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Comparative Study of Systematization Procedures Applied to K-level Electron Binding Energies in X-ray Spectra

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Abstract

X-ray and photoelectron spectroscopic studies have led to the measurement of accurate K level binding energy values in atoms. Since these experiments are conducted at various laboratories all over the globe using different instruments, there is every possibility that the results deviate from reality more than the probable errors. Consequently when these energy values are used for some other applications, their results obtained will be different from what is being expected. Therefore these energy values need to be systematized and corrected for errors if any. Various systematization procedures available in X-rays spectroscopy are (i) Mosley Law (ii) Modified Mosley Plot (iii) Hagstrom doubly modified Mosley plot (iv) Iterative self-consistent doubly modified Mosley plot. A detailed comparative study of all these systematization procedures is performed as applied to the K level binding energies with a view to ascertain their applicability for the purpose.

Keywords

Mosley Plot, Parabolic Shape, Iterative Procedure, Systematization, Energy Levels

1. Introduction

The experimental measurements and the theoretical calculations of atomic electron binding energy values for almost all the elements and all the levels have been completed thoroughly in the last century. These binding energies have been observed in different laboratories, using varied experimental procedures and calculated adopting different theoretical models, there is every possibility of numerous unknown errors and uncertainties in the final results. Therefore it becomes necessary to systematize these energy values to bring them on the same standards from the precision and accuracy point of view. Accurate and precise values of these binding energies are the utmost requirement of experimentalists and theoreticians alike working in different disciplines and thus their refinement and systematization become an absolute necessity of the hour.

The present paper presents a detailed description of different empirical systematization procedures, namely Mosley Law [1-2], Modified Mosley Plot [3], doubly modified Mosley plot [4] and Iterative self-consistent doubly modified Mosley plot [5]. These methods can be applied to eliminate the inherent errors which are unknown and hidden in these energy values, thus leading to obtaining the precise and accurate atomic electron binding energies for atoms. We also examine the relative merit of these procedures with a view to decide which method is best suited for the purpose and undertake as an illustration of such calculations, the systematization of these energies for the K level in the atomic number range 21-30. The results so obtained are reported and discussed.

2. Systematization Procedures

2.1. Mosley's Historical Approach

Using a crystal of potassium ferrocyanide Mosley [1] photographed the K and L spectra of a number of elements. Consequent upon this he was able to enunciate the celebrated law, which bears his name and states that the square root of the frequency of a line is approximately a linear function of the atomic number. In his own words:

"From the approximate linear relation between $\upsilon^{1/2}$ and Z for each line we obtain the general equation:

$$\upsilon = A(Z-b)^2$$

where A and b are constants characteristic of each line. For the Kα line:

$A = R(1/1^2-1/2^2)$ and $b = 1$

For the Lα line approximately,

$A = R(1/2^2-1/3^2)$ and $b = 7.4$

The fact that b is much larger for the Lα lines than for the Kα lines suggests that the L system is situated the farther from nucleus." However, this method cannot be applied for precise and for an accurate calculation of these atomic electron binding energy values because as is very well established, the Mosley Plot systematically deviates from the straight linear behavior. Since these deviations are very small and therefore to make them discernible the Mosley Plot has to be drawn on a very large scale.

2.2. Modified Mosley Method

An elegant way to surpass the above mentioned difficulty was suggested by Idei [6] who devised the method of the " Modified Mosley Plot " which consists in drawing the ($\sqrt{E}$ -AZ-B) versus Z graph, where E is the energy of the level under consideration for the element with atomic number Z and A and B are constants. The modified Mosley Plot generally has a roughly

parabolic shape and the small deviations in the Mosley Plot caused by wrongly measured or calculated energy values now become discernible. The corrected energy values can, therefore, be obtained from this modified Mosley Plot. However, like the conventional Mosley Plot, the modified Mosley Plot also does not take into account the Z^4 and higher terms in the series expansion of the well-known Sommerfeld relativistic energy formula [7-8]. This is very remarkable that the Sommerfeld energy formula is exactly equivalent to the energy formula later derived by Darwin [9] and Gordon [10] independently using Dirac's advanced quantum mechanics [11-12].

2.3. Doubly Modified Mosley Approach

In order to take the Z^4 and higher terms, of the series expansion of the well-known Sommerfeld-Dirac energy formula into account, Hagstrom [4] proposed a further modification. He suggested to Plot $(\sqrt{E}$ -AZ-B$)^{1/2}$ – CZ, as a function of Z, where C is also a constant. This new type of curve known as doubly modified Mosley Plot is found to be very well represented by a straight line and any anomaly in the energy values will certainly be reflected as a scatter from the regular trend of the graph. Hagstrom found that there exist changes of slope in the straight line whenever a new subshell starts filling or is completed, however the points corresponding to the energy values of an individual subshell do fall upon a straight line.

2.4. Iterative Self Consistent Doubly Modified Mosley Plot Method

Misra et al [5] developed the method known as the "iterative self-consistent doubly modified Mosley plot method" based on Hagstrom's [4] doubly modified Mosley plot approach. This iterative self-consistent doubly modified Mosley Plot method can be profitably applied in different atomic number ranges to data which in the first approximation obey the Mosley law. A detailed description of the method can be found in the works of Mathew [13] and Kumar [14] who have used this method for the systematization of energy levels as well as of the diagram lines.

3. Results

The present study has been carried out for the systematization of the energy values of the K-level atomic electron binding energies in the atomic number range Z= 21 to 30. The results obtained in the manner described above are presented in table 1 which contains results after applying the Mosley's Law, the Hagstrom's modification and Misra et al's iterative procedure.

The table contain three entries, in each of the three columns, being the sum of the squares of the deviation from experimentally observed energy values for elements (i) from beginning of the range i.e. Z = 21 to Z = Z_0 where Z_0 presents the atomic number for the vertex of the parabola. (ii) for the elements from Z = Z_0 to the end of the atomic number range i.e. Z = 30 and (iii) for all the elements of the subshell under consideration. The value for Z_0 is 27 in the present study of Z=21-30 for the K level binding energies.

4. Discussion

A close scrutiny of the results presented in the table 1 reveals many very interesting features which not only throw light on applicability of various systematization procedures i.e. Mosley law, modified Mosley Plot, doubly modified Mosley Plot and Iterative self-consistent doubly modified Mosley plot, but also enlightens how the inner 3d sub shell is being filled. A detailed study of the entire process of the systematization of the K-level binding energies for Z= 21-30 clearly shows that the successive application of these procedures does not lead to any significant modification to the experimentally observed K-level atomic electron binding energies, establishing the fact that these energy values were measured accurately. Further it is observed that**:**

(i) the sum of the squares of deviations from experimentally observed K level binding energy values for all the elements in the atomic number range Z=21-30 after applying iterative self- consistent doubly modified Mosley plot is minimum whereas after applying Mosley law is maximum.

(ii) a Scrutiny of the values obtained in various stages further revels that the agreement between the experimentally observed energy values and the theoretically calculated energy values in each cycle is much better for Z=21-27 than for Z=27-30. Similar is the observation for agreement between the theoretically calculated energy values in a particular cycle to the theoretically calculated energy values in the previous cycle. This becomes clear if one analyses the entire process.

5. Conclusion

From the observation that the sum of the squares of deviations from experimentally observed energy values remains almost same, it may be concluded/ realized that these experimentally observed atomic electron binding energies for the K level in the atomic number range Z=21-30 are very carefully measured precise values and need no refinement or systematization. This fact is also established from the error analysis done by Bearden and Burr [15] as in their compilation, the maximum reported error in this range is for 26Fe equal to 0.9Ev.

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Table 1. Results of K-Level Atomic Electron Binding Energies For Z= 21-30

Cycle	Sum of the squares of deviation from experimentally observed k-level binding energy values for the elements in the atomic number range Z=21-30 after applying		
	Mosley Law	Hagstrom's modification	Misra et al's iterative procedure
After 1st Cycle	56.18, 92.42 **136.69**	3.75, 34.35 **37.91**	6.41, 8.21 **14.62**
After 2nd Cycle	56.63, 89.90 **134.94**	3.87, 34.72 **38.45**	6.30, 7.97 **14.26**
After 3rd Cycle	56.67, 89.87 **134.94**	3.86,34.69 **38.42**	6.24,7.89 **14.13**
After 4th Cycle	56.80, 89.79 **134.91**	3.88, 34.80 **38.55**	6.21,7.87 **14.08**
After 5th Cycle	56.27, 90.20 **135.06**	3.88, 34.80 **38.55**	6.21, 7.85 **14.06**
After 6th Cycle	56.27, 90.20 **135.06**	3.88, 34.80 **38.54**	6.21, 7.85 **14.06**
After 7th Cycle	56.31, 90.17 **135.05**	3.89, 34.82 **38.57**	6.20, 7.85 **14.06**
After 8th Cycle	56.33, 90.16 **135.05**	3.90, 34.86 **38.62**	6.20, 7.85 **14.06**

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