L X-RAY SATELLITE LINES USING WAVELENGTH DISPERSION X-RAY FLUORESCENCE FOR STRONTIUM AND MOLYBDENUM

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Abstract

X-Ray fluorescence (XRF) is a technique to analysis of various materials. We have two types of techniques in XRF.They are Energy dispersive X Ray Flouroscence (EDXRF) and Wave length dispersive X Ray flouroscence. The effective method to find the chemical profile of the element is WDXRF. This wavelength dispersive X ray fluorescence (WDXRF) will be used to check the nuclear design of different compounds. The study of relative intensity ratios of various satellite peaks of different elements is associated with their atomic spectral structures. The intensity ratios will give the validity of the Hatree-slater model of different combinations. In this paper, we will present energy versus intensity and data obtained using WDXRF of strontium in addition to the previous work on Molybdenum and its compounds.

Keywords: Wavelength Dispersive X-Ray fluorescence (WDXRF), Satellite peaks, Relative intensity ratio.

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Introduction

The emission of fluorescent X-Rays from a material when it is bombarded with high energy X-rays is called X-Ray fluorescence (XRF). This method is used to analyze chemical compounds. Wavelength Dispersive X-Ray fluorescence (WDXRF) is a modified version of XRF method that is useful to make measurements at a specific wavelength emission.

In the present study we use WDXRF to determine L X-Ray satellite lines of different compounds. We have selected WDXRF over EDXRF due to its sensitivity, and non-damaging nature. Also, this method allows us to decide the relative force proportions on X-Ray beams spectra.

The elements having energy less than 3.2KeV, can be studied by WDXRF method which is not possible by regular detection methods. That is the elements that have atomic numbers in which have $35 \leq Z \leq 53$.

For a better understanding atomic parameters of compounds, the WDXRF technique is used because of its sensitivity to the composition of mixtures and flexibility with the chosen material. We can decide the relative force proportions on L X beams spectra with a non-damaging procedure.

In this paper, we studied the L Spectral lines of Molybdenum (Mo) and Molybdenum trioxide (MoO_3) and strontium (Sr) and Strontium Nitric trioxide (Sr NO$_3$) compounds. Through these spectral lines the satellite peaks will obtain for a particular region through the energy versus intensity plots. They are having strong reduced intensity when compared to normal transition lines which are formed due to radiative electron transition in multiply ionized atoms. This study is carried out on these compounds due to their applications in various research fields.

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Experimental Details

For elemental analysis, two types of X-Ray fluorescence instrumentation are used. They are Energy dispersive X-Ray fluorescence (EDXRF) and Wavelength dispersive X-Ray florescence (WDXRF).

We prefer WDXRF over EDXRF because of the following reasons: The spectrum of EDXRF applies peak deconvolution, whereas the range of WDXRF can resolve the peaks and doesn't require post-processing. By the WDXRF spectrum, we can achieve higher precession in elemental identification and qualification. An elite presentation WDXRF spectrometer (Model: S8 Tiger, Bruker, Germany) braced with Rh anode X-Ray container of 4KW gave an example charger containing PET and XS-Ge dispersive gems and corresponding counter identifier was utilized to concentrate on the L shell spectra in the current work .

Figure 1 shows various parts of WDXRF spectrometer. By this schematic diagram X-Rays are ejected from the X-Ray tube of 20kV-60kV voltage with a power of 4KW. This power passes through the filter wheel, which will filter the bremsstrahlung radiation from the sample. And the rays fall on the molybdenum and go to the collimator through the vacuum seal, which will not allow the environmental conditions to affect it as the sample is in the solid phase. The X- Rays deflected from the sample will be passed to a crystal changer in the collimator. We use XS Ge (2.0keV-2.5keV) with the crystal distance (2d=0.653nm) to analyze the X- Rays. These crystals are suitable for 1.5KeV to 3.5KeV. We will decide the step size to 1/10th part according to the optical collimator value. By this, we can get a resolution. There is a better resolution for low step size, and for high step size, they will be better intensity. The X-Rays are deflected from the crystal changer to the gas flow proportional detector (90% Ar-10% CH4) used to record the low and high characteristic X-Ray intensities [10].
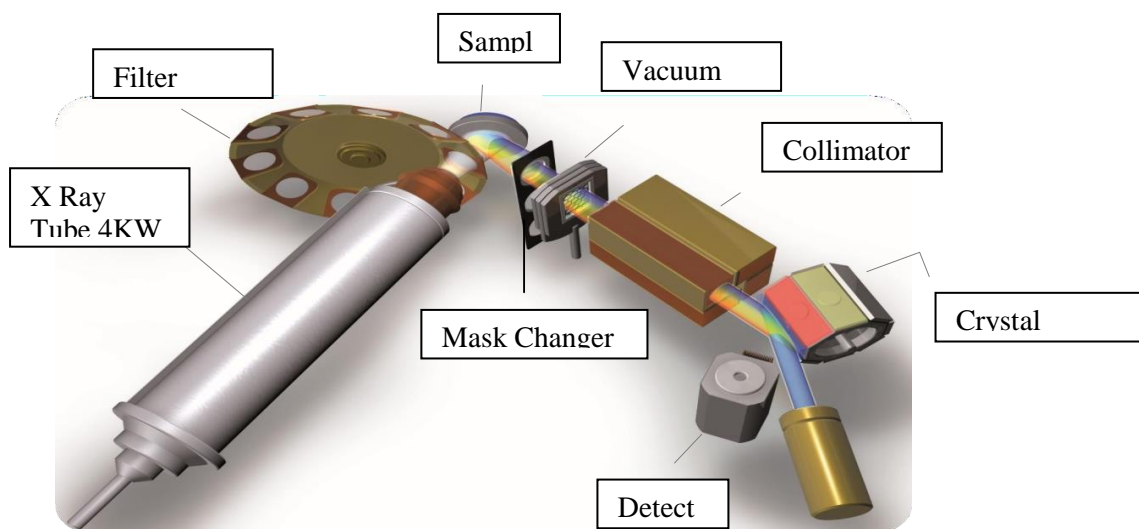

Figure 1: Schematic view of WDXRF spectrometer (Model: S8 Tiger, Bruker, Germany)

By using this device, the intensity ratios of taken compounds is calculated. During data collection the energy scan mode is set with 0.15sec per step.

Evaluation Method

L shell X ray's intensity ratios of measured intensity is calculated by using L_i/L_α is given by

$L_i/L_\alpha = [N(L_i)/N(L_\alpha)][\beta(L_\alpha)/\beta(L_i)][\varepsilon(L_\alpha)/\varepsilon(L_i)]$

Where $N(L_i)/N(L_\alpha)$ represents ratio of counting rates under L_i and L_α peaks

$\beta(L_\alpha)/\beta(L_i)$ represents the ratio of self absorption correction factor of the target

$\varepsilon(L_\alpha)/\varepsilon(L_i)$ Represents the ratio of detector efficiency values of L_α and L_i peaks X rays

respectively.

Measured intensity is given by $(Im)i=QR$ $\beta\,\varepsilon f_\beta$ (Iuc)i

Where Q=Geometrical element and not entirely settled during XRF analysis utilizing

standard example and taken as solidarity.

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(Iuc) i=uncorrected intensity $(i = L_\alpha, L_\beta, L_{\beta 3}, L_{\beta 4}, L_{\beta 15,2}, L_{\gamma 1})$ through spectrometer

R=Reflection efficiency parameter of Xs-Ge crystal

Self-absorption correction factor for the incident and scattered X- ray emission lines is

$$\beta = \frac{[1 - e^{-(sec\theta_E + sec\theta_{SC})m\mu}]}{[sec\theta_E + sec\theta_{SC}]m\mu}$$

θ_E , θ_{sc} refers to bragg incidence and emission angles

m is mass thickness of targets

μ is mass attenuation

The intensity is measured experimentally and it is denoted by counts per second.

Results and Discussions

In this section we will present intensities and normalized intensities of Mo and MoO_3. The L X Ray spectrum is fitted under necessary conditions by using Origin software. By this, we observe 12 peaks of the both elements 6 peaks each. From these satellite peaks are observed.
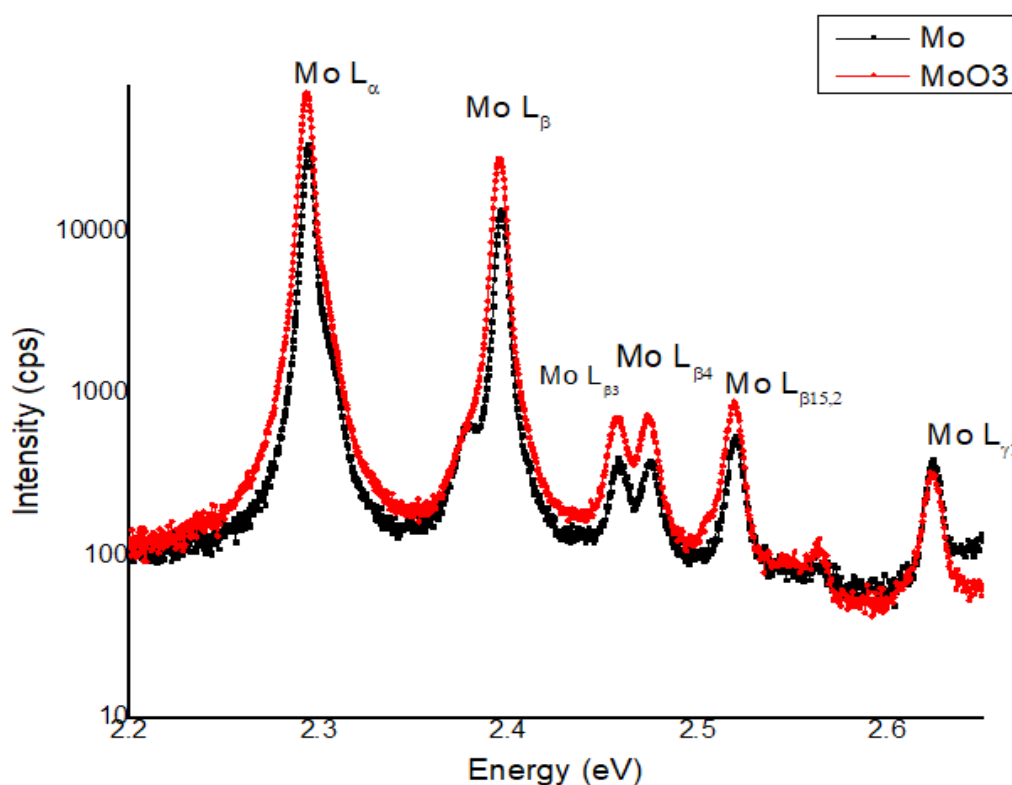

Figure 2: Energy in electron volts versus intensity in counts per second

Figure 2 shows plot of energy in electron volts versus intensity in counts per seconds. The purpose of this plot is to find the intensity ratios. In this plot red line corresponds to Molybdenum trioxide and black line corresponds to

Molybdenum. For both compounds the plot shows 6 peaks. In the plot the height of the left most peak is L_α, the height of the second, third, fourth, fifth and sixth peaks from left is L_β, $L_{\beta 3}$, $L_{\beta 4}$, $L_{\beta 15,2}$ and $L\gamma_1$ respectively. Three satellite peaks ($L_{\beta 3}$, $L_{\beta 4}$, $L_{\beta 15,2}$) in L_β region are detected.

Table 1: Relative Intensity of Mo and MoO_3

S No	Name of the Composition	L_β / L_α	$L_{\beta 3} / L_\alpha$	$L_{\beta 4} / L_\alpha$	$L_{\beta 15,2} / L_\alpha$
1	Molybdenum (Mo)	0.414	0.0105	0.0108	0.0125

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| 2 | MolybdenumTrioxide (MoO3) | 0.4057 | 0.0115 | 0.011 | 0.0157 |

Table 1 shows relative intensity of Mo and MoO_3 in L_β region. As shown in figure L_α is the main peak which is used to calculate the relative intensity of individual compounds. The relative intensity is calculated by the L_β region (L_β, $L_{\beta3}$, $L_{\beta4}$, $L_{\beta15,2}$) with respect to the main peak L_α region.

Table 2: Variation of Intensities of Mo and MoO_3

S No	Name of the Composition	$L_\beta(Mo)/$ $L_\beta(MoO_3)$	$L_{\beta3}(Mo)/$ $L_{\beta3}(MoO_3)$	$L_{\beta4}(Mo)/$ $L_{\beta4}(MoO_3)$	$L_{\beta15,2}(Mo)/$ $L_{\beta15,2}(MoO_3)$
1	Molybdenum Trioxide (MoO3) relative to Molybdenum (Mo)	0.467	0.566	0.543	0.564

Table 2 shows the variation of intensities between Molybdenum (Mo) and Molybdenum trioxide (MoO_3) by plot which it can be calculated by taking the ratios of both the compounds in the same region.
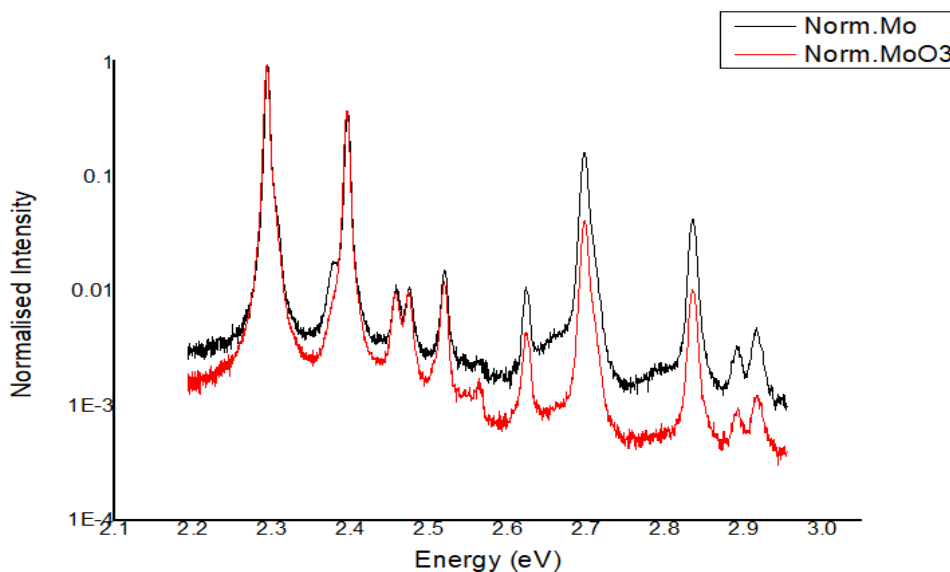

Figure 3: Energy in Electron Volts versus Normalized intensity

Figure 3 shows plot of energy in electron volts versus normalized intensity. The purpose of this plot is to find the relative intensity ratios. In this plot red line corresponds to Molybdenum trioxide and black line corresponds to Molybdenum. The intensity ratios by the plot energy versus Normalized intensity as to divide the whole spectra by relative intensity for the better plot. In this the black line denotes the molybdenum and red line denotes molybdenum trioxide. From Figure 3 Energy versus Normalized intensity plot is taken to find out the changes due to Mo-O bonding in MoO_3, it is apparent.

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Table 3: Normalized relative Intensity of Mo and MoO$_3$

S No	Name of the Composition	Lβ/ Lα	L $\beta3$/ L α	L β 4/ L α	L $\beta15,2$/ L α
1	Molybdenum (Mo)	0.3904	0.0108	0.0114	0.0154
2	Molybdenu mTrioxide (MoO3)	0.3904	0.0098	0.0106	0.0124

Table 3 shows Normalized relative intensity of Mo and MoO$_3$ in L$_\beta$ region. As shown in figure L$_\alpha$ is the main peak which is used to calculate the Normalized relative intensity of individual compounds. The Normalized relative intensity is calculated by the L$_\beta$ region (L$_\beta$, L$_{\beta3}$, L$_{\beta4}$, L$_{\beta15,2}$) with respect to the main peak L$_\alpha$ region.

Table 4: Variation of Normalized Intensity of Mo and MoO$_3$

S No	Name of the Composition	L$_\beta$(Mo)/ L$_\beta$(MoO$_3$)	L$_{\beta3}$(Mo)/ L$_{\beta3}$(MoO$_3$)	L$_{\beta4}$(Mo)/ L$_{\beta4}$(MoO$_3$)	L$_{\beta15,2}$(Mo)/ L$_{\beta15,2}$(MoO$_3$)
1	Molybdenum Trioxide (MoO3) relative to Molybdenum (Mo)	1	1.1042	1.082	1.195

Table 4 shows the variation of intensities are normalized between Molybdenum (Mo) and Molybdenum trioxide (MoO3) by plot which it can be calculated by taking the ratios of both the compounds in the same region.

In this section we will present intensities and normalized intensities of Sr and SrNO$_3$. The L X Ray spectrum is fitted under necessary conditions by using Origin software. By this, we observe 16 peaks of the both elements 8 peaks each. From these satellite peaks are observed.

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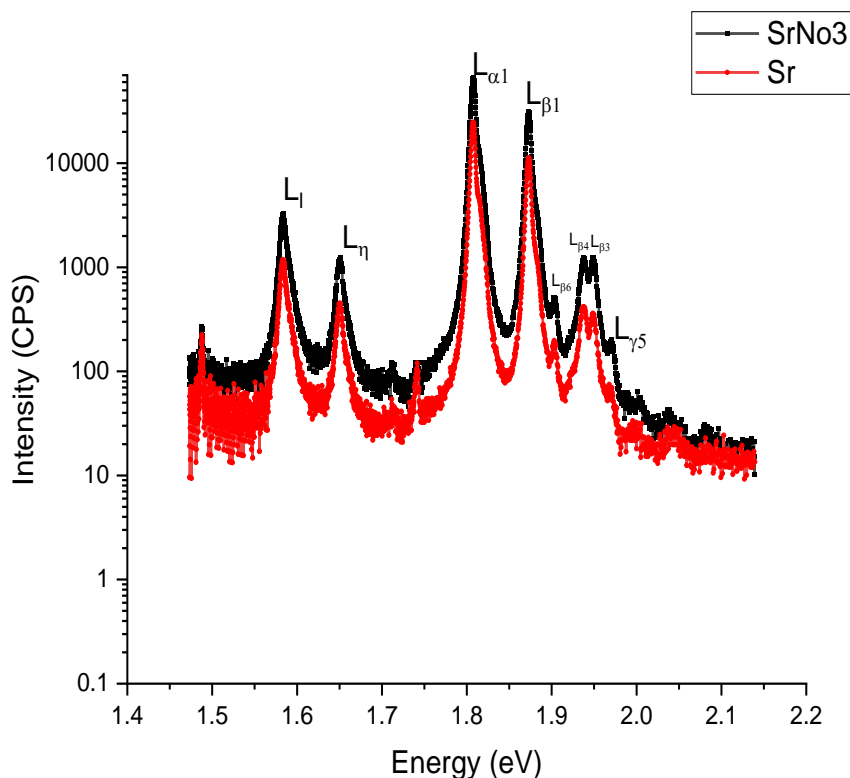Eur. Chem. Bull. 2023, 12(Issue 8),1380-1388

Figure 2 shows plot of energy in electron volts versus intensity in counts per seconds. The purpose of this plot is to find the intensity ratios. In this plot red line corresponds to Strontium and black line corresponds to Strontium nitric trioxide. For both compounds the plot shows 8 peaks. In the plot the height of the left most peak is L_l, the height of the second, third, fourth, fifth, sixth and seventh peaks from left is L_η, $L_{\alpha 1}$, $L_{\beta 1}$, $L_{\beta 6}$, $L_{\beta 4}$, $L_{\beta 3}$ and $L\gamma_5$ respectively. Four satellite peaks ($L_{\beta 1}$, $L_{\beta 6}$, $L_{\beta 4}$, $L_{\beta 3}$) in L_β region are detected.

Table 1: Relative Intensity of Sr and SrNO$_3$

S No	Name of the Composition	$L_{\beta 1}/L_{\alpha 1}$	$L_l/L_{\alpha 1}$	$L\eta/L_{\alpha 1}$	$L_{\beta 3}/L_{\alpha 1}$	$L_{\beta 4}/L_{\alpha 1}$	$L_{\beta 6}/L_{\alpha 1}$	$L_{\gamma 5}/L_{\alpha 1}$
1	Strontium (Sr)	0.4546	0.0456	0.0186	0.0131	0.0159	0.00752	0.00289
2	Strontium nitric trioxide (SrNO3)	0.48316	0.04846	0.01876	0.0179	0.01848	0.00764	0.00312

Table 1 shows relative intensity of Sr and SrNO$_3$. As shown in figure $L_{\alpha 1}$ is the main peak which is used to calculate the relative intensity of individual compounds. The relative intensity is calculated by the L_β region ($L_{\beta 1}$, $L_{\beta 3}$, $L_{\beta 4}$, $L_{\beta 6}$) with respect to the main peak $L_{\alpha 1}$ region.

Table 2: Variation of Intensities of Sr and SrNO$_3$

S No	Name of the Composition	$L_{\beta 1}(Sr)/$ $L_{\beta 1}(SrNO_3)$	$L_l(Sr)/$ $L_l(SrNO_3)$	$L\eta (Sr)/$ $L\eta (SrNO_3)$	$L_{\beta 3}(Sr)/$ $L_{\beta 3}(SrNO_3)$	$L_{\beta 4}(Sr)/$ $L_{\beta 4}(SrNO_3)$	$L_{\beta 6}(Sr)/L_{\beta 6}(SrNO_3)$	$L_{\gamma 5}(Sr)/L_{\gamma 5}(SrNO_3)$

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1	Strontium Nitric $(Sr(NO3)_2)$ relative to Strontium (Sr)	0.941	0.941	0.992	0.7318	0.8604	0.9843	0.9263

Table 2 shows the variation of intensities between Strontium (Sr) and Strontium Nitric trioxide ($SrNO_3$) by plot which it can be calculated by taking the ratios of both the compounds in the same region.
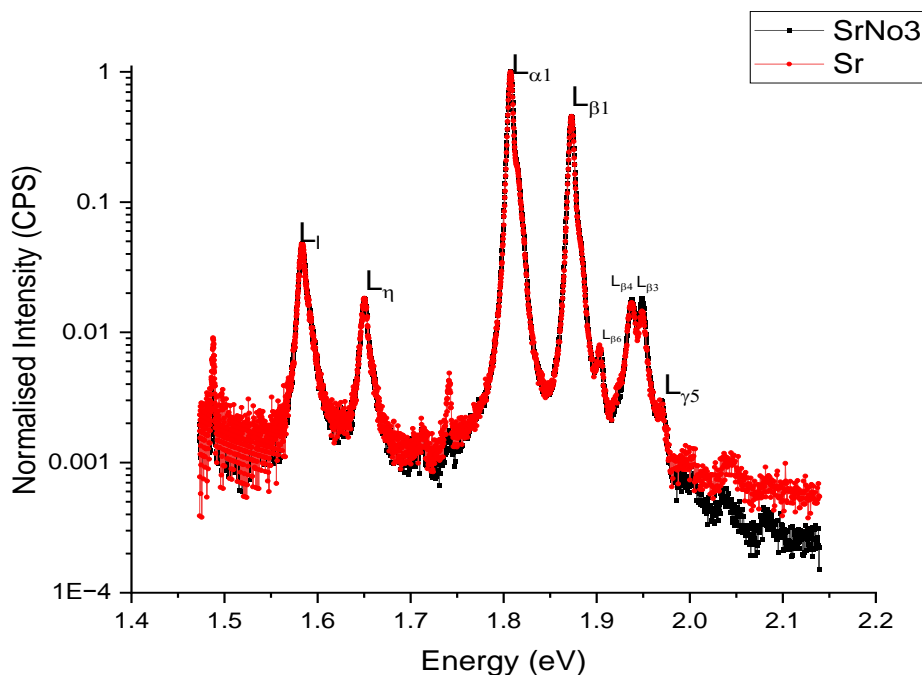

Figure 3: Energy in Electron Volts versus Normalized intensity

Figure 3 shows plot of energy in electron volts versus normalized intensity. The purpose of this plot is to find the relative intensity ratios. In this plot red line corresponds to Strontium and black line corresponds to Strontium Nitric Trioxide. The intensity ratios by the plot energy versus Normalized intensity as to divide the whole spectra by relative intensity for the better plot. In this the black line denotes the Strontium Nitric Trioxide and red line denotes Strontium. From Figure 3 Energy versus Normalized intensity plot is taken to find out the changes due to bonding in $SrNO_3$, it is apparent.

Table 3: Normalized relative Intensity of Sr and $SrNO_3$

S No	Name of the Composition	$L_{\beta1}/L_{\alpha1}$	$L_l/L_{\alpha1}$	$L\eta/L_{\alpha1}$	$L_{\beta3}/L_{\alpha1}$	$L_{\beta4}/L_{\alpha1}$	$L_{\beta6}/L_{\alpha1}$	$L_{\gamma5}/L_{\alpha1}$
1	Srontium (Sr)	0.4623	0.04702	0.0184	0.01741	0.01702	0.00787	0.00306
2	Strontium nitrate $(Sr(NO3)_2)$	0.4623	0.04702	0.0184	0.01741	0.01784	0.00787	0.00306

Table 3 shows Normalized relative intensity of Sr and $SrNO_3$ in $L_{\alpha1}$ region. As shown in figure $L_{\alpha1}$ is the main peak which is used to calculate the Normalized relative intensity of individual compounds. The Normalized relative intensity is calculated by the L_β region ($L_{\beta1}$, $L_{\beta3}$, $L_{\beta4}$, $L_{\beta6}$) with respect to the main peak $L_{\alpha1}$ region.

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Table 4: Variation of Normalized Intensity of Sr and SrNO$_3$

S No	Name of the Composition	$L_{\beta 1}$(Sr)/ $L_{\beta 1}$(SrNO$_3$)	L_l(Sr)/ L_l(SrNO$_3$)	$L\eta$ (Sr)/ $L\eta$ (SrNO$_3$)	$L_{\beta 3}$(Sr)/ $L_{\beta 3}$(SrNO$_3$)	$L_{\beta 4}$(Sr)/$L_{\beta 3}$(SrNO$_3$)	$L_{\beta 6}$(Sr)/$L_{\beta 6}$(SrNO$_3$)	$L_{\gamma 5}$(Sr)/ $L_{\gamma 5}$(SrNO$_3$)
1	Strontium nitrate (SrNO3) relative to Strontium (Sr)	1	1	1	1	0.95454	1	1

Table 4 shows the variation of intensities are normalized between Strontium (Sr) and Strontium Nitric oxide (SrNO3) by plot which it can be calculated by taking the ratios of both the compounds in the same region.

We have got the values of relative intensities of each plot and also varied the intensities of both the compounds.

Conclusion

In this paper we have collected intensity data by varying the energy for the compounds Mo and MoO$_3$, Sr and SrNo$_3$ using WDXRF. The data has plotted and observed that each of the compounds Mo and MoO$_3$ display six peaks viz., L_α ,L_β,$L_{\beta 3}$,$L_{\beta 4}$,$L_{\beta 15,2}$ and $L\gamma_1$.It is observed that L_α peak is main peak for both the compounds and the remaining peaks have less intensity in comparison to L_α peak. The data plotted and observed that each compound of Sr and SrNo$_3$ display eight peaks viz., L_l,L_η,$L_{\alpha 1}$,$L_{\beta 1}$,$L_{\beta 6}$,$L_{\beta 4}$,$L_{\beta 3}$,$L_{\gamma 5}$. It is observed that $L_{\alpha 1}$ peak is the main peak for both the compounds and remaining peaks have less intensity in comparison to $L_{\alpha 1}$ peak.

In Molybdenum three satellite peaks ($L_{\beta 3}$,$L_{\beta 4}$,$L_{\beta 15,2}$) that are having reduced intensity transitions are observed. The satellite lines $L_{\beta 3}$,$L_{\beta 4}$ are due to coaster-kronig transitions L_1-L_1M_2, L_1-L_1M_3 which are offset, and $L_{\beta 15,2}$ is due to coaster-kronig transitions L_2-$L_3N_{4,5}$ which has double vacancy states of L_3N_4 and L_3N_5.Coaster-Kronig transitions are the transitions in the same shell. In this the electron transforms from one subshell to another subshell before the vacancy is filled by another electron transition. When comparing the molybdenum trioxide with molybdenum intensity ratios relatively normalized.

In strontium four satellite peaks ($L_{\beta 1}$,$L_{\beta 3}$,$L_{\beta 4}$,$L_{\beta 6}$) are observed and which are with reduced intensity. In which the satellite lines $L_{\beta 3}$,$L_{\beta 4}$ are due to coaster-kronig transitions L_1-L_1M_2, L_1-L_1M_3 which are offset and $L_{\beta 1}$ is due to the transition of L_2M_5, $L_{\beta 6}$ is due to the transition of L_3N_1. When comparing the Strontium nitric oxide with strontium element intensity ratios are normalized.

Through this results of these both elements are presented here to benefit those using this WDXRF Technique can achieve the higher precision in elemental identification and qualification.

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