



## A Study on Radiation Shielding Abilities of Some Compounds of 3d Transition Elements by Using Phy-X/PSD Code

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### Highlights

- Photon attenuation parameters of the compounds have been determined by Phy-X/PSD.
- The radiation shielding potentials of the compounds have been evaluated.
- Fast neutron shielding performances of the compounds have been studied.

### Article Info

Received: 18 Aug 2021

Accepted: 01 Apr 2022

### Keywords

Radiation attenuation parameters  
Radiation shielding  
3d transition elements

### Abstract

In the present study, it was aimed to calculate the radiation-matter interaction parameters of some compounds of 3d transition elements. The radiation attenuation parameters, which are important to have knowledge about the radiation shielding potentials, were calculated by using Phy-X/PSD code in the energy range of 0.01-15 MeV. The calculated mass attenuation coefficient and effective atomic number results were compared with the experimental data which were measured at 19.63 and 22.10 keV previously and, a good agreement was achieved. In order to evaluate the shielding properties of the compounds, we also compared the mass attenuation coefficients of the compounds with ordinary concrete, steel-scrap, ilmenite-limonite and basalt-magnetite, which are widely used as radiation protective materials. According to the obtained results, it is concluded that the studied compounds have radiation shielding potentials.

## 1. INTRODUCTION

Recently, protection of all living creatures from the harms of radiation becomes more important due to the increase in application fields of radiation such as agriculture, technology, industry, medicine, medical imaging and radiotherapy etc. There has been an enormous interest in researches including radiation attenuation parameters that can assure significant knowledge about radiation shielding potentials of materials [1-5]. These parameters consist of mass attenuation coefficient (MAC), linear attenuation coefficient (LAC), mean free path (MFP), half-value layer (HVL), tenth-value layer (TVL), total atomic and electronic cross-sections (ACS and ECS), effective atomic number ( $Z_{eff}$ ), effective electron density ( $N_{eff}$ ), effective conductivity ( $C_{eff}$ ) and fast neutron removal cross section (FNRCs). Several methods are developed in order to calculate the photon interaction coefficients of materials such as, XCOM [6], WinXCom [7,8], XMuDat [9], Phy-X/PSD [10], Py-MLBUF [11], EpiXS [12] and simulation code Geant4 [13]. Recently, researchers widely use the codes for determination of the shielding potentials of various materials such as alloys, glasses, rocks, soils, etc. [2-5,14-18].

The 3d transition elements and their compounds have a considerable effect in the development of technologic applications because of the well-known features such as hardness, high density, good thermal conductivity, high melting-boiling temperatures and having more than one oxidation state. Due to the diversity of physical properties of the 3d transition elements, many applications of these elements and their compounds indicate the need to get information about various physical parameters [19]. Many studies have

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been done about coefficients,  $Z_{eff}$  of the 3d transition metal elements, their compounds and alloys at several photon energies before [19-23]. But these works are limited only by some parameters in several energies. We believe that it would be important to determine the radiation attenuation parameters such as MAC, LAC, HVL, TVL, MFP, ACS, ECS,  $Z_{eff}$ ,  $N_{eff}$ ,  $C_{eff}$  and FNRCs, hence, radiation shielding potentials of 3d transition metal compounds for different energy values. By this comprehensive investigation, we can conclude that which compound has better radiation shielding potential.

In this work, it is aimed to calculate radiation attenuation parameters of some compounds of the 3d transition elements (CoO, CoF<sub>2</sub>, CoF<sub>3</sub>, Cr<sub>2</sub>O<sub>3</sub>, CrF<sub>2</sub>, CrF<sub>3</sub>, FeO, Fe<sub>2</sub>O<sub>3</sub>, MnO<sub>2</sub>, TiO<sub>2</sub>, V<sub>2</sub>O<sub>3</sub>, VF<sub>3</sub>, V<sub>2</sub>O<sub>5</sub>, VF<sub>4</sub> and ZnO) in the photon energy range of 0.01-15 MeV theoretically by using Phy-X/PSD software which can calculate quickly and accurately all specified shielding parameters for different materials in the continuous energy range and selected energies [10]. At 19.63 and 22.10 keV energies, calculated MAC and  $Z_{eff}$  values of the compounds were also compared with the experimental MAC and  $Z_{eff}$  results given by Yilmaz et al., [23].

## 2. MATERIAL METHOD

The MAC is a quantity that defines the interaction possibility between gamma photons and the mass per unit area for a particular medium and can be calculated by the Beer–Lambert formulated as:

$$I = I_0 e^{-\mu t} \quad (1)$$

$$\mu_m = \frac{\mu}{\rho} = \ln(I_0/I)/\rho t = \ln(I_0/I)/t_m \quad (2)$$

where  $I_0$  and  $I$  are incident and attenuated photon intensities,  $\rho$  (g/cm<sup>3</sup>) is the density of material,  $\mu_m$ (cm<sup>2</sup>/g) and  $\mu$ (cm<sup>-1</sup>) are mass and linear attenuation coefficients,  $t_m$  (g/cm<sup>2</sup>) and  $t$  (cm) are sample mass thickness (the mass per unit area) and the thickness, respectively.

If the sample has various elements, we can write the total mass attenuation coefficient for any compound as follows [24];

$$\mu/\rho = \sum_i w_i (\mu/\rho)_i \quad (3)$$

where  $w_i$  and  $(\mu/\rho)_i$  are the weight fraction and the mass attenuation coefficient of the  $i$ th constituent element, respectively.

The total atomic cross-section ( $\sigma_a$ ) for any sample can be calculated using the equation formulated as;

$$ACS = \sigma_a = \frac{N}{N_A} (\mu/\rho) \quad (4)$$

where  $N_A$  and  $N$  respectively are the Avogadro's number and the atomic mass of materials.

The total electronic cross-section ( $\sigma_e$ ) is formulated by the following equation [7];

$$ECS = \sigma_e = \frac{\sigma_a}{Z_{eff}} \quad (5)$$

By using the Equations (4) and (5), we can find the effective atomic number,  $Z_{eff}$ , of the material as follows;

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} \quad (6)$$

We can calculate the effective electron number,  $N_{eff}$ , as follows [21],

$$N_{eff} = \frac{\mu_m}{\sigma_e} \quad (7)$$

HVL and TVL are the thicknesses parameters that are used to reduce the radiation intensities by one half and one tenth, respectively. MFP is the average distance at which a photon travels through the material between two interactions. The  $\mu$  is used to obtain the parameters given by

$$HVL = \frac{\ln(2)}{\mu} \quad (8)$$

$$MFP = \frac{1}{\mu} \quad (9)$$

$$TVL = \frac{\ln 10}{\mu} \quad (10)$$

Effective conductivity ( $C_{eff}$ ) of materials can be given by the following equation [25]:

$$C_{eff} = \left(\frac{N_{eff} \rho e^2 \tau}{m_e}\right) 10^3 \quad (11)$$

where  $m_e$  (kg) and  $e$  (C) are mass and charge of electron, respectively.

FNRCS ( $\sum R$ ) values of the materials can be calculated by the following equation [26,27]:

$$\sum R = \sum_i \rho_i (\sum R / \rho)_i \quad (12)$$

where  $(\sum R / \rho)_i$  and  $\rho_i$  are the mass removal cross-section of the  $i$ th constituent element and partial density of the material, respectively.

### 3. THE RESEARCH FINDINGS AND DISCUSSION

The radiation shielding parameters of the compounds of the 3d transition elements which were reported previously by Yilmaz et al. [23] are theoretically calculated by using Phy-X/PSD code [10]. The theoretically calculated and experimentally reported MAC and  $Z_{eff}$  values of the compounds are given at photon energies 19.63 and 22.10 keV and listed in Table 1. It is clearly seen in the Table 1 that the calculated parameters are in good agreement with those obtained experimentally [23]. Due to the good agreement between calculated and experimental MAC and  $Z_{eff}$  results at 19.63 and 22.10 keV, we also wanted to obtain all radiation-matter interaction parameters theoretically in the energies of 0.015-15 MeV. Variations of the calculated values versus photon energies are given in Figures 1-5.

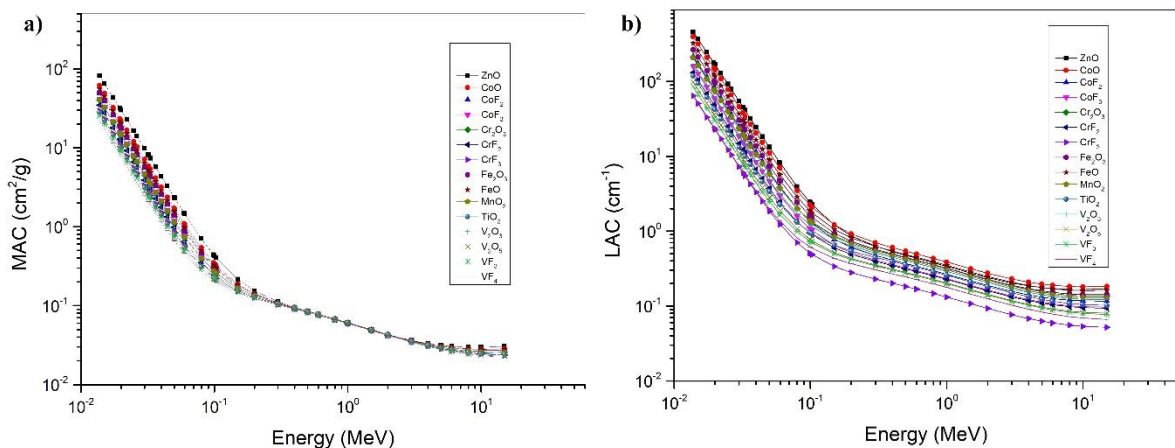


Figure 1. The changes of MAC (a) and LAC (b) as a function of incident photon energy

**Table 1.** Comparison of the calculated and experimental values of MAC and  $Z_{eff}$  for 3d transition elements compounds

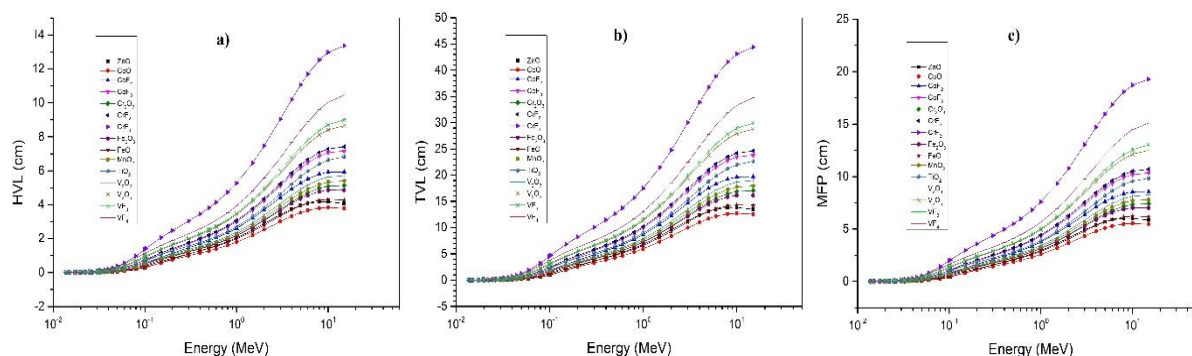
Comp	Phy-X/PSD MAC values		Experimental MAC values (Yılmaz <i>et al.</i> 2016)		Phy-X/PSD $Z_{eff}$ values		Experimental $Z_{eff}$ values (Yılmaz <i>et al.</i> 2016)	
	19.63 (keV)	22.1 (keV)	19.63 (keV)	22.1 (keV)	19.63 (keV)	22.1 (keV)	19.63 (keV)	22.1 (keV)
CoO	23.41	16.82	21.347±0.949	15.467±1.314	26.48	26.45	24.457±1.078	24.327±1.508
CoF <sub>2</sub>	18.41	13.23	17.297±0.778	12.597±1.070	25.70	25.66	24.157±1.065	24.097±1.494
CoF <sub>3</sub>	15.59	11.21	13.827±0.622	10.717±0.910	25.12	25.07	23.277±1.026	23.077±1.430
Cr <sub>2</sub> O <sub>3</sub>	14.98	10.73	14.947±0.672	10.737±0.912	23.12	23.07	23.027±1.015	22.997±1.425
CrF <sub>2</sub>	12.91	9.25	11.937±0.536	8.2927±0.705	22.54	22.49	20.797±0.916	20.127±1.247
CrF <sub>3</sub>	10.86	7.79	10.367±0.466	6.5827±0.559	21.91	21.85	20.237±0.892	18.377±1.138
FeO	21.23	15.23	22.077±0.993	16.207±1.377	25.46	25.43	26.907±1.186	26.607±1.649
Fe <sub>2</sub> O <sub>3</sub>	19.20	13.77	20.337±0.915	14.657±1.245	25.20	25.15	26.637±1.174	26.057±1.615
MnO <sub>2</sub>	15.33	10.99	13.677±0.615	9.4547±0.803	23.90	23.84	21.347±0.941	20.507±1.271
TiO <sub>2</sub>	10.38	7.41	10.327±0.464	7.3127±0.621	20.73	20.66	20.657±0.911	20.197±1.252
V <sub>2</sub> O <sub>3</sub>	12.96	9.26	13.997±0.629	9.8647±0.838	22.07	22.02	23.897±1.097	23.467±1.454
VF <sub>3</sub>	9.42	6.74	11.137±0.456	7.8927±0.585	20.84	20.77	22.447±1.039	21.187±1.317
V <sub>2</sub> O <sub>5</sub>	10.84	7.75	10.367±0.556	7.3217±0.622	21.52	21.44	21.567±0.989	20.247±1.251
VF <sub>4</sub>	8.19	5.86	7.3817±0.332	5.0027±0.425	20.26	20.18	18.277±0.806	17.227±1.067
ZnO	31.62	22.84	29.557±1.329	22.427±1.906	29.54	29.52	27.637±1.218	29.017±1.799

**Table 2.** Calculated MAC values of the investigated compounds and widely used shielding materials

Energy (MeV)	ZnO	CoO	FeO	Fe <sub>2</sub> O <sub>3</sub>	CoF <sub>2</sub>	CoF <sub>3</sub>	MnO <sub>2</sub>	Cr <sub>2</sub> O <sub>3</sub>	V <sub>2</sub> O <sub>3</sub>	CrF <sub>2</sub>	CrF <sub>3</sub>	V <sub>2</sub> O <sub>5</sub>	TiO <sub>2</sub>	VF <sub>3</sub>	VF <sub>4</sub>	OC [28]	SS [28]	IL [28]	BM [28]
1.50x10 <sup>-02</sup>	65.57	49.16	44.78	40.47	38.68	32.74	32.44	31.86	27.65	27.46	23.11	23.11	22.23	20.11	17.47	7.079	37.92	29.64	20.47
2.00x10 <sup>-02</sup>	30.05	22.22	20.15	18.22	17.49	14.80	14.55	14.21	12.29	12.25	10.31	10.28	9.848	8.941	7.772	3.105	17.02	13.28	9.156
3.00x10 <sup>-02</sup>	9.769	7.129	6.440	5.832	5.625	4.776	4.652	4.521	3.903	3.907	3.304	3.283	3.131	2.863	2.502	1.048	5.445	4.250	2.971
4.00x10 <sup>-02</sup>	4.377	3.186	2.879	2.616	2.531	2.162	2.098	2.035	1.763	1.769	1.510	1.499	1.430	1.316	1.161	0.541	2.446	1.907	1.295
5.00x10 <sup>-02</sup>	2.366	1.732	1.569	1.433	1.391	1.199	1.162	1.129	0.984	0.990	0.856	0.849	0.813	0.753	0.673	0.358	1.345	1.074	0.789
6.00x10 <sup>-02</sup>	1.452	1.074	0.979	0.900	0.874	0.762	0.740	0.720	0.635	0.638	0.560	0.557	0.536	0.500	0.454	0.241	0.849	0.690	0.526
8.00x10 <sup>-02</sup>	0.705	0.540	0.500	0.467	0.454	0.407	0.397	0.389	0.351	0.353	0.320	0.319	0.310	0.293	0.274	0.204	0.445	0.378	0.309
1.00x10 <sup>-01</sup>	0.430	0.344	0.324	0.307	0.299	0.274	0.270	0.266	0.245	0.246	0.229	0.229	0.225	0.215	0.205	0.172	0.296	0.261	0.227
1.50x10 <sup>-01</sup>	0.215	0.188	0.183	0.178	0.174	0.167	0.166	0.165	0.158	0.158	0.153	0.154	0.153	0.148	0.145	0.142	0.176	0.165	0.157
2.00x10 <sup>-01</sup>	0.154	0.142	0.141	0.139	0.136	0.133	0.133	0.133	0.129	0.129	0.127	0.128	0.128	0.124	0.123	0.127	0.139	0.134	0.132
3.00x10 <sup>-01</sup>	0.113	0.109	0.109	0.109	0.106	0.106	0.106	0.107	0.105	0.104	0.104	0.105	0.105	0.102	0.102	0.108	0.109	0.108	0.109
4.00x10 <sup>-01</sup>	0.095	0.094	0.094	0.095	0.092	0.092	0.093	0.093	0.092	0.092	0.091	0.092	0.093	0.090	0.090	0.096	0.095	0.095	0.096
5.00x10 <sup>-01</sup>	0.085	0.084	0.085	0.085	0.083	0.083	0.084	0.084	0.083	0.083	0.083	0.084	0.084	0.082	0.082	0.088	0.085	0.085	0.087
6.00x10 <sup>-01</sup>	0.078	0.077	0.078	0.078	0.076	0.076	0.077	0.077	0.076	0.076	0.076	0.077	0.077	0.075	0.076	0.079	0.079	0.079	0.080
8.00x10 <sup>-01</sup>	0.067	0.067	0.068	0.068	0.066	0.067	0.067	0.068	0.067	0.067	0.067	0.067	0.068	0.066	0.066	0.071	0.068	0.069	0.072
1.00x10 <sup>0</sup>	0.060	0.060	0.061	0.061	0.060	0.060	0.060	0.061	0.060	0.060	0.060	0.060	0.061	0.059	0.059	0.064	0.063	0.061	0.063
1.50x10 <sup>0</sup>	0.049	0.049	0.050	0.050	0.049	0.049	0.049	0.049	0.049	0.049	0.049	0.049	0.050	0.048	0.048	0.052	0.051	0.050	0.050
2.00x10 <sup>0</sup>	0.043	0.043	0.043	0.043	0.042	0.042	0.043	0.043	0.042	0.042	0.042	0.043	0.043	0.042	0.042	0.045	0.045	0.043	0.044
3.00x10 <sup>0</sup>	0.036	0.036	0.036	0.036	0.035	0.035	0.036	0.036	0.035	0.035	0.035	0.035	0.035	0.034	0.034	0.036	0.037	0.036	0.036
4.00x10 <sup>0</sup>	0.033	0.032	0.033	0.032	0.032	0.031	0.032	0.032	0.031	0.031	0.031	0.031	0.031	0.030	0.030	0.031	0.033	0.032	0.031
5.00x10 <sup>0</sup>	0.031	0.031	0.031	0.030	0.029	0.029	0.029	0.030	0.029	0.029	0.029	0.029	0.029	0.028	0.028	0.028	0.031	0.029	0.029
6.00x10 <sup>0</sup>	0.030	0.029	0.029	0.029	0.028	0.028	0.028	0.028	0.028	0.027	0.027	0.027	0.027	0.026	0.026	0.026	0.030	0.028	0.027
8.00x10 <sup>0</sup>	0.030	0.028	0.028	0.028	0.027	0.026	0.026	0.027	0.026	0.026	0.025	0.025	0.026	0.025	0.024	0.024	0.028	0.026	0.025
1.00x10 <sup>1</sup>	0.030	0.028	0.028	0.027	0.026	0.025	0.026	0.026	0.025	0.025	0.024	0.025	0.025	0.024	0.023	0.022	0.027	0.025	0.024
1.50x10 <sup>1</sup>	0.030	0.028	0.028	0.027	0.026	0.025	0.026	0.026	0.025	0.025	0.024	0.024	0.024	0.023	0.022	0.021	0.027	0.025	0.023

The variations of the MAC values versus the incident photon energies for all compounds are shown in Figure 1(a). It was obtained that the highest three MAC values are found for ZnO, CoO and FeO compounds both at high and low energies, respectively. It is clearly seen that MAC values decrease with the increasing photon energy which affects the penetration of the photon. In order to evaluate the shielding properties of the compounds, the calculated MAC values were compared with the widely used shielding materials (ordinary concrete, steel-scrap, ilmenite-limonite and basalt-magnetite) reported by Bashter [28], and the results are given in Table 2. It can be mentioned that all the studied compounds show higher shielding features than ordinary concrete (OC). ZnO, CoO, FeO, Fe<sub>2</sub>O<sub>3</sub>, and CoF<sub>2</sub> have higher shielding potentials than steel-scrap. The obtained MAC values of ZnO, CoO, FeO, Fe<sub>2</sub>O<sub>3</sub>, CoF<sub>2</sub>, CoF<sub>3</sub>, MnO<sub>2</sub>, and Cr<sub>2</sub>O<sub>3</sub> are greater than those of ilmenite-limonite, while except from VF<sub>3</sub> and VF<sub>4</sub> all the other compounds show higher shielding abilities than basalt magnetite.

LAC is one of the parameters for defining the photon-matter interaction, but it is not sufficient. Additionally, it is evaluated to calculate MAC, HVL and MFP shielding parameters. The value of LAC depends on both MAC and density of compound. We can see the dependence of LAC values on photon energies in Figure 1(b). We observed the highest LAC value for ZnO at low energies while this was observed for CoO compound at high energies. Due to the density effect, differences of LAC values are greater than those of MAC values.



**Figure 2.** Dependence of HVL (a) TVL (b) and MFP (c) versus incident photon energy

The HVL and TVL are the parameters to understand the ability of radiations to penetrate materials. HVL, TVL and MFP parameters changing with the incident photon energies are given in Figure 2(a-c). It is desirable to have low HVL, TVL and MFP values in the high energy regions. It is seen that the lowest HVL, TVL and MFP values were obtained for CoO, ZnO and FeO compounds in high energy regions. Due to the obtained HVL, TVL and MFP values, it can be concluded that the best radiation shielding property is shown by CoO compound.

The interaction possibility of per atom and per electron in a unit volume of any material is given by ACS and ESC, respectively. In Figure 3(a-b), changing of ACS and ECS values as a function of incident photon energies are given. If the ACS and ECS values are high, the compounds with these values can be evaluated as better shielding compounds. According to these parameters, we can mention that the highest shielding properties belong to ZnO, CoO and FeO compounds, respectively and the lowest shielding capacity is determined for VF<sub>4</sub>. This result is compatible with the mentioned parameters above.

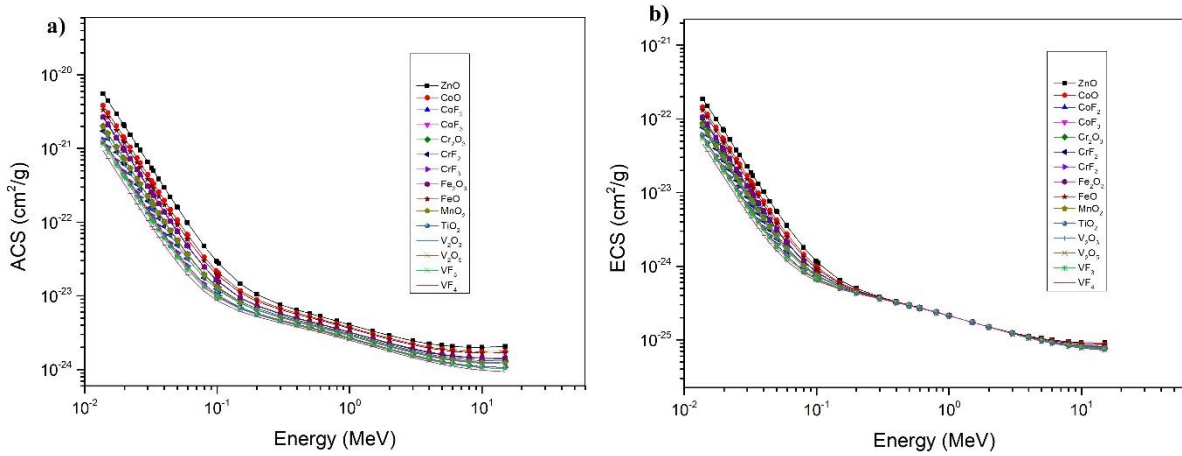


Figure 3. The variations of ACS (a) and ECS (b) as a function of incident photon energy

The energy dependence of  $Z_{eff}$  and  $N_{eff}$  are given in Figure 4(a-b).  $Z_{eff}$  values are high for ZnO, CoO and FeO compounds while those are low for  $VF_4$  compound in the all energies. Due to the higher  $Z_{eff}$  values, it can be said that ZnO has the highest shielding potential among others.  $N_{eff}$  is one of the most important parameter that represents the effective conductivity of the compound depending on the excitatory photon energy [5]. As seen in the figure, the dependence of the  $N_{eff}$  values on the incident photon energies is similar with the variations of  $Z_{eff}$  values.

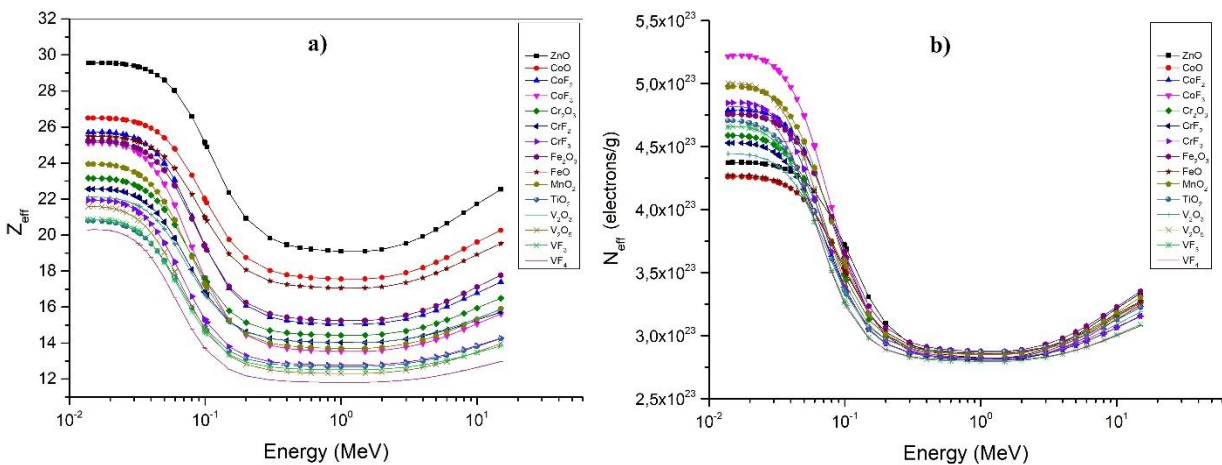


Figure 4. The changes of  $Z_{eff}$  (a) and  $N_{eff}$  (b) as a function of incident photon energy

The interactions between photons and material with photo-electric effect, Compton scattering, and pair production interaction processes cause changes in the number of free electrons in the material. This change depends on the  $N_{eff}$  values because of the conduction electron numbers. Hence,  $C_{eff}$  is proportional to  $N_{eff}$  of the compounds. Change of  $C_{eff}$  values versus photon energies is given in Figure 5. CoO, compound has the highest  $C_{eff}$  values in all energies compared to others.

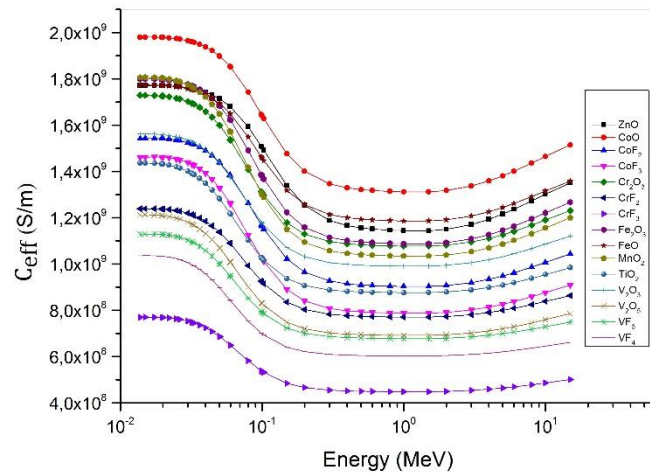


Figure 5. The variations of  $C_{eff}$  versus photon energy

Additionally, it is important to learn the neutron shielding capacity of the compounds for neutron applications. The fast neutron attenuation capabilities of the compounds were also determined by Phy-X/PSD. FNRCS and densities of the studied compounds are given in Figure 6. It was concluded that there is a direct relation between the densities and FNRCS values of the compounds. The lowest FNRCS (0,063) is observed for  $CrF_3$  and the highest one (0.154) is observed for  $CoO$ . It can be noted that  $CoO$  compound has the best neutron shielding ability among the compounds, while  $CrF_3$  has the least.

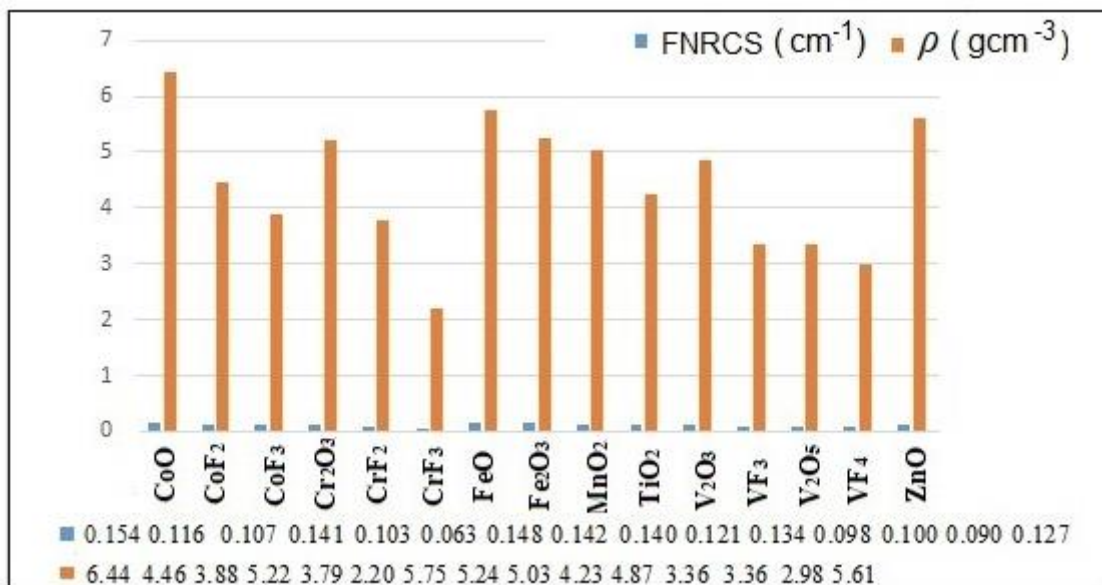


Figure 6. The changes of FNRCS values and densities of the compounds

#### 4. RESULTS

In the present study, radiation-matter interaction parameters of compounds of 3d transition elements were calculated to determine the radiation shielding capabilities. For the purpose of determining the parameters Phy-X / PSD software was applied. The MAC and  $Z_{eff}$  parameters were calculated and compared with experimental results at 19.63 and 22.10 keV energies. In addition, MAC, LAC, HVL, TVL, MFP, ACS, ECS,  $Z_{eff}$ ,  $N_{eff}$ ,  $C_{eff}$  and FNRCS values of the present compounds were calculated in the range of 0.01-15 MeV. According to the obtained results in the present study, it was concluded that  $ZnO$ ,  $CoO$  and  $FeO$  compounds have the highest probabilities of interacting with photon and so have highest shielding



potentials compared to other compounds. According to the obtained FNRCS values of the compounds, CoO, FeO and Fe<sub>2</sub>O<sub>3</sub> have more neutron shielding performances among the studied compounds.

#### CONFLICTS OF INTEREST

No conflict of interest was declared by the authors.

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