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Study of Chemical State Analysis of Rubidium Compounds in Lα, $L\beta_1$, $L\beta_{3,4}$ and $L\gamma_{2,3}$ X-Ray Emission Lines with Wavelength Dispersive X-Ray Fluorescence Spectrometer

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Abstract : Rubidium salts have been commonly used as an electrolyte to improve the efficiency cycle of Li-ion batteries. In recent years, it has been implemented into the large scale for further technological advances to improve the performance rate and better cyclability in the batteries. X-ray absorption spectroscopy (XAS) is a powerful tool for obtaining the information in the electronic structure which involves the chemical state analysis in the active materials used in the batteries. However, this technique is not well suited for the industrial applications because it needs a synchrotron X-ray source and special sample file for in-situ measurements. In contrast to this, conventional wavelength dispersive X-ray fluorescence (WDXRF) spectrometer is nondestructive technique used to study the chemical shift in all transitions (K, L, M, …) and does not require any special pre-preparation planning. In the present work, the fluorescent Lα, $L\beta_1$, $L\beta_{3,4}$ and $L\gamma_{2,3}$ X-ray spectra of rubidium in different chemical forms (Rb_2CO_3 , RbCl, RbBr, and RbI) have been measured first time with high resolution wavelength dispersive X-ray fluorescence (WDXRF) spectrometer (Model: S8 TIGER, Bruker, Germany), equipped with an Rh anode X-ray tube (4-kW, 60 kV and 170 mA). In $_{37}$Rb compounds, the measured energy shifts are in the range (-0.45 to - 1.71) eV for Lα X-ray peak, (0.02 to 0.21) eV for $L\beta_1$, (0.04 to 0.21) eV for $L\beta_3$, (0.15 to 0.43) eV for $L\beta_4$ and (0.22 to 0.75) eV for $L\gamma_{2,3}$ X-ray emission lines. The chemical shifts in rubidium compounds have been measured by considering Rb_2CO_3 compounds taking as a standard reference. A Voigt function is used to determine the central peak position of all compounds. Both positive and negative shifts have been observed in L shell emission lines. In Lα X-ray emission lines, all compounds show negative shift while in $L\beta_1$, $L\beta_{3,4}$, and $L\gamma_{2,3}$ X-ray emission lines, all compounds show a positive shift. These positive and negative shifts result increase or decrease in X-ray energy shifts. It looks like that ligands attached with central metal atom attract or repel the electrons towards or away from the parent nucleus. This pulling and pushing character of rubidium affects the central peak position of the compounds which causes a chemical shift. To understand the chemical effect more briefly, factors like electro-negativity, line intensity ratio, effective charge and bond length are responsible for the chemical state analysis in rubidium compounds. The effective charge has been calculated from Suchet and Pauling method while the line intensity ratio has been calculated by calculating the area under the relevant emission peak. In the present work, it has been observed that electro-negativity, effective charge and intensity ratio ($L\beta_1/L\alpha$, $L\beta_{3,4}/L\alpha$ and $L\gamma_{2,3}/L\alpha$) are inversely proportional to the chemical shift (RbCl > RbBr > RbI), while bond length has been found directly proportional to the chemical shift (RbI > RbBr > RbCl).

Keywords : chemical shift in L emission lines, bond length, electro-negativity, effective charge, intensity ratio, Rubidium compounds, WDXRF spectrometer
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