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# Exploring the metal tungstate oxides ( $MWO_4$ ; M = Ca, Sr, Ba, and Pb) as radiation shielding materials: a simulation study

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## ABSTRACT

Environmentally hazardous radiation sources can negatively affect human health. For example, tumors, cancer, a decrease in lymphocyte cell count, and severe cases of fatalities. Because of this, the present work aims to explore the radiation-protecting performances of the metal-tungstate oxides:  $CaWO_4$ ,  $SrWO_4$ ,  $BaWO_4$ , and  $PbWO_4$  as a comparative study that provides effective strategy for developing sustainable and alternative shield material. The mean track length of incoming photons inside four distinct metal tungstate oxides has been determined using the Monte Carlo simulation code. Then, other significant gamma-ray shielding characteristics were computed based on the predicted track length. For all samples, attenuation coefficients are estimated by MCNP5 simulation code, which showed satisfactory agreement with the Phy-X/PSD results. It also used to figure out the half-value layer, mean free path, effective atomic number, and effective electron density. The mass attenuation coefficient and effective atomic number are energy and density dependency, have maximum values at the lowest energies and minimum values at the highest energies. The study findings imply that the atomic density and metal tungstate oxide composition of the material determine the correlation between the photon and the shield material. The results showed that the maximum mass attenuation coefficient was achieved for  $PbWO_4$  that is a superior candidate for radiation shielding applications.

## 1. Introduction

Since ionizing radiation is used so often in the medical field, the military, and numerous other businesses, the problem is presently growing worse. It is significant that ionizing radiation may cause harm to human health. Many studies on radiation-protective materials have been conducted in an effort to address these shortcomings [1-3]. Lead, however, is a highly dangerous material for both people and their surroundings. Due to its large atomic number  $Z$  (82), higher density ( $11.29 \text{ g/cm}^3$ ), and inexpensive cost, lead is frequently employed in radiation shields [2]. As a result, it is necessary to identify and create substitutes that provide equally effective radiation protection. In the last few years, a wide range of compositions have been suggested and investigated for radiation shielding [3].

Structure of a perovskite with the general chemical formula  $ABX_3$ . The X atoms (usually oxygen), the B atoms (a smaller metal cation, such as W, V, Mn, etc.), and the A atoms (a larger metal cation, such as Ca, Ba, Fe, Sr, Pb, La, etc.) [4-6]. Among those materials, the metal tungstate based on the perovskite-structured  $ABO_3$  might be capable of radiation protection. Among the well-known metal tungstate oxides  $ABO_3$  perovskites form,  $PbWO_4$  and  $BaWO_4$  exhibit remarkable multifunctional properties [4]. In addition to being non-organic in structure, metal tungstate oxides are hard, less porous, long-lasting, and environmentally friendly [7-12].

To enhance the polymer composite's radiation shielding capabilities, for example,  $Bi_2(WO_4)_3$  was reinforced into the polyester composite has been recently reported. The metal tungstate oxides have better performance in radiation protecting [13]. An investigation of metal composites series based on tungsten ( $Bi_2WO_6$ ,  $PbWO_4$ , and  $Pb_{0.82}Bi_{0.12}WO_4/W_{0.5}Pb_{0.5}Bi_{1.2}O_{20}$ ) has been studied as effective protective blocks against gamma radiation [14]. Also evaluate the validity of LDPE/SBR polymer bland with 5, 10, 15, and 20 wt.% of  $BaWO_4/B_2O_3$  nanofillers against radiation [15]. The radiation shielding parameters of  $BaWO_4$  metal tungstate oxides doped with  $Ho_2O_3$  oxides have been assessed using the MCNP code for gamma rays [16]. Very recently,

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E-mail address: [saidmoawad2@gmail.com](mailto:saidmoawad2@gmail.com) (Said M. Kassem); Tel.: +201091878513DOI: [10.21608/IFJSIS.2024.273401.1067](https://doi.org/10.21608/IFJSIS.2024.273401.1067)

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Vishnu et al. [17] studied the addition of barium tungsten (BaWO<sub>4</sub>) to natural rubber, which significantly improved the characteristics of gamma radiation shielding.

This search might encourage researchers to do experimental research on different kinds of metal tungstate oxides so that our results can be compared to those of future investigations. Researchers in technological fields who want to create novel chemicals for protecting themselves from radiation can benefit from this work. To accomplish this work, the desired metal tungstate oxides are CaWO<sub>4</sub> (CWO), SrWO<sub>4</sub> (SWO), BaWO<sub>4</sub> (BWO), and PbWO<sub>4</sub> (PWO) by theoretical investigation to examine their radiation attenuation properties.

## 2. Attenuation theory

### 2.1. Simulation procedures

A Monte Carlo simulation code (MCNP-5) input file is necessary for an adequate simulation procedure with an acceptable relative error value that can be used to estimate the average track length for various forms of ionizing radiation [18]. The shielding properties of the metal tungstate oxides were evaluated by instruction as displayed in Fig. 1. The elemental composition and the density of metal tungstate oxide samples are listed in Table 1. The input file consists of many cards, including surface, cell, material, importance, source, and physical cards. Regarding the surface card, it is used to describe the boundaries and dimensions of each cell. The cell is considered the smallest unit in geometry, where each consists of many cells arranged together. Besides, the material card is used to describe the chemical composition and density of each cell used in the geometry [2]. The F4 tally is used for detector to evaluation the average track length [19]. In addition, the results of simulation compared with theoretical values using the Phy-X/PSD software [20].

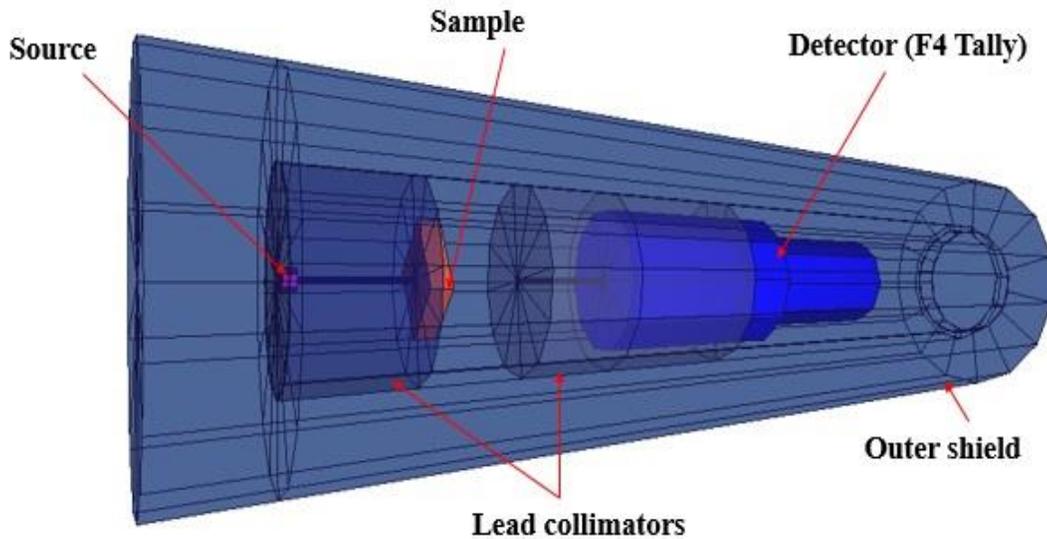


Fig.1. MCNP simulation geometry.

Table 1: The density, molar volume and elemental composition of metal tungsten oxides.

Metal tungstate oxides Code	Elements Fraction (wt. %)			Density (g/cm <sup>3</sup> )	Molar Volume (cm <sup>3</sup> .mol <sup>-1</sup> )
	M	W	O		
CWO (M=Ca)	0.1392	0.6385	0.2223	6.10	47.202
SWO (M=Sr)	0.2612	0.5480	0.1908	6.31	53.163
BWO (M=Ba)	0.3565	0.4773	0.1662	6.25	61.626
PWO (M=Pb)	0.4553	0.4040	0.1406	7.96	57.166

### 2.2. Attenuation parameters calculation

To assess the gamma-ray absorption abilities, the current study used the gamma-ray attenuation equations for MWO<sub>4</sub> perovskite oxides (M = Ca, Sr, Ba, and Pb) as detailed below [21-25]. The narrow beam transport radiation setup could determine the attenuation coefficients for the studied shield material as follows:

$$I_x = I_0 e^{-LAC x} \tag{1}$$

$$MAC = \left(\frac{LAC}{\rho}\right) = \frac{\ln\left(\frac{I_0}{I_x}\right)}{\rho x}, \tag{2}$$

Where; I<sub>0</sub> and I<sub>x</sub> are the without shield and attenuated intensities.

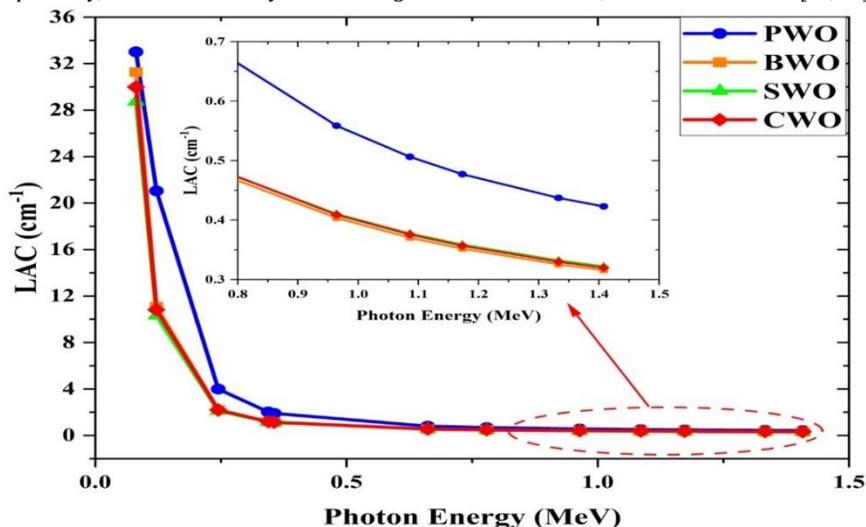
For theoretical computations, using the Phy-X/PSD software's program, the MFP, Z<sub>eff</sub>, N<sub>eff</sub>, HVL, and TVL values were obtained using measurements of LAC and MAC, which has been discussed in detail in references [2, 20].

### 3. Results and discussion

#### 3.1. Radiation shielding parameters

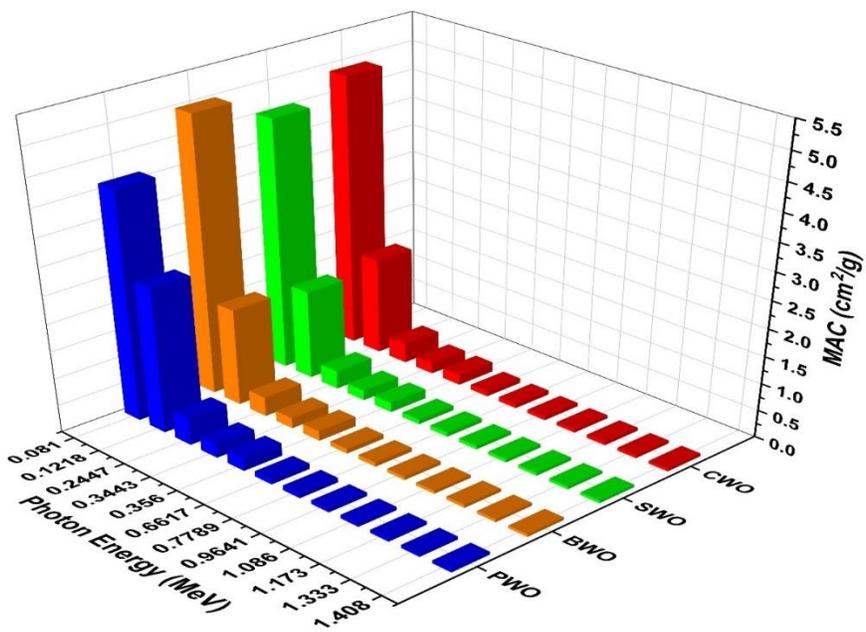
Herein, the  $MWO_4$  (M =Ca, Sr, Ba, and Pb) metal oxides capability to shield the gamma photons in the 0.081-1.408 MeV energy range using gamma sources ( $^{60}Co$ ,  $^{137}Cs$ ,  $^{133}Ba$ , and  $^{152}Eu$ ) was studied using the MCNP simulation code and Phy-X program 26. **Fig. 2** shows the LAC against gamma photon energy to adequately understand the shielding features of the metal tungstate oxides. **Table 2** depicts this comparison for the metal tungstate oxides with different compositions. Apparently, the MCNP and Phy-X values of the four metal tungstate oxides agreed highly with each other [26].

As the energy increases from 0.081 to 1.408 MeV, the LAC shows a decreasing pattern (**Fig. 2**). This decrease in LAC is brought on by radiation with relatively high energy since it penetrates the sample more readily. This indicates that the CWO, SWO, BWO, and PWO metal tungstate oxides possess the least (maximum) shield proficiency against high (lower) energy of radiation. The LAC values exhibit a tendency to rise as the MWO density of metal oxides rises, with the lowest (highest) value of  $28.722\text{ cm}^{-1}$  ( $0.4229\text{ cm}^{-1}$ ) at 0.081 MeV (1.408 MeV) for SWO and PWO, and the highest (lowest) value of  $33.0154\text{ cm}^{-1}$  ( $0.3157\text{ cm}^{-1}$ ) at 0.081 MeV (1.408 MeV) for PWO and BWO composite, respectively. The LAC increases with increasing atomic numbers from Ca, Sr, Ba, and Pb respectively, as does the density of metal tungstate oxides increases, as shown in **Table 1** [27, 28].



**Fig. 2.** Variation of the  $MWO_4$  metal tungstate oxides LAC versus the gamma photon energy.

The metal tungstate oxide’s mass attenuation coefficients are listed in **Table 2**, compared to values obtained from Phy-X calculations, which give a good agreement together. The MACs of the CWO, SWO, BWO, and PWO metal oxides were all compared at energies of  $^{60}Co$ ,  $^{137}Cs$ ,  $^{133}Ba$ , and  $^{152}Eu$  gamma ray sources to situate their protective the PWO abilities into perspective. When looking at the prepared metal tungstate oxides, BWO metal tungstate oxides have the greatest MAC, while CWO and SWO ceramics are practically slightly behind. The MAC values at 0.081 (1.408) MeV are equal to 4.917 (0.05245), 4.552 (0.05107), 5.006 (0.05052), and 4.148 (0.05313)  $\text{cm}^2/\text{g}$  for CWO, SWO, BWO, and PWO metal tungstate oxides, respectively, as shown in **Fig. 3**.

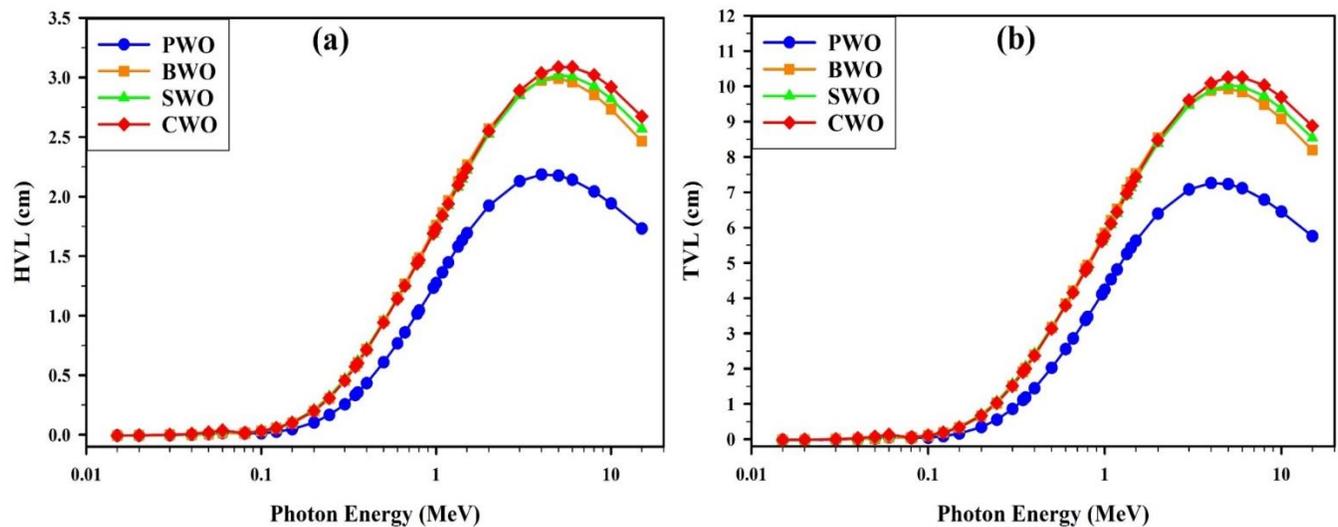


**Fig. 3.** The variation of MAC of  $MWO_4$  metal-tungstate oxides versus the gamma photon energy.

**Table 2:** The MAC of metal-tungstate oxides.

Energy (MeV)	CaWO <sub>4</sub>			SrWO <sub>4</sub>			BaWO <sub>4</sub>			PbWO <sub>4</sub>		
	MCNP	Phy-x	RD%									
0.0810	4.91700	4.91694	0.0011	4.55200	4.55186	0.0030	5.00600	5.00544	0.0111	4.14800	4.14766	0.0082
0.1218	1.77400	1.77366	0.0192	1.63500	1.63492	0.0051	1.77400	1.77393	0.0037	2.64300	2.64342	0.0160
0.2447	0.35920	0.35924	0.0122	0.33420	0.33419	0.0025	0.35180	0.35177	0.0094	0.50150	0.50147	0.0065
0.3443	0.19630	0.19631	0.0040	0.18480	0.18477	0.0177	0.19070	0.19071	0.0051	0.25440	0.25443	0.0111
0.3560	0.18650	0.18651	0.0071	0.17580	0.17578	0.0121	0.18110	0.18109	0.0069	0.23980	0.23976	0.0157
0.6617	0.09047	0.09047	0.0022	0.08704	0.08704	0.0050	0.08721	0.08721	0.0010	0.10060	0.10056	0.0398
0.7789	0.07883	0.07883	0.0056	0.07612	0.07612	0.0043	0.07592	0.07592	0.0013	0.08509	0.08509	0.0056
0.9641	0.06707	0.06707	0.0028	0.06502	0.06502	0.0054	0.06457	0.06457	0.0029	0.07017	0.07017	0.0064
1.0860	0.06158	0.06160	0.0322	0.05980	0.05981	0.0221	0.05925	0.05927	0.0278	0.06358	0.06360	0.0328
1.1730	0.05851	0.05851	0.0030	0.05687	0.05687	0.0032	0.05630	0.05630	0.0085	0.05995	0.05995	0.0033
1.3330	0.05410	0.05410	0.0017	0.05265	0.05265	0.0000	0.05209	0.05209	0.0052	0.05492	0.05492	0.0044
1.4080	0.05245	0.05245	0.0017	0.05107	0.05107	0.0073	0.05052	0.05052	0.0069	0.05313	0.05313	0.0073

**Fig. 4(a)** shows the half-value layers (HVL) of the metal tungstate oxides as a function of gamma photon energy. HVL grows with energy; this clear trend indicates that in order to attenuate the same number of photons at higher energy, the graph also shows that, of the examined metal tungstate oxides, the PWO sample has a lower HVL than the MWO<sub>4</sub> samples, making them the more efficient barriers [29]. HVL values at 0.081 MeV (the minimum) and highest (1.408 MeV) gamma ray energy were equaled to 0.023 (2.166), 0.024 (2.151), 0.022 (2.195), and 0.021 (1.639) cm for CWO, SWO, BWO, and PWO metal tungstate oxides, respectively. Tenth-value layer (TVL) values are shown in **Fig. 4 (b)**. Herein, according to the TVL values at 0.081 MeV (lower) and highest (1.408 MeV) gamma ray energy, it was found to be 0.077 (7.197) cm, 0.080 (7.146) cm, 0.074 (7.293) cm, and 0.070 (5.445) cm for CWO, SWO, BWO, and PWO, respectively.



**Fig. 4.** Variation of the (a) HVL, (b) TVL for MWO<sub>4</sub> oxides versus the gamma photon energy.

The mean free path (MFP), another significant shield metric that is utilized to calculate the effective shield against ionizing radiation. In practical applications, it is preferred for metal tungstate oxides to have a lower MFP since it indicates greater photon contact with the material [30]. **Fig. 5** illustrates MFP results varying with investigated gamma source energies for the CWO, SWO, BWO, and PWO metal tungstate oxides. It was also revealed that the MFP energy dependent on the atomic number of metals added with WO<sub>3</sub> in the MWO<sub>4</sub> (M= Ca (z=20), Sr (z=38), Ba (z=56), and Pb (z=82)) metal tungstate oxides, as well as the density of the composite. The minimum MFP at PWO while the maximum MFP was reported at CWO ceramic. By contrast, the MFP at 0.662 MeV energy is 1.812, 1.821, 1.853, and 1.249 cm for CWO, SWO, BWO, and PWO metal tungstate oxides, respectively [31, 32].

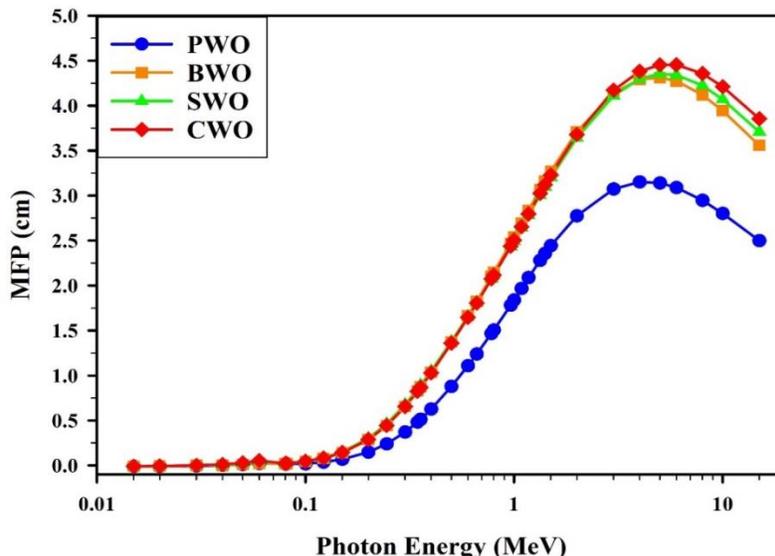


Fig. 5. Variation of MFP values for MWO<sub>4</sub> oxides versus the photon energies.

The effective atomic number ( $Z_{eff}$ ) was also ascertained in order to understand the efficacy of the shielding material attenuation abilities. At high  $Z_{eff}$  values, the sample with the highest atomic number of heavy elements demonstrated a growing efficacy in attenuating gamma rays [33]. The  $Z_{eff}$  has relatively high values at first (< 0.8 MeV) with the PWO metal tungstate oxides with Pb concentrations having the largest and SWO having the lowest values. Following that, there is a significant decrease in  $Z_{eff}$  up to around 0.8 MeV. In the energy range of 0.8–1.4079 MeV,  $Z_{eff}$  achieves its lowest values, as seen in Fig. 6(a). We observed that with higher energy (> 1 MeV) the PWO have large  $Z_{eff}$  values and CWO has the lowest. Fig. 6(b) demonstrates the variation of effective electron density ( $N_{eff}$ ) with the photon energies.  $N_{eff}$  showed a commensurate response to the increase in metal at the MWO<sub>4</sub> composite, with a pattern that was similar to  $Z_{eff}$ 's.

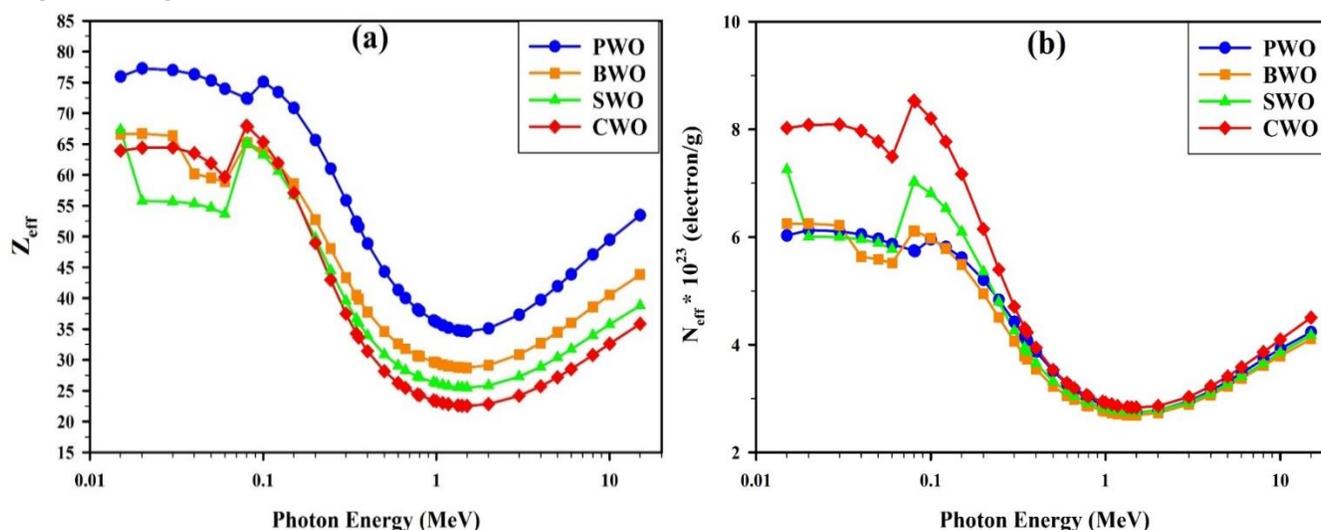


Fig. 6. Variations of the (a)  $Z_{eff}$  and (b)  $N_{eff}$  with photon energy for the MWO<sub>4</sub> metal tungstate oxides.

#### 4. Conclusions

This work briefs the shielding features for metal tungstate oxides of MWO<sub>4</sub>, where M =Ca, Fe, Sr, Ba, and Pb. The radiation protective parameters were examined using the MCNP code and Phy-X/PSD software in the gamma-ray energy range of 0.081-1.4079 MeV for gamma radiation sources <sup>60</sup>Co, <sup>137</sup>Cs, <sup>133</sup>Ba and <sup>152</sup>Eu. We also examined the LAC and MAC in the same energy range and observed a tendency for the attenuation ability to decrease from 0.81 to 1.4079 MeV. The LAC values exhibit a tendency to rise as the MWO density of metal oxides rises, with the lowest (highest) value of 28.722 cm<sup>-1</sup> (0.4229 cm<sup>-1</sup>) at 0.081 MeV (1.408 MeV) for SWO and PWO, and the highest (lowest) value of 33.0154 cm<sup>-1</sup> (0.3157 cm<sup>-1</sup>) at 0.081 MeV (1.408 MeV) for PWO and BWO composite, respectively. HVL values at 0.081 MeV (the minimum) and highest (1.408 MeV) gamma ray energy were equaled to 0.023 (2.166), 0.024 (2.151), 0.022 (2.195), and 0.021 (1.639) cm for CWO, SWO, BWO, and PWO metal tungstate oxides, respectively. The research results suggest that the correlation between the photon and the material depends upon the material's atomic density and composition of metal tungstate oxides. In addition,  $N_{eff}$  showed a commensurate response to the increase in metal at the MWO<sub>4</sub> composite, with a pattern that was similar to  $Z_{eff}$ 's. The results of this comparison study showed that the MWO<sub>4</sub> metal tungstate oxides could work well for radiation shielding applications.

**Author Contributions**

Said M. Kassem: Data curation, Investigation, Methodology, Writing - original draft, Writing - review & editing. Adel M. El Sayed: Data curation, Investigation, Writing - original draft. S. Ebraheem: Data curation, Supervision. A. I. Helal: Data curation, Supervision. Y. Y. Ebaïd: Data curation, Supervision.

**Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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