

*Full Length Research Paper*

# The novel terms on the basis of some photon interaction parameters for some barium compounds

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Accepted 3 August, 2012

**The molecular ( $\sigma_M$ ), atomic ( $\sigma_A$ ), electronic ( $\sigma_E$ ) cross-sections and the total mass attenuation coefficient ( $\mu_t$ ) values of barium compounds are determined both experimentally and theoretically. The most interesting result of this study is that the effective  $\sigma_M$ ,  $\sigma_A$ ,  $\sigma_E$  cross-section values are not as expected near the absorption edge. The results have been compared with some other theoretical values in literature due to these unexpected behaviours. The link between the  $J\sigma_M$ ,  $J\sigma_A$ ,  $J\sigma_E$  values and the cross-section  $\sigma_M$ ,  $\sigma_A$ , and  $\sigma_E$  values are also investigated with the absorption jump factor (J).**

**Key words:** Mass attenuation coefficient, molecular, atomic and electronic cross-sections, jump ratio.

## INTRODUCTION

Barium compounds have been chosen for their wide range of use in technology, especially in medical and diagnostic industries (David, 2009). It is important to measure the total effective atomic ( $\sigma_A$ ), molecular ( $\sigma_M$ ), electronic ( $\sigma_E$ ) cross-sections and absorption jump factor (J) of barium compounds. Moreover, absorption jump factors and ratios are important parameters in energy dispersive X-ray fluorescence spectroscopy (EDXRF). Those parameters are necessary in a variety of areas: nuclear industries, medical applications, biological tissue analyses, crystal

characterizations, dosimetric computations for health physics and in many fields of scientific applications. To obtain the jump factors, the total mass attenuation coefficients must be measured. Those coefficients depend on the incident photon energy and the nature of the absorbing material.

Various methods have been used by researchers to determine the jump ratio and factor for materials and for elements (Sidhu et al., 2001; Budak and Polat, 2004; Ayala and Mainardi, 1996).

There are no studies related to absorption jump factor and total effective  $\sigma_A$ ,  $\sigma_M$ ,  $\sigma_E$  cross-sections near the K-absorption edge of compounds in the literature. The aim of the present study is to fill the mentioned gap in the literature by determining  $J\sigma_M$ ,  $J\sigma_A$  and  $J\sigma_E$  terms which are new and are called the jump factors of  $\sigma_A$ ,

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**Table 1.** The studied compounds with the bond structure, oxidation state and crystalline form.

Sample	Bond structure	Oxidation number	Crystalline form
BaO	Ionic	+2	Octahedral
BaO <sub>2</sub>	Ionic	+4	Tetragonal
Ba(NO <sub>3</sub> ) <sub>2</sub>	Ionic	+2	Cubic
BaCrO <sub>4</sub>	Ionic	+2	Orthorhombic

$\sigma_M$ ,  $\sigma_E$  cross-sections. Furthermore, these terms can be obtained directly from the experimental or theoretical total effective cross-sections, and the calculation of  $\sigma_M$ ,  $\sigma_A$  and  $\sigma_E$  values near the absorption edge can be difficult, generally.

The absorption jump factor of the total effective  $\sigma_A$ ,  $\sigma_M$ ,  $\sigma_E$  cross-sections has been measured in this study by using the mass attenuation coefficient near the absorption edge for some barium compounds. The absorption coefficients exhibit discontinuities or deviations like steps when a photon energy is sufficient to expel electrons from a specific inner level in the atom. This fine structure consists of deviations in each simple step and includes deviations not only in the abrupt rise but also in the high energy side of the rise. The fine structure is limited to ~200 eV of the edge in general (Zabinsky et al., 1995; Prins and Köninsberger, 1988).

One of the main purposes of this study is to demonstrate the  $J\sigma_M$ ,  $J\sigma_A$  and  $J\sigma_E$  terms in the literature. The studied properties of the barium compounds are given in Table 1 with the bond structure, oxidation state and crystalline form.

The present study claims that there is an almost a linear correlation between the total effective  $\sigma_A$ ,  $\sigma_M$ ,  $\sigma_E$  cross-sections and absorption jump factor. This is the first time that we have measured the  $J\sigma_M$ ,  $J\sigma_A$  and  $J\sigma_E$  values for the selected barium compounds at energies < 100 keV. Our literature search shows that there has been no available data in the literature for the comparison. Therefore, we think that it is important to calculate the  $J\sigma_M$ ,  $J\sigma_A$  and  $J\sigma_E$  terms.

## METHODS OF CALCULATION

### The total mass attenuation coefficients

The total mass attenuation coefficient  $\mu_t$  (in cm<sup>2</sup>/g) is given as follows:

$$\mu_t = \frac{\mu}{\rho} = \left( \frac{1}{\rho \cdot x} \right) \ln \left( \frac{I_0}{I} \right) \quad (1)$$

Here  $I_0$  and  $I$  are the intensities of the beam before and after passing through an absorber compound.  $x$  and  $\rho$  are the thickness and density of the sample, respectively. The theoretical values for the total mass attenuation coefficients were obtained from the state of the art program XCOM and from the database (Berger and Hubbell, 1999). These tools are later used for developing the WinXCom software (Gerward et al., 2001). The software applies the mixture rule to calculate the partial and total mass attenuation coefficients for elements, mixtures, and chemicals compounds at standard and also at selected energies.

### The total effective molecular cross-section

The total effective molecular cross-section ( $\sigma_M$ ) can be calculated by using the values of mass attenuation coefficients with:

$$\sigma_M = \frac{1}{N} (\mu_t)_{comp} \sum_i (n_i A_i) \quad (2)$$

Here  $N$  is the Avogadro's number,  $n_i$  is the number of atoms and  $A_i$  is the  $i^{\text{th}}$  element in a molecule.

### The total effective atomic cross-section

The total effective atomic cross-section ( $\sigma_A$ ) can be calculated easily from Equation 2.

$$\sigma_A = \sigma_M \frac{1}{\sum_i n_i} \quad (3)$$

### The total effective electronic cross-section

The total effective electronic cross-section ( $\sigma_E$ ) for a mixture or compound is expressed by the following formula:

$$\sigma_E = \frac{1}{N} \sum_i \frac{f_i A_i}{Z_i} (\mu_t)_i \quad (4)$$

Here  $f_i$  is the number of atoms of element  $i$  relative to the total number of atoms for all elements in the molecular formula, that is  $(n_i / \sum_i n_i)$ .  $Z_i$  is the atomic number and  $(\mu_i)_i$  is the total mass attenuation coefficient of the  $i^{\text{th}}$  element in a molecule (Kaur et al., 2000).

**The absorption jump factors**

The total effective molecular, atomic and electronic cross-sections of any compounds vary with the wavelength or energy of the absorbed X-rays. An increase is expected towards the longer or softer wavelength if  $J\sigma_M$ ,  $J\sigma_A$  and  $J\sigma_E$  values are plotted against wavelength for any chosen absorber compound. In some regions, however, the variation in the plots is not continuous. It is marked by a series of abrupt discontinuities which are called absorption edges.

The difference between the upper and lower edge values gives us directly the photoelectric effect cross-section for a particular shell without necessarily assuming any other partial cross-section. This situation is significant since it is a measurement of the photoelectric effect due to a particular shell relative to other interaction processes.

The three physical phenomena, which are the photoelectric absorption, the Compton scattering and the pair production, constitute the total absorption. The absorption curve may be taken as additive effects of photoelectric absorption for each absorption edge, if the scattering component is neglected. The pair production does not occur and the photoelectric absorption predominates over scatter in the wavelength region of X-ray spectrochemistry.

Consequently,  $\mu_i$  can be calculated by the total photoelectric mass absorption coefficients ( $\tau_{total}$ ). In the wavelengths shorter than the K-edge,  $\tau_{total}$  is the sum of a series of coefficients representing the photon absorption due to electron expulsion for each atomic level. Therefore,  $\tau_{total}$  can be written as:

$$\tau_{total} = \tau_K + (\tau_{LI} + \tau_{LII} + \tau_{LIII}) + (\tau_{MI} + \tau_{MII} \dots) + \dots \quad (5)$$

The  $\tau_K$  component becomes negligible as the K-absorption edge is presented at lower energies or longer wavelength. Therefore, the ratio  $r_K$  of absorptions on either side of the edge can be written as:

$$r_K = \frac{\tau_K + \tau_L + \tau_M + \dots}{\tau_L + \tau_M + \dots} \quad (6)$$

This equation is called absorption jump ratio for the K-absorption edge (Bertin, 1985a). It can be written in a simpler manner as:

$$r_K = \frac{\tau_S}{\tau_L} \text{ or } r_K = \frac{\tau_+}{\tau_-}$$

Here  $S$ ,  $L$  and  $(+, -)$  refer to the short-and long-wavelength sides of the edge, the "top" and "bottom" or "maximum" and "minimum" values of  $\tau$  respectively.

In the subsequent developments, the absorption jump ratio ( $r_K$ ) will be used to calculate absorption jump factors. The symbol  $J$ , that is  $J_{\lambda_i}$  which refers to the probability of ejection of any electron from K, L, M, ... energy levels by an incident photon. For example, the ejection probability of an electron from K energy level for element  $i$  can be given as:

$$J_K = \frac{(r_K - 1)}{r_K} \quad (7)$$

The  $\sigma_M$ ,  $\sigma_A$  and  $\sigma_E$  values versus energy of the absorbed X-rays are plotted in Figures 1 to 3. The absorption jump factors of the total effective molecular, atomic and electronic cross-sections can be given in terms of the related upper and lower edges

$$J\sigma_M = \frac{(J\sigma_M)_+ - (J\sigma_M)_-}{(J\sigma_M)_+}$$

$$J\sigma_A = \frac{(J\sigma_A)_+ - (J\sigma_A)_-}{(J\sigma_A)_+}$$

$$J\sigma_E = \frac{(J\sigma_E)_+ - (J\sigma_E)_-}{(J\sigma_E)_+} \quad (8)$$

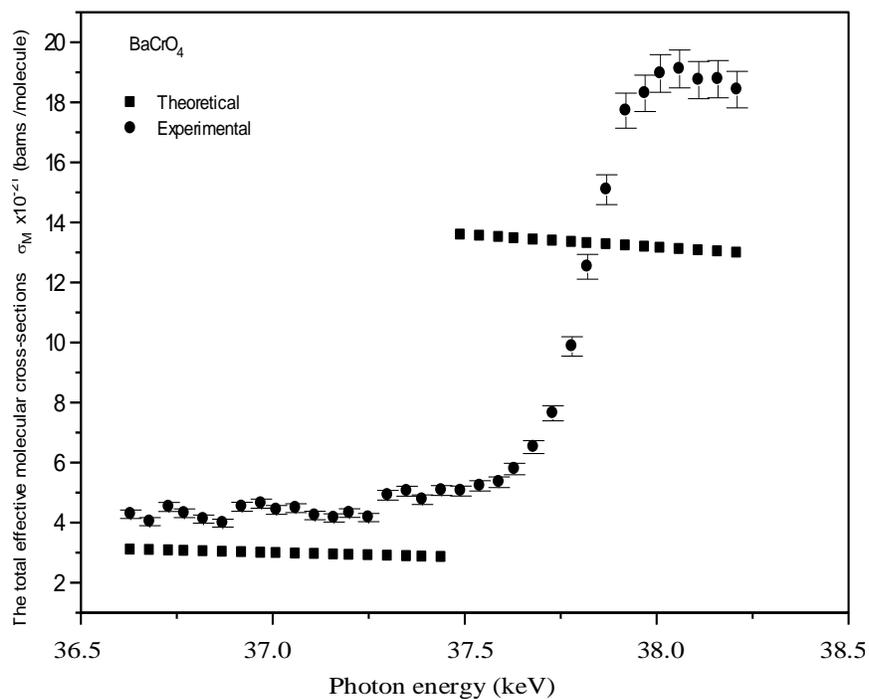
Here,  $(J\sigma)_+$  and  $(J\sigma)_-$  represent the upper and lower edge of the total effective molecular, atomic, and electronic cross-sections related to subscript of  $\sigma$ . The graphs fitted the first degree linear regression for both  $(J\sigma)_+$  and  $(J\sigma)_-$  as seen in Figures 1 to 3. Each fit for the K-absorption edges shows almost the first degree linear regression. The appropriate equation can be written as

$$y = ax + b \quad (9)$$

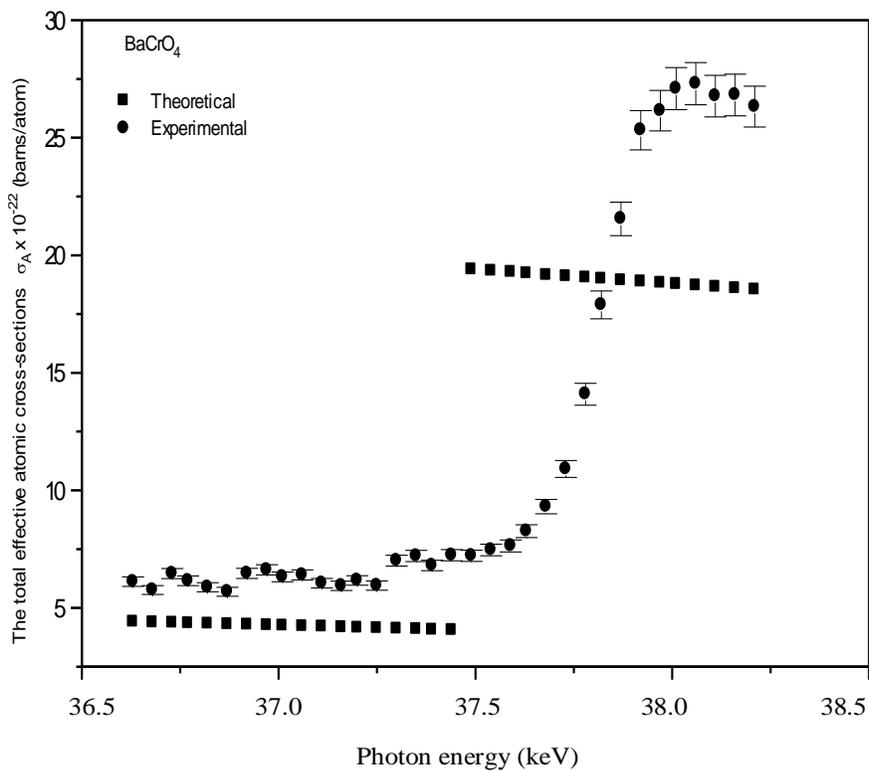
Here,  $a$  and  $b$  are constant coefficients,  $x$  represents the K-absorption edge of absorber compound and  $y$  is the total effective atomic number. Although the jump factors  $J\sigma_M$ ,  $J\sigma_A$  and  $J\sigma_E$  are labeled with  $\sigma_M$ ,  $\sigma_A$  and  $\sigma_E$ , they are not the total effective molecular, atomic, and electronic cross-sections. They can be derived from those parameters. They can also be evaluated as a measurement of  $\sigma_M$ ,  $\sigma_A$ ,  $\sigma_E$  and  $J\sigma_M$ ,  $J\sigma_A$ ,  $J\sigma_E$  terms have a specific value. We have measured these parameters experimentally except for the  $J\sigma_E$ . Moreover, those parameters have been compared with the theoretically predicted values.

**EXPERIMENTAL PROCEDURE**

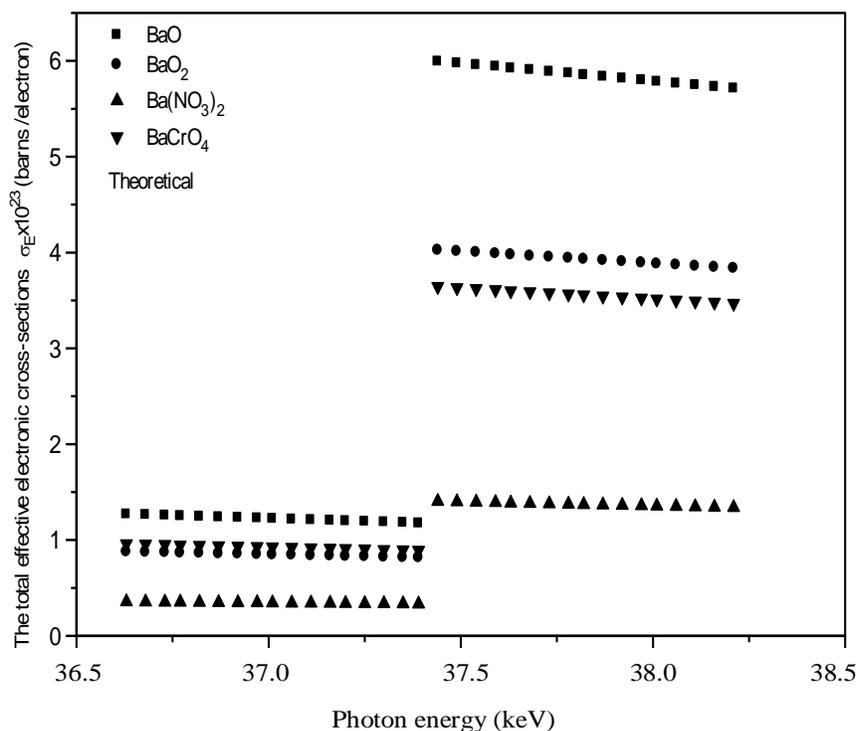
The mass attenuation coefficients for compounds BaO, BaO<sub>2</sub>, Ba(NO<sub>3</sub>)<sub>2</sub> and BaCrO<sub>4</sub> with high purity (99%) were measured to the X-ray with energy ranging from 36.63 keV up to 38.21 keV.



**Figure 1.** The total effective molecular cross sections of BaCrO<sub>4</sub> versus photon energy, near K-absorption edge.



**Figure 2.** The total effective atomic cross sections of BaCrO<sub>4</sub> versus photon energy, near K-absorption edge.



**Figure 3.** The total effective electronic cross sections of compounds versus photon energy near K-absorption edge.

Si(Li) detector has 12 mm<sup>2</sup> detector area, 4 mm in active diameter, 3 mm insensitive crystal depth, a thin (25 μm) Be window. The γ-rays from Am-241 source were stopped in Nd target material to produce Kα<sub>1</sub> and Kα<sub>2</sub>, Kβ<sub>1</sub> and Kβ<sub>2</sub> X-ray emissions. The energies of Kα and Kβ X-rays emitted from secondary source (Nd) must be within the range of K<sub>abs</sub> values of absorber compounds (BaO, BaO<sub>2</sub>, Ba(NO<sub>3</sub>)<sub>2</sub> and BaCrO<sub>4</sub>). We investigated different energy ranges and separated Kα<sub>1</sub> and Kα<sub>2</sub>, Kβ<sub>1</sub> and Kβ<sub>2</sub> peaks by calculating the absorption coefficients. The calculations have been carried out by considering the intensities of the photons dropped to each energy channel for whole peaks, before and after the absorption. The experimental arrangement is presented in Polat et al. (2011).

The total attenuation coefficients and K-absorption jump factors were calculated by using transmission geometry. In the present experiment, a Si(Li) detector was used with a nuclear data (ND) 581 analog-digital converter interfaced with a personal computer provided with suitable software for data acquisition and with the peak analysis for the detection of X-rays. FWHM value is 160 eV in 5.96 keV. This detector was coupled to a 1024-multichannel analyzer through a spectroscopy automatic, fine-tuning research amplifier. The statistical errors in the X-ray intensities, in unit of time rising originating from radioisotope and in unit of time characteristic X-rays rising originating from secondary source had been minimized by taking the counting time long enough. The errors were always less than 1%. In order to obtain statistical accuracy, each sample was measured by collecting the spectra from selected elements for a period of 72 × 10<sup>3</sup> s. High purity (99.9%) samples of BaO, BaO<sub>2</sub>, Ba(OH)<sub>2</sub>, Ba(NO<sub>3</sub>)<sub>2</sub> and BaCrO<sub>4</sub> were measured by using a radioactive annular source of Am-241 in the strength of 3.7 × 10<sup>9</sup> Bq (100 mCi) and γ-photon energy of 59.5 keV. The mass thicknesses of these mixtures were calculated to be 8.49 × 10<sup>-2</sup> g/cm<sup>2</sup>. The measurements of mass thickness values

with gravimetric method (in g/cm<sup>2</sup> units) are always the same. In this experiment, the net data without absorber ( $I_0$ ) and with absorber ( $I$ ) were obtained at the same time and under the same experimental conditions. We have considered the change in the detector efficiency as there was no change in the absorbed and unabsorbed peaks.

The multiple scattering and continual X-ray production have been reduced to ensure the  $\mu t < 1$  condition (where  $\mu$  is the linear attenuation coefficients and  $t$  is the thickness of the absorber compound). There was a built-in provision for deadtime correction. The percentage dead time correction was always < 2%.

## RESULTS AND DISCUSSION

There is only one specific value for the terms  $J\sigma_M$ ,  $J\sigma_A$  and  $J\sigma_E$  appearing in Table 6; although  $\sigma_M$ ,  $\sigma_A$  and  $\sigma_E$  have different values for each energy level as seen in Tables 2 to 5. This situation gives an excellent excuse to simplify the calculations.

The experimental and theoretical  $\sigma_M$  and  $\sigma_A$ , and theoretical  $\sigma_E$  values are listed together in Tables 2 to 5. Both experimental and theoretical  $\sigma_M$  and  $\sigma_A$  of BaCrO<sub>4</sub> around K-absorption edges versus the photon

**Table 2.** The total effective molecular, atomic and electronic cross-sections of BaO.

Energy (keV)	Theoretical			Experimental	
	$\sigma_M \times 10^{-21}$ (barns/molecule)	$\sigma_A \times 10^{-22}$ (barns/atom)	$\sigma_E \times 10^{23}$ (barns/electron)	$\sigma_M \times 10^{-21}$ (barns/molecule)	$\sigma_A \times 10^{-22}$ (barns/atom)
36.63	1.369	6.846	1.266	2.189±0.0418	10.94±0.2090
36.68	1.362	6.814	1.260	2.091±0.0399	10.45±0.1997
36.73	1.356	6.718	1.254	2.029±0.0387	10.14±0.1937
36.77	1.349	6.749	1.248	1.949±0.0372	9.748±0.1862
36.82	1.343	6.716	1.243	1.870±0.0357	9.350±0.1785
36.87	1.337	6.684	1.237	1.817±0.0347	9.085±0.1735
36.92	1.330	6.652	1.231	1.809±0.0345	9.048±0.1728
36.97	1.324	6.619	1.225	1.818±0.0347	9.091±0.1736
37.01	1.317	6.587	1.219	1.875±0.0358	9.379±0.1791
37.06	1.311	6.556	1.213	1.996±0.0381	9.981±0.1906
37.11	1.304	6.523	1.208	2.105±0.0402	10.52±0.2011
37.16	1.297	6.489	1.202	2.180±0.0416	10.90±0.2082
37.20	1.291	6.459	1.196	2.204±0.0421	10.52±0.2011
37.25	1.285	6.426	1.190	2.145±0.0409	10.72±0.2048
37.30	1.278	6.394	1.184	2.109±0.0402	10.54±0.2014
37.35	1.272	6.361	1.178	2.046±0.0390	10.23±0.1954
37.39	1.265	6.329	1.173	2.009±0.0383	10.04±0.1918
37.44	6.666	33.33	5.990	1.990±0.0380	9.950±0.1901
37.49	6.647	33.23	5.973	1.982±0.0378	9.912±0.1893
37.54	6.628	33.14	5.955	2.023±0.0386	10.11±0.1932
37.59	6.608	33.04	5.938	2.098±0.0400	10.49±0.2004
37.63	6.587	32.93	5.920	2.270±0.0433	11.35±0.2167
37.68	6.567	32.83	5.903	2.557±0.0488	12.78±0.2442
37.73	6.547	32.73	5.885	2.999±0.0572	14.99±0.2864
37.78	6.529	32.64	5.868	3.873±0.0739	19.36±0.3699
37.82	6.509	32.54	5.850	4.916±0.0939	24.58±0.4695
37.87	6.488	32.44	5.833	5.923±0.1131	29.61±0.5656
37.92	6.468	32.34	5.815	6.958±0.1329	34.79±0.6645
37.97	6.447	32.23	5.797	7.185±0.1372	35.92±0.6861
38.01	6.427	32.13	5.780	7.444±0.1421	37.22±0.7109
38.06	6.409	32.04	5.762	7.502±0.1432	37.51±0.7164
38.11	6.386	31.93	5.745	7.356±0.1405	36.78±0.7025
38.16	6.369	31.84	5.727	7.369±0.1407	36.84±0.7037
38.21	6.348	31.74	5.710	7.233±0.1381	36.16±0.6908

energy are plotted in Figures 1 to 2, as an example. Theoretical  $\sigma_E$  values of all compounds around K-absorption edges are plotted in Figure 3. As seen in Figure 3, while theoretical  $\sigma_E$  values of BaO have the maximum value, Ba(NO<sub>3</sub>)<sub>2</sub> is located in the minimum value. The figures clearly show that the total effective molecular, atomic, and electronic cross-sections depend on the photon energy. The same cross-sections of the barium compounds increased up to the absorption edge energy but they sharply increased up near to the absorption edge as shown in Figures 1 to 3. These

discontinuities can be attributed to resonant at energies corresponding to K-edge of present barium compounds with Ba (Ba K<sub>abs</sub> = 37.41 keV). The total effective molecular, atomic and electronic cross-sections of each barium compounds generally increased with the increasing energy near the absorption edges as shown in Tables 2 to 5. This can be attributed to the absorber compounds that predominantly absorb the incident photons in those regions. The tendency of  $\sigma_M$ ,  $\sigma_A$  and  $\sigma_E$  versus energy in Figures 1 to 3 indicates that  $\sigma_M$ ,  $\sigma_A$  and  $\sigma_E$  increase near the absorption edge. The

**Table 3.** The total effective molecular, atomic and electronic cross-sections of BaO<sub>2</sub>.

Energy (keV)	Theoretical			Experimental	
	$\sigma_M \times 10^{-21}$ (barns/molecule)	$\sigma_A \times 10^{-22}$ (barns/atom)	$\sigma_E \times 10^{23}$ (barns/electron)	$\sigma_M \times 10^{-21}$ (barns/molecule)	$\sigma_A \times 10^{-22}$ (barns/atom)
36.63	1.377	4.590	0.876	1.855±0.0272	6.185±0.0909
36.68	1.370	4.568	0.872	1.747±0.0265	5.826±0.0885
36.73	1.363	4.546	0.868	1.678±0.0262	5.595±0.0873
36.77	1.357	4.525	0.864	1.590±0.0255	5.303±0.0851
36.82	1.351	4.504	0.860	1.502±0.0250	5.009±0.0835
36.87	1.344	4.481	0.856	1.444±0.0248	4.814±0.0827
36.92	1.338	4.460	0.852	1.440±0.0245	4.800±0.0819
36.97	1.331	4.438	0.848	1.445±0.0247	4.818±0.0824
37.01	1.325	4.418	0.844	1.509±0.0252	5.030±0.0842
37.06	1.318	4.396	0.841	1.712±0.0262	5.708±0.0874
37.11	1.312	4.374	0.837	1.763±0.0272	5.877±0.0907
37.16	1.306	4.353	0.833	1.846±0.0278	6.153±0.0928
37.20	1.299	4.330	0.829	1.870±0.0279	6.235±0.0931
37.25	1.292	4.309	0.825	1.801±0.0277	6.005±0.0925
37.30	1.286	4.287	0.821	1.767±0.0273	5.892±0.0912
37.35	1.280	4.267	0.817	1.720±0.0271	5.734±0.0904
37.39	1.273	4.244	0.813	1.623±0.0268	5.411±0.0895
37.44	1.267	4.224	4.022	1.692±0.0266	5.640±0.0889
37.49	6.639	22.13	4.010	1.844±0.0267	6.147±0.0891
37.54	6.640	22.13	4.000	1.953±0.0269	6.512±0.0899
37.59	6.600	22.00	3.986	2.317±0.0275	7.724±0.0918
37.63	6.580	21.93	3.975	2.506±0.0288	8.356±0.0960
37.68	6.563	21.87	3.963	2.824±0.0309	9.414±0.1032
37.73	6.541	21.80	3.951	3.287±0.0348	10.95±0.1162
37.78	6.524	21.74	3.939	4.201±0.0412	14.00±0.1374
37.82	6.504	21.68	3.928	4.948±0.0500	16.49±0.1668
37.87	6.485	21.61	3.916	5.429±0.0631	18.09±0.2104
37.92	6.468	21.56	3.904	6.260±0.0747	20.86±0.2491
37.97	6.445	21.48	3.892	7.534±0.0798	25.11±0.2662
38.01	6.428	21.42	3.881	7.900±0.0840	26.33±0.2800
38.06	6.406	21.35	3.869	8.284±0.0845	27.61±0.2819
38.11	6.389	21.29	3.857	8.018±0.0826	26.72±0.2755
38.16	6.369	21.23	3.845	8.052±0.0818	26.84±0.2727
38.21	6.350	21.16	3.834	7.988±0.0822	26.62±0.2742

difference between the values of  $\sigma_M$ ,  $\sigma_A$  and  $\sigma_E$  near the absorption edge (37.39 to 37.44) is roughly 80%; although the incident photon energies lie within approximately 1.58 keV below/above absorption edge, as seen in Table 2. This situation confirms that  $\sigma_M$ ,  $\sigma_A$  and  $\sigma_E$  is impressed near the absorption edge. Therefore, researchers must take into account this confirmation in measuring the atomic parameters such as the total effective molecular, atomic, and electronic cross-sections. The experimental and theoretical  $J\sigma_M$ ,  $J\sigma_A$ ,

and theoretical  $J\sigma_E$  are listed in Table 6. The most interesting result of this study is that both experimental and theoretical values of  $J\sigma_M$  and  $J\sigma_A$  are equal for each barium compound. The present results can be interpreted as a discovery since no similar result is published in the literature before. Hence, the results are not compared with the results of other experiments. The results include the measurement of absorption jump ratio of the total effective molecular, atomic and electronic cross-sections and the accuracy of the mixture rule near the absorption edge of the absorber compounds.

**Table 4.** The total effective molecular, atomic and electronic cross-sections of Ba(NO<sub>3</sub>)<sub>2</sub>.

Energy (keV)	Theoretical			Experimental	
	$\sigma_M \times 10^{-21}$ (barns/molecule)	$\sigma_A \times 10^{-22}$ (barns/atom)	$\sigma_E \times 10^{23}$ (barns/electron)	$\sigma_M \times 10^{-21}$ (barns/molecule)	$\sigma_A \times 10^{-22}$ (barns/atom)
36.63	1.421	1.578	0.355	2.411±0.0226	2.678±0.0252
36.68	1.414	1.571	0.353	2.388±0.0223	2.653±0.0248
36.73	1.407	1.564	0.352	2.310±0.0218	2.567±0.0243
36.77	1.401	1.556	0.351	2.330±0.0213	2.589±0.0236
36.82	1.394	1.549	0.349	2.270±0.0206	2.523±0.0229
36.87	1.388	1.542	0.348	2.310±0.0202	2.567±0.0224
36.92	1.381	1.534	0.346	2.302±0.0197	2.558±0.0219
36.97	1.374	1.527	0.345	2.470±0.0196	2.744±0.0218
37.01	1.368	1.520	0.343	2.560±0.0199	2.844±0.0221
37.06	1.361	1.513	0.342	2.603±0.0207	2.892±0.0230
37.11	1.355	1.505	0.341	2.546±0.0218	2.829±0.0242
37.16	1.348	1.498	0.339	2.351±0.0226	2.612±0.0251
37.20	1.342	1.491	0.338	2.429±0.0230	2.699±0.0256
37.25	1.335	1.484	0.336	2.428±0.0229	2.698±0.0254
37.30	1.328	1.476	0.335	2.485±0.0226	2.762±0.0251
37.35	1.322	1.469	0.333	2.568±0.0222	2.854±0.0247
37.39	1.315	1.461	0.332	2.643±0.0219	2.937±0.0243
37.44	1.309	1.454	1.402	3.191±0.0214	3.545±0.0238
37.49	6.702	7.447	1.398	3.581±0.0211	3.979±0.0234
37.54	6.680	7.422	1.394	4.322±0.0206	4.802±0.0229
37.59	6.666	7.403	1.390	4.882±0.0207	5.424±0.0230
37.63	6.641	7.379	1.386	5.650±0.0210	6.278±0.0234
37.68	6.619	7.355	1.382	6.667±0.0217	7.408±0.0241
37.73	6.598	7.331	1.378	7.358±0.0239	8.176±0.0265
37.78	6.576	7.307	1.374	8.004±0.0280	8.893±0.0312
37.82	6.563	7.292	1.370	8.729±0.0356	9.699±0.0396
37.87	6.537	7.263	1.366	9.931±0.0456	11.03±0.0507
37.92	6.520	7.244	1.362	10.78±0.0557	11.98±0.0619
37.97	6.498	7.220	1.358	11.40±0.0646	12.67±0.0718
38.01	6.476	7.196	1.354	12.19±0.0689	13.54±0.0766
38.06	6.459	7.177	1.350	11.65±0.0690	12.95±0.0767
38.11	6.437	7.153	1.346	11.76±0.0691	13.07±0.0768
38.16	6.416	7.128	1.342	12.19±0.0707	13.54±0.0786
38.21	6.398	7.109	1.338	11.99±0.0688	13.32±0.0764

The predicted values for the total effective molecular, atomic, and electronic cross-sections of the absorber compounds are generally consistent except the absorption edge. These discontinuities can be attributed to the absorption edge of present absorber compounds. The theoretical and experimental total effective molecular and atomic cross-sections of absorber compound (BaCrO<sub>4</sub>) versus the photon energy incident are in Figures 1 and 2. These effects may be considered as simple abrupt discontinuities. The  $\sigma_M$ ,  $\sigma_A$  and  $\sigma_E$  values for an absorber compound may vary substantially for

incident photon energies that lie within 1.58 keV above absorption edge as seen in Figures 1 to 3. The theoretical total effective electronic cross-section was plotted versus photon energy in Figure 3 since the total effective electronic cross-sections are not measured experimentally.

An identical state was not obtained experimentally; although there is an instantaneous jump after 37.44 keV theoretically, as seen in Tables 2 to 5 and Figures 3. A linear decrease, however, for the theoretical total effective electronic cross-section is observed from the

**Table 5.** The total effective molecular, atomic and electronic cross-sections of BaCrO<sub>4</sub>.

Energy (keV)	Theoretical			Experimental	
	$\sigma_M \times 10^{-21}$	$\sigma_A \times 10^{-22}$	$\sigma_E \times 10^{23}$	$\sigma_M \times 10^{-21}$	$\sigma_A \times 10^{-22}$
	(barns/molecule)	(barns/atom)	(barns/electron)	(barns/molecule)	(barns/atom)
36.63	3.080	4.401	0.960	4.280±0.0650	0.115±0.0929
36.68	3.065	4.379	0.956	4.032±0.0613	5.761±0.0875
36.73	3.051	4.359	0.952	4.521±0.0687	6.459±0.0981
36.77	3.036	4.337	0.947	4.310±0.0655	6.157±0.0935
36.82	3.026	4.322	0.943	4.115±0.0625	5.879±0.0893
36.87	3.007	4.296	0.939	3.980±0.0605	5.687±0.0864
36.92	2.993	4.275	0.935	4.529±0.0688	6.470±0.0983
36.97	2.978	4.254	0.930	4.632±0.0704	6.617±0.1005
37.01	2.963	4.234	0.926	4.423±0.0672	6.319±0.0960
37.06	2.948	4.212	0.922	4.483±0.0681	6.404±0.0973
37.11	2.934	4.192	0.917	4.236±0.0643	6.051±0.0919
37.16	2.919	4.171	0.913	4.158±0.0632	5.941±0.0903
37.20	2.905	4.150	0.909	4.318±0.0656	6.169±0.0937
37.25	2.890	4.129	0.905	4.165±0.0633	5.951±0.0904
37.30	2.876	4.108	0.900	4.909±0.0746	7.013±0.1066
37.35	2.861	4.087	0.896	5.045±0.0766	7.208±0.1095
37.39	2.847	4.067	0.892	4.764±0.0724	6.805±0.1034
37.44	2.832	4.045	3.644	5.069±0.0770	7.242±0.1100
37.49	13.57	19.39	3.633	5.051±0.0767	7.215±0.1096
37.54	13.53	19.33	3.622	5.224±0.0794	7.464±0.1134
37.59	13.49	19.28	3.611	5.346±0.0812	7.637±0.1160
37.63	13.45	19.22	3.600	5.783±0.0879	8.262±0.1255
37.68	13.41	19.15	3.589	6.516±0.0990	9.308±0.1414
37.73	13.37	19.10	3.578	7.642±0.1161	10.91±0.1659
37.78	13.33	19.04	3.567	9.868±0.1500	14.09±0.2142
37.82	13.29	18.99	3.556	12.52±0.1900	17.89±0.2720
37.87	13.25	18.93	3.545	15.09±0.2293	21.55±0.3276
37.92	13.21	18.88	3.534	17.72±0.2694	25.32±0.3849
37.97	13.17	18.82	3.523	18.30±0.2782	26.15±0.3974
38.01	13.13	18.77	3.513	18.96±0.2883	27.09±0.4118
38.06	13.09	18.70	3.502	19.11±0.2905	27.30±0.4150
38.11	13.05	18.65	3.491	18.74±0.2846	26.77±0.4069
38.16	13.01	18.59	3.480	18.77±0.2853	26.82±0.4077
38.21	12.97	18.53	3.469	18.42±0.2801	26.32±0.4001

jump region. The values of  $\sigma_M$ ,  $\sigma_A$  and  $\sigma_E$  in near absorption edge region are very sensitive to the incident photon energies. The secondary source (Nd) is producing K $\alpha$  and K $\beta$  X-ray emission from the interaction of Am-241 gamma rays with the secondary source in the present method used. It is important to obtain convenient selection for the energies near the absorption edges of absorber compounds (BaO, BaO<sub>2</sub>, Ba(NO<sub>3</sub>)<sub>2</sub> and BaCrO<sub>4</sub>) with an ideal transmission geometry. The choice of suitable secondary source is very important to set up an ideal transmission geometry. The success of the

present method is related to the consistency between the regulated energy values in K $\alpha$  and K $\beta$  X-ray emission of secondary source and K<sub>abs</sub> absorber values obtained by the help of X-ray critical-absorption and emission energies chart. It is shown that agreements have not been obtained with WinXCom for elements, compounds and mixtures (Berger and Hubbell, 1999; Gerward et al., 2001). WinXCom program uses the mixture rule to predict the related parameters from the total mass attenuation coefficients. Hence the mixture rule may be responsible for the experimental and theoretical

**Table 6.** Experimental and theoretical absorption jump factors for total effective molecular  $J\sigma_M$ , atomic  $J\sigma_A$  and electronic cross  $J\sigma_E$  sections.

Jump factor	BaO	BaO <sub>2</sub>	Ba(NO <sub>3</sub> ) <sub>2</sub>	BaCrO <sub>4</sub>
<b>Theoretical</b>				
$J\sigma_M$	0.810	0.809	0.804	0.791
$J\sigma_A$	0.810	0.809	0.804	0.791
$J\sigma_E$	0.804	0.797	0.763	0.755
<b>Experimental</b>				
$J\sigma_M$	0.732	0.795	0.738	0.750
$J\sigma_A$	0.732	0.795	0.738	0.750

differences. We note that a few studies have been made on the reliability of mixture rule (Lakshminarayana et al., 1986; Tan et al., 1988; Kerur et al., 1994; Söğüt et al., 2001; Turgut et al., 2002; İçelli and Erzeneoğlu, 2004).

They have shown that for a given incident photon energy the mixture rule breaks down not only for the compounds which contain an element whose K-edge energy is less than the photon energy around 1500 eV but also for those with K-edge energy slightly more than the photon energy around 100 eV. In other words, the mixture rule breaks down for photon energies ranging from 100 eV below to 1500 eV above the K-edge.

In this case, we concluded that these deviations may not be directly explained by the number of atoms which varies with the type of absorber compound. BaO, BaO<sub>2</sub>, Ba(NO<sub>3</sub>)<sub>2</sub> and BaCrO<sub>4</sub> still have a large Z's from 1 (H) to 56 (Ba) due to the fact that the variation in its effective atomic number with energy is inevitable. Thus, it can be concluded that these deviations cannot be directly explained with the molecular weight of absorber compounds.

The differences between the present experimental and theoretical values may be attributed to the different chemical compositions of the barium compounds and the nature of mixture rule neglects the interactions between atoms in barium compounds. The thickness values of absorber compounds are different from each other even if the mass thickness values are the same. It is expected that the differences in thickness values have an effect on experimental results. This effect may be attributed to the effect of chemical environment on absorber compounds prepared as pellet samples.

We may conclude that for compounds, the mixture rule is not applicable near the absorption edge. This result may be attributed to chemical, molecular, and thermal environment of present absorber compounds. We believe that the principal explanation is originated from the fact

that the chemical effects are appreciable for only near the absorption edges.

As seen in Tables 1, it can be stated that the crystalline form and oxidation number of barium compounds also affect the involvement of outer orbital in the emission of K X-rays when vacancy is created in a shell. It is known that different bonding energies and interatomic distances depend on different interactions between central atom and ligands in the chemical compounds. These effects play a role in the K X-ray transitions. The outer energy levels are sensitive to the chemical environment and they are strongly influenced by ligands in terms of crystal field theory. In the bond formation, valence state of atom has important effect on the related parameters of the spectrum in terms of relative and transmitted intensity. Oxidation number is the most important chemical feature that contributes to a wavelength shift in an X-ray spectral line (Bertin, 1985b). Therefore, it can be concluded that there is an indirect or direct chemical effect on the  $J\sigma_M$ ,  $J\sigma_A$  and  $J\sigma_E$ .

It is estimated that the maximum errors in calculations are less than 3.3%. These errors are attributed to the statistical errors in I and I<sub>0</sub> (≤ 1%), in sample thickness (≤ 1%), sample weighing (≤ 1%), geometric factor (≤ 1%), source intensity (≤ 1%) and systematic errors (≤ 2%).

## Conclusion

In this study, both the experimental and the theoretical values for  $\sigma_M$ ,  $J\sigma_M$ ,  $\sigma_A$ ,  $J\sigma_A$  and only the theoretical values for  $\sigma_E$ ,  $J\sigma_E$  are presented near the absorption edge of the selected barium compounds. The measured values are compared with the theoretical values which were obtained by using WinXCom, a Windows version of XCOM on the basis of the mixture rule. It is clearly visible

from Figures 1 to 3 that the  $\sigma_M$ ,  $\sigma_A$  and  $\sigma_E$  depend on photon energies of < 100 keV, especially, energies near the absorption edge. The present study indicates that there is a considerable relationship between  $J\sigma_M$ ,  $J\sigma_A$  and  $J\sigma_E$  and energy of the X-rays near the absorption edge.

The most interesting result of this study is that both experimental and theoretical values of  $J\sigma_M$  and  $J\sigma_A$  are equal for each barium compound. This fact would be verified for other compounds, alloys and mixtures hereafter. We note that the  $J\sigma_E$  term could not be measured, experimentally.

This study shows the existence of the terms  $J\sigma_M$ ,  $J\sigma_A$  and  $J\sigma_E$ . The present results constitute the best of our knowledge, so we could not compare the results reported in the literature. The most crucial finding of this study is the demonstration of the validity of Equation (8) that is used for calculating  $J\sigma_M$ ,  $J\sigma_A$ , and  $J\sigma_E$  values. As a result, those terms can be measured in a direct way, reliably and quickly with the help of an ideal transmission geometry and with the help of an appropriate selection of the energy range of K $\alpha$  and K $\beta$  X-rays that are published from the secondary sources within the range of  $K_{\text{abs}}$  values of absorbers.

To sum up, absorption jump factors of the effective molecular  $J\sigma_M$ , atomic  $J\sigma_A$  and electronic  $J\sigma_E$  cross-sections are not the total effective molecular  $\sigma_M$ , atomic  $\sigma_A$ , and electronic  $\sigma_E$  cross-sections but they are the calculation of those terms and have a specific value. As seen in Tables 2 to 5, although the total effective  $\sigma_M$  and  $\sigma_A$  cross-sections are different, absorption jump factors of  $J\sigma_M$  and  $J\sigma_A$  are identical. From Table 6 it can be seen that both experimental and theoretical absorption jump factors of  $J\sigma_M$  and  $J\sigma_A$  are also identical. This situation enhances the importance of the results and it can give the opportunity of expanding the scope of our study to various other compounds.

## ACKNOWLEDGEMENT

This work was supported by the Yildiz Technical University under award number 2011-01-01-KAP02.

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