	1.391	1.351
Er	57.483	9.776	9.263	8.364	2.207	2.006	1.812	1.453	1.409
Tm	59.335	10.144	9.628	8.652	2.307	2.090	1.885	1.515	1.468
Yb	61.303	10.486	9.977	8.943	2.398	2.173	1.950	1.576	1.528
Lu	63.304	10.876	10.345	9.241	2.491	2.263	2.024	1.639	1.589

Table 2. Total mass attenuation coefficient (μ/ρ) (cm^2/g), effective atomic number and electron density (electrons/g) of oxides of lanthanides in 59.54 keV.

Compound	(μ/ρ)	Z_{eff}[a]	Z_{eff}[b]	Z_{eff}[c]	Z_{eff}[d]	Z_{eff}[e]	N_{eff}[a] ($x10^{23}$)	N_{eff}[b] ($x10^{23}$)	N_{eff}[c] ($x10^{23}$)
Pr_6O_{11}	8.459	56.95	57.57	57.57			5.709	5.770	5.768
Nd_2O_3	9.058	58.19	58.84	58.85	50.03	55.39	5.208	5.270	5.264
Gd_2O_3	10.427	62.24	62.93	62.93			5.170	5.230	5.225
Tb_4O_7	10.637	63.07	63.78	63.77			5.589	5.650	5.648
Ho_2O_3	11.683	65.24	65.99	65.99			5.200	5.260	5.257
Er_2O_3	12.163	66.23	67.01	67.01			5.214	5.280	5.273
La_2O_3	7.827			55.77	54.33	51.57			

[a]Experimentally measured values from G. Singh et al. (2015).
[b]Calculated values by using Ratio method from G. Singh et al. (2015).
[c]Calculated values of the present work by using Direct method.
[d]Experimentally measured values by using coherent to Compton scattering ratio method from İçelli (2006).
[e]Calculated values by using coherent to Compton scattering ratio method from İçelli (2006).

In general, the agreement is good between experiments and our presented results except for values of İçelli (2006) because of that the used (coherent to Compton scattering ratio) method for calculation of Z_{eff}. Thus Z_{eff} may have significantly different values in different energy regions. Coherent to Compton scattering ratio method is based on directly proportional to the areas of Rayleigh (N_R) and Compton (N_C) peaks of sample in the measured spectrum (R/C method) and For a fixed momentum transfer, R/C is a function of only the Z_{eff} of the sample (Duvauchelle et al. 1999; Del Lama et al. 2015). On the other hand, ratio method is based on proportional of the total atomic cross-section to total electronic cross-section of sample (Demir and Han 2009).

4. Conclusions

Below conclusions can be deduced from the present study:

- Z_{PEAeff}, Z_{PIeff}, Z_{Reff}, N_{PEAeff} and N_{PIeff} of compound of oxides of lanthanides have been calculated for total photon interaction and photon energy-absorption in an extended energy range 1 keV–20 MeV.
- Because of the high element present in compounds (lanthanide elements of compounds), the Z_{eff}s show strong energy dependence.
- In the low energy region, where photoelectric absorption is more dominant, significant variations and maximum values were observed for Z_{eff}. The minimum values of Z_{eff} have been observed in intermediate energies where Compton scattering is dominant, but there is no energy region where Compton scattering is totally dominating.
- At the K, L, M-absorption edge energies of lanthanide elements of compounds, more than a single value of Z_{eff} could be obtained due to the non-uniform variation of mass attenuation coefficients.
- The N_{eff} is closely related to the Z_{eff} and has the same qualitative energy dependence as Z_{eff}.
- We have shown that Z_{eff} and N_{eff} for both photon energy-absorption and photon interaction are useful parameters for compounds at all energies greater than 1 keV.
- In the second region, significant differences exist between Z_{PEAeff} and Z_{PIeff}, and it is preferable to use Z_{PEAeff} or Z_{PIeff} in the radiation dosimetry according to the purpose. Thus the results of the present work may be useful for applications of the compounds in the fields where radiation is used.

Highlights

(i) Effective atomic number and electron density of some lanthanide oxide compounds were calculated in continuous energy range using direct method.

(ii) The significant differences for Z_{eff} and N_{eff} were determined in different energy region.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

References

Atomic weight softh elements, IUPAC, 2007, The table is based on the 2005 table at Pure Appl. Chem. 78 (2006) 2051-2066 with 2007 changes to the values forlutetium, molybdenum, nickel, ytterbium and zinc. /http://www. chem.qmul.ac.uk/iupac/AtWt/S.

Del Lama LS, Soares LDH, Antoniassi M, Poletti ME (2015). Effective atomic numbers for materials of medical interest at low photon energy using the Rayleigh to Compton scattering ratio. Nucl. Instrum. Methods A 784, 597–601.

Demir L, Han I (2009). Mass atternuation coefficients, effective atomic numbers and electron densities of undoped and differently doped GaAs and InP crystals. Ann. Nucl. Energy 36, 869-873.

Duvauchelle P, Peix G, Babot D (1999). Effective atomic number in the Rayleigh to Compton scattering Ratio. Nucl. Instrum. Methods B 155, 221-229.

El-Kateb AH, Rizk R, Abdul-Kader AM (2000). Determination of atomic cross-sections and effective atomic numbers for some alloys. Ann. Nucl. Energy 27, 1333-1343.

Gowda S, Krishnaveni S, Gowna R (2005). Studies on effective atomic numbers and electron densities in amino acids and sugars in the energy range 30–1333 keV. Nucl. Instr. Methods B 239, 361-369.

Gowda S, Krishnaveni S, Yashoda T, Umesh TK, Gowda R (2004). Photon mass attenuation coefficients, effective atomic numbers and electron densities of some thermoluminescent dosimetric compounds. Parmana 63, 529-531.

Hine GJ (1952). The effective atomic numbers of materials for various gamma interactions. Physics Review 85, 725-737.

İçelli O, Erzeneoglu S, Karahan İH, Cankaya G (2005). Effective atomic numbers for CoCuNi alloys using transmission experiments. JQSRT 91, 485–491.

İçelli O (2006). Practical method for experimental effective atomic number in the coherent to Compton scattering ratio. Journal of Quantitative Spectroscopy and Radiative Transfer 101, 151-158.

Jackson DF, Hawkes DJ (1981). X-ray attenuation coefficients and elements and mixtures. Physics report 70, 169-233.

Kaewkhao J, Laopaiboon J, Chewpraditkul W (2008). Determination of effective atomic numbers and effective electron densities for Cu/Zn alloy. JQSRT 109, 1260-1265.

Kaewkhao J, Limsuwan P (2010). Mass attenuation coefficients and effective atomic numbers in phosphate glass containing Bi_2O_3, PbO and BaO at 662 keV. Nucl. Instr. Methods Phys. Res. A 619, 295-297.

Kirdsiri K, Kaewkhao J, Pokaipisit A, Chewpraditkul

W, Limsuwan P (2009). Gamma-rays shielding properties of xPbO:(100 Àx)B_2O_3 glasses system at 662 keV. Ann. Nucl. Energy 36, 1360-1365.

Kurudirek M, Büyükyıldız M, Özdemir Y (2010). Effective atomic number study of various alloys for total photon interaction in the energy region of 1 keV-100 GeV. Nucl. Instrum. Methods B 613, 251-256.

Kurudirek M (2014a). Effective atomic numbers of different types of materials for proton interaction in the energy region 1 keV–10 GeV. Nucl. Instrum. Methods B 336, 130-134.

Kurudirek M (2014b). Effective atomic numbers and electron densities of some human tissues and dosimetric materials for mean energies of various radiation sources relevant to radiotherapy and medical applications. Radiation Physics and Chemistry 102, 139-146.

Kurudirek M. and Kurudirek SV (2015). Collisional, radiative and total electron interaction in compound semiconductor detectors and solid state nuclear track detectors: Effective atomic number and electron density. Applied Radiation and Isotopes. 99, 54-59.

Manohara SR, Hanagodimath SM, Gerward L (2009). Photon interaction and energy absorption in glass: a transparent gamma ray shield. J. Nucl. Mater 393, 465-472.

Manohara SR, Hanagodimath SM (2007). Studies on effective atomic numbers and electron densities of essential amino acids in the energy range in energy range 1 keV-100 GeV. Nucl Instrum. Methods B 258, 321-328.

Manohara SR, Hanagodimath SM, Thind KS, Gerward L (2008). On the effective atomic number and electron density: a comprehensive set of formulas for all types of materials and energies above 1 keV. Nucl Instrum. Methods B 266, 3906-3912.

Murty VRK (2004). Effective atomic numbers for W/Cu alloy for total photon attenuation. Radiat. Phys. Chem 71, 667-669.

Niranjan RS, Rudraswamy B, Dhananjayan N (2012). Effective atomic number, electron density and kerma of gamma radiation for oxides of lanthanides. Pramana J. Phys. 78, 451-458.

Önder P, Tursucu A, Demir D, Gürol A (2012). Studies on mass attenuation coefficient, effective atomic number and electron density of some thermoluminescent dosimetric compounds. Nucl. Instrum. Methods B 292, 1-10.

Petrucci PH, Herring FG, Madura JD, Bissonnette, C (2007). General Chemistry: Principles and Modern Applications (10th Edition).

Shivaramu V. Ramprasath (2000). Effective atomic numbers for photon energy absorption and energy dependence of some thermoluminescent dosimetric compounds. Nucl. Instrum. Methods B 168, 294-304.

Singh G, Kumar Gupta M, Dhaliwal AS, Kahlon KS (2015). Measurement of attenuation coefficient, effective atomic number and electron density of oxides of lanthanides by using simplified ATM-method. Journal of Alloys and Compounds 619, 356-360.

Singh K, Singh H, Sharma G, Gerward L, Khanna A, Kumar R, Nathuram R, Sahota HS (2005). Gamma-ray shielding properties of CaO–SrO–B2O3 glasses. Radiat. Phys. Chem. 72, 225–228.

Singh K, Singh H, Sharma V, Nathuram R, Khanna A, Kumar R, Bhatti SS, Sahota HS (2002). Gamma-ray attenuation coefficients in bismuth borate Glasses, Nucl. Instrum Methods B 194, 1-6.

Tengku Kamarul Bahri TNH, Wagiran H, Hussin R, Saeed MA, Hossain I, Ali H, (2014). Dosimetric properties of germanium doped calcium borate glass subjected to 6 MV and 10 MV X-ray irradiations. Nucl. Instrum. Methods B 336, 70-73.