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Research Article

Measurement of K Level Natural Line Widths, Kα$_1$ and Kα$_2$ X-Ray Line Widths

Ömer SÖĞÜT[1]*

[1]Kahramanmaraş Sütçü Imam University Faculty of Arts and Science Department of Physics, 46100 Kahramanmaraş.

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Abstract

In this study, the K shell natural line widths with Kα$_1$ and Kα$_2$ X-ray line widths of Ti, V, Cr, Mn, Fe, Co, Ni, Cu and Zn elements and compounds were semi-experimentally calculated by using the values of K shell fluorescence yield. An ^{241}Am radioisotope source, emitting in 75 mCi intensity and 59.5 keV energy gamma rays was used to stimulate the samples. A solid state Si(Li) detector have a resolution 155 eV at 5.96 keV, was used to count K X-rays emitted from the specimens. It was determined that the X-ray line widths of $\Gamma_{K\alpha1}$ and $\Gamma_{K\alpha2}$ and the natural line width of the Γ_K K level vary depending on the chemical structure. The results show that Γ_K, $\Gamma_{K\alpha1}$ and $\Gamma_{K\alpha2}$ line widths measured in compounds deviated up to 5-48% from according to values of the pure element. The present results, for pure elements, are in good agreement with the results of other researchers in the literature within the limits of error.

Keywords: K X-rays, chemical effect, fluorescence yield, line width, Kα$_1$ and Kα$_2$.

K Kabuğu Flüoresans Verimleri Kullanılarak K Seviyesi Doğal Çizgi Genişlikleri ile Kα$_1$ ve Kα$_2$ X-Işını Çizgi Genişliklerinin Ölçülmesi

Öz

Bu çalışmada Ti, V, Cr, Mn, Fe, Co, Ni, Cu ve Zn element ve bileşiklerinin K kabuğu doğal çizgi genişlikleri ile Kα$_1$ ve Kα$_2$ X-ışını çizgi genişlikleri yarı deneysel olarak, K kabuk flüoresans verimi değerleri kullanılarak hesaplandı. Numuneleri uyarmak için 75mCi şiddetinde ve 59. 5 keV enerjili gama ışınları yayınlayan ^{241}Am radyoizotop kaynağı kullanıldı. Numunelerden yayınlanan K X-ışınlarını saymak için çözünürlüğü 5.96 keV'de 155 eV olan katı hal Si(Li) detektörü kullanıldı. Kimyasal yapıya bağlı olarak K seviyesi doğal çizgi genişliği ile Kα$_1$ ve Kα$_2$ X-ışını çizgi genişliklerinin değiştiği tespit edildi. Sonuçlar bileşiklerde ölçülen Γ_K, $\Gamma_{K\alpha1}$ and $\Gamma_{K\alpha2}$ çizgi genişliklerinin saf element değerlerine göre % 5-48 kadar değiştiğini göstermektedir. Ancak, saf elementler için ölçülen deneysel sonuçlar, literatürdeki diğer araştırmacıların sonuçlarıyla hata sınırları dâhilinde iyi bir uyum içinde olduğu bulunmuştur.

Anahtar Kelimeler: K X-ışınları, kimyasal etki flüoresans verimi, çizgi genişliği, Kα$_1$ ve Kα$_2$.

1. Introduction

Various researchers have shown that the characteristic K X-rays are more affected by the chemical state of the X-ray emitting atom than L X-rays (Söğüt et al., 2002 and 1997; Cevik et al., 2005; Sögüt, 2009; Boydaş et al., 2015). However, the peak widths and energies, the satellite peaks and the formation of the dependent emission rates are affected by the detector element speciation. In addition to this, it is well known that the width of bottom atomic levels is affected, by means of multiplet splitting, by the different possible configurations of outermost electrons in unfilled shells. The measurement of X-ray line width constitutes an important application of X-Ray Fluorescence Spectroscopy (XRF). The widths of Kα$_1$ and Kα$_2$ X-ray lines yield important information on the L$_1$ and L$_2$ subshells. For example, for

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*Corresponding Author: omersogut@gmail.com transition metals, many computations have been done for the width of the $K\alpha_{1,2}$ (from L_2 and L_3 subshell to K shell transitions) X-ray lines, the considering all potential arrangements of outermost shell electrons, and the calculated line widths have been compared with experimental values (Schönfeld and Janßen,1996). In 1979, Krause and Oliver, 1979, Krause and Oliver reported that it is possible the values of fluorescence yield, along with calculated theoretically radiative rates, to obtain credible semi empirical values of K and L levels natural widths with, from these, Kα X-ray natural line widths and KLL Auger lines (Krause and Oliver, 1979). When K shell ionisation occurs with additional outer shell excitation or ionisation, as frequently happens, Kα X-rays are relocated in energy according to the diagram lines. When the M shell is excited, the shift in Kα X-ray energy is commonly less than the diagram lines natural width, which can then become mightily polluted and deteriorated as was proved speculatively (Krause and Oliver, 1979). The strong discontinuities in the L_3- $M_{4,5}M_{4,5}$ / L_2-$M_{4,5}M_{4,5}$ Auger intensity ratios for Zn, Cu, Ni, and Co was determined by Yin et al.(Yin et al., 1973). They have reported that an irregular decrease in the widths of L_2 level as the atomic number goes from 20 to 30. L_2-$L_3M_{4,5}$ Coster-Kronig transition rates of 3d transition metals were empirically defined by analysing the extra L_2 hole life span width broadening by the Coster-Kronig transition compared with one of the L_3 holes and one of the spectral intensity singles L_2-$M_{4,5}M_{4,5}$ (Nyholm et al., 1981). Ertuğrul and Şimşek have determined L_2 and L_3 subshell fluorescence yields, and $K\alpha_1$ and $K\alpha_2$ line widths in $22 \leq Z \leq 62$ atomic number range (Ertuğrul and Şimşek, 2002). Their experimental results, K, L_2 and L_3 level widths, agree with those of Krause and Oliver (Krause and Oliver, 1979). In a study conducted by Mauran and his companions in 1979, they revised again the L_3 and M_1 subshell atomic level widths of elements with atomic numbers between 54 and 77 (Mauron et al., 2003). Many authors have experimentally studied K X-ray and L level line widths with various methods or different spectroscopic area from the 1960s until today (Durak and Özdemir, 1998; Salem and Lee, 1976; Raboud et al., 2002; John and DuMond, 1961). The ingredient intensity ratios $K\alpha_2/K\alpha_1$ and the natural line widths for all elements in the range of Z = 70-82, were measured by Campbell and Schulte (Campbell and Schulte, 1980). Bamynek et al. have explained K- and L-level widths (Bambynek et al., 1972).

The purpose of this research is to compute semi-experimentally $K\alpha_1$ and $K\alpha_2$ X-ray line widths and K shell natural line widths of elements and compounds of Zn, Cu, Ni, Fe, Co, Mn, Cr, Ti and V by using the values of the K shell fluorescence yield. In addition to these, the chemical effects of Zn, Cu, Ni, Fe, Co, Mn, Cr, Ti and V compounds on $K\alpha_1$ and $K\alpha_2$ X-ray line widths and K shell natural line widths were studied.

2. Experimental Procedure

Samples consisting of elements and its compounds of Cr, Ti, V, Mn, Co, Fe, Ni, Zn and Cu were excited with an ^{241}Am radioactive source emitting gamma rays by an intensity of 75 mCi and 59.5 keV energy. A Si (Li) detector which is a resolution of 155 eV at 5.96 keV was used to count the characteristic K X rays emitted from the samples. All samples were shifted by 400 mesh sieves after being powdered. The samples were prepared as $2\text{-}10\text{x}10^{-3}$ g/cm^2 mass thickness on a scotch tape as the amount of substance per unit area for the measurements. The shape of the experimental setup and the typical K X-ray spectrum of copper which excited with the 241Am source and counted with the Si (LI) detector in Figure 1 and Figure 2, respectively are given. As seen from Figure 1, the lead shield prevents the detector from directly irradiating with radiation from the source. In order to prevent the L X rays of the lead, an iron lining was used. An aluminium collimator was also used to block the K X-rays emitted from the iron.

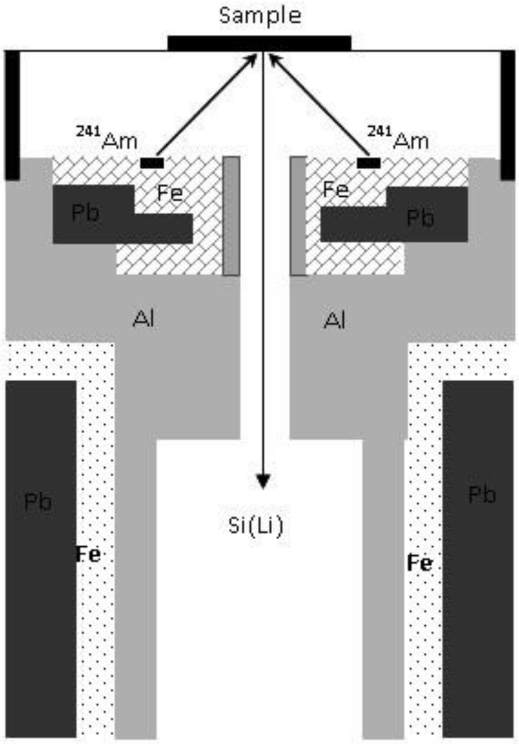

Figure 1. Experimental set up

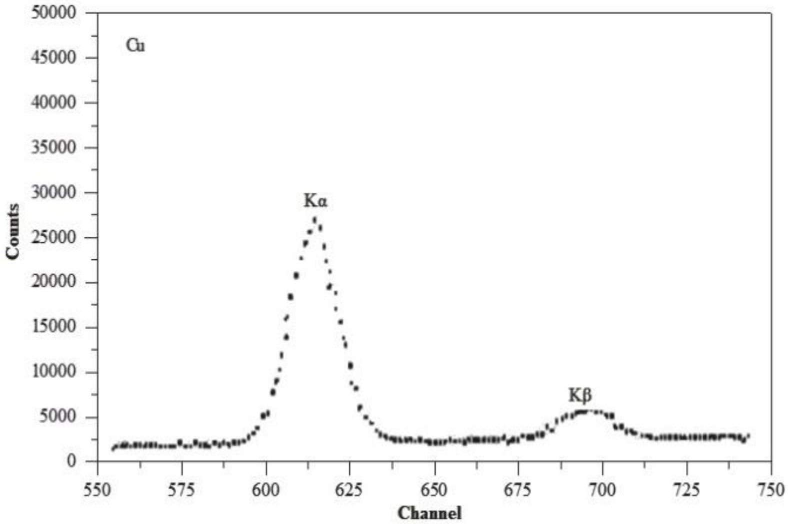

Figure 2. A typical Cu spectrum excited with a ^{241}Am radioactive source and detected with a Si (Li) detector

The experimental K shell fluorescence yield values can be calculated as follows (Apaydın and Tırasoğlu, 2006; Söğüt, 2010),

$$\omega_K = \frac{\sigma_{K_i}}{\sigma_K(E)} \qquad (i=\alpha,\beta) \tag{1}$$

where $\sigma_K(E)$ is the K-shell photoionization cross-section for the concerned at element at 59.5 keV (Scofield, 1973), σ_{Ki} is the experimental K shell fluorescence cross-section, and σ_{Ki} is given as the following (Aylikci et al., 2010; Söğüt et al., 2003):

$$\sigma_{K_i} = \frac{I_{K_i}}{I_0 G \varepsilon_{K_i} \beta\, t} \tag{2}$$

where I_{Ki} ($i=\alpha, \beta$) is the net area under the corresponding photo peak, t is the thickness of the sample as the amount of substance per unit area (g/cm^2), ε_{Ki} is the detector efficiency (Söğüt, 2010), I_0 is the stimulate radiation coming to the sample surface, G is a geometric factor, and β is the self-absorption correction factor of the sample. β was computed by using the following equation written by supposing the coming angle of the fluorescence radiation equalled of the detector to be approximately 90^0 (Söğüt, 2009),

$$\beta = \frac{1-\exp\left[-\left(\mu_{inc}\sec\theta + \mu_{emt}\right)t\right]}{\left(\mu_{inc}\sec\theta + \mu_{emt}\right)t} \tag{3}$$

where μ_{inc} (cm^2 g^{-1}) and μ_{emt} (cm^2 g^{-1}) are the total mass absorption coefficients for the stimulating radiation, and the emitted characteristic X-rays, respectively. The total mass absorption coefficients were calculated from the table of Hubbell and Seltzer (Hubbell and Seltzer, 1995). K level natural line widths (Γ_K), $K\alpha_1$ and $K\alpha_2$ X-ray line widths ($\Gamma_{K\alpha1}$ and $\Gamma_{K\alpha2}$) were calculated from the equations given in below (Campbell and Schulte, 1980; Scofield, 1974; Krause and Oliver, 1979;).

$$\Gamma_K = \frac{\Gamma_K(R)}{\omega_K} \tag{4}$$

$$\Gamma_{K\alpha_1} = \Gamma_{L_3} + \Gamma_K \tag{5}$$

$$\Gamma_{K\alpha_2} = \Gamma_{L_2} + \Gamma_K \tag{6}$$

where $\Gamma_K(R)$ is radiative transition rate (Scofield, 1974)), Γ_{L2} and Γ_{L3} are the L_2 and L_3 line widths (Krause and Oliver,1979), respectively, and ω_K is K shell fluorescence yield which computed from equation (1).

3. Results and Discussion

The obtained values of K shell natural line widths with $K\alpha_1$ and $K\alpha_2$ X-ray line widths of Ti, V, Cr, Mn, Fe, Co, Ni, Cu and Zn elements and compounds were shown in Table 1. It can be seen from Table 1 that the K shell level widths for pure elements are in good agreement with the results of other researchers in the literature within the limits of error. The measured values of Γ_K, $\Gamma_{K\alpha1}$ and $\Gamma_{K\alpha2}$ line widths in the atomic number range $22 \leq Z \leq 58$ defined experimentally using equation (4-6), and are listed in Table 1. Possible sources of error include: $I_0G\varepsilon$ determination (2-3%); background determination (1-2%); self-absorption correction factor (2-3%), counting statistics (1-2%). When all error sources are added together, the total experimental relative error is 6-10%.

As seen from Table 1 and Figure 3-5, the values of K level natural line width (Γ_K), $K\alpha_1$ and $K\alpha_2$ X-ray line widths ($\Gamma_{K\alpha1}$ and $\Gamma_{K\alpha2}$) of the present study are in good agreement both the experimental values of Kundeyi and Aylikci and the theoretical values of Krause and Oliver, within error limits. As seen from Figure 3-5, the K level natural line widths (Γ_K) and $K\alpha_1$ and $K\alpha_2$ X-ray line widths ($\Gamma_{K\alpha1}$ and $\Gamma_{K\alpha2}$) increase with increasing atomic number. As seen from Table 1, for pure element values of samples, K level natural line width (Γ_K) from the values of Kundeyi and Aylikci are different 0.56% for Ti, 6% for V, 9% for Cr, and 9% for Mn, 3% for Fe, 12% for Co, 6% for Ni, 3% for Cu and Zn 8%. According to the values of Krause and Oliver, this difference is 11% for Ti, 17% for V, 4% for Cr, 3% for Mn, 13% for Fe, 10% for Co, 15% for Ni, 13% for Cu and 15% for Zn. According to the values of Kundeyi and Aylikci, $\Gamma_{K\alpha1}$ and $\Gamma_{K\alpha2}$ X-ray line widths are different 0.53% for Ti, 5% for V, 7% for Cr, 7% for Mn, 2% for Fe, 21% for Co, 4% for Ni, 2% for Cu and 7% for Zn. According to Krause and Oliver's values, these differences are as follows: are 8% for Ti; 15% for V; 3% for Cr; 3% for Mn; 10% for Fe; 7% for Co; 12% for Ni; 10% for Cu and 13% for Zn. As seen from Table 1, the experimental Γ_K, $\Gamma_{K\alpha1}$ and $\Gamma_{K\alpha2}$ line widths measured for the compounds were found to differ 5-52% according to the values of Kundeyi and Aylikci. This difference is 3-41% according to Krause and Oliver's theoretical values.

Table 1. K shell natural line widths with $K\alpha_1$ and $K\alpha_2$ X-ray line widths of Ti. V. Cr. Mn. Fe. Co. Ni. Cu and Zn elements and compounds

Sample	**Oxidation number**	**Symmetry structure**	**Present work**			**Kundeyi and Aylikci, 2019**			**Krause and Oliver, 1979**		
			Γ_K	$\Gamma_{K\alpha1}$	$\Gamma_{K\alpha2}$	Γ_K	$\Gamma_{K\alpha1}$	$\Gamma_{K\alpha2}$	Γ_K	$\Gamma_{K\alpha1}$	$\Gamma_{K\alpha2}$
Ti	0		0.841±0.067	1.062±0.069	1.082±0.070	0.8363	1.0563	1.0763	0.94	1.16	1.18
TiO_2	4		0.501 ±0.031	0.721±0.044	0.741±0.045	-					
V	0		0.835 ±0.075	1.075±0.086	1.095±0.088	0.8920	1.1320	1.1520	1.01	1.26	1.28
VO	2		0.539 ±0.045	0.779±0.054	0.799±0.059	-					
V_2O_3	3		0.491 ±0.030	0.731±0.046	0.751±0.048	-					
V_2O_4	4		0.535 ±0.044	0.775±0.048	0.795±0.049	-					
V_2O_5	5	O_h	0.573 ±0.037	0.813±0.058	0.833±0.061	-					
Cr	0		1.042 ±0.085	1.312±0.082	1.332±0.086	0.9531	1.2231	1.2431	1.08	1.35	1.37
Cr_2O_3	3		0.532 ±0.033	0.802±0.059	0.822±0.060	-					
$Cr(NO_3)_3$	3	O_h	0.523 ±0.045	0.780±0.065	0.819±0.069	-					
$Cr(NO_3)_3x9H_2O$	3		0.519 ±0.045	0.789±0.069	0.809±0.071	-					
$Cr_2O_7(NH_4)_2$	6	T_h	0.847 ±0.055	1.117±0.087	1.137±0.020	-					
$CrCl_2$	2	O_h	0.656 ±0.043	0.926±0.072	0.945±0.084	-					
$CrCl_3x6H_2O$	3	O_h	0.659 ±0.040	0.929±0.059	0.949±0.607	-					
$Na_2Cr_2O_7$	6		0.844 ±0.073	1.114±0.071	1.134±0.077	-					
$K_2Cr_2O_7$	6	T_h	0.933 ±0.089	1.203±0.118	1.223±0.107	-					
$Cr_2(SO_4)_3xH_2O$	3		0.675 ±0.045	0.945±0.064	0.965±0.065	-					
Mn	0		1.121 ±0.100	1.441±0.092	1.461±0.095	1.0278	1.3478	1.3678	1.16	1.48	1.50
MnO_2	4	O_h	0.713 ±0.057	1.033±0.069	1.053±0.076	-					
$MnCl_2x2H_2O$	2		0.812 ±0.055	1.132±0.072	1.152±0.074	-					
$MnSO_4\ H_2O$	2		0.762 ±0.066	1.082±0.067	1.102±0.090	-					
$Mn(CH_3COO)_3$	3		0.785 ±0.069	1.1053±0.095	1.125±0.097	-					
$MnCO_3$	2		0.858 ±0.066	1.178±0.095	1.198±0.103	-					
$KMnO_4$	7		0.773 ±0.773	1.093±0.075	1.113±0.070	-					
$MnCl_4$	4	T_h	0.697 ±0.065	1.017±0.121	1.037±0.081	-					
$MnCl_2x4H_2O$	2		0.658 ±0.056	0.978±0.080	0.998±0.078	-					
Fe	0		1.082 ±0.081	1.441±0.091	1.451±0.094	1.1102	1.4702	1.4802	1.25	1.61	1.62
Fe_2O_3	3	O_h	0.835 ±0.056	1.195±0.076	1.205±0.077	-					

$FeCl_2x4H_2O$	2		1.005 ±0.074	1.365±0.101	1.375±0.089	-					
FeS	2	O_h	0.894 ±0.079	1.254±0.017	1.264±0.079	-					
$Fe(NO_3)_3x9H_2O$	3		0.843 ±0.071	1.203±0.076	1.213±0.079	-					
$FePO_4$	3		0.959 ±0.071	1.319±0.100	1.329±0.101	-					
FeF_3	3		0.822 ±0.063	1.812±0.111	1.192±0.079	-					
Co	0		1.199 ±0.103	1.629±0.106	1.629±0.105	1.2004	1.6304	1.6304	1.33	1.76	1.76
CoO	2	O_h	0.861 ±0.061	1.291±0.09	1.291±0.105	-					
Co_2O_3	3		0.929 ±0.082	1.359±0.117	1.359±0.117	-					
$CoSO_4$	2		1.446 ±0.136	1.878±0.174	1.878±0.175	-					
CoF_2	2	O_h	1.093 ±0.090	1.523±0.124	1.523±0.124	-					
CoF_3	3		1.086 ±0.104	1.516±0.139	1.516±0.139	-					
$CoCl_2$	2		1.538 ±0.133	1.968±0.161	1.968±0.161	-					
$Co(CH_3COO)_2$	2		1.466 ±0.107	1.896±0.147	1.896±0.133	-					
$Co(SCN)_2$	2		1.750 ±0.144	2.180±0.178	2.180±0.179	-					
Ni	0		1.222 ±0.092	1.701±0.110	1.741±0.114	1.3001	1.7801	1.8201	1.44	1.94	1.96
$NiCl_2$	2	T_h	1.148 ±0.080	1.628±0.133	1.668±0.138	-					
$NiSO_4$	2		0.929 ±0.073	1.409±0.101	1.449±0.104	-					
Cu	0		1.345 ±0.128	1.905±0.148	1.965±0.157	1.3879	1.9479	2.0079	1.55	2.11	2.17
CuO	2	O_h	0.957±0.057	1.517±0.101	1.577±0.102	-					
Cu_2O	1	O_h	0.865 ±0.074	1.425±0.119	1.485±0.125	-					
$CuCl$	1		0.723 ±0.054	1.283±0.095	1.343±0.106	-					
$CuCl_2$	2		0.935 ±0.078	1.495±0.122	1.555±0.132	-					
$CuCl_2x2H_2O$	2	T_h	1.620 ±0.151	2.179±0.205	2.239±0.211	-					
CuC_2O_4	2		1.159 ±0.103	1.719±0.141	1.779±0.146	-					
$Cu(CN)_2$	2		1.161 ±0.160	1.721±0.165	1.781±0.167	-					
$CuBr$	1	T_h	0.976 ±0.070	1.536±0.111	1.596±0.124	-					
$CuBr_2$	2	T_h	1.237±0.081	1.797±0.120	1.857±0.119	-					
$CuCO_3$	6		0.937±0.081	1.497±0.124	1.557±0.134	-					
Zn	0		1.423 ±0.116	2.070±0.161	2.142±0.167	1.5440	2.1940	2.2640	1.67	2.32	2.39
ZnS	2		1.363 ±0.099	2.013±0.179	2.083±0.175	-					
$ZnSO_4$	2		2.349 ±0.216	2.999±0.284	3.069±0.298	-					

Mukoyama have measured $K\alpha_{1,2}$ X-ray line widths for 3d elements and have explained the results according to asymmetry index of the compounds of 3d elements (Mukoyama, 2000). They have also discussed chemical effect on $K\alpha$ X-ray line widths and CK transition differences between $K\alpha_1$ and $K\alpha_2$ line widths due to L_2-L_3 $M_{4,5}$ CK transition probabilities. Söğüt et al (Söğüt et al., 2002) have measured the chemical effect on K X-ray intensity ratios of 3d elements and they reported that the chemical effects play an important role in K X-ray transitions. In 1986, Broll has investigated accurate X-ray fluorescence analysis for compact or diluted specimens and calculated some X-ray fluorescence parameters such as ω_K, $f_{K\alpha}$, and J_K for elements in the range Z = 11-70 (Broll, 1986). Campbell et al. (Campbell and Papp, 2001) have measured widths of the atomic K-N7 levels. They have given in tables the experimental and theoretical Γ_K values for the K shell of some elements in the atomic range $3 \leq Z \leq 92$. In addition, $K\alpha_1$, $K\alpha_2$, $K\beta_1$ and $K\beta_3$ line widths have been measured by Kessler et al (Kessler et al., 1982) for some elements in the atomic region $13 \leq Z \leq 92$. They stimulated the samples by accelerated electrons which have the energy of 2.5 MeV.

As seen in Figure 3-5, in the results of this study, $K\alpha_1$ and $K\alpha_2$ X-ray line widths and K level natural line widths vary approximately linearly with respect to atomic number. The reason of this may be while the atomic number increases the value of the K shell fluorescence yield values increase.

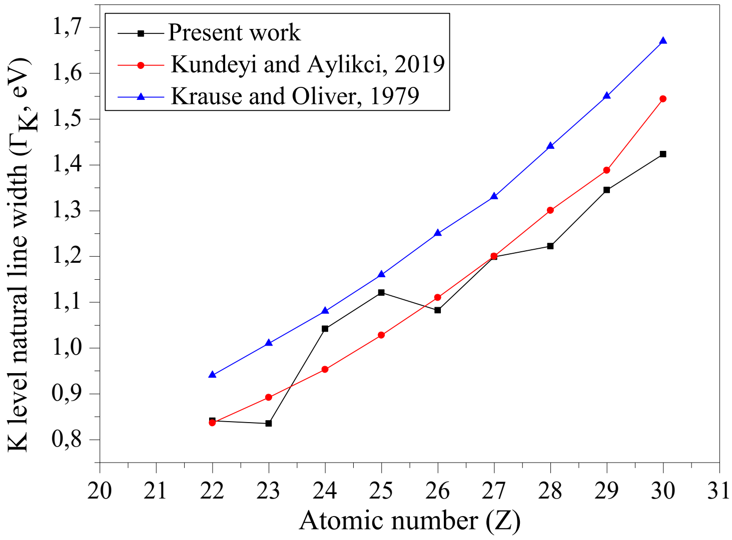

Figure 3. K level natural line width (Γ_K) as a function of atomic number.

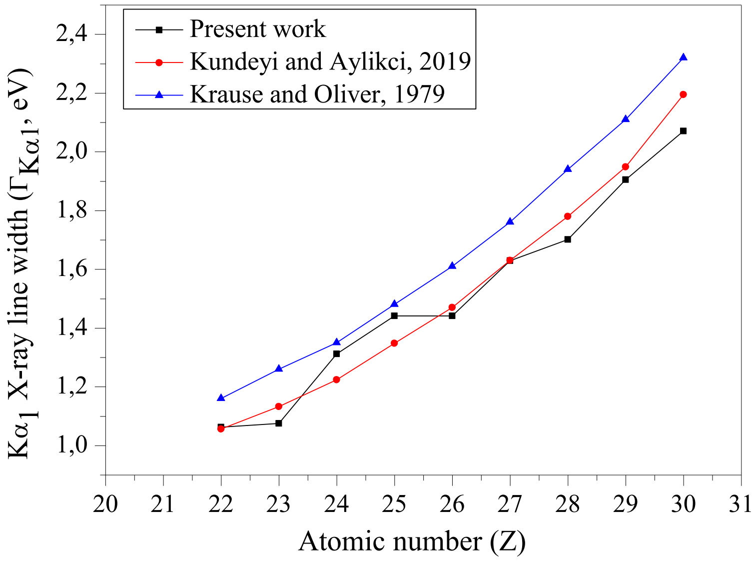

Figure 4. $K\alpha_1$ X-ray lines width as a function of atomic number

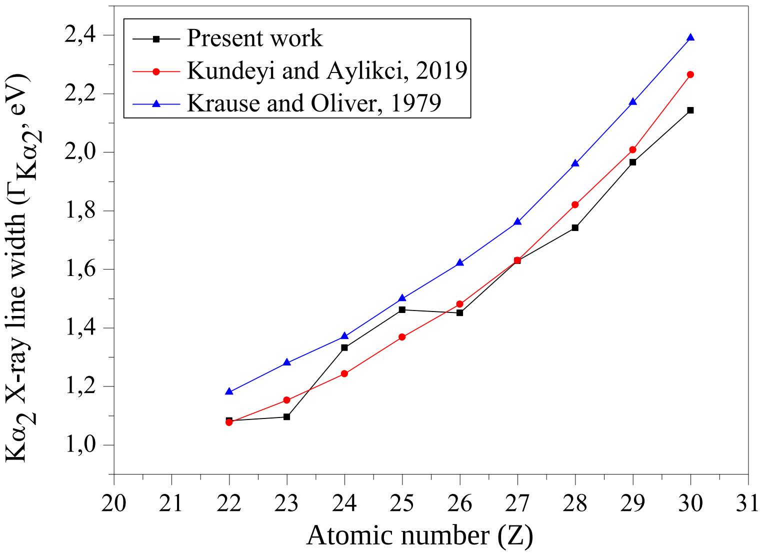

Figure 5. $K\alpha_2$ X-ray lines width as a function of atomic number

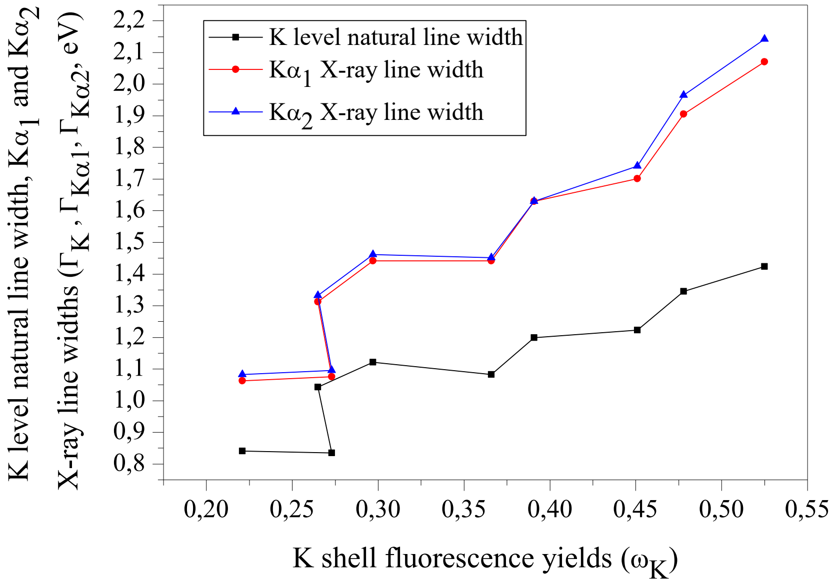

Figure 6. The variation of K level natural line width, $K\alpha_1$ and $K\alpha_2$ X-ray line widths as a function of fluorescence yield

As seen from Figure 6, the changes of K level natural line width, $K\alpha_1$ and $K\alpha_2$ X-ray line widths with respect to fluorescence yield are approximately the same as the change of Γ_K, $\Gamma_{K\alpha1}$ and $\Gamma_{K\alpha2}$ line widths according to atomic number. This result shows that the change in fluorescence yields will change the natural line width of the K level, and the X-ray line widths of $K\alpha_1$ and $K\alpha_2$.

As seen from Table 1, the chemical effects were detected in K level line widths with $K\alpha_1$ and $K\alpha_2$ X-ray line widths. The results show that Γ_K, $\Gamma_{K\alpha1}$ and $\Gamma_{K\alpha2}$ line widths of the compounds changes according to pure element values. The reason for this is because the outer electrons of the elements in the chemical compound structure (especially the 3d group elements) are weakly bound to the ligand atoms, and as a result, it is the increase in the possibility of transition from the outer shells to the inner shells, which occurs according to the electric dipole selection rules. In addition, one of the most important factors related to chemical effects on X-ray emission possibilities is the bond types of the elements. That is to say, the chemical bonding types such as ionic, metallic and covalent bond significantly affect the characteristic K X-ray emission probabilities. The changing of X-ray emission probabilities affects K shell fluorescence yield (ω_K), and as a result of this, K level line widths with $K\alpha_1$ and $K\alpha_2$ X-ray line widths are affected. The electron density changes depending on the type of bonding in close to atoms in the molecule. Changing the valence electron density changes the K X-ray emission probabilities. This phenomenon affects the K shell fluorescence efficiency. The more change in chemical bond causes to the more change in its valence electron density. In a study conducted by Mukoyama in 2000, it was shown that for Cr compounds there is a relation between the $K\alpha_1$ and $K\alpha_2$ emission line widths and the 3d electrons number (Mukoyama, 2000).

Depending on the possibilities of K X-ray emission, ω_K is also affected by the change of the electronegativity around the central X-ray emitter atom in the chemical bond. Since the outermost electron cloud of the central atom in the chemical bond will be attracted by the ligands due to increase the value of the electronegativity, the binding energies of the electrons in the outermost shell may also be affected. Some of the factors that can cause this change are the ligand structure, the electronegativity effect and the distribution of the ligands around the X-ray emitting central atom (Sawhney et al., 2000). In a 2002 study, it was reported that a chemical bond with tetrahedral (T_d) symmetry is more covalent than a bond with octahedral (O_h) symmetry, and the bond length in the tetrahedral symmetric structure is shorter according to the bond length in octahedral symmetry (Söğüt et al., 2002). However, in another study conducted in the same year, in the tetrahedral symmetry was reported to increase the interaction between the ligands and the central atom in both effects (Mukoyama et al., 1986). Generally, it is known that the change of the K X-ray emission probabilities for O_d symmetry compounds are less than those for T_d symmetry compounds.

4. Conclusion

In this study, the chemical effects on $K\alpha_1$ and $K\alpha_2$ X-ray line widths and K shell natural line widths of Ti, Cr, V, Fe, Mn, Ni, Co, Cu and Zn compounds were investigated. It was determined that $K\alpha_1$ and $K\alpha_2$ X-ray line widths and K shell natural line widths changed approximately linearly with increasing atomic number (Figure 3-5). $K\alpha_1$ and $K\alpha_2$ X-rays and K shell natural line widths were found to vary approximately linearly with increasing fluorescence yield values, except for Ti and V. The chemical effects on $K\alpha_1$ and $K\alpha_2$ X-ray and K shell natural line widths were determined, and factors such as electronegativity, chemical bond type, valence electron density and symmetrical structures of chemical molecules were found to be effective in the formation of chemical effects. Consequently, while the experimental Γ_K, $\Gamma_{K\alpha 1}$ and $\Gamma_{K\alpha 2}$ line widths for the compounds were calculated 5-48% difference according to the values of Kundeyi and Aylikci, 3-41% difference was computed according to the theoretical values of Krause and Oliver.

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