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The detection of effective atomic numbers of some potassium compounds using direct and linear differential scattering methods

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Abstract. In this work, the direct method and the linear differential scattering method were used to detect the experimental effective atomic numbers of some potassium compounds (KH_2PO_4, KNO_3, $K_2S_2O_8$, KOH, K_2HPO_4, K_2SO_4, KCl, KIO_3 and KI). The experiment has been done by using ^{241}Am radioactive source, a Si(Li) detector and an energy-dispersive X-ray fluorescence spectrometer (EDXRFS). The experimental effective atomic numbers were compared with the effective atomic numbers obtained using WinXCom, FFAST, non-relativistic theory (NRT) and relativistic theory (RT).

Keywords. Effective atomic number; potassium; WinXCom; FFAST; non-relativistic theory; relativistic theory.

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1. Introduction

Absorption and scattering events occur by the interaction of a photon with matter. The attenuation, scattering coefficients, and cross-sections play important roles in explaining the absorption and scattering events. Scattering and absorption of γ-photon is related to the density and atomic numbers of matter [1]. The interaction of gamma radiations with matter is investigated with important parameters such as mass attenuation coefficient, atomic cross-section, electronic cross-section, effective atomic number, electron density and scattering cross-section. In particular, the effective atomic number is a suitable parameter for understanding the attenuation of X- and γ-rays in matter [2]. The effective atomic number is the ratio of the total atomic cross-section to the total electronic cross-section [3]. The effective atomic number of a sample is very important in nuclear industry, space research programmes, engineering and in many fields of scientific, biological applications, in designing radiation shielding, computing absorbed dose, medical physics, radiation dosimetry and build-up factor [4]. It can be determined by various methods such as Rayleigh/Compton scattering ratio (R/C), direct method and linear differential scattering method [5]. The R/C ratio is used in the fields of physics. The R/C ratio depends only on the studied mixture and based on the proven measurement of complex functions, the atomic number and effective atomic number. The experimental differential scattering coefficient and effective atomic number were measured with the help of R/C ratio and the mass attenuation coefficients. The mass attenuation coefficient is an important parameter that describes the interaction of a photon with a sample. These coefficients are widely used in industrial, biological, agriculture and medical applications [6]. Also, the attenuation coefficients are important to form the region that the theory is valid in theoretical studies. In this case, the results of theoretical studies can be used to assist the experimental findings [7]. According to the National Committee for Clinical Laboratory Standards, potassium (K) is an essential major element [8]. It is very important for the life of living things. Therefore, in this study compounds of potassium were chosen.

In the literature, researches for effective atomic numbers of different samples are available. İçelli and Erzeneoglu [9] determined the effective atomic number of some of the vanadium and nickel compounds at 15.746–40.930 keV. İçelli [10] measured the effective atomic numbers of some oxide compounds by using linear differential scattering coefficients. Kumar and Umesh [11] reported a new method to obtain the effective atomic number of composite materials at 280–1200 keV energy. Akça and Erzeneoğlu [12] investigated

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cross-sections of compounds of some biomedically important elements at 59.54 keV energy. Manjunatha and Umesh [13] determined the effective atomic number of several rare-earth compounds by using external bremsstrahlung. Gowda [14] determined the effective atomic number of some halides. Singh and Badiger [15] obtained the effective atomic number for some dosimetric organic compounds by using different methods. Hosamani and Badiger [16] reported a novel method to obtain effective atomic number of composite materials by using backscattering gamma photons at 180°. Revathy *et al* [17] obtained effective atomic numbers by using Cs-137 γ-ray for mixtures of graphite, aluminum and selenium powders in different proportions, commercial and home-made edible powders, fruit and vegetable juices as well as certain allopathic and ayurvedic medications.

In this study, the mass attenuation coefficients of some potassium compounds have been measured at 59.54 keV energy. The effective atomic number has been obtained by using the mass attenuation coefficients. Experimental effective atomic numbers have been compared with atomic numbers from WinXCom and FFAST. Also, the linear differential scattering coefficients of some potassium compounds have been measured at 90° and 59.54 keV energy. The R/C ratios have been obtained by using experimental and theoretical linear differential scattering coefficients. The fit equations have been obtained by using the R/C ratio for non-relativistic theory (R/C_{NRT}) and the R/C ratio for a relativistic theory (R/C_{RT}) of some elements. The experimental and theoretical effective atomic number (Z_{eff}) have been determined by using these fit equations. The experimental effective atomic numbers ($Z_{eff\,Exp}$) have been compared with effective atomic numbers from non-relativistic theory (NRT) and relativistic theory (RT).

2. The theoretical and experimental basis

2.1 *The effective atomic number using the direct method*

In the direct method, the mass attenuation coefficients have been measured. The effective atomic numbers have been obtained by using the measured values, and such studies have been made by earlier investigators [12]. The theoretical mass attenuation coefficients have been detected by WinXCom [18] and FFAST [19]. The effective atomic number (Z_{eff}) of the sample is the ratio of the total atomic cross-section ($\sigma_{t,a}$) and the total electronic cross-section ($\sigma_{t,el}$) [20]:

$$Z_{eff} = \frac{\sigma_{t,a}}{\sigma_{t,el}}. \tag{1}$$

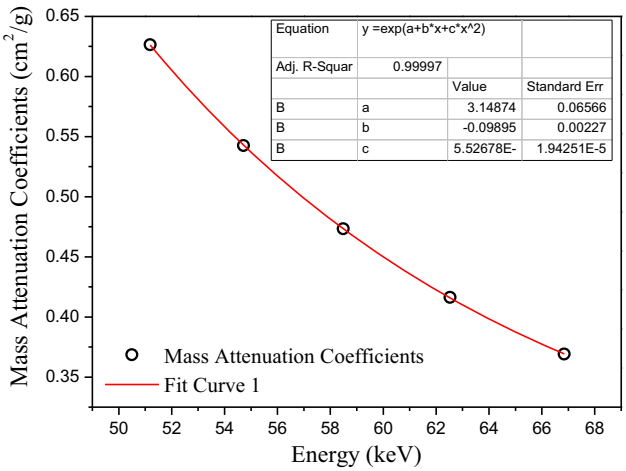

Figure 1. A sample interpolation graph for FFAST values of KOH.

The FFAST does not have values of the mass attenuation coefficients at 59.54 keV energy. Therefore, theoretical values were obtained by using the interpolation method. In this method, values close to 59.54 keV energy were selected. The interpolation formula was obtained by plotting the graph (with the help of Origin Pro8). The interpolation graph is shown in figure 1.

2.2 *The effective atomic number using the linear differential scattering method*

R/C is calculated theoretically as follows [21]:

$$\frac{R}{C} = \frac{N_{Rayleigh}}{N_{Compton}}(Z) \approx \frac{[\mu_s(E,q) - N_A.\rho[\frac{d\sigma_{KN}(E,\theta)}{d\Omega}\sum_i \frac{w_i}{A_i}S_i(q)]]}{[\mu_s(E,q) - N_A.\rho[\frac{d\sigma_{TH}(\theta)}{d\Omega}\sum_i \frac{w_i}{A_i}F_i^2(q)]]}, \tag{2}$$

where $\mu_s(E,q)$ is the linear differential scattering coefficient, Z is the atomic number, q is the photon momentum transfer ($q = 3.38\,\text{Å}^{-1}$ for this study), w_i and A_i are, respectively, the mass fraction and the atomic mass of the ith element in the target, N_A is the Avogadro constant, ρ is the sample density, E is the energy, $F_i(q)$ is the molecular form factor of the ith element in the material, $S_i(q)$ is the molecular incoherent scattering function, $[d\sigma/d\Omega]_{TH}$ is the Thomson cross-section and $[d\sigma/d\Omega]_{KN}$ is the Klein–Nishina cross-section. The NRT and RT do not have values of $F_i(q)$ and $S_i(q)$ at

59.54 keV energy. $F_i(q)$ and $S_i(q)$ values were obtained using the interpolation method from tables in [22–24] for 90°. The interpolation formula was obtained by plotting the graph (with the help of Origin Pro8). The interpolation graphs for NRT are shown in figures 2 and 3.

In order to determine the experimental R/C, the experimental values of $\mu_s(E, q)$ have been used. $\mu_s(E, q)$ is

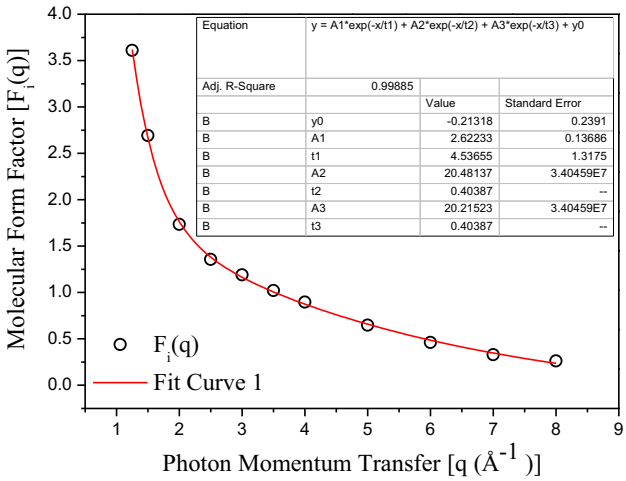

Figure 2. A sample interpolation graph for NRT-$F_i(q)$ of potassium (K).

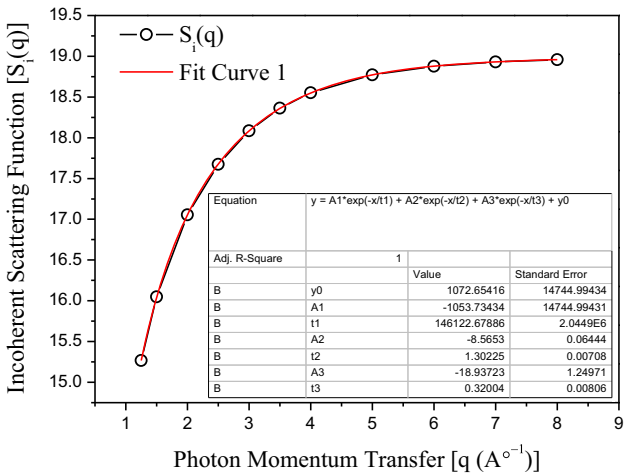

Figure 3. A sample interpolation graph for NRT-$S_i(q)$ of K.

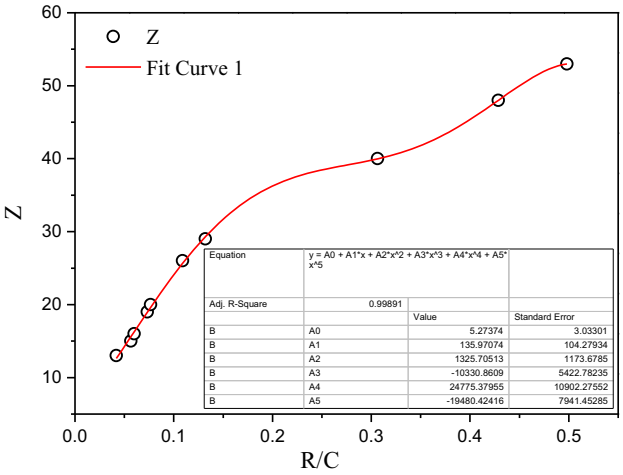

Figure 4. Z vs. R/C for NRT at 90°.

calculated experimentally as follows [25]:

$$\mu_s(E, q) = \frac{N(\theta)}{TK(\theta)B(\theta)}, \tag{3}$$

where $N(\theta)$ is the total area of Rayleigh and Compton peaks, $K(\theta)$ is a constant which is the characteristic of experimental geometry, $B(\theta)$ is a constant and T is the collecting time. Also, the theoretical linear differential scattering coefficient of a sample with molecular weight M is given [26]:

$$\mu_s(E, q) = N_A\rho\left\{\frac{d\sigma_{TH}(\theta)}{d\Omega}\sum_i \frac{w_i}{A_i}F_i^2(q) + \frac{d\sigma_{KN}(E, \theta)}{d\Omega}\sum_i \frac{w_i}{A_i}S_i(q)\right\}. \tag{4}$$

In order to obtain fit equations, R/C_{NRT} and R/C_{RT} values have been calculated using eq. (2) for some elements. The findings are given in table 1.

The graph has been drawn by using table 1 for NRT and RT values of R/C. This graph is shown in figures 4 and 5. Figures 4 and 5 have been fitted to fifth-order polynomial.

The fifth-order polynomial fit formula was obtained by plotting the graph. The fifth-order polynomial fit formula for the best-fit curve is (where $y = Z$ and $x = R/C$)

Table 1. Computed theoretical R/C for some elements to achieve a fit equality.

Element (Atomic number)	Al (13)	P (15)	S (16)	K (19)	Ca (20)	Fe (26)	Cu (29)	Zr (40)	Cd (48)	I (53)
R/C_{NRT}	0.04195	0.05664	0.05992	0.07317	0.07661	0.10903	0.13195	0.30641	0.42872	0.49821
R/C_{RT}	0.03815	0.05230	0.05848	0.07255	0.07603	0.10486	0.13078	0.33477	0.49759	0.56905

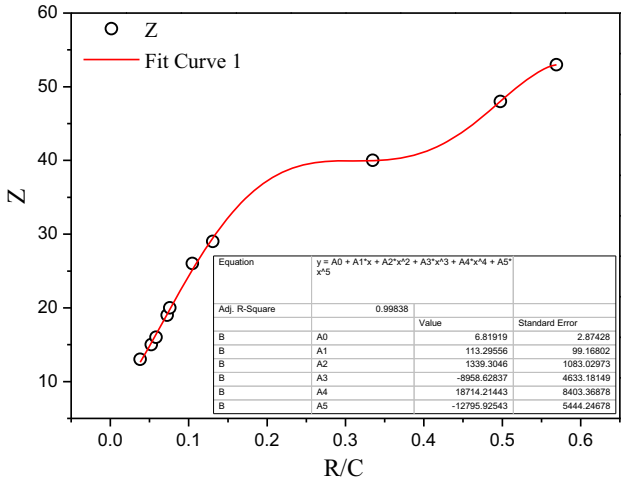

Figure 5. Z vs. R/C for RT at 90°.

$$y_{\mathrm{NRT}} = 5.27374 + 135.97074x + 1325.70513x^2 - 10330.8609x^3 + 24775.37955x^4 - 19480.42416x^5 \quad (5)$$

$$y_{\mathrm{RT}} = 6.81919 + 113.29556x + 1339.3046x^2 - 8958.62837x^3 + 18714.21443x^4 - 12795.92543x^5. \quad (6)$$

The experimental linear differential scattering coefficients have been calculated using eq. (3) and the theoretical linear differential scattering coefficients have been calculated using eq. (4). Later, the theoretical and experimental R/C values have been determined by using eq. (2) for some potassium compounds. Lastly, experimental and theoretical effective atomic number values have been calculated with help of the fifth-order polynomial fit formula (eqs (5) and (6)).

2.3 *Experimental procedure*

The experimental set-up used in the direct method is shown in figure 6. The experiment has been done by using 100 mCi ^{241}Am radioactive source, a Si(Li) detector and an energy-dispersive X-ray fluorescence spectrometer (EDXRFS). The spectra for the direct method were collected for a period of 1800 s. The powder samples were compressed into pellets by using a manual hydraulic press. The target had a diameter of 1.3 cm. The powder samples to obtain the best experimental values were prepared in four different masses (≈0.500, 0.600, 0.700 and 0.800 g). ln $I-t$ graphs have been drawn by using Origin Pro8. The mass attenuation coefficients have been obtained by using the slope of the ln $I-t$ graph. The net unattenuated (I_0) and attenuated (I) counts were obtained in the same period and geometry. A representative spectrum of 59.54 keV γ-rays passed through KNO_3 is shown in figure 7.

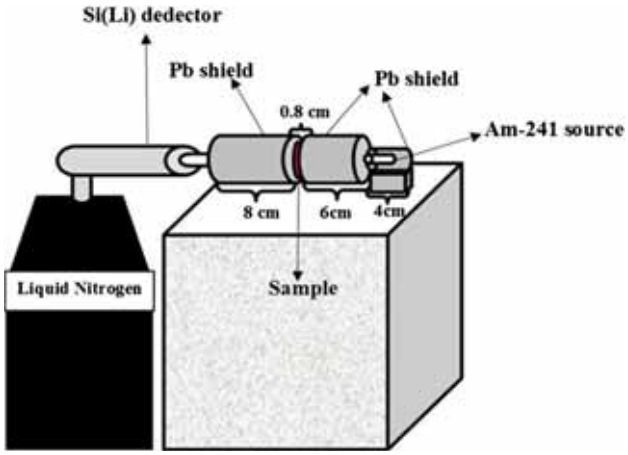

Figure 6. Experimental geometry for the direct method.

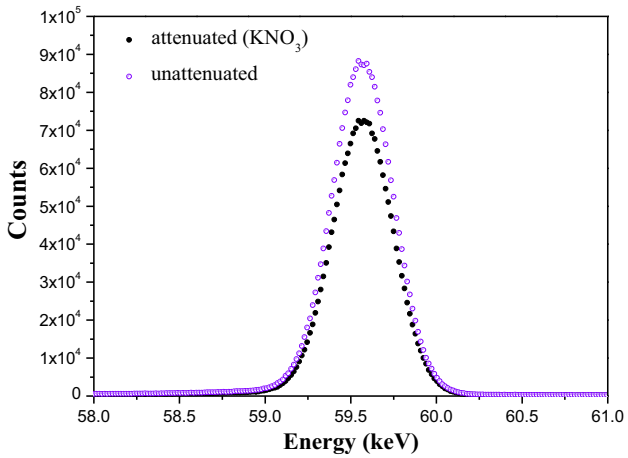

Figure 7. A sample spectrum for the direct method.

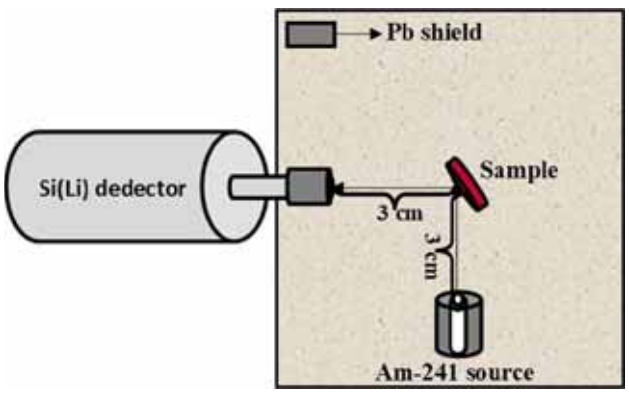

Figure 8. Experimental geometry for the linear differential scattering method.

Also, the experimental set-up used in the linear differential scattering method is shown in figure 8. The spectra for the linear differential scattering method have been collected for a period of 5400 s. The bore radius of the source-collimator is 0.1 cm. The length of the source-collimator is 4 cm. A sample spectrum of 59.54 keV γ-rays scattered by KNO_3 is shown in figure 9.

To decrease statistical errors, the experiment was repeated at least three to four times. The deviations from the mean value in the peak areas were about 4% and, this value for the target thickness was about 2%.

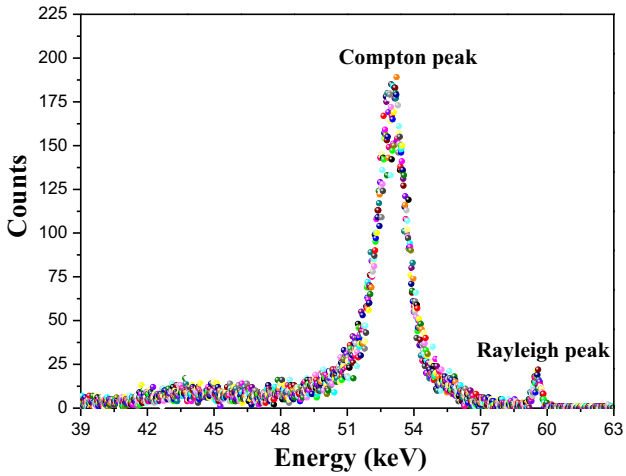

Figure 9. A sample spectrum of KNO_3 using the linear differential scattering method.

3. Results and discussion

In this study, the experimental effective atomic numbers for some potassium compounds have been determined by using the direct method and the linear differential scattering method. Also, experimental effective atomic numbers have been compared with WinXCom, FFAST, NRT and RT values. Experimental determination by using different methods of effective atomic numbers are very important, and such experimental works have been done by earlier investigators [2–16,21,27–33]. To the best of our knowledge, no previous studies of energy and scattering angle for the mentioned compounds were done earlier. Ours is the first experimental results on the potassium-based compounds. The theoretical and experimental effective atomic numbers, the ratios of

Table 2. The theoretical and experimental effective atomic numbers of some potassium compounds using the direct method.

Compounds	Direct method			Percent error (%)		T/E	
	Z_{eff}(WinXCom)	Z_{eff}(FFAST)	Z_{eff}(Exp)	Z_{eff}(WinXCom)	Z_{eff}(FFAST)	Z_{eff}(WinXCom)	Z_{eff}(FFAST)
KH_2PO_4	11.283	11.184	11.945±0.335	5.865	6.798	0.945	0.936
KNO_3	12.703	12.601	12.741±0.042	0.294	1.112	0.997	0.989
$K_2S_2O_8$	13.514	13.476	12.448±0.493	7.887	7.627	1.086	1.083
KOH	13.660	13.534	16.964±1.587	24.190	25.343	0.805	0.798
K_2HPO_4	13.796	13.731	13.761±0.001	0.254	0.220	1.003	0.998
K_2SO_4	14.900	14.819	15.893±0.487	6.667	7.251	0.938	0.932
KCI	18.119	18.130	17.556±0.268	3.107	3.167	1.032	1.033
KIO_3	48.650	48.516	41.496±3.341	14.705	14.469	1.172	1.169
KI	50.984	50.972	52.990±0.948	3.934	3.959	0.962	0.962

Table 3. The theoretical and experimental effective atomic numbers of some potassium compounds using the linear differential scattering method.

Compounds	Linear differential scattering method				Percent error (%)		T/E	
	Z_{eff}(Theo-NRT)	Z_{eff}(Exp-NRT)	Z_{eff}(Theo-RT)	Z_{eff}(Exp-RT)	Z_{eff}(NRT)	Z_{eff}(RT)	Z_{eff}(NRT)	Z_{eff}(RT)
KH_2PO_4	11.510	13.654±0.565	12.562	14.031±0.630	18.630	11.694	0.843	0.895
KNO_3	10.626	10.745±0.154	11.702	11.492±0.203	1.122	1.794	0.989	1.018
$K_2S_2O_8$	11.936	15.076±0.874	13.095	15.344±0.855	26.304	17.170	0.792	0.853
KOH	14.540	15.147±0.181	15.780	15.292±0.059	4.175	3.089	0.960	1.032
K_2HPO_4	13.186	13.789±0.158	14.305	14.069±0.134	4.570	1.651	0.956	1.017
K_2SO_4	13.442	14.032±0.150	14.654	14.288±0.106	4.391	2.497	0.958	1.026
KCI	18.153	20.501±0.653	19.724	20.137±0.294	12.931	2.095	0.885	0.979
KIO_3	39.233	34.885±1.930	39.958	36.608±0.613	11.083	8.382	1.125	1.091
KI	43.663	41.088±0.233	42.274	40.131±0.957	5.897	5.068	1.063	1.053

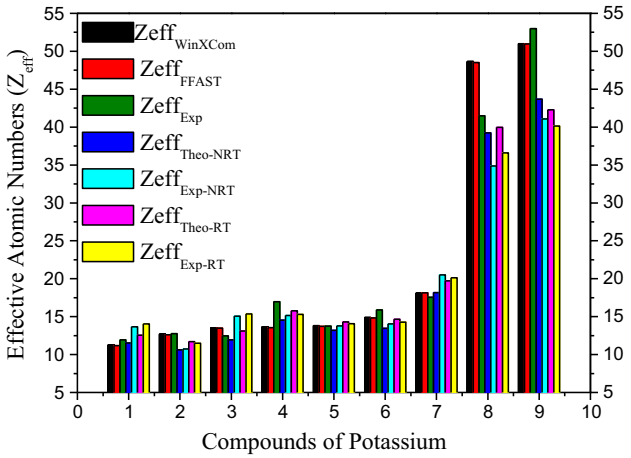

Figure 10. Experimental (Exp) and theoretical (Theo) effective atomic numbers for some potassium compounds.

theoretical (T) and experimental (E) effective atomic number (T/E) and percent error (%) are listed for some potassium compounds in tables 2 and 3. The standard deviation was added to the experimental values. A comparison graph of experimental and theoretical effective atomic numbers for some potassium compounds is shown in figure 10. In the graph, compounds of potassium were numbered KH_2PO_4 (1), KNO_3 (2), $K_2S_2O_8$ (3), KOH (4), K_2HPO_4 (5), K_2SO_4 (6), KCI (7), KIO_3 (8) and KI (9).

As seen in tables 2 and 3 and figure 10, the linear differential scattering coefficients increase in compounds with high density. The ratios of theoretical (T) and experimental (E) effective atomic numbers (T/E) are between 0.792 and 1.172. There is a very good agreement between experimental and theoretical results. According to percent error (%), generally, RT gives good results for the linear differential scattering method and, WinXCom gives good results for the direct method. Also, generally RT values are bigger than NRT values for the differential scattering method and, WinXCom values are bigger than FFAST values for the direct method. Such results have been observed in [12,27,34,35]. WinXCom is a program based on the mixture rule. For any compound, effects such as molecular bonds and chemical environment are important, but these effects are ignored by the mixture rule. The values in the FFAST program have been calculated by different methods and may produce different results. Therefore, there are small differences between the results. Important differences between the experimental and theoretical values have not been observed when changing the number of atoms. Similar results have been observed in [12,36]. Also, as seen in tables 2 and 3, the effective atomic number is greater in iodine (I) compounds. The reason for this is that elements with large atomic numbers interact more with the photon.

4. Conclusions

In conclusion, these two methods can be used for the accurate determination of the effective atomic number. But, the direct method is more easy, fast and convenient than the linear differential scattering method for the determination of the effective atomic number.

In future, this experimental work can be repeated for different scattering angles, energies, samples and methods. Also, experimental results can be compared with different theoretical results.

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