Calculation of Absorption Parameters for Some Selected Minerals in the Energy Range of 1 KeV to 100 GeV

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Abstract— Theoretical information about the absorption parameters for different material is very useful for the different research areas such as trace element analysis, medicine, physics, environmental science, etc. In this study, mass attenuation coefficients, molecular cross sections, atomic cross sections, electronic cross sections, effective atomic numbers and effective electron densities were calculated in the energy range from 1 keV to 100 GeV for $MnCO_3$, $ZnCO_3$, $SrCO_3$ and CdCO3. It has been observed that photoelectric effect, Compton scattering and pair production process are predominate in different energy regions.

Index Terms—mineral, gamma, WinXCOM, absorption, linear, coefficient.

1 INTRODUCTION

MANGANESE Carbonate ($MnCO_3$), Zinc Carbonate ($ZnCO_3$), Strontium Carbonate ($SrCO_3$) and Cadmium Carbonate ($CdCO_3$) are very important minerals used in daily life. Manganese Carbonate ($MnCO_3$) is observed in granite and other igneous rock. Manganese Carbonate ($MnCO_3$) minerals are used in agriculture, food productions, ceramics, etc. Zinc Carbonate ($ZnCO_3$) occurs in zinc-bearing ore deposits and carbonate rocks. Zinc Carbonate minerals are utilized in the chemistry, agriculture, paint industry, medicine, television industry, rubber industry, etc. Both Strontium Carbonate ($SrCO_3$) and Cadmium Carbonate ($CdCO_3$) minerals are existed in granite and other igneous rock. Strontium Carbonate ($SrCO_3$) minerals are used in ceramics, electronics, glass industry, paint industry, superconductor, electroluminescent materials, etc. Cadmium Carbonate ($CdCO_3$) minerals are utilized in pharmaceutical industry, applications of physics, chemical reagents, etc. Determination of photon interaction parameters of minerals such as mass absorption coefficients, molecular cross sections, atomic cross sections, electronic cross sections, active atomic numbers, effective electron densities are help us to understand the physical properties of minerals.

The various theoretical and experimental studies related to the absorption parameters are available in literature for elements, compounds, alloys, etc. Berger *et al.*[1] developed a computer program called XCOM to determine the cross-sections and mass absorption coefficients of any compound, element or mixture. XCOM program was modified a Windows version called WinXCOM by Gerward *et al.* [2]. Mass absorption coefficients, molecular, atomic, electronic cross-sections, effective atomic numbers and electron densities for some enzyme inhibitors, some drugs used in chemotherapy, various alloys, composite materials, different shielding materials, some perovskites compounds in the energy range from 1 keV to 100 GeV were calculated by Kaçal *et al.* [3], Akman and Kaçal [4], Kurudirek *et al.* [5], Hosamani and Badiger [6], Elmahroug *et al.* [7], Oto *et al.* [8]. Pawar and Bichile [9], Kore and Pawar [10], Gaikvad *et al.* [11] measured the mass attenuation coefficients, atomic cross sections, electronic cross sections, effective atomic numbers and effective electron densities for some enzymes, proteins, amino acids and fatty acids in the energy range from 122 keV to 1330 keV. Polat and İçelli [12], Polat *et al.* [13], Akman *et al.* [14,15], investigated mass absorption coefficients, atomic, molecular, electronic cross-sections, effect atomic numbers, electron densities and absorption jump factors for some cerium, barium, indium and samarium compounds. Photon interaction parameters such as mass attenuation coefficient, effective atomic number, electron density, buildup factor were measured for $Fe(NO_3)_3$, V_4O_2, $NaCO_3.H_2O$, $C_6H_5FeO_7.H_2O$ and CuCI compounds in the energy range from 32.2 keV to 59.5 keV by Levent and Özdemir [16]. Akman *et al.* [17] measured the effective atomic numbers and electron densities of some synthesized triazoles using mass attenuation coefficients in the energy range from 13.93 keV to 59.54 keV. The mass attenuation coefficients, half value layers, mean free paths and effective atomic numbers for $BaZrO_3$, $BaTiO_3$, Mg_3N_2, $Ba_2P_2O_7$, SiC were investigated by Sayyed *et al.* [18]. Mass and linear attenuation coefficients, half value layers, tenth value layers, mean free paths, effective atomic numbers, electron densities, exposure buildup factors and fast neutron removal cross sections for peridot, aluminum nitride, ruby, yttrium oxide, magnesium silicate, and silicon nitride ceramics were examined by Kaçal *et al.* [19].

Although mass absorption coefficient, molecular cross section, atomic cross section, electronic cross section, effective atomic number and electron density values for various materials such as elements, compounds, mixture, alloys, etc. are sufficient in the literature, these theoretical

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parameters are very limited for minerals. In this study, we calculated the mass absorption coefficients, molecular cross section, atomic cross section, electronic cross sections, effective atomic numbers and electron densities in the energy range from 1 keV to 100 GeV for Manganese Carbonate ($MnCO_3$), Zinc Carbonate ($ZnCO_3$), Strontium Carbonate ($SrCO_3$) and Cadmium Carbonate ($CdCO_3$).

Total mass absorption coefficient is given by;

$$I = I_0 e^{-(\mu/\rho)x} \tag{1}$$

where, I_0 and I represent the primary intensity and transmitted intensity respectively, μ represents the linear absorption coefficient, ρ represents the density of the absorber and x represents the thickness of the absorber.

The mass attenuation coefficient for any alloy, mixture or compound is computed using the following equation;

$$\left(\frac{\mu}{\rho}\right)_{Comp} = \sum W_i \left(\frac{\mu}{\rho}\right)_i \tag{2}$$

where, W_i represents the weight fraction and $(\mu/\rho)_i$ represents the mass attenuation coefficient of the *ith* constituent element.

$$W_i = \frac{n_i A_i}{\sum_j n_j A_j} \tag{3}$$

A_i represents the atomic weight of the *ith* element and n_i represents the number of atoms of *ith* constituent element in the compound.

Molecular cross section is calculated using the total mass absorption coefficients and given by;

$$\sigma_{t,m} = \frac{1}{N}(\mu/\rho)_{Comp} \sum (n_i A_i) \tag{4}$$

where, N represents the Avogadro's constant. Total atomic cross section can be calculated the following equation;

$$\sigma_{t,a} = \sigma_{t,m} \frac{1}{\sum_i n_i} \tag{5}$$

The total electronic cross section is computed using the following equation;

$$\sigma_{t,e} = \frac{1}{N} \sum \frac{f_i A_i}{Z_i} \left(\frac{\mu}{\rho}\right)_i \tag{6}$$

where, f_i represents the fractional abundance of the *ith* element with respect to number of atoms, Z_i represents the atomic number for the *ith* element in a compound.

Effective atomic number and electron density are computed using the equation (7) and equation (8), respectively.

2 Theoretical Calculation

$$Z_{Eff} = \frac{\sigma_{t,a}}{\sigma_{t,e}} \tag{7}$$

$$N_{eff} = \frac{Z_{Eff.}}{A_{tot}} (N n_{tot}) \tag{8}$$

A_{tot} represents the atomic weight of compound and n_{tot} represents the total number of atoms.

3 Result and Discussion

Total mass absorption coefficient values for the Manganese Carbonate ($MnCO_3$), Zinc Carbonate ($ZnCO_3$), Strontium Carbonate ($SrCO_3$) and Cadmium Carbonate ($CdCO_3$) were taken from WinXCOM program (Gerward et al., 2001). The molecular cross sections, atomic cross sections and electronic cross sections were determined from eq. 4-6 with the help of the theoretical total mass absorption coefficients from WinXCOM, Avogadro's constant, the atomic weight of the elements in the minerals, the number of atoms of the elements in the minerals, fractional abundance of the elements in the minerals and the atomic number for the elements in the minerals. The effective atomic numbers and electron densities for $MnCO_3$, $ZnCO_3$, $SrCO_3$ and $CdCO_3$ were obtained from eq. 7 and eq. 8, respectively. The theoretical total mass absorption coefficients, molecular cross sections, atomic cross sections, electronic cross sections, effective atomic numbers and electron densities for $MnCO_3$ are listed in Table 1.

Mass absorption coefficients, molecular cross sections, atomic cross sections and electronic cross sections for $MnCO_3$, $ZnCO_3$, $SrCO_3$ and $CdCO_3$ are presented as a function of energy in Figure 1-4. As seen from Figure 1-4, it is clearly observed that the absorption parameters for minerals change with changing in the studied energy region. Also, as clearly seen from Figure 1-4 and Table 1, mass absorption coefficient, molecular cross section, atomic cross section and electronic cross section values for Manganese Carbonate, Zinc Carbonate, Strontium Carbonate and Cadmium Carbonate decrease with increasing energy. But absorption parameters sharply increase at the *K*, *L*,… edge energies for elements and then decrease continue with the increasing energy. Thus a saw-tooth structure around the *K*, *L*,… edge was formed as seen Figure 1-4. It is clearly seen Figure 1-4 and Table 1, sharply increase at the *K* edge is at 6.539 keV, 9.6586 keV, 16.105 keV, 26.7112 keV for $MnCO_3$, $ZnCO_3$, $SrCO_3$ and $CdCO_3$, respectively.

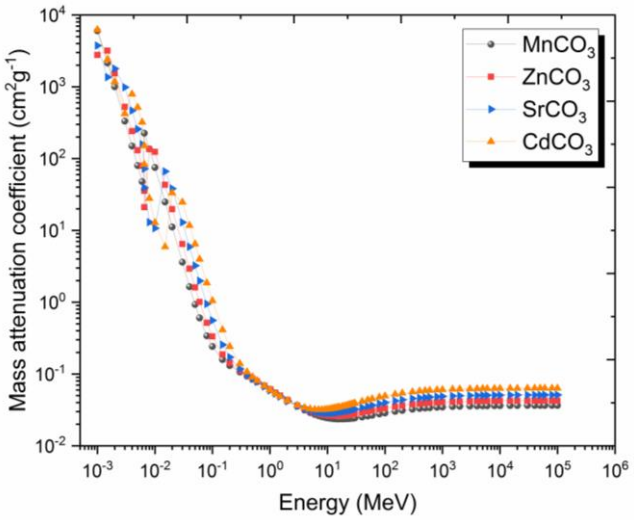

Figure 1. Mass attenuation coefficients of $MnCO_3$, $ZnCO_3$, $SrCO_3$ and $CdCO_3$ versus photon energy.

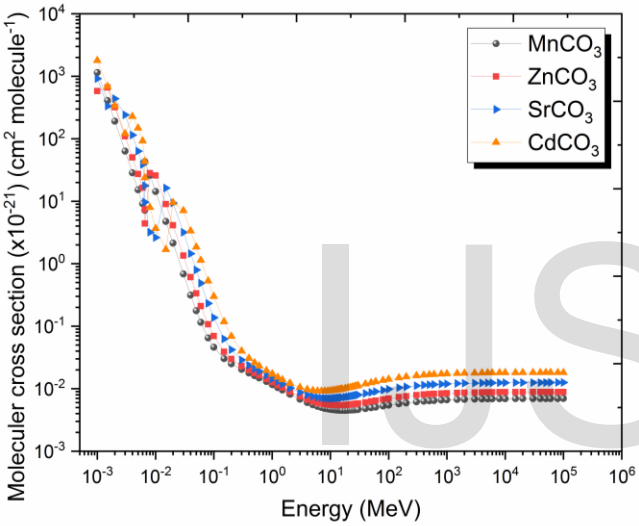

Figure 2. Molecular cross sections of $MnCO_3$, $ZnCO_3$, $SrCO_3$ and $CdCO_3$ versus photon energy.

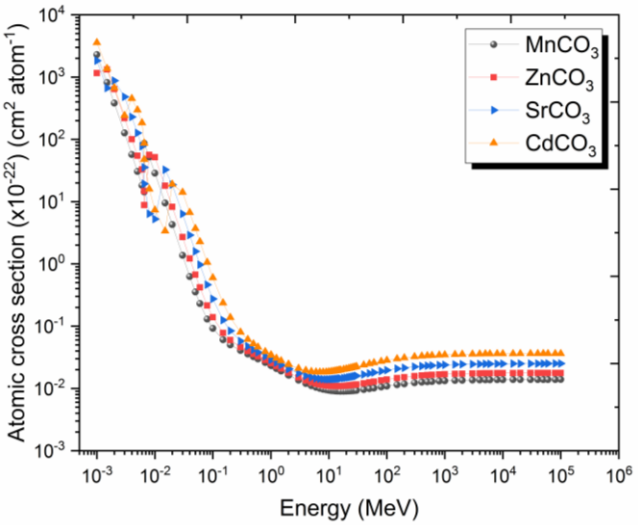

Figure 3. Atomic cross sections of $MnCO_3$, $ZnCO_3$, $SrCO_3$ and $CdCO_3$ versus photon energy.

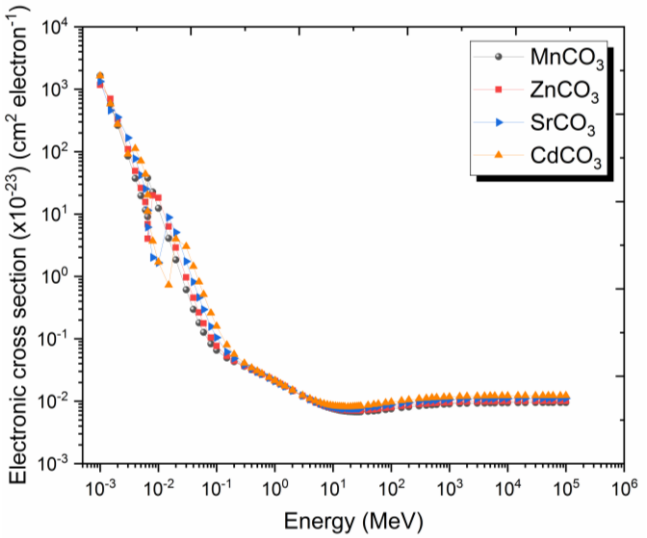

Figure 4. Electronic cross sections of $MnCO_3$, $ZnCO_3$, $SrCO_3$ and $CdCO_3$ versus photon energy.

The effective atomic numbers and effective electron densities as a function of energy are given in Figure 5 and Figure 6 for $MnCO_3$, $ZnCO_3$, $SrCO_3$ and $CdCO_3$. As clearly seen from Figure 5, 6 and Table 1, the effective atomic numbers and effective electron densities for minerals display different characteristic futures at different energy regions. Also, effective atomic numbers and effective electron densities decrease with increasing energy in low energy region. This is why the photoelectric interaction is dominant in this energy region. The proportions between photoelectric absorption and energy and atomic number are $1/E^{3.5}$ and Z^{4-5}, respectively (Akman and Kaçal, 2018). The effective atomic numbers and effective electron densities of the $MnCO_3$, $ZnCO_3$, $SrCO_3$ and $CdCO_3$ in the middle energy region were the smallest due to the Compton scattering. The proportions between Compton scattering and energy, and atomic number are $1/E$ and Z, respectively. In the high energy region, the effective atomic number and electron density values increase with increasing energy. The proportions between pair production and energy, and atomic number are E and Z^2, respectively.

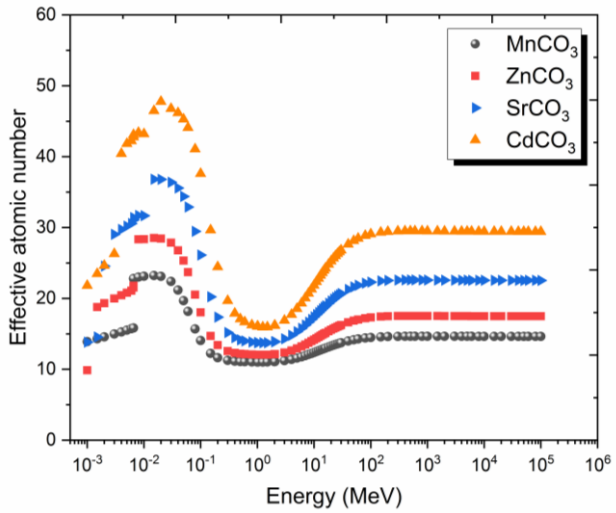

Figure 5. Effective atomic numbers of $MnCO_3$, $ZnCO_3$, $SrCO_3$ and $CdCO_3$ versus photon energy.

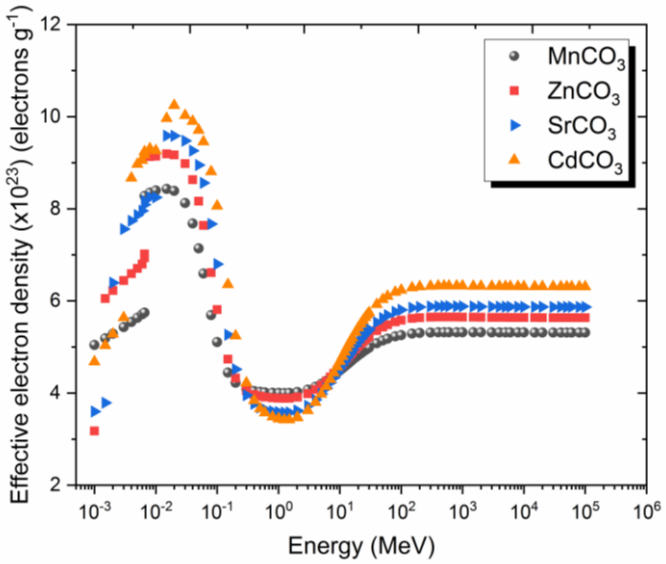

Figure 6. Effective electron densities of $MnCO_3$, $ZnCO_3$, $SrCO_3$ and $CdCO_3$ versus photon energy.

TABLE 1

μ/ρ (cm²/g), $\sigma_{t,m}$ (cm²/molecule), $\sigma_{t,a}$ (cm²/atom), $\sigma_{t,e}$ (cm²/electrons), Z_{eff} and N_{eff} (electrons/g) at some selected energies for $MnCO_3$ mineral

Energy (MeV)	μ/ρ	$\sigma_{t,m}$ (x10^{-21})	$\sigma_{t,a}$ (x10^{-22})	$\sigma_{t,e}$ (x10^{-23})	Z_{eff}	N_{eff} (x10^{23})
0,001	6015,469	1148,195	2296,390	1652,148	13,899	5,046
0,002	1000,982	191,061	382,122	262,304	14,568	5,288
0,003	331,932	63,357	126,714	84,661	14,967	5,433
0,004	149,365	28,510	57,020	37,338	15,271	5,544
0,005	79,927	15,256	30,512	19,662	15,519	5,633
0,006	47,838	9,131	18,262	11,610	15,729	5,710
0,006539	37,539	7,165	14,330	9,053	15,830	5,746
0,006539	225,830	43,105	86,210	37,805	22,804	8,278
0,008	136,023	25,963	51,927	22,578	22,999	8,349
0,01	75,075	14,330	28,660	12,390	23,131	8,397
0,02	11,173	2,133	4,265	1,846	23,109	8,389
0,04	1,644	0,314	0,628	0,297	21,164	7,682
0,06	0,604	0,115	0,231	0,127	18,169	6,595
0,08	0,340	0,065	0,130	0,083	15,685	5,694
0,1	0,241	0,046	0,092	0,066	14,065	5,106
0,2	0,131	0,025	0,050	0,043	11,636	4,224
0,4	0,094	0,018	0,036	0,032	11,137	4,043
0,6	0,078	0,015	0,030	0,027	11,063	4,016
0,8	0,068	0,013	0,026	0,024	11,038	4,007
1	0,061	0,012	0,023	0,021	11,026	4,003
2	0,043	0,008	0,016	0,015	11,074	4,020
4	0,031	0,006	0,012	0,011	11,396	4,137
6	0,027	0,005	0,010	0,009	11,754	4,267
8	0,025	0,005	0,010	0,008	12,081	4,385
10	0,024	0,005	0,009	0,008	12,367	4,489
12	0,024	0,005	0,009	0,007	12,610	4,577
16	0,024	0,005	0,009	0,007	12,992	4,716
20	0,024	0,005	0,009	0,007	13,279	4,820
24	0,024	0,005	0,009	0,007	13,494	4,898
28	0,024	0,005	0,009	0,007	13,663	4,960
30	0,024	0,005	0,009	0,007	13,734	4,985
40	0,025	0,005	0,010	0,007	13,995	5,080
80	0,028	0,005	0,010	0,007	14,408	5,230
100	0,029	0,005	0,011	0,008	14,485	5,258

200	0,031	0,006	0,012	0,008	14,613	5,305
400	0,033	0,006	0,013	0,009	14,650	5,318
600	0,034	0,006	0,013	0,009	14,655	5,320
800	0,034	0,007	0,013	0,009	14,656	5,320
1000	0,035	0,007	0,013	0,009	14,655	5,320
2000	0,035	0,007	0,014	0,009	14,651	5,319
4000	0,036	0,007	0,014	0,009	14,647	5,317
6000	0,036	0,007	0,014	0,009	14,644	5,316
8000	0,036	0,007	0,014	0,009	14,643	5,316
10000	0,036	0,007	0,014	0,009	14,643	5,316
15000	0,036	0,007	0,014	0,009	14,641	5,315
20000	0,036	0,007	0,014	0,009	14,641	5,315
30000	0,036	0,007	0,014	0,009	14,640	5,314
40000	0,036	0,007	0,014	0,010	14,639	5,314
50000	0,036	0,007	0,014	0,010	14,639	5,314
60000	0,036	0,007	0,014	0,010	14,639	5,314
80000	0,036	0,007	0,014	0,010	14,639	5,314
100000	0,036	0,007	0,014	0,010	14,638	5,314

4 CONCLUSION

In this study, Total mass absorption coefficient, molecular cross sections, atomic cross sections, electronic cross sections, effective atomic numbers and electron densities were theoretically determined some selected energy in the energy range 1 keV≤E≤100 GeV for $MnCO_3$, $ZnCO_3$, $SrCO_3$ and $CdCO_3$. We observed that the absorption parameters exhibit distinct characteristic futures in different energy regions. Also, it can be conclude that $CdCO_3$ display the best radiation shielding futures in investigated compounds. Absorption parameter studies for minerals are very limited in literature. We believe that theoretical absorption parameters of the Manganese Carbonate ($MnCO_3$), Zinc Carbonate ($ZnCO_3$), Strontium Carbonate ($SrCO_3$) and Cadmium Carbonate ($CdCO_3$) are very important in different research areas such as agriculture, medicine, chemistry, applications of physic, pharmaceutical industry, paint industry, etc.

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